Dimorphism of Ortho-Positronium in Relativistic Schrödinger Theory

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Abstract

The non-relativistic energy levels of ortho-positronium are calculated in the quadrupole and octupole approximations for the interaction potential. For this purpose, the RST eigenvalue problem of angular momentum is illustratively solved for the quantum numbers \( j_0 = 0, 1, 2, 3, 4 \) and \( (b) j_z = \pm 1 \). This eigenvalue problem admits ambiguous solutions for \( 0 < |(b) j_z| < j_0 \) whereas the solutions for \( (b) j_z = 0 \) and \( (b) j_z = \pm j_0 \) are unique. In order to attain some (at least approximative) solutions of the energy eigenvalue problem one tries a factorized ansatz for the wave function and thus splits off the angular problem (with its ambiguous solutions) from the residual radial problem. The latter does, as usual, finally fix the energy eigenvalues. But it is just by this procedure that the ambiguity of the angular problem is transferred to most of the energy levels which thereby become doubled. The corresponding doubling energy amounts to (roughly) one percent of the total binding energy and is, however, of purely electric origin, since magnetism is completely neglected. Indeed, the charge distributions of both positronium constituents (i.e. electron and positron) do inherit their ambiguity from the ambiguous solution of the angular eigenvalue problem (\( \sim \) charge “dimorphism”); and naturally the dimorphic configurations must then possess slightly different interaction energies of the electrostatic type.
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I Introduction and Survey of Results

The present paper aims at the further elaboration of Relativistic Schrödinger Theory (RST), i.e. a fluid-dynamic version of relativistic few-particle quantum theory [1,2]. This fluid-dynamic approach is applied here in order to study the non-relativistic energy spectrum of ortho-positronium; and it is found that there does occur a somewhat strange phenomenon, i.e. the doubling of the number of the energy levels. But since such a fluid-dynamic view on the physics of elementary particles is rather unusual, it may perhaps appear desirable to first premise some conceptual and epistemic remarks about its relation to the conventional quantum theory which is strongly dominated by the probabilistic point-particle picture of quantum matter.

As desirable and instructive as such a comparison of our fluid-dynamic concepts to the conventional point-particle logic may be, there unfortunately arises a certain difficulty here because the point-particle proponents seem still to disagree about their fundamental notions.

The birth of quantum mechanics, some nine decades ago, has first been accompanied by considerable confusion and many controversies about the epistemic status of the new theory, see ref. [3] for a historic account of the notorious Bohr-Einstein debate. But now that almost a century has passed away, and a considerable technical and cultural progress could be made thanks to the overwhelming applications of the new theory (think, e.g., of nuclear and laser technology, semiconductors, materials science, supernovae astrophysics, big bang cosmology etc.) one should nowadays think that the teething troubles of the theory’s childhood have been successfully overcome already long time ago. Indeed, it is hardly conceivable how such an immense civilizing progress could have been made without possessing a correspondingly profound theoretical basis. In this sense, one expects that present-day quantum theory has been anchored in the mean time on solid fundaments, comparable to the situation with classical electromagnetism or thermodynamics, and thus will be able to provide us with hopeful future developments.
However, this impression is grossly fallacious. Indeed, a superficial inspection of some modern presentations of the fundamentals of conventional quantum theory is sufficient in order to ascertain that the controversies about the true meaning of this theory and its conceptional framework are becoming now rather more violent than dying out. This regrettable fact is brought to light mostly on the occasions of celebrating the very birth of quantum mechanics, e.g. Heisenberg’s \textit{matrix mechanics} of 1925. Usually, the inventor (or discoverer) of a new fruitful theory (such as, e.g., Galilei [4], Newton [5] or Maxwell [6]) enjoys later on much reputation by the scientific descendants; and the corresponding first texts about the original new idea are frequently celebrated by historic reprints. However, concerning Heisenberg’s \textit{matrix mechanics} of 1925, the situation is rather ambiguous: whereas some people do hold it adequate to celebrate Heisenberg’s invention (discovery) by dedicating a book to his original proposal of matrix mechanics [7], others argue that this proposal “consisted essentially in the introduction of novel algorithms (i.e. his matrix mechanics) and even renowned and formalistic physicists do nowadays confirm that this paper is actually unintelligible” (ref.[8], p. 39; authors’ translation).

A further subject of never-ending controversies concerns even the central concept of quantum theory: i.e. the \textit{wave function} (or more generally: \textit{quantum state}). Is the wave function to be associated to some real property of the observed system and thus does exist also when the system is not observed? Or does the wave function merely reflect the state of information of the observer? In the latter case, the wave function is thought to “collapse” whenever the observer’s state of information undergoes a sudden change (e.g. by reading off the pointer of some measurement device). A competent opinion looks as follows: “In the first place, it is often argued that the wave function itself should not be regarded as giving an objective description of the world (or part of it) but as providing information merely of ‘one’s state of knowledge’ about the world. This view I really cannot accept.” (R. Penrose in ref. [9], p. 121). Another opinion is the following: “The claim, that the wave function be not real but describe ‘information’, reminds me of arguments
which are widespread in homeopathy” (ref. [8], p. 79; authors’ translation).

Some co-authors do also frankly concede that they disagree even about the fundamental quantum concepts: “Although we have tried to write a ‘coherent’ book, our reader will soon notice that our conceptions vary on some basic notions. Characteristic are our different opinions on the relevance of mathematical concepts for the interpretation of quantum mechanics and hence different inclinations to make active use of these concepts in physical arguments.” [10]

It should be evident that such a loose bedrock is not suited to erect on it a continual scientific and technological progress; and it seems that already the fathers of the new theory (especially Bohr and Heisenberg) were aware of such a grave drawback of their new theory and therefore they tried to cobble together some minimalistic interpretation of their quantum formalism (i.e. the kopenhagen interpretation, see, e.g., ref. [9]) which should suffice to handle with the quantum formalism “for all practical purposes”. However, the Bohr-Heisenberg interpretative proposal of their formalism evokes nowadays some harsh critique: “If a physicist declares that he consistently applies the kopenhagen interpretation, then this does mean nothing else than that he consistently always refers to the same kind of conceptual inconsistency – but this does not yield a consistent theory” (ref.[8], p. 51; authors’ translation).

Wave-Particle Duality

One of the key concepts of the kopenhagen interpretation does refer to the complementarity principle, with the wave-particle duality representing the most conspicuous exemplification thereof. Indeed, the progress of the past decades was made by extensive use of both the particle and the wave concept in like manner. Both concepts have been thought to be unrenouncable for the description of elementary matter and its interactions. This fact becomes immediately evident by merely glimpsing at the titles of some of the competent text books, see ref.s [11]–[25]. On the other hand, there seem to arise now seri-
ous arguments which point to the possibility that 'particles' (in the classical and quantum sense) do not really exist but merely are some kind of fiction (if not illusion): "There are no quantum jumps, nor are there particles" [8,26]. That might be true. But even if the long-lived concept of a 'particle' (classical and quantum) ultimately should turn out as a mere fiction, then it is surely a very useful fiction since it advanced the progress of the past decades considerably. If now a new time should dawn with the particle concept being superseded by some novel, more powerful concept (perhaps decoherence [8,10]? or emergence [27]? then that novel concept will also possess the epistemic status of being not more than a fiction! Indeed, it is hold quite generally that the limited epistemic abilities of a human being admits to describe 'reality' at most in terms of fictions [28] which, however, must then of course be required to be free of logical and observational contradictions.

* 

Thus it seems to us that the notorious quantum controversies are nothing else than some kind of useless struggles for domination among different fictions. In place of opposing these different fictions against each other in an irreconcilable way, one should rather consider them as helpful complementations of each other, so that they together can mediate to us a more integral picture of what is really going on in the quantum world.

Bearing this situation in mind, one may doubt whether the ardently desired and unique 'theory of everything' [29] will ever be discovered (or invented, resp.) in order to supersede Bohr’s complementarity principle. So long as we must be content with theories having a loose end, we should rather recall Bohr’s viewpoint on this question to our mind. Indeed, it seems that Bohr was the first who noticed clearly that the behaviour of elementary particles could not be satisfactorily described in terms of one single logical framework. More concretely, he thought that the (self-suggesting) probabilistic point-particle description of an elementary particle should be complemented by a fluid-dynamic wave description,
namely in order to better understand and manage the notorious \textit{wave-particle duality}. This original idea of Bohr is now known as the ‘\textit{complementarity principle}’ [9] (see also the corresponding remarks in the precedent paper [1]). According to this principle (if it is understood in the right sense) one needs two logical systems (or “pictures”), excluding one another to a certain degree, in order to become able to predict and ‘understand’ the outcomes of the considered experiments.

For instance, in the well-known two-slit interference experiment for electrons one becomes forced to find some plausible explanation why the electrons do form the well-known interference pattern on the detection screen after having passed the two-slit arrangement. The solution of this problem is based upon the postulate that the electrons do pass the two-slit region in form of a wave (with appropriate wave length); but their arrival on the detection screen occurs in form of point-like particles [30].

In order to manage intellectually such a highly ambiguous phenomenon it seems wise to us to resort to Bohr’s complementarity principle and develop two complementary logical systems (or ‘pictures’), i.e. the probabilistic point-particle picture and the fluid-dynamic wave picture. This means that we have to specify two mathematical formalisms together with their associated physical interpretations so that we can ‘understand’ and predict the outcomes of physical experiments and/or observations. Whether or not a future \textit{theory of everything} will be able to incorporate simultaneously both pictures (or create a completely new picture) must be left unclarified for the time being.

\textit{Probabilistic Point-Particle Picture}

The necessity for developing additionally also a fluid-dynamic picture of the quantum objects becomes perhaps most clear when one reconsiders the somewhat artificial manner in which the point-particle theory tries to explain the undeniable wave-like aspects which become evident in the notorious double-slit experiment.

A closer inspection of the interference pattern and the associated double-slit geometry
in terms of the particle picture may suggest the following conclusion: The confining of the particle position to a spatial volume measured by a certain linear dimension (slit distance $\Delta x$, say) must induce in some (mysterious) way a momentum uncertainty ($\Delta p_x$, say) so that both point-particle quantities will obey the Heisenberg uncertainty relation

$$\Delta x \cdot \Delta p_x \gtrsim \frac{\hbar}{2},$$

being needed for explaining the appearance of the interference pattern (see any textbook about elementary quantum mechanics which treats the double-slit experiment in the point-particle picture, e.g. [31]). Furthermore, since the interference pattern on the detection screen is built up by a huge number of particle-like impacts, one thought that one must describe such a phenomenon in terms of a statistical theory. For such a purpose, the appropriate mathematical formalism appeared to be the Hilbert space of quantum states $|\Psi>$ with the classical observables (such as position $x$ and momentum $p$) being transcribed to the corresponding operators (here $\hat{x}$ and $\hat{p}$) acting over that Hilbert space. The particles passing through the double slit and striking at the detection screen do then build up a statistical ensemble which is to be characterized by the statistical operator (density matrix) $\hat{\rho}$, with $\text{tr} \hat{\rho} = 1$. Thus, let the quantum state of a point particle, located point-like at $\xi$ ($0 \lesssim \xi \lesssim \Delta x$), be denoted by the Hilbert space vector $|\xi>$

$$\hat{x} |\xi> = \xi |\xi>,$$

then the statistical operator $\hat{\rho}$ for such an ensemble of particles with unknown (but well determined) locations in the double-slit region ($0 \lesssim \xi \lesssim \Delta x$) is adopted as

$$\hat{\rho} = \int_0^{\Delta x} d\xi \, w(\xi) \, |\xi><\xi|.$$

Here, the probability $w(\xi)$ for the space point $\xi$ ($0 \lesssim \xi \lesssim \Delta x$) being occupied by some particle is to be normalized to unity as usual

$$\int_0^{\Delta x} d\xi \, w(\xi) = 1.$$
Finally, it remains to demonstrate how the desired Heisenberg uncertainty relation (I.1) can arise from such a mathematical construction. For this purpose, one merely has to interpret the position and momentum uncertainties $\Delta x$ and $\Delta p$ as the corresponding mean square deviations (“variances”)

\[
(\Delta x)^2 \doteq \text{tr} \left[ \hat{\rho} (\hat{x} - <x>)^2 \right], \quad (I.5a)
\]
\[
(\Delta p)^2 \doteq \text{tr} \left[ \hat{\rho} (\hat{p}_x - <p_x>)^2 \right], \quad (I.5b)
\]

and additionally one postulates the Heisenberg commutation relations for the operators $\hat{x}$ and $\hat{p}$ as follows:

\[
[\hat{x}, \hat{p}_x] = i\hbar \cdot 1. \quad (I.6)
\]

But the crucial point is now that this probability construction (I.2)-(I.6) cannot bring forth that desired uncertainty relation (I.1) which one would like to see being validated in order to become able to explain the appearance of the interference pattern. Here, the problematic constituent of the whole probability construction is the assumption (I.3) which means that anyone of the point particles does occupy a unique (albeit unknown) point of space. Namely, such a collection of pure point particles does not develop the right lateral pressure for generating a transverse momentum $p_x$ across their direction of flight ($y$-axis, say) which is necessary in order to produce just the observed interference pattern on the detection screen. Indeed, if this assumption (I.3) is rejected and replaced by the assumption that any “point particle” is in a (exotic) state $|\Psi>$ which is some “superposition” of the states $|\xi>$ (I.2), being themselves due to the classical localization of a real point particle, then it is no problem to deduce the wanted uncertainty relation (I.1). Namely, the statistical operator $\hat{\rho}$ becomes now

\[
\hat{\rho} = |\Psi> <\Psi|
\]

with the superposition $|\Psi>$ of the classical configurations $|\xi>$ being defined through

\[
|\Psi> = \int_0^{\Delta x} d\xi \psi(\xi) |\xi> . \quad (I.8)
\]
Obviously, this is just the place where the point-particle picture has to introduce fluid-
dynamic concepts, since the particle’s spatial presence is (in some mysterious way) now
smeared out over some finite region. And consequently, the variances $I.5a$–$I.5b$ emerge
now in the position representation as

\[
(\Delta x)^2 = \int_0^{\Delta x} dx \, \psi^*(x) \left( x - <x> \right)^2 \psi(x) 
\] (I.9a)

\[
(\Delta p_x)^2 = \int_0^{\Delta x} dx \, \psi^*(x) \left( \hat{p}_x - <p_x> \right)^2 \psi(x) , 
\] (I.9b)

where the mean values $<x>$, $<p_x>$ are defined as usual through

\[
<x> = \frac{1}{\Delta x} \int_0^{\Delta x} dx \, \psi^*(x) \, x \psi(x) 
\] (I.10a)

\[
<p_x> = \frac{1}{\Delta x} \int_0^{\Delta x} dx \, \psi^*(x) \, \hat{p}_x \psi(x) 
\] (I.10b)

\[
\left( \hat{p}_x = \hbar \frac{i}{\hbar} \frac{\partial}{\partial x} \right) .
\]

Now, whenever the considered system (here: a point particle confined to the one-
dimensional interval $[0, \Delta x]$) is in such a superposition $|\Psi\rangle$ of classical configurations
$|\xi\rangle$ and therefore can be described by a “wave function” $\psi(x)$ ($\approx <x|\Psi\rangle$), then a quite
general theorem ensures that an inequality of the following type must hold (Schwarz’
inequality, e.g. [32])

\[
(\Delta x)^2 \cdot (\Delta p)^2 \geq \left( \frac{1}{2} |<C>| \right)^2 , 
\] (I.11)

where $<C>$ is the expectation value of the commutator $\hat{C}$

\[
\hat{C} \triangleq [\hat{x}, \hat{p}_x] = i\hbar \, \mathbf{1} .
\] (I.12)

Obviously, the result $I.11$–$I.12$ for the variances $\Delta x$, $\Delta p_x$ is now just the wanted
uncertainty relation $I.1$. 

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It appears natural that such a successful invention of a mathematical formalism (together with the physical interpretation of the inherent mathematical quantities) will be celebrated as a great progress in ‘understanding’ the working in the micro-world. So much the more the formalism can be extended in order to deal with all possible physical situations. It is merely necessary to set up a Hilbert space whose basis vectors may be selected in such a way that they describe the classically realizable configurations (\(|\xi >\), say); but other basis systems are also possible. The Hilbert space for the many-particle systems is the tensor product of the one-particle Hilbert spaces. Next, one writes down the general state vector \(|\Psi >\), if desired as a superposition of the classical states \(|\xi >\), cf. (I.8); and then one lets this state vector \(|\Psi >\) evolve in time according to the time-dependent Schrödinger equation

\[
i \hbar \frac{\partial}{\partial t} |\Psi > _t = \hat{H} |\Psi >_t .\tag{I.13}
\]

For the stationary states one puts

\[
|\Psi >_t = e^{-iEt/\hbar} |\Psi >_0 \tag{I.14}
\]

which then yields the time-independent Schrödinger equation

\[
\hat{H} |\Psi >_0 = E |\Psi >_0 \tag{I.15}
\]

which, e.g., admits to determine the energy spectrum \(\{E\}\) of bound systems. This quantization formalism may not only be applied to mechanical systems but also to field systems and then entails the well-known quantum field theory. But despite its overwhelming success the latter quantum-formalism continues to own the epistemic status of a probabilistic point-particle fiction; and therefore the question must be asked whether there do perhaps exist other ‘fictions’ which, after thorough elaboration, do also yield a comprehensive and consistent picture of the micro-world?
As already mentioned at various occasions, the precedent point-particle picture seems to us to be plagued by a certain deficiency: i.e. the very concept of a “point” particle. In the original classical sense, a point particle does occupy some point $\vec{x}$ of 3-space and possesses a definite momentum $\vec{p}$. Concerning the precise position, the corresponding state vector $|\xi> \in$ the one-particle Hilbert-space obeys the eigenvalue equation (I.2). However, by means of the set (I.3) of such state vectors one cannot explain the interference pattern on the detection screen! Therefore one brings into play the conception of a coherent superposition $|\Psi> \in$ (I.8) of all classically possible positions $\xi$ ($0 \leq \xi \leq \Delta x$) so that this range $\Delta x$ of all those possible locations together with the range of all possible momenta $\Delta p$ can obey the required uncertainty relation (I.1). It seems that such a strange superposition of classical locations has been considered because one felt being forced to take account of the particle’s finite “extension” within the logical framework of point particles! Indeed, this auxiliary construction may be understood in the sense that the point particle becomes somehow “smeared” over the whole interval $\Delta x$ and thus appears as a kind of droplet of some esoteric fluid; whereas on other occasions it may be treated as a true point particle! It surely does not come as a surprise that such a self-contradictory and mysterious idea of a point particle has provoked the question: “Is this now profound thoughtfulness or the ultimate degree of craziness?” (ref.[8], p. 52; authors’ translation).

Most textbook authors prefer to evade the notion of a point particle with unknowable position and momentum and they rather try to explain the double-slit experiment completely in terms of the wave picture [30]. But then the problem becomes urgent anew when one resolves microscopically the interference pattern, being thought to arise in the wave picture by the superposition of different wave trains. However, one finds the pattern being composed of point-like impacts on the detection screen. So one feels oneself being thrown back again to the notorious phenomenon of wave-particle duality.

In such a confused situation it seems reasonable to suppose that the dominance of
either the particle aspect or the wave aspect is brought forth cooperatively by the object itself plus its surroundings. Such a holistic theory (if feasible) could then interpolate between the pure particle-like and the pure wave-like aspects of the considered physical situation. But when one cuts the system off its environment (⇒ closed system) the balance of the particle-like and wave-like aspect goes lost and one has to decide whether one wants to neglect the particle aspect or the wave aspect. In many situations, one of both aspects will be the dominant one and therefore suggests itself to become preferred over the other one for the description of the isolated system. In other instances, both aspects may be mutually counterbalanced; and if one nevertheless cuts the system off its surroundings and favours only one of the complementary aspects, then there will arise those notorious “quantum paradoxes”, e.g. the mentioned double-slit phenomenon. In recent time, there were put forth some proposals of treating the system in combination with its surroundings (see, e.g., ref.s [8,10,27]) but presently a final judgement seems premature.

Historically, the method of neglecting the system’s environment, together with the preference of the probabilistic point-particle picture, has been the prevailing world view and the corresponding success is impressive, see ref.s [11]–[25]. But, if concentrating on the system alone by neglecting its surroundings, one should not despise the possibility of describing the isolated system also in fluid-dynamic terms according to the complementary wave picture. One cannot exclude that the more comprehensive view on “system plus environment” can also be built up by starting from the side of the fluid-dynamic approach.

A proposal of the latter kind is the “Relativistic Schrödinger Theory” [1,2], i.e. a fluid-dynamic version of relativistic few-particle quantum mechanics. The subsequent investigation is an application of this theory to ortho-positronium to be conceived as a closed system (para-positronium has been the subject of the preceding paper [2]). More concretely, the present paper is a study of the question to what extent the non-relativistic RST spectrum of ortho-positronium does coincide with that of the conventional quantum
theory (which is a probabilistic point-particle theory). The main result of this study is that most of the conventional energy levels become duplicated as an indirect consequence of the specific way in which the angular momenta of the constituents (i.e. electron and positron) are to be composed in RST to the total angular momentum. Unfortunately, the corresponding energy eigenvalue problem is in RST much more complicated than in the conventional quantum theory so that we have to resort to appropriate perturbation techniques which we develop up to the “octupole” approximation [33]. Thus our obtained result of level duplication emerges here in the quadrupole and octupole approximations and therefore might eventually be an artefact of those perturbation orders, i.e. possibly not being present in the exact RST solution of the eigenvalue problem for ortho-positronium. However, the main effect of level doubling occurs in the quadrupole approximation (Fig. VII.A on p.108) and the relative doubling energy amounts to more than 1%; on the other hand, the octupole correction of the levels in the quadrupole approximation amounts to less than 1 percent (table on p.145). This hints at level doubling being a true effect in RST which receives merely some minor corrections from the higher-multipole approximations.

* It is true, the origin of this level duplication can be traced back to the fact that ortho-positronium has unity of spin ($\sim s_\Omega = 1$); whereas para-positronium has zero spin ($\sim s_P = 0$) and therefore does not undergo that phenomenon of level duplication. But it is important to note that the energy difference of both levels (emerging by duplication) is not of magnetic but rather of electric origin! Namely, for the ortho-spin $s_\Omega = 1$, the eigenvalue problem for angular momentum admits (mostly) two different solutions belonging to the same values of total angular momentum $j_\Omega$ and its $z$-component $(b)j_z$. This then yields two different angular distributions of the corresponding charge densities ($\sim$ dimorphism, see Fig.IV.B on p.75) which thereby acquire different interaction energies of the electrostatic type.
Subsequently, these results will be elaborated in detail along the following arrangement.

Fluid-Dynamic Character of RST

As proponents of a fluid-dynamic description of the elementary matter we tend to the hypothesis that ‘matter’ (in its most general sense) is always spread out over some finite region of three-space and can never be concentrated in a truly point-like manner. The fiction of a point-like particle appears to us as a (more or less realistic) idealization; and consequently the finite-size effects of matter must be somehow simulated in the point-particle picture, preferably by saying that the state $|\Psi>$ of the point-particle refers to a “superposition” of states being due to really point-like positions $|\xi>$, see equation (I.8). By this construction it may seem now that the concept of wavefunction $\psi(x)$ ($\equiv <x|\Psi>$) is the crucial point in the probabilistic approach and thus must be made responsible for its overwhelming success.

But actually RST is also based essentially on the use of wavefunctions $\Psi(x)$, namely in order to generate the physical densities of the considered system such as, e.g., the total current density $j_{\mu}$ or the energy-momentum density $T_{\mu\nu}$ of the considered system, see equations (II.29) and (II.35) below. Thus, in contrast to the situation with the point-particle case, the RST wave function $\Psi$ owns a well-defined meaning, namely to generate all the physical densities of the considered system (Sect.s II and III are taken over from the precedent paper [2] in order to elucidate the common basis of both para- and orthopositronium $\rightarrow$ ortho/para dichotomy). The RST handling with the wave functions $\Psi(x)$ is quite different from the probabilistic point-particle case when many-particle systems are considered: here, the conventional theory relies on the tensor product of the one-particle Hilbert spaces and therefore sets up the dynamics (I.13) in the configuration space. However, RST adopts the Whitney sum of the one-particle fibre bundles

$$\Psi(x) = \psi_1(x) \oplus \psi_2(x) \oplus \psi_3(x) \oplus \ldots$$

(I.16)
which then admits to set up the dynamics in the real four-dimensional space-time, namely in form of the Relativistic Schrödinger Equation for the wave function $\Psi(x)$ in combination with the (non-abelian) Maxwell equations for the bundle connection $A_\mu(x)$, see equations (II.1) and (II.15) below.

This formal difference of the dynamical equations of both approaches entails an important physical consequence: whereas (in the non-relativistic approximation) the probabilistic conventional approach takes the predetermined Coulomb potential as the basis for the interaction mechanism, the corresponding RST mechanism retains the interaction field as a truly dynamical object being equipped with its own field equation. For instance, for the positronium system (to be considered subsequently) the non-relativistic Hamiltonian $\hat{H}$ (I.15) contains the non-dynamical Coulomb potential in a manifest way

$$\hat{H} = \frac{\hat{p}_1^2}{2M} + \frac{\hat{p}_2^2}{2M} - \frac{e^2}{||\vec{r}_1 - \vec{r}_2||}.$$ (I.17)

On the other hand, the corresponding RST interaction potential $({}^{(b)}A_0(\vec{r}))$, say, must obey the Poisson equation (IV.19) below, where the source is given by the electric charge density $({}^{(b)}k_0(\vec{r}))$ generated by the RST wave function $\Psi$. Through this arrangement the RST eigenvalue problem becomes a system of coupled differential equations, which (in the spherically symmetric approximation) consists of the Schrödinger equation (IV.17) and the Poisson equation (IV.18). Naturally, such a coupled eigenvalue system is much more difficult to solve than the simple conventional problem (I.15) which for the positronium Hamiltonian (I.17) admits to determine exactly the energy spectrum $E_C^{(n)}$ in terms of the principal quantum number $n$:

$$E_C^{(n)} = -\frac{e^2}{4a_B} \cdot \frac{1}{n^2} = -\frac{6.8029}{n^2} \ [\text{eV}].$$ (I.18)

Ortho-Dimorphism

In contrast to this simple situation in the conventional probabilistic theory, the solution of the corresponding RST eigenvalue problem can be worked out only approximately. The
difficulty refers here to the fact that the wave function becomes considerably anisotropic, according to the value of angular momentum \( ^{(b)}j_z \); as an example see Fig.IV.A below. But since the wave function generates the charge density which then acts as the source of the interaction potential, the anisotropy of the wave function is transferred to the interaction potential via the Poisson equation so that we ultimately have to solve the (RST form of the) Schrödinger equation for an \textit{anisotropic} potential. Clearly, this can be attained only in an approximative way; and most of the paper is concerned with setting up an adequate approximation procedure (Sect.VIII) for managing this anisotropy effect. The key point is here a suitable factorization of the wave function in a radial part and an angular-dependent part which then also becomes transferred to the charge density, cf. its product form (IV.19)–(IV.21) below.

As usual, the (approximate) product form of the wave function splits up the energy eigenvalue problem in two subproblems, namely (i) the radial problem which depends upon the specific physical system to be considered and which ultimately yields the energy eigenvalues, and (ii) the eigenvalue problem of angular momentum which is of quite general nature and thus is independent of the details of the considered system. Now it is just this latter problem, cf. (IV.6a)–(IV.6b), which provides us with the origin of the ortho-dimorphism. Namely, for the same values of the angular-momentum quantum numbers \( \{j_\text{o}, ^{(b)}j_z\} \) with \((-j_\text{o}) \leq ^{(b)}j_z \leq j_\text{o} \) there do exist \textit{two} solutions of the eigenvalue problem. This ambiguity then is transferred to the angular part \( ^{(b)}k_0(\vartheta) \) of the charge density, see Fig.IV.B below.

\textbf{Induced Energy Difference of Dimorphic Partners}

Since the charge density is the source of the electrostatic interaction potential, cf. the Poisson equation (II.43), the angular ambiguity of the charge density is immediately transferred to the interaction potential which thereby inherits the anisotropy of the charge density. More precisely, for any pair of angular-momentum quantum numbers \( \{j_\text{o}, ^{(b)}j_z\} \)
the interaction potential \( \langle b \rangle A_0(\vec{r}) \) acquires a corresponding angular dependence; and the elaboration of this interconnection necessitates an extensive search for the most rational representation of the angular dependency of the interaction potential (Sect. VII–VIII). There are various possibilities, but ultimately it turns out that the separative method provides the most pleasant representation of the wanted multipole expansion because here the energy contributions of the various multipole modes can be clearly separated. Consequently, one can subdivide the total anisotropy energy into the set of contributions of any mode (\( \sim \) quadrupole energy, octupole energy, \ldots).

But if once the anisotropy energy is determined, one can substitute this (together with the isotropy energy and the kinetic energy) in the RST energy functional and try to extremalize this by use of an appropriate trial ansatz. For our present purpose, we are satisfied with a very simple ansatz for the radial part \( \hat{\Omega}(r) \) of the wave amplitude, cf. (VI.1a)–(VI.1b), with only two trial parameters \( (\beta, \nu) \). The value of the RST energy functional \( \tilde{E}_{\{j\}} \) (VI.25) on the chosen trial configuration yields the corresponding energy function \( \tilde{E}\{IV\}(\beta, \nu) \) as a function of both trial parameters \( \beta \) and \( \nu \), cf. (VI.36). After minimalization of this function with respect to the first trial parameter \( \beta \) we are left with the problem of determining the minimal value of the reduced energy function \( \tilde{E}_{\{O\}\{j\}}(\nu) \) (VIII.106) or, resp., the maximal value of the associated spectral function \( S_{\{O\}\{j\}}(\nu) \) (VIII.108). This function contains both quantum numbers \( j_O \) and \( \langle b \rangle j_z \iff \langle b \rangle m_1, \langle b \rangle m_2 \) of angular momentum while the principal quantum number \( n_O \) is restricted to \( n_O = j_O + 1 \) on account of our too simple ansatz (VI.1a)–(VI.1b). Thus, one finally obtains the energy spectrum of ortho-positronium simply by looking for the maximal value of the spectral function \( S_{\{O\}\{j\}}(\nu) \) (VIII.108), namely by admitting all possible quantum numbers \( j_O = 0, 1, 2, 3, \ldots \) and \( \langle b \rangle j_z, \) with \( -j_O \leq \langle b \rangle j_z \leq j_O \). This may be performed by means of some appropriate numerical program, and the most important results are the following (Fig.VII.A and table on p. 145):

The energy spectrum resembles the conventional one (118) but its \((n^2)\)-fold degeneracy...
becomes eliminated. Such a result has already been found for the spectrum of para-positronium [2]; but for ortho-positronium there additionally occurs now a doubling of most of the energy levels. The origin of this strange effect traces back to the specific spin composition for ortho-positronium ($s_O = 1$), where two different solutions of the eigenvalue problem for angular momentum are mostly possible for fixed values of quantum numbers $j_O$ and $\langle j \rangle_j z$. The corresponding energy difference (due to level splitting) amounts to (roughly) 1% of the binding energy, see the table on p.145; it is not caused by magnetism but is a purely electric effect due to the ambiguity of the electric charge distribution, see Fig.IV.B, p. 75.
II Positronium Eigenvalue Problem

In order that the paper be sufficiently self-contained, it may appear useful to mention briefly some fundamental facts about RST. As its very notation says, the central idea is the Relativistic Schrödinger Equation (II.1) which leads one in a rather straight-forward way to the Dirac equation (II.13) for few-particle (or many-particle) systems. In order to ultimately end up with a closed dynamical system for the fluid-dynamic quantum matter, one adds the (generally non-Abelian) Maxwell equations (II.15) where this coupled system of matter and gauge field dynamics automatically entails certain conservation laws, such as those for charge (II.25) or energy-momentum (II.32). This fundamental structure of RST is then subsequently specialized down to the non-relativistic positronium system, especially to its ortho-form, with the main interest aiming at its energy spectrum.

1. Relativistic Schrödinger Equation

A subset of problems within the general framework of RST concerns the (stationary) bound systems. The simplest of those systems is positronium which consists of two oppositely charged particles of the same rest mass ($M$). The physical behaviour of its matter subsystem is assumed here to obey the \textit{Relativistic Schrödinger Equation}

\begin{equation}
  i\hbar c \mathcal{D}_\mu \Psi = \mathcal{H}_\mu \Psi \tag{II.1}
\end{equation}

where the two-particle wave function $\Psi(x)$ is the direct sum of the two one-particle wave functions $\psi_a(x)$ ($a = 1, 2$)

\begin{equation}
  \Psi(x) = \psi_1(x) \oplus \psi_2(x). \tag{II.2}
\end{equation}

The gauge-covariant derivative $\mathcal{D}$ on the left-hand side of the basic wave equation (II.1) is defined in terms of the $u(2)$-valued gauge potential $A_\mu$ as usual

\begin{equation}
  \mathcal{D}_\mu \Psi = \partial_\mu \Psi + A_\mu \Psi, \tag{II.3}
\end{equation}

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or rewritten in component form

\[ D_\mu \psi_1 = \partial_\mu \psi_1 - i A^2_\mu \psi_1 \]  
(II.4a)

\[ D_\mu \psi_2 = \partial_\mu \psi_2 - i A^1_\mu \psi_2 . \]  
(II.4b)

Here, the electromagnetic four-potentials \( A^a_\mu \) \((a = 1, 2)\) are the components of the original gauge potential \( A_\mu \) with respect to some suitable basis \( \tau_\alpha \) \((\alpha = 1, \ldots, 4)\) of the \( u(2) \)-algebra

\[ A_\mu(x) = A^a_\mu(x) \tau_a = A^a_\mu(x) \tau_a + B_\mu(x) \chi - B^*_\mu(x) \bar{\chi} . \]  
(II.5)

Here, the electromagnetic generators \( \tau_a \) \((a = 1, 2)\) do commute

\[ [\tau_1, \tau_2] = 0 \]  
(II.6)

and the exchange potential \( B_\mu \) is put to zero \((\leadsto B_\mu(x) \equiv 0)\) because the two positronium constituents (i.e. electron and positron) do count as non-identical particles. Recall that the exchange effects, being mediated by the exchange potential \( B_\mu(x) \), do occur exclusively for identical particles so that \( B_\mu(x) \) is inactive for the positronium constituents \((\leadsto B_\mu(x) \equiv 0)\). Thus the bundle connection \( A_\mu(x) \) \((II.5)\) becomes reduced to its \( u(1) \oplus u(1) \) projection

\[ A_\mu(x) \Rightarrow A^a_\mu(x) \tau_a . \]  
(II.7)

2. **Dirac Equation**

For Dirac particles, which are to be described by four-spinors \( \psi_a(x) \), the Hamiltonian \( H_\mu \) in the Relativistic Schrödinger Equation \((II.1)\) obeys the relation

\[ \Pi^\mu H_\mu = MC^2 , \]  
(II.8)

where \( \Pi^\mu \) is the total velocity operator and thus is the direct sum of the Dirac matrices \( \gamma^\mu \)

\[ \Pi^\mu = (-\gamma^\mu) \oplus \gamma^\mu . \]  
(II.9)
The mass operator $\mathcal{M}$ specifies the two particle masses $M^a$ ($a = 1, 2$)

$$\mathcal{M} = i M^a \tau_a$$  \hspace{1cm} (II.10)

and is required to be Hermitian ($\mathcal{M} = \mathcal{M}^\dagger$) and covariantly constant

$$D_\mu \mathcal{M} = 0 .$$  \hspace{1cm} (II.11)

This requirement is trivially satisfied for particles of identical rest masses ($M^1 = M^2 \equiv M$) since for such a situation the mass operator becomes proportional to the identity operator

$$\mathcal{M} = M 1 .$$  \hspace{1cm} (II.12)

Thus the result is that, by virtue of the relation (II.8), the Relativistic Schrödinger Equation (II.1) becomes the two-particle Dirac equation

$$i \hbar c \Gamma^\mu D_\mu \Psi = M c^2 \Psi ,$$  \hspace{1cm} (II.13)

or in component form

$$i \hbar c \gamma^\mu D_\mu \psi_1 = - M c^2 \psi_1 ,$$  \hspace{1cm} (II.14a)

$$i \hbar c \gamma^\mu D_\mu \psi_2 = M c^2 \psi_2 ,$$  \hspace{1cm} (II.14b)

where the gauge-covariant derivatives ($D$) of the single-particle wave functions $\psi_a(x)$ are given by equations (II.4a)–(II.4b).

For identical particles, the Dirac equations (II.14a–II.14b) would couple both particles much more directly since the exchange potential $B_\mu$ is generated cooperatively by both particles and simultaneously does act back on any individual particle which then entails the phenomenon of self-coupling. However, for the present situation of non-identical particles the coupling is more indirect: any particle does generate a Dirac four-current $k_{a \mu}(x)$ ($a = 1, 2$) which is the source of the four-potential $A^a_\mu(x)$ (see below). And then this four-potential $A^a_\mu$ of the $a$-th particle acts on the wave-function $\psi_b(x)$ of the other particle ($b \neq a$) as shown by equations (II.14a–II.14b) in connection with the gauge-covariant derivatives $D$ (II.4a–II.4b).
3. Maxwell Equations

The bundle connection $A_\mu(x)$ (II.5) is itself a dynamical object of the theory (just as is the wave function $\Psi(x)$) and therefore must be required to obey some field equation. This is the (generally non-Abelian) Maxwell equation

$$\mathcal{D}^\mu F_{\mu\nu} = -4\pi i\alpha_s J_\nu$$ (II.15)

$$\left(\alpha_s \doteq \frac{e^2}{\hbar c}\right).$$

Here, the bundle curvature $F_{\mu\nu}$ is defined in terms of the bundle connection $A_\mu$ as usual, i.e.

$$F_{\mu\nu} = \nabla_\mu A_\nu - \nabla_\nu A_\mu + [A_\mu, A_\nu].$$ (II.16)

For the present situation of non-identical particles, the connection $A_\mu$ becomes reduced to its (Abelian) $u(1) \oplus u(1)$ projection, cf. (II.7), which then also holds for its curvature $F_{\mu\nu}$

$$F_{\mu\nu} \Rightarrow \nabla_\mu A_\nu - \nabla_\nu A_\mu.$$ (II.17)

Decomposing here both the curvature $F_{\mu\nu}$ and current operator $J_\mu$ with respect to the chosen basis of commuting generators $\tau_a$ ($a = 1, 2$)

$$F_{\mu\nu} \Rightarrow F_{\mu\nu}^a \tau_a$$ (II.18a)

$$J_\nu \Rightarrow i j_{\nu}^a \tau_a,$$ (II.18b)

one obtains the Maxwell equations (II.15) in component form as

$$\nabla^\mu F_{\mu\nu}^a = 4\pi \alpha_s j^a_\nu.$$ (II.19)

Since for the present Abelian situation the curvature components $F_{\mu\nu}^a$ (II.18a) are linked to the connection components $A_a^\mu$ (II.7) as usual in Maxwellian electrodynamics (in its Abelian form)

$$F_{\mu\nu}^a = \nabla_\mu A_\nu^a - \nabla_\nu A_\mu^a,$$ (II.20)
the Maxwell equations (II.19) for the field strengths $F_{\mu\nu}^a$ become converted to the d'Alembert equations for the four-potentials $A_{\mu}^a$

$$\Box A_{\mu}^a = 4\pi\alpha_s j_{\mu}^a,$$  \hspace{1cm} (II.21)

provided the gauge potentials $A_{\mu}^a$ do obey the Lorentz gauge condition

$$\nabla^{\mu} A_{\mu}^a \equiv 0 .$$  \hspace{1cm} (II.22)

4. Conservation Laws

One of the most striking features in the description of physical systems is that both classical and quantum matter do obey certain conservation laws. For the presently considered Relativistic Schrödinger Theory, as a fluid-dynamic theory, this means that there should exist certain local conservation laws, preferably concerning charge and energy-momentum. Moreover, these local laws should turn out as an immediate consequence of the basic dynamical equations, i.e. the Relativistic Schrödinger Equation (II.1) and the Maxwell equations (II.15).

In this regard, a very satisfying feature of the Relativistic Schrödinger Theory is now that such conservation laws are automatically implied by the dynamical equations themselves. In order to elaborate this briefly, consider first the conservation of total charge which as a local law reads

$$\nabla^\mu j_{\mu} \equiv 0 .$$  \hspace{1cm} (II.23)

But such a continuity equation for the total four-current $j_{\mu}$ can easily be deduced from both the matter equation (II.1) and the gauge field equations (II.15); and this fact signals the internal consistency of the RST dynamics. First, consider the gauge field dynamics (II.15) and observe here the identity

$$D^\mu D^\nu F_{\mu\nu} \equiv 0$$  \hspace{1cm} (II.24)
which holds in any flat space-time. Obviously, the combination of this identity with the Maxwell equations (II.15) yields the following continuity equation in operator form

$$D^\mu J_\mu \equiv 0.$$  \hspace{1cm} (II.25)

Decomposing here the current operator in component form yields

$$D^a j_\mu^a \equiv 0$$  \hspace{1cm} (II.26)

which furthermore simplifies to

$$\nabla^\mu j_\mu^a \equiv 0$$  \hspace{1cm} (II.27)

under the Abelian reduction (II.18a)–(II.18b). But when the individual Maxwell currents $j_\mu^a$ do obey such a continuity equation (II.27), then the total current $j_\mu$

$$j_\mu \doteq \sum_{a=1}^{2} j_\mu^a$$  \hspace{1cm} (II.28)

must also obey a continuity equation which is just the requirement (II.23).

On the other hand, we can start also from the matter dynamics (II.1) and can define the total current $j_\mu$ by

$$j_\mu \doteq \bar{\Psi} \Pi_\mu \Psi.$$  \hspace{1cm} (II.29)

The divergence of this current is

$$\nabla^\mu j_\mu = (D^\mu \bar{\Psi}) \Pi_\mu + \bar{\Psi} \Pi_\mu (D^\mu \Psi) + \bar{\Psi} (D^\mu \Pi_\mu) \Psi.$$  \hspace{1cm} (II.30)

Here, one requires that the gauge-covariant derivative of the total velocity operator $\Pi_\mu$ is covariantly constant

$$D^\mu \Pi_\mu \equiv 0,$$  \hspace{1cm} (II.31)

and furthermore one evokes the Relativistic Schrödinger equation together with the Hamiltonian condition (II.8) which then ultimately yields again the desired continuity equation.
Thus, the conservation of total charge is actually deducible from both subdynamics of the whole RST system; and this fact supports the mutual compatibility of both subdynamics (i.e. the matter dynamics (II.11) and the gauge field dynamics (II.15)).

A further important conservation law does refer to the energy-momentum content of the considered physical system. Aiming again at a local law, one may think of a continuity equation of the following form

$$\nabla \mu \left( T_{\mu \nu} \right) \equiv 0 ,$$

(II.32)

where \( T_{\mu \nu} \) is the total energy-momentum density, i.e. the sum of the Dirac matter part \( (D)T_{\mu \nu} \) and the gauge field part \( (G)T_{\mu \nu} \):

\[
(T)T_{\mu \nu} = (D)T_{\mu \nu} + (G)T_{\mu \nu} .
\]

(II.33)

Clearly, the validity of the total law (II.32) does not require an analogous law for the subdensities but merely requires the right balance of the energy-momentum exchange between the subsystems, i.e.

\[
\nabla \mu (D)T_{\mu \nu} = -\nabla \mu (G)T_{\mu \nu} .
\]

(II.34)

Indeed, the matter part has been identified as

\[
(D)T_{\mu \nu} = \frac{i\hbar c}{4} \left[ \bar{\Psi} \Gamma_{\mu} (D_{\nu} \Psi) - (D_{\nu} \bar{\Psi}) \Gamma_{\mu} \Psi + \bar{\Psi} \Gamma_{\nu} (D_{\mu} \Psi) - (D_{\mu} \bar{\Psi}) \Gamma_{\nu} \Psi \right]
\]

(II.35)

and the gauge field part by

\[
(G)T_{\mu \nu} = \frac{\hbar c}{4\pi \alpha_s} K_{\alpha\beta} \left( F_{\mu\lambda}^\alpha F_{\nu}^{\beta\lambda} - \frac{1}{4} g_{\mu\nu} F_{\sigma}^\alpha F_{\sigma}^{\beta\lambda} \right) ,
\]

(II.36)

where \( K_{\alpha\beta} \) is the fibre metric in the associated Lie algebra bundle. The (local) conservation law (II.32) comes now actually about through the mutual annihilation (II.34) of the sources of both energy-momentum densities, i.e.

\[
\nabla \mu (D)T_{\mu \nu} = -\nabla \mu (G)T_{\mu \nu} = \hbar c F_{\mu \nu} j_\mu .
\]

(II.37)
Obviously the sources of the partial densities \((D)T_{\mu\nu}\) and \((G)T_{\mu\nu}\) are just the well-known Lorentz forces in non-Abelian form.

It should now appear self-suggesting that the definition of the total energy \((E_T)\) of an RST field configuration is to be based upon the time component \((T)T_{00}\) of the energy-momentum density \((T)T_{\mu\nu}\), i.e.

\[
E_T \doteq \int d^3 \vec{r} \, (T)T_{00}(\vec{r}) .
\]  

(II.38)

But since the total density \((T)T_{\mu\nu}\) is the sum of a matter part and a gauge field part, cf. (II.33), the total energy \(E_T\) [II.38] naturally breaks up in an analogous way

\[
E_T = E_D + E_G ,
\]  

(II.39)

with the self-evident definitions

\[
E_D \doteq \int d^3 \vec{r} \, (D)T_{00}(\vec{r})
\]  

(II.40a)

\[
E_G \doteq \int d^3 \vec{r} \, (G)T_{00}(\vec{r}) .
\]  

(II.40b)

But clearly, such a preference of the time component \(T_{00}\) among all the other components \(T_{\mu\nu}\) entails the selection of a special time axis for the space-time manifold. This then induces a similar space-time splitting of all the other objects in the theory, i.e. we have to consider now stationary field configurations which are generally thought to represent the basis of the energy spectra of the bound systems.

5. Stationary Field Configurations

In the present context, the notion of stationarity is coined with regard to the time-independence of the physical observables of the theory, i.e. the physical densities and the electromagnetic fields generated by them. In contrast to this, the wave functions do not count as observables and therefore are not required to be time-independent. But their time-dependence must be in such a way that the associated densities become truly time-independent.
Gauge-Field Subsystem

The simplest space-time splitting refers to the four-potentials $A^\mu_a$, which for the stationary states become time-independent and thus appear in the following form:

$$A^\mu_a(x) \Rightarrow \left\{ (a)A_0(\vec{r}); -\vec{A}_a(\vec{r}) \right\} \quad (a = 1, 2) .$$

A similar arrangement does apply also to the Maxwell four-currents $j^\mu_a$

$$j^\mu_a \Rightarrow \left\{ (a)j_0(\vec{r}); -\vec{j}_a(\vec{r}) \right\} ,$$

so that the d’Alambert equations (II.21) become split up into the Poisson equations, for both the scalar potentials $(a)A_0(\vec{r})$

$$\Delta (a)A_0(\vec{r}) = -4\pi\alpha_s (a)j_0(\vec{r})$$

and the three-vector potentials $\vec{A}_a(\vec{r})$

$$\Delta \vec{A}_a(\vec{r}) = -4\pi\alpha_s \vec{j}_a(\vec{r}) .$$

Recall here that the standard solutions of these equations are formally given by

$$(a)A_0(\vec{r}) = \alpha_s \int d^3\vec{r}' \frac{(a)j_0(\vec{r}')}||\vec{r} - \vec{r}'||$$

$$(II.45a)\quad \vec{A}_a(\vec{r}) = \alpha_s \int d^3\vec{r}' \frac{\vec{j}_a(\vec{r}')}||\vec{r} - \vec{r}'|| .$$

Similar arguments would apply also to the exchange potential $B_\mu = \left\{ B_0, -\vec{B} \right\}$ but since we are dealing with non-identical particles the exchange potential must be put to zero ($B_\mu(x) \equiv 0$).

It is true, the particle interactions are organized here via the (electromagnetic and exchange) potentials which, according to the principle of minimal coupling, are entering
the covariant derivatives $D_\mu \psi_a$ of the wave functions $\psi_a$ as shown by equations \((\text{II.4a)}-\text{(II.4b)})$. But nevertheless it is very instructive to glimpse also at the field strengths $F^a_{\mu\nu}$. Their space-time splitting is given by

\[
\vec{E}_a = \{^{(a)}E^j\} \div \{F^a_{0j}\} \quad \text{ (II.46a)}
\]
\[
\vec{H}_a = \{^{(a)}H^j\} \div \{ \frac{1}{2} \varepsilon^{jk}_{\ l} F^a_{\ l k}\} \quad \text{ (II.46b)}
\]

and thus the \textit{linear} Maxwell equations \((\text{II.19)}) do split up in three-vector form ($a = 1, 2$) to the scalar equations for the electric fields

\[
\nabla \cdot \vec{E}_a = 4\pi \alpha_s (^{(a)}j_0) \quad \text{ (II.47)}
\]

and to the curl equations for the magnetic fields

\[
\nabla \times \vec{H}_a = 4\pi \alpha_s \vec{j}_a . \quad \text{ (II.48)}
\]

There is a pleasant consistency check for these linearized (but still relativistic) field equations in three-vector form; namely one may first link the field-strengths to the potentials in three-vector notation (cf. \((\text{II.20)}) for the corresponding relativistic link):

\[
\vec{E}_a(\vec{r}) = -\nabla (^{(a)}A_0(\vec{r})) \quad \text{ (II.49a)}
\]
\[
\vec{H}_a(\vec{r}) = \nabla \times \vec{A}_a(\vec{r}) \quad \text{ (II.49b)}
\]

and then one substitutes these three-vector field strengths into their source and curl equations \((\text{II.47)}-\text{(II.48)}). In this way one actually recovers the Poisson equations \((\text{II.43)}-\text{(II.44)}\) for the electromagnetic potentials $(^{(a)}A_0, \vec{A}_a$.\

\textit{Matter Subsystem}

Concerning now the stationary form of the matter dynamics, one resorts of course to the generally used factorization of the wave functions $\psi_a(\vec{r},t)$ into a time and a space factor

\[
\psi_a(\vec{r},t) = \exp \left[ -i \frac{Ma^2}{\hbar} t \right] \cdot \psi_a(\vec{r}) . \quad \text{ (II.50)}
\]
Here, the mass eigenvalues $M_a (a = 1, 2)$ are the proper objects to be determined from the mass eigenvalue equations which we readily put forward now. For this purpose, observe first that the Dirac four-spinors $\psi_a$ may be conceived as the direct sum of Pauli two-spinors $(a)\varphi_{\pm}$:

$$\psi_a(\vec{r}) = (a)\varphi_+(\vec{r}) \oplus (a)\varphi_-(\vec{r}) .$$  \hspace{1cm} (II.51)

Consequently, the Dirac mass eigenvalue equations (to be deduced from the general Dirac equations (II.14a)–(II.14b) by means of the factorization ansatz (II.50)) are recast to their equivalent Pauli form for the two-spinors $(a)\varphi_{\pm}(\vec{r})$

$$i \vec{\sigma} \cdot \vec{\nabla} (1)\varphi_\pm(\vec{r}) + (2)A_0(\vec{r}) \cdot (1)\varphi_\mp(\vec{r}) = \pm \frac{M_p - M_1}{\hbar} c \cdot (1)\varphi_\mp(\vec{r}) \hspace{1cm} (II.52a)$$

$$i \vec{\sigma} \cdot \vec{\nabla} (2)\varphi_\pm(\vec{r}) + (1)A_0(\vec{r}) \cdot (2)\varphi_\mp(\vec{r}) = - \frac{M_2 \pm M_e}{\hbar} c \cdot (2)\varphi_\mp(\vec{r}) . \hspace{1cm} (II.52b)$$

(Observe here that we do neglect for the moment the magnetic effects by putting the three-vector potentials $\vec{A}_a(\vec{r})$ (II.41) to zero: $\vec{A}_a(\vec{r}) \Rightarrow 0$). The mass eigenvalue for the positron (with rest mass $M_p$) is denoted by $M_1$ and for the electron (with rest mass $M_e$) by $M_2$.

Summarizing, the RST eigenvalue system consists of the mass eigenvalue equations (II.52a)–(II.52b) for the Pauli spinors $(a)\varphi_{\pm}(\vec{r})$ in combination with the Poisson equations (II.43). Since the magnetic effects are neglected, the Poisson equations (II.44) need not be considered here. But what is necessary in order to close the whole eigenvalue problem is the prescription for the link of the Pauli spinors $(a)\varphi_{\pm}(\vec{r})$ to the Maxwell charge densities $(a)j_0(\vec{r})$, or more generally to the Maxwellian four-currents $j^a_\mu$ (II.42) as the sources of the four-potentials $A^a_\mu$, cf. the d’Alembert equations (II.21). Surely, such a link between the wave functions $\psi_a$ and the currents $j^a_\mu$ will have something to do with the Dirac four-currents $k_{a\mu}$ which are usually defined by $(a = 1, 2)$

$$k_{a\mu} \Rightarrow \bar{\psi}_a \gamma_\mu \psi_a . \hspace{1cm} (II.53)$$
Indeed, a more profound scrutiny reveals the following link [33]

\[ j^1_\mu \equiv k_{1\mu} = \bar{\psi}_1 \gamma_\mu \psi_1 \]  
\[ j^2_\mu \equiv -k_{2\mu} = -\bar{\psi}_2 \gamma_\mu \psi_2. \]  

(II.54a)  

(II.54b)

The change in sign of both Dirac currents reflects the positive and negative charge of both particles. In terms of the Pauli spinors \( (a)\varphi_{\pm}(\vec{r}) \) \( (a = 1, 2) \) the space and time components of the Dirac currents read

\[ (a)k_0(\vec{r}) = (a)\varphi^\dagger_+(\vec{r}) (a)\varphi_+(\vec{r}) + (a)\varphi^\dagger_-(\vec{r}) (a)\varphi_-(\vec{r}) \]  
\[ \vec{k}_a(\vec{r}) = (a)\varphi^\dagger_+(\vec{r}) \vec{\sigma} (a)\varphi_-(\vec{r}) + (a)\varphi^\dagger_-(\vec{r}) \vec{\sigma} (a)\varphi_-(\vec{r}). \]  

(II.55a)  

(II.55b)

Although the magnetic effects, which originate from the three-currents \( \vec{k}_a(\vec{r}) \) via the magnetic Poisson equations (II.44), are neglected in the present paper these current densities nevertheless play now an important part for identifying two essentially different kinds of positronium.
In the conventional theory, the manifestation of two principally different kinds of positronium is traced back to the two possibilities of combining the spins of the electron (e) and positron (p); if both spins $s_e$ and $s_p$ add up to the total Spin $S = 1$

$$s_O = s_p + s_e = 1$$  \hspace{1cm} (III.1)

one has ortho-positronium; and zero spin

$$s_p = s_p - s_e = 0$$  \hspace{1cm} (III.2)
yields para-positronium. This is the well known ortho/para dichotomy mentioned in any textbook on relativistic quantum mechanics. In contrast to this (generally valid) composition rule for angular momenta, the ortho/para dichotomy in RST is based upon the (anti) parallelity of the Maxwellian three-currents $\vec{j}_a(\vec{r})$. Here, it is assumed that both particles do occupy physically equivalent one-particle states $\psi_a(\vec{r}) \hspace{0.5cm} (a = 1, 2)$ in the sense that the Dirac currents (and therefore also the Maxwell currents) are either parallel or antiparallel. Thus we propose the following characterization of ortho-positronium $[33]$:

$$\vec{k}_1(\vec{r}) \equiv -\vec{k}_2(\vec{r}) \doteq \vec{k}_b(\vec{r})$$  \hspace{1cm} (III.3a)

$$\vec{j}_1(\vec{r}) \equiv \vec{j}_2(\vec{r}) \doteq \vec{j}_b(\vec{r}) \equiv \vec{k}_b(\vec{r})$$  \hspace{1cm} (III.3b)

$$\vec{A}_1(\vec{r}) \equiv \vec{A}_2(\vec{r}) \doteq \vec{A}_b(\vec{r})$$  \hspace{1cm} (III.3c)

$$\vec{H}_1(\vec{r}) \equiv \vec{H}_2(\vec{r}) \doteq \vec{H}_b(\vec{r})$$  \hspace{1cm} (III.3d)

and analogously for para-positronium:

$$\vec{k}_1(\vec{r}) \equiv \vec{k}_2(\vec{r}) \doteq \vec{k}_p(\vec{r})$$  \hspace{1cm} (III.4a)

$$\vec{j}_1(\vec{r}) \equiv -\vec{j}_2(\vec{r}) \doteq \vec{j}_p(\vec{r}) \equiv \vec{k}_p(\vec{r})$$  \hspace{1cm} (III.4b)

$$\vec{A}_1(\vec{r}) \equiv -\vec{A}_2(\vec{r}) \doteq \vec{A}_p(\vec{r})$$  \hspace{1cm} (III.4c)

$$\vec{H}_1(\vec{r}) \equiv -\vec{H}_2(\vec{r}) \doteq \vec{H}_p(\vec{r})$$  \hspace{1cm} (III.4d)
The interesting point with such a subdivision of positronium into two classes is the fact that this subdivision is based upon the magnetic effects which however are neglected for the present paper; but despite this neglect the subdivision is of great relevance also for the presently considered electrostatic approximation! Namely, even within the framework of the latter approximation scheme, there do emerge different distributions of electrostatic charge \((a)k_0(\vec{r})\) for ortho- and para-positronium with corresponding quantum numbers \(\sim ortho/para\) dichotomy); and moreover there does arise also a certain ambiguity of the electric charge distribution even within the subclass of the ortho-configurations due to the same quantum number \(\sim ortho\)-dimorphism). In order to elaborate these effects it is necessary to first specify the general eigenvalue problem down to the subcases and then to look for the corresponding solutions.

1. Mass Eigenvalue Equations

The hypothesis of physically equivalent states for both positronium constituents entails that both mass eigenvalues \(M_a\) are actually identical, i.e.

\[
M_1 = -M_2 = -M_* .
\] (III.5)

Next, one considers the Maxwellian charge densities \((a)j_0(\vec{r})\) which must of course differ in sign for oppositely charged particles

\[
(1)j_0(\vec{r}) = -(2)j_0(\vec{r})
\] (III.6)

and this must be true for both ortho- and para-positronium. On the other hand, the link \((II.54a)\sim(II.54b)\) of the Maxwellian currents \(j^\alpha_\mu\) to the Dirac currents \(k_\alpha^\mu\) shows that the requirement \((II.6)\) demands the identity of the Dirac densities \((a)k_0(\vec{r})\), i.e.

\[
(1)k_0(\vec{r}) \equiv (2)k_0(\vec{r}) ,
\] (III.7)

or rewritten in terms of the Pauli spinors \((II.55a)\)

\[
(1)\varphi_+^\dagger(\vec{r}) (1)\varphi_+(\vec{r}) + (1)\varphi_-^\dagger(\vec{r}) (1)\varphi_-(\vec{r}) = (2)\varphi_+^\dagger(\vec{r}) (2)\varphi_+(\vec{r}) + (2)\varphi_-^\dagger(\vec{r}) (2)\varphi_-(\vec{r}) .
\] (III.8)

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However, the situation is different for the Dirac three-currents \( \vec{k}_a(\vec{r}) \), since they may differ in sign, cf. (III.3a) vs. (III.4a). Expressing the (anti) parallelity of both Dirac currents in terms of the Pauli spinors, cf. (II.55b), one requires

\[
(1) + (1, \vec{r}) \sigma^{(1)} (1, \vec{r}) = \mp \left\{ (2) + (2, \vec{r}) \sigma^{(2)} (2, \vec{r}) + (2, \vec{r}) \sigma^{(2)} (2, \vec{r}) \right\},
\]

where the upper/lower sign refers to the ortho/para case, resp. Both conditions (III.8) and (III.9) can be satisfied by putting

\[
\begin{align*}
(1, \vec{r}) = \mp i (2, \vec{r}) \sigma^{(2)} (2, \vec{r}) \\
(1, \vec{r}) = i (2, \vec{r}) \sigma^{(2)} (2, \vec{r})
\end{align*}
\]

where the upper/lower sign refers again to ortho/para-positronium, resp.

It is true, the disposal (III.10a)–(III.10b) satisfies both algebraic requirements (III.8) and (III.9), but additionally there must be satisfied also a differential requirement: actually, the spinor identifications (III.10a)–(III.10b) leave us with just one spinor field (i.e. \((b/p) \varphi_\pm (\vec{r})\) for ortho-positronium and \((p/b) \varphi_\pm (\vec{r})\) for para-positronium); and therefore both spinor equations (II.52a)–(II.52b) must collapse without contradiction to only one spinor equation (either for \((b/p) \varphi_\pm (\vec{r})\) or \((p/b) \varphi_\pm (\vec{r})\)). In order to validate this requirement, we have to make a disposal also for the electrostatic gauge potentials \((a)A_0(\vec{r})\). But this can easily be done by observing the link between the Dirac densities \((a)k_0(\vec{r})\) and \((a)A_0(\vec{r})\) as it is implemented by the Poisson equations (II.43). Indeed, this link entails that the potentials \((a)A_0(\vec{r})\) must differ (or not) in sign when this is (or is not) the case also for the Maxwell densities \((a)j_0(\vec{r})\). Therefore one concludes that for the positronium situation both electrostatic potentials must \emph{always} differ in sign

\[
(1) A_0(\vec{r}) = -(2) A_0(\vec{r}) \mp (b/p) A_0(\vec{r}).
\]

But when this circumstance is duly respected, both mass eigenvalue equations (II.52a)–
\[ (\text{III.52b}) \text{ actually do collapse to a single one for ortho-positronium:} \]

\[ i \vec{\sigma} \cdot \vec{\nabla} (b) \varphi_{\pm}(\vec{r}) - (b) A_0(\vec{r}) \cdot (b) \varphi_{\mp}(\vec{r}) = \frac{M_e \pm M}{\hbar} c \cdot (b) \varphi_{\mp}(\vec{r}). \]  

\text{(III.12)}

The existence of one and the same eigenvalue equation (\text{III.12}) for both ortho-positronium constituents thus validates our original hypothesis that both the electron and the positron should occupy physically equivalent states.

The relativistic pair (\text{III.12}) of Pauli equations has a single Schrödinger-like equation as its non-relativistic limit. Indeed, assuming that the “negative” Pauli-spinor \((b) \varphi_{-}(\vec{r})\) is always considerably smaller than its “positive” companion \((b) \varphi_{+}(\vec{r})\) one can solve the upper one of the equations (\text{III.12}) for \((b) \varphi_{-}(\vec{r})\) approximately in the following form:

\[ (b) \varphi_{-}(\vec{r}) \approx \frac{i \hbar}{2Mc} \vec{\sigma} \cdot \vec{\nabla} (b) \varphi_{+}(\vec{r}), \]  

\text{(III.13)}

and if this is substituted into the lower equation (\text{III.12}) one finally ends up with the following non-relativistic eigenvalue equation of the Pauli form

\[ -\frac{\hbar^2}{2M} \Delta (b) \varphi_{+}(\vec{r}) - (b) A_0(\vec{r}) \cdot (b) \varphi_{+}(\vec{r}) = E_* \cdot (b) \varphi_{+}(\vec{r}). \]  

\text{(III.14)}

Here, the non-relativistic eigenvalue \(E_*\) emerges as the difference of the rest mass \(M\) and the relativistic mass eigenvalue \(M_*\), i.e.

\[ E_* \equiv (M_* - M) c^2. \]  

\text{(III.15)}

Subsequently, we will be satisfied with clarifying the phenomenon of the ortho-dimorphism in the non-relativistic version (\text{III.14}) of the original relativistic eigenvalue equation (\text{III.12}).

But the case of para-positronium is a little bit more complicated. To begin with the positron equation (\text{II.52a}), this becomes transcribed by the identifications (\text{III.10a}–(\text{III.10b}), lower case, to the following form (para-positronium):

\[ i \vec{\sigma} \cdot \vec{\nabla} (p) \varphi_{\pm}(\vec{r}) - (p) A_0(\vec{r}) \cdot (p) \varphi_{\mp}(\vec{r}) = \frac{M_e \pm M}{\hbar} c \cdot (p) \varphi_{\mp}(\vec{r}). \]  

\text{(III.16)}
Obviously, this positron equation is just of the same form as the joint positron/electron equation (III.12) for ortho-positronium. However, the electron equation (II.52b) of para-positronium becomes transcribed by the identifications (III.10a)–(III.10b) to a somewhat different form:

\[ i \vec{\sigma} \cdot \vec{\nabla} (p) \varphi_{\pm}(\vec{r}) + (p)A_0(\vec{r}) \cdot (p)\varphi_{\mp}(\vec{r}) = -\frac{M \pm M}{\hbar} c \cdot (p)\varphi_{\mp}(\vec{r}). \]  

(III.17)

Since the sign of the potential term (\( \sim (p)A_0(\vec{r}) \)) is reversed here in comparison to the positron equation (III.16), the latter electron equation (III.17) is the ”charge conjugated” form of the first equation (III.16).

The charge conjugation is defined here by the following replacements:

\[ (p)\varphi_{+}(\vec{r}) \Rightarrow (p)\varphi_{-}(\vec{r}), \quad (p)\varphi_{-}(\vec{r}) \Rightarrow (p)\varphi_{+}(\vec{r}) \]  

(III.18a)

\[ (p)A_0(\vec{r}) \Rightarrow - (p)A_0(\vec{r}) \]  

(III.18b)

\[ M \Rightarrow - M. \]  

(III.18c)

Indeed, one is easily convinced that the two forms of eigenvalue equations (III.16) and (III.17) for para-positronium are transcribed to one another by these replacements (III.18a)–(III.18c). This means that any solution of the positron equation (III.16) can be interpreted also to be a solution of the electron equation (III.17); however, the charge conjugation does not leave invariant the Poisson equations, cf. (III.21)-(III.22) below. Therefore, we prefer here the use of solutions with the same non-relativistic limit! Indeed, it follows from both equations (III.16) and (III.17) that the “negative” Pauli spinor \( (p)\varphi_{-}(\vec{r}) \) can be approximately expressed in terms of the “positive” spinor \( (p)\varphi_{+}(\vec{r}) \) through

\[ (p)\varphi_{-}(\vec{r}) \approx \pm \frac{\hbar c}{2M} \vec{\sigma} \cdot \vec{\nabla} (p)\varphi_{+}(\vec{r}), \]  

(III.19)

where the upper case refers to (III.16) and the lower case to (III.17). This result may then be substituted in either residual equation (III.16) and (III.17) which in both cases yields the same Schrödinger-like equation for the “positive” spinor \( (p)\varphi_{+}(\vec{r}) \):

\[ -\frac{\hbar^2}{2M} \Delta (p)\varphi_{+}(\vec{r}) - \hbar c (p)A_0(\vec{r}) \cdot (p)\varphi_{+}(\vec{r}) = E \cdot (p)\varphi_{+}(\vec{r}). \]  

(III.20)
Thus it becomes again evident that the corresponding solutions of (III.16) and (III.17) do actually describe physically equivalent states. The notion of “physical equivalence” is meant here to refer in first line to the numerical identity of the energy being carried by anyone of the constituents of para-positronium, see below.

2. Poisson Equations

The mass eigenvalue equations do not yet represent a closed system and therefore cannot be solved before an equation for the interaction potential \((b/p) A_0(\vec{r})\) has been specified. On principle, this has already been done in form of equation (II.43) so that we merely have to further specify that equation in agreement with the ortho/para dichotomy. Observing here the circumstance that the Maxwellian current of the first particle \((a = 1, \text{ positron})\) agrees with the Dirac current, cf. (II.54a) and (II.55a), the Poisson equation (II.43) reads in terms of the Pauli spinors

\[
\Delta \frac{(b/p)}{A_0(\vec{r})} = -4\pi \alpha_s \left\{ (b/p) \varphi_+^\dagger(\vec{r}) (b/p) \varphi_+(\vec{r}) + (b/p) \varphi_-^\dagger(\vec{r}) (b/p) \varphi_- (\vec{r}) \right\}.
\]

This Poisson equation closes the relativistic eigenvalue systems, both for ortho-positronium (III.12) and for para-positronium (III.16)–(III.17). For the non-relativistic limit, one merely suppresses the “negative” Pauli spinors \((b/p) \varphi_-(\vec{r})\) so that the relativistic Poisson equations (III.21) simplify to

\[
\Delta \frac{(b/p)}{A_0(\vec{r})} = -4\pi \alpha_s \left\{ (b/p) \varphi_+^\dagger(\vec{r}) (b/p) \varphi_+(\vec{r}) \right\}
\]

which then closes both the non-relativistic eigenvalue equations (III.14) for ortho-positronium and (III.20) for para-positronium.

Clearly, these coupled systems of eigenvalue and Poisson equations cannot be solved exactly (though exact solutions do surely exist), and consequently we have to resort to some adequate approximation procedure. But this suggests itself when we subsequently will establish the variational principle of minimal energy.
3. Non-Unique Spinor Fields

Despite the fact that we originally subdivided the whole set of positronium configurations into two subclasses, i.e. ortho- and para-positronium (III.3a–(III.4d), it may seem now that by the neglection of the magnetic forces we ended up with an eigenvalue problem, which does no longer offer any handle for sticking to that original subdivision into two peculiar subsets. Indeed, the adopted electrostatic approximation does admit exclusively an interaction force of the purely electric type (being described by the electric potential \( (b/p)A_0(\vec{r}) \)), whereas the original ortho/para dichotomy was based upon the three-currents \( \vec{k}_a(\vec{r}) \) as the curls of the magnetic fields, cf. (II.48). As a result of this neglection of magnetism, the Poisson equation (III.21), or (III.22), resp., holds equally well for both the ortho-configurations (b) and the para-configurations (p). But also the mass eigenvalue equations, especially in their non-relativistic forms (III.14) and (III.20) are formally the same for ortho- and para-positronium. Does this mean that, through passing over to the electrostatic approximation, the difference between ortho- and para-positronium has gone lost? This is actually not the case because the difference of total angular momentum (in combination with the hypothesis of the physical equivalence of both constituent states) leaves its footprint also on the electrostatic approximation.

The crucial point here refers to the fluid-dynamic character of RST, as opposed to the probabilistic character of the conventional quantum theory. This entails that in RST the angular momenta of the subsystems cannot be combined (to the total angular momentum of the whole system) in such a way as it is the case in the conventional theory (\( \Rightarrow \) addition theorem for angular momenta). More concretely: if we wish to insist on the viewpoint that the (observable) angular momentum of the considered two-particle system should emerge as the eigenvalue \( j_z \) of the angular momentum operator \( \hat{J}_z = \hat{L}_z + \hat{S}_z \), i.e.

\[
\hat{J}_z \Psi_{b/p}(\vec{r}) = (b/p)j_z \hbar \cdot \Psi_{b/p}(\vec{r}) ,
\]

then the quantum number \( (b/p)j_z \) due to the whole two-particle system must be carried
already by any individual particle! Namely, the wave function $\Psi_{b/p}(\vec{r})$ refers here to the two-particle system as a whole and thus, according to the RST philosophy, is to be conceived as the direct (Whitney) sum of the one-particle constituent wave functions $\psi_a(\vec{r})$ ($a = 1, 2$)

$$\Psi_{b/p}(\vec{r}) = (b/p)\psi_1(\vec{r}) \oplus (b/p)\psi_2(\vec{r}) . \quad \text{(III.24)}$$

According to this sum structure, the total angular momentum $\hat{J}_z$ is also the sum of the individual angular momenta

$$\hat{J}_z = (^{(1)}\hat{J}_z) \oplus (^{(2)}\hat{J}_z) . \quad \text{(III.25)}$$

Therefore the eigenvalue equations (III.23) for the total angular momentum $\hat{J}_z$ can be decomposed as follows

$$\hat{J}_z \Psi_{b/p}(\vec{r}) = (^{(1)}\hat{J}_z \psi_1(\vec{r})) \oplus (^{(2)}\hat{J}_z \psi_2(\vec{r})) . \quad \text{(III.26)}$$

Consequently both one-particle spinors $\psi_1(\vec{r})$ and $\psi_2(\vec{r})$ must obey the same eigenvalue equation as the total wave function (III.24), i.e.

$$^{(1)}\hat{j}_z (b/p)\psi_1(\vec{r}) = (b/p)\hat{j}_z \hbar \cdot (b/p)\psi_1(\vec{r}) \quad \text{(III.27a)}$$

$$^{(2)}\hat{j}_z (b/p)\psi_2(\vec{r}) = (b/p)\hat{j}_z \hbar \cdot (b/p)\psi_2(\vec{r}) . \quad \text{(III.27b)}$$

Furthermore, the Dirac four-spinors $\psi_a(\vec{r})$ can also be conceived as the direct sum of Pauli two-spinors $^{(a)}\varphi_+ (\vec{r})$ and $^{(a)}\varphi_- (\vec{r})$, i.e.

$$\psi_a(\vec{r}) = ^{(a)}\varphi_+(\vec{r}) \oplus ^{(a)}\varphi_- (\vec{r}) . \quad \text{(III.28)}$$

Therefore the same eigenvalue equation must also hold for the individual Pauli spinors, especially after those identifications (III.10a)–(III.10b):

$$^{(+)\hat{j}_z} (b/p)\varphi_+ (\vec{r}) = (b/p)\hat{j}_z \hbar \cdot (b/p)\varphi_+ (\vec{r}) \quad \text{(III.29a)}$$

$$^{(-)\hat{j}_z} (b/p)\varphi_- (\vec{r}) = (b/p)\hat{j}_z \hbar \cdot (b/p)\varphi_- (\vec{r}) . \quad \text{(III.29b)}$$
This means mathematically that the eigenvalue \((b/p)j_z\) of the two-particle state \(\Psi_{b/p}\) becomes transferred to any individual Pauli component of this two-particle state! In physical terms, the bosonic or fermionic character of the two-particle state \(\Psi\) becomes thus incorporated in any individual constituent of the two-particle system.

But now it is clear that positronium as a whole carries bosonic properties \((\sim j_z\) is integer-valued); and this must therefore hold also for any Pauli constituent \((^a)\varphi_\pm(\vec{r})\) of both particles \((a = 1, 2)\), cf. (III.29a)–(III.29b). On the other hand, it is well known that the Pauli spinors do form a half-integer representation of the rotation group \(\text{SO}(3)\).

This means that one can select in any two-dimensional spinor space a certain spinor basis \(\{\zeta^{j, m}\}\) with the following eigenvalue properties:

\[
\begin{align*}
\hat{J}^2 \zeta^{j, m} &= j(j + 1)\hbar^2 \zeta^{j, m} \\
\hat{J}_z \zeta^{j, m} &= m\hbar \zeta^{j, m} \\
\hat{L}^2 \zeta^{j, m} &= \ell(\ell + 1)\hbar^2 \zeta^{j, m} \\
\hat{S}^2 \zeta^{j, m} &= s(s + 1)\hbar^2 \zeta^{j, m}.
\end{align*}
\]

(III.30a) (III.30b) (III.30c) (III.30d)

Here the electron/positron spin is \(s = \frac{1}{2}\); the orbital angular momentum is \(\ell = 0, 1, 2, 3, \ldots\) and thus the lowest possible value of \(j(=\ell \pm s)\) is \(j = \frac{1}{2}\) with \(\ell = 0\) or \(\ell = 1\). Therefore we have two basis systems for \(j = \frac{1}{2}\), namely \(\{\zeta^{\frac{1}{2}, \frac{1}{2}}_0; \zeta^{\frac{1}{2}, -\frac{1}{2}}_0\}\) and \(\{\zeta^{\frac{1}{2}, \frac{1}{2}}_1; \zeta^{\frac{1}{2}, -\frac{1}{2}}_1\}\).

**Fermionic States**

The existence of these two basis systems admits us to decompose now a fermionic state in the following way

\[
\begin{align*}
(^a)\varphi_+(\vec{r}) &= (^a)\mathcal{R}_+(\vec{r}) \cdot \zeta^{\frac{1}{2}, \frac{1}{2}}_0 + (^a)\mathcal{S}_+(\vec{r}) \cdot \zeta^{\frac{1}{2}, -\frac{1}{2}}_0 \\
(^a)\varphi_-(\vec{r}) &= -i \left\{ (^a)\mathcal{R}_-(\vec{r}) \cdot \zeta^{\frac{1}{2}, \frac{1}{2}}_1 + (^a)\mathcal{S}_-(\vec{r}) \cdot \zeta^{\frac{1}{2}, -\frac{1}{2}}_1 \right\}.
\end{align*}
\]

(III.31a) (III.31b)
The action of the angular momentum operator $\hat{J}_z$ on such a fermionic state is obviously

$$
\hat{J}^{(+)}_{z} (a) \varphi_{+}(\vec{r}) = \left( \hat{L}_{z} (a) \mathcal{R}_{+}(\vec{r}) \right) \cdot \zeta_{\frac{1}{4}, \frac{1}{4}} + \left( \hat{L}_{z} (a) \mathcal{S}_{+}(\vec{r}) \right) \cdot \zeta_{0, \frac{1}{2}} + \left( \hat{J}^{(+)}_{z} \zeta_{\frac{1}{4}, \frac{1}{4}} \right) \cdot \zeta_{0, \frac{1}{2}} + \left( \hat{L}_{z} - \frac{\hbar}{2} \right) (a) \mathcal{S}_{+}(\vec{r}) \cdot \zeta_{0, \frac{1}{2}} \tag{III.32a}
$$

$$
\hat{J}^{(-)}_{z} (a) \varphi_{-}(\vec{r}) = -i \left( \hat{L}_{z} (a) \mathcal{R}_{-}(\vec{r}) \right) \cdot \zeta_{\frac{1}{4}, \frac{1}{4}} - i \left( \hat{L}_{z} (a) \mathcal{S}_{-}(\vec{r}) \right) \cdot \zeta_{\frac{1}{4}, \frac{1}{4}} - i \left( \hat{J}^{(-)}_{z} \zeta_{\frac{1}{4}, \frac{1}{4}} \right) \cdot \zeta_{\frac{1}{4}, \frac{1}{4}} - i \left( \hat{L}_{z} - \frac{\hbar}{2} \right) (a) \mathcal{S}_{-}(\vec{r}) \cdot \zeta_{\frac{1}{4}, \frac{1}{4}} \tag{III.32b}
$$

The required results (III.29a)–(III.29b) of the action of the angular momentum operator $\hat{J}_z$ on the Pauli spinors $(a)\varphi_{\pm}(\vec{r})$ (with $a = 1, 2$ or $a = b/p$) are now deducible from the present equations (III.32a)–(III.32b) by making the following arrangements:

$$
\hat{L}_{z} (a) \mathcal{R}_{\pm}(\vec{r}) = \ell_{z} \hbar \cdot (a) \mathcal{R}_{\pm}(\vec{r}) \tag{III.33a}
$$

$$
\hat{L}_{z} (a) \mathcal{S}_{\pm}(\vec{r}) = (\ell_{z} + 1) \hbar \cdot (a) \mathcal{S}_{\pm}(\vec{r}) \tag{III.33b}
$$

Indeed, with these disposals the equations (III.32a)–(III.32b) adopt the required form of the eigenvalue equations (III.29a)–(III.29b) with the eigenvalue of angular momentum being found as

$$
(a)j_{z} = \ell_{z} + \frac{1}{2} \tag{III.34}
$$

Since the quantum number of orbital angular momentum is adopted as integer ($\ell_{z} = 0, \pm 1, \pm 2, \pm 3, \ldots$), we actually end up with half-integer quantum numbers $(a)j_{z}$ (III.34) for fermionic states!

These fermionic states can obviously be realized by use of unique amplitude fields $(a)\mathcal{R}_{\pm}(\vec{r})$, $(a)\mathcal{S}_{\pm}(\vec{r})$ and also unique spinor basis fields $\zeta_{\frac{1}{4}, \frac{1}{4}}$, $\zeta_{\frac{1}{4}, \frac{1}{4}}$. Evidently, the latter fields work as the carriers of the spin, whereas the amplitude fields do contribute the orbital angular momentum. If this philosophy is tried also for the bosonic states we are forced to give up the uniqueness of the spinor basis!
Joining here the general conviction that bosonic states should have integer quantum numbers \( (a) j_z \) (III.29a)–(III.29b), i.e. \( (a) j_z = 0, \pm 1, \pm 2, \pm 3, \ldots \), it suggests itself to think that the amplitude fields should furthermore carry integer quantum numbers \( (\ell) z \) of orbital angular momentum; i.e. such equations as (III.33a)–(III.33b) should persist also for the bosonic states. Thus the necessary modification must refer to the basis spinor fields \( \zeta_{j, m} \) (III.30a)–(III.30d). More concretely, we think of four basis spinor fields \( \zeta_{0,0}^{(+)} \), \( \zeta_{0,0}^{(-)} \), \( \zeta_{1,0}^{(+)} \), \( \zeta_{1,0}^{(-)} \) for para-positronium which obey the following eigenvalue equations

\[
\hat{J}_z^{(+)} \zeta_{0,0}^{(+)} = \zeta_{0,0}^{(+)} = \hat{J}_z^{(-)} \zeta_{1,0}^{(+)} = \hat{J}_z^{(-)} \zeta_{1,0}^{(-)} = 0 ;
\]

(III.35)

and similarly for ortho-positronium one wishes to work with a spinor basis \( \eta_{0,0}^{(+)}, \eta_{0,0}^{(-)}, \eta_{1,0}^{(+)}, \eta_{1,0}^{(-)} \) of the following kind:

\[
\hat{J}_z^{(+)} \eta_{0,0}^{(+)} = \hbar \eta_{0,0}^{(+)} \quad \text{(III.36a)}
\]
\[
\hat{J}_z^{(+)} \eta_{0,0}^{(-)} = -\hbar \eta_{0,0}^{(-)} \quad \text{(III.36b)}
\]
\[
\hat{J}_z^{(-)} \eta_{1,0}^{(+)} = \hbar \eta_{1,0}^{(+)} \quad \text{(III.36c)}
\]
\[
\hat{J}_z^{(-)} \eta_{1,0}^{(-)} = -\hbar \eta_{1,0}^{(-)} \quad \text{(III.36d)}
\]

This says that for the para-case (III.35) the spins \( s_a \) \( (a = 1, 2) \) do combine to zero spin quantum number \( s_P \) of the para-type \( s_P \div s_1 - s_2 = 0, s_1 = s_2 = \frac{1}{2} \); whereas for the ortho-case (III.36a)–(III.36d) the individual spins combine to unity \( s_O \div s_1 + s_2 = 1 \). Thus both basis systems (III.35) and (III.36a)–(III.36d) carry integer spin and therefore may be used for the corresponding decomposition of the Pauli spinors \( (a) \varphi_{\pm}(\vec{r}) \) due to a bound two-particle system.

For para-positronium \( s_P = 0 \) one has now in place of the fermionic situation (III.31a)–(III.31b) the following decomposition

\[
^{(p)} \varphi_+^{(+)}(\vec{r}) = (p) \mathcal{R}_+(\vec{r}) \cdot \xi_0^{(+)} + (p) \mathcal{S}_+(\vec{r}) \cdot \xi_0^{(-)}
\]

(III.37a)

\[
^{(p)} \varphi_-^{(+)}(\vec{r}) = -i \left\{ (p) \mathcal{R}_-(\vec{r}) \cdot \xi_1^{(+)} + (p) \mathcal{S}_-(\vec{r}) \cdot \xi_1^{(-)} \right\} .
\]

(III.37b)
Here, the action of the angular momentum operator $\hat{J}_z$ looks now as follows

$$
\hat{J}_z^+ (p) \varphi_+ (\vec{r}) = \left( \hat{L}_z (p) \mathcal{R}_+ (\vec{r}) \right) \cdot \xi_0^{(+)} + \left( \hat{L}_z (p) \mathcal{S}_+ (\vec{r}) \right) \cdot \xi_0^{(-)} \quad \text{(III.38a)}
$$

$$
\hat{J}_z^- (p) \varphi_- (\vec{r}) = -i \left( \hat{L}_z (p) \mathcal{R}_- (\vec{r}) \right) \cdot \xi_1^{(+)} - i \left( \hat{L}_z (p) \mathcal{S}_- (\vec{r}) \right) \cdot \xi_1^{(-)}. \quad \text{(III.38b)}
$$

Consequently in order to satisfy again the para-form $(p)$ of the eigenvalue equations \((\text{III.29a}−\text{III.29b})\) one puts here

$$
\hat{L}_z (p) \mathcal{R}_\pm (\vec{r}) = \ell_z \hbar \cdot (p) \mathcal{R}_\pm (\vec{r}) \quad \text{(III.39a)}
$$

$$
\hat{L}_z (p) \mathcal{S}_\pm (\vec{r}) = \ell_z \hbar \cdot (p) \mathcal{S}_\pm (\vec{r}), \quad \text{(III.39b)}
$$

so that the quantum number $(p)j_z \ (\text{III.29a}−\text{III.29b})$ is solely due to orbital angular momentum:

$$
(p)j_z \equiv \ell_z \quad \text{(III.40)}
$$

$$(\ell_z = 0, \pm 1, \pm 2, \pm 3, \ldots)$$

For ortho-positronium $(s_O = 1)$, the situation is somewhat different. First, the decomposition of the ortho-spinors $(b)\varphi_\pm (\vec{r})$ looks quite similar to the para-case \((\text{III.37a}−\text{III.37b})\):

$$
(b)\varphi_+ (\vec{r}) = (b)\mathcal{R}_+ (\vec{r}) \cdot \eta_0^{(+)} + (b)\mathcal{S}_+ (\vec{r}) \cdot \eta_0^{(-)} \quad \text{(III.41a)}
$$

$$
(b)\varphi_- (\vec{r}) = -i \left\{ (b)\mathcal{R}_- (\vec{r}) \cdot \eta_1^{(+)} + (b)\mathcal{S}_- (\vec{r}) \cdot \eta_1^{(-)} \right\}. \quad \text{(III.41b)}
$$

But the action of the angular momentum operator $\hat{J}_z^\pm$ on these ortho-states looks now as follows

$$
\hat{J}_z^+ (b) \varphi_+ (\vec{r}) = \left[ \left( \hat{L}_z + \hbar \right) (b)\mathcal{R}_+ (\vec{r}) \right] \cdot \eta_0^{(+)} + \left[ \left( \hat{L}_z - \hbar \right) (b)\mathcal{S}_+ (\vec{r}) \right] \cdot \eta_0^{(-)} \quad \text{(III.42a)}
$$

$$
\hat{J}_z^- (b) \varphi_- (\vec{r}) = -i \left\{ \left[ \left( \hat{L}_z + \hbar \right) (b)\mathcal{R}_- (\vec{r}) \right] \cdot \eta_1^{(+)} + \left[ \left( \hat{L}_z - \hbar \right) (b)\mathcal{S}_- (\vec{r}) \right] \cdot \eta_1^{(-)} \right\}. \quad \text{(III.42b)}
$$
For satisfying here again the eigenvalue requirement (III.29a)–(III.29b) in its ortho-form (b) one puts in a self-evident way
\[
\hat{L}_z^{(b)R_\pm} = \ell_z \hbar \cdot (b) R_\pm \\
\hat{L}_z^{(b)S_\pm} = (\ell_z + 2) \hbar \cdot (b) S_\pm.
\]
This arrangement yields then the following eigenvalue equations for the ortho-spinors
\[
\hat{J}_z^{(b)} \varphi_\pm (\vec{r}) = (\ell_z + 1) \hbar \cdot (b) \varphi_\pm (\vec{r}).
\]
Thus one finds the quantum numbers of the ortho-system:
\[
^{(b)}j_z = \ell_z + 1
\]
\[
^{(b)}j_z = 0, \pm 1, \pm 2, \pm 3, \ldots.
\]

For a realization of the required basis spinors one takes the fermionic basis \( \{ \zeta_{\frac{1}{2} \pm \frac{1}{2}}, \zeta_{\frac{1}{2} \mp \frac{1}{2}} \} \) as the point of departure and introduces a general spinor basis \( \{ \omega_0^{(+)}, \omega_0^{(-)}, \omega_1^{(+)}, \omega_1^{(-)} \} \) through
\[
\omega_0^{(+)} = e^{-ib\phi} \cdot \zeta_{\frac{1}{2} \pm \frac{1}{2}}
\]
\[
\omega_0^{(-)} = e^{ib\phi} \cdot \zeta_{\frac{1}{2} \mp \frac{1}{2}}
\]
\[
\omega_1^{(+)} = e^{-ib\phi} \cdot \zeta_{\frac{3}{2} \pm \frac{1}{2}}
\]
\[
\omega_1^{(-)} = e^{ib\phi} \cdot \zeta_{\frac{3}{2} \mp \frac{1}{2}}.
\]
Here it is easy to see emerging the following relations concerning angular momentum
\[
\hat{J}_z^{(+)} \omega_0^{(+)} = - \left( b - \frac{1}{2} \right) \hbar \cdot \omega_0^{(+)}
\]
\[
\hat{J}_z^{(+)} \omega_0^{(-)} = \left( b - \frac{1}{2} \right) \hbar \cdot \omega_0^{(-)}
\]
\[
\hat{J}_z^{(-)} \omega_1^{(+)} = - \left( b - \frac{1}{2} \right) \hbar \cdot \omega_1^{(+)}
\]
\[
\hat{J}_z^{(-)} \omega_1^{(-)} = \left( b - \frac{1}{2} \right) \hbar \cdot \omega_1^{(-)}.
\]
Obviously, this \( \omega \)-basis contains some free parameter \( \tilde{b} \) (i.e. the boson number) and if this is chosen as \( \tilde{b} = \frac{1}{2} \) we obtain the desired \( \xi \)-basis (III.35) for para-positronium; and if \( \tilde{b} \) is chosen as \( \tilde{b} = -\frac{1}{2} \) we obtain the \( \eta \)-basis (III.36a)–(III.36d) for ortho-positronium. For \( \tilde{b} = 0 \) we get back the purely fermionic \( \zeta \)-basis (III.30a)–(III.30d).

With the choice of the \( \omega \)-basis (III.46a)–(III.46d) the loss of uniqueness becomes now evident: since the original \( \zeta \)-basis (III.30a)–(III.30d) is unique (i.e. the \( \zeta_j^m(\vartheta, \phi) \) constitute a "unique" spinor field on the 2-sphere \( S^2 \)), the other two basis systems \( \xi \) (III.35) and \( \eta \) (III.36a)–(III.36d) are double-valued. More concretely, for both the \( \xi \)- and the \( \eta \)-basis \((\sim \tilde{b} = \pm \frac{1}{2})\) one finds by performing one revolution around the \( z \)-axis \((0 \leq \phi \leq 2\pi)\):

\[
\xi_{0,1}^{(\pm)}(\phi + 2\pi) = e^{\pm i\pi} \xi_{0,1}^{(\pm)}(\phi) = -\xi_{0,1}^{(\pm)}
\]

(III.48a)

\[
\eta_{0,1}^{(\pm)}(\phi + 2\pi) = e^{\pm i\pi} \eta_{0,1}^{(\pm)}(\phi) = -\eta_{0,1}^{(\pm)},
\]

(III.48b)

and this says that we need two revolutions around the \( z \)-axis \((0 \leq \phi \leq 4\pi)\) in order to return to the original basis configurations. Since we adopt all the amplitude fields \((b/p)R_{\pm}(\vec{r}), (b/p)S_{\pm}(\vec{r})\) to be unique scalar fields, the double-valuedness of the para- and ortho-basis becomes transferred to the para-spinors \((p,\varphi_{\pm}(\vec{r})\) (III.37a)–(III.37b) and ortho-spinors \((b,\varphi_{\pm}(\vec{r})\) (III.41a)–(III.41b) and from here ultimately to the Dirac spinors \(\Psi_P, \Sigma\)

\[
\Psi_P(\vec{r}) = (p,\varphi_+)(\vec{r}) \oplus (p,\varphi_-)(\vec{r})
\]

(III.49a)

\[
\Psi_\Sigma(\vec{r}) = (b,\varphi_+)(\vec{r}) \oplus (b,\varphi_-)(\vec{r}).
\]

(III.49b)

Summarizing, the Dirac wave functions \(\Psi_P(\vec{r})\) and \(\Psi_\Sigma(\vec{r})\) for ortho- and para-positronium must in RST be double-valued in the following sense:

\[
\Psi_P(r, \vartheta, \phi + 2\pi) = -\Psi_P(r, \vartheta, \phi)
\]

(III.50a)

\[
\Psi_\Sigma(r, \vartheta, \phi + 2\pi) = -\Psi_\Sigma(r, \vartheta, \phi).
\]

(III.50b)
Uniqueness of the Physical Densities

Naturally, in a fluid-dynamic theory (such as the present RST) the proper observable objects are the physical densities, such as those of charge, current, energy, linear and angular momentum, etc. A plausible condition on these densities is surely given by the demand that these physical densities should be single-valued tensor fields. But, as we will readily demonstrate, this condition can be satisfied also by non-unique wave functions; and this fact allows us to actually deal with such non-unique wave functions, as given for example by the double-valued positronium states (III.50a)–(III.50b). Therefore one wishes to have some condition on the wave functions which on the one hand admits their non-uniqueness but on the other hand ensures the uniqueness of the associated physical densities!

Now according to the present RST philosophy, the non-uniqueness of the (Dirac) wave functions is to be traced back to the spinor basis, whereas the amplitude fields are furthermore required to be unique. Therefore the non-uniqueness of the wave functions is measured by the boson number \( \tilde{b} \), cf. (III.46a)–(III.46d); and thus the condition of uniqueness of the densities is to be retraced to some condition for the fixation of the boson number \( \tilde{b} \). Such a fixation may be attained now by considering specifically the Dirac density \( \langle a \rangle k_0 (\vec{r}) \) and the three-current \( \vec{k}_a (\vec{r}) \) which read in terms of the Pauli spinors \( \langle a \rangle \varphi_\pm (\vec{r}) \) as shown by equations (II.55a)–(II.55b). Decomposing these Pauli spinors with respect to the \( \omega \)-basis (III.46a)–(III.46d) lets then appear the (Dirac) charge densities (II.55a) in the following form:

\[
\langle a \rangle k_0 (\vec{r}) = \frac{\langle a \rangle \vec{R}_+ \cdot \langle a \rangle \vec{R}_+ + \langle a \rangle \vec{S}_+ \cdot \langle a \rangle \vec{S}_+ + \langle a \rangle \vec{R}_- \cdot \langle a \rangle \vec{R}_- + \langle a \rangle \vec{S}_- \cdot \langle a \rangle \vec{S}_-}{4\pi}.
\]

Evidently, these charge densities are unique in any case and therefore do not yet provide an immediate handle for fixing the parameter \( \tilde{b} \).

This situation changes now when one considers also the Dirac currents \( \vec{k}_a \) (III.55b), which by their very definitions are always real-valued objects:

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\[(a)\kappa_r = \frac{i}{4\pi} \left\{ (a)\mathcal{R}_+ \cdot (a)\mathcal{R}_- + (a)\mathcal{S}_+ \cdot (a)\mathcal{S}_- - (a)\mathcal{R}_- \cdot (a)\mathcal{R}_+ - (a)\mathcal{S}_- \cdot (a)\mathcal{S}_+ \right\} \quad (\text{III.52a})\]

\[(a)\kappa_\phi = -\frac{i}{4\pi} \left\{ e^{2i(b-\frac{1}{2})\phi} \cdot \mathcal{C}_{(a)} - e^{-2i(b-\frac{1}{2})\phi} \cdot \mathcal{C}_{(a)}^* \right\} \quad (\text{III.52b})\]

\[(a)\kappa_\phi = \sin \frac{\vartheta}{4\pi} \left\{ (a)\mathcal{R}_+ \cdot (a)\mathcal{R}_- + (a)\mathcal{S}_+ \cdot (a)\mathcal{S}_- - (a)\mathcal{S}_- \cdot (a)\mathcal{S}_+ \right\} - \cos \frac{\vartheta}{4\pi} \left\{ e^{2i(b-\frac{1}{2})\phi} \cdot \mathcal{C}_{(a)} + e^{-2i(b-\frac{1}{2})\phi} \cdot \mathcal{C}_{(a)}^* \right\}. \quad (\text{III.52c})\]

But here a nearby restriction upon the parameter \(b\) suggests itself, namely through the plausible demand that the Dirac currents \(\vec{k}_a\) (II.55b), with their components being specified by \text{III.52a}–\text{III.52c}, must be \text{unique} (!) vector fields over three-space (albeit only apart from the origin \(r = 0\) and the \(z\) axis \(\vartheta = 0, \pi\)). Evidently this demand of uniqueness reads in terms of the spherical polar coordinates \(\{r, \vartheta, \phi\}\)

\[
\vec{k}_a(r, \vartheta, \phi + 2\pi) = \vec{k}_a(r, \vartheta, \phi),
\]

and thus the values of \(b\) become restricted to the range

\[
b = \frac{1}{2} (n + 1) \quad (n = 0, \pm1, \pm2, \pm3, \ldots)
\]

which then entails also \text{(half-)integer} quantum numbers for the \(z\) component of the angular momentum \text{III.47a}–\text{III.47d} of the spinor basis:

\[
s_z = \pm \left( b - \frac{1}{2} \right) = \pm \frac{n}{2}. \quad (\text{III.55})
\]

Here it will suffice to admit for the spinor basis (of the two-particle systems) exclusively the values \(b = \pm \frac{1}{2}\); other values of \(b\) come into play for bound systems of more than two fermions.

Notice here that this \text{(half-)integrity} arises as a consequence of the demand of uniqueness with respect to certain physical \text{densities} (i.e. Dirac current), whereas the corresponding \text{integral} quantum numbers of conventional non-relativistic quantum mechanics.
are mostly traced back in the textbooks to the uniqueness requirement for the wave functions themselves (not the densities). The lowest values of $s_z$ (III.55) are $s_z = \pm \frac{1}{2}$ for $\tilde{b} = 0$ and $s_z = 0, \pm 1$ for $\tilde{b} = \pm \frac{1}{2}$. Thus for the first case ($\tilde{b} = 0$) we have a fermionic basis and for the second case ($\tilde{b} = \pm \frac{1}{2}$) one deals with a bosonic basis. In this sense, a Dirac particle is said to occupy a fermionic quantum state $\psi$ if the “boson number” $\tilde{b}$ of its spinor basis is zero ($\tilde{b} = 0$), and a bosonic quantum state if the boson number $\tilde{b}$ equals $\pm \frac{1}{2}$. Observe that through this arrangement the fermionic or bosonic character of the quantum state of a Dirac particle is defined by reference to the corresponding spinor basis.
IV Ortho-Positronium \((b = -\frac{1}{2})\)

After the general RST logic for the occurrence of the ortho/para dichotomy is sufficiently displayed, we will now turn (for the remainder of the paper) to ortho-positronium. For this specific two-particle system there occurs a further ambiguity, i.e. the “ortho-dimorphism”, which is not present in the para-configuration. The effect of dimorphism consists in the circumstance that the angular momentum quantization admits the emergence of two different charge distributions \({^b}k_0(\vec{r})\) which, however, are both due the same configuration of quantum numbers! Since these two electrostatic charge distributions are differing slightly, they carry a slightly different electrostatic interaction energy, and this causes a slightly different binding energy. In this way, ortho-positronium does appear in RST in form of electrostatic doublets. Observe here that, for our subsequent discussion of this ortho-dimorphism, we will be satisfied with the electrostatic approximation, where magnetic effects are neglected completely!

1. Mass Eigenvalue Equations for the Amplitude Fields

The point of departure for our quantization of angular momentum is the mass eigenvalue equation (III.12) in Pauli form. Here, we will adopt for the moment the spherically symmetric approximation where the interaction potential \({^b}A_0(\vec{r})\) appears to be spherically symmetric (i.e. \({^b}A_0(\vec{r}) \Rightarrow {^b}A_0(r), r = ||\vec{r}||\)). For this situation, the amplitude fields \({^b}\mathcal{R}_\pm, {^b}\mathcal{S}_\pm\) (III.41a)–(III.41b) can be assumed to be the product of a purely angular-dependent factor and a purely radial factor which then entails the splitting of the original eigenvalue system into a purely angular and a purely radial problem. As usual, the solution of the radial problem yields then the energy spectrum (i.e. quantization of energy).

To begin with, one inserts the decomposition of the Pauli spinors \({^b}\varphi_{\pm}(\vec{r})\) (III.41a)–(III.41b) into the Pauli equations (III.12) and thereby obtains the following system of
eigenvalue equations for the amplitude fields \((b)\mathcal{R}_\pm(r, \vartheta, \phi), (b)\mathcal{S}_\pm(r, \vartheta, \phi)\) \[\text{(IV.1a)}\]

\[
\frac{\partial (b)\mathcal{R}_+}{\partial r} + \frac{i}{r} \frac{\partial (b)\mathcal{R}_+}{\partial \phi} - \frac{1}{2r} (b)\mathcal{R}_+ - (b)A_0 \cdot (b)\mathcal{R}_- \\
e^{-2i\phi} \left\{ \frac{1}{r} \frac{\partial (b)\mathcal{S}_+}{\partial \vartheta} - \frac{\cot \vartheta}{r} \cdot \left[ \frac{1}{2} (b)\mathcal{S}_+ + i \frac{\partial (b)\mathcal{S}_+}{\partial \phi} \right] \right\} = \frac{M + M_*}{\hbar} c \cdot (b)\mathcal{R}_-
\]

\[
\frac{\partial (b)\mathcal{S}_+}{\partial r} - \frac{i}{r} \frac{\partial (b)\mathcal{S}_+}{\partial \phi} - \frac{1}{2r} (b)\mathcal{S}_+ - (b)A_0 \cdot (b)\mathcal{S}_- \\
e^{2i\phi} \left\{ \frac{1}{r} \frac{\partial (b)\mathcal{R}_+}{\partial \vartheta} - \frac{\cot \vartheta}{r} \cdot \left[ \frac{1}{2} (b)\mathcal{R}_+ - i \frac{\partial (b)\mathcal{R}_+}{\partial \phi} \right] \right\} = \frac{M + M_*}{\hbar} c \cdot (b)\mathcal{S}_-
\]

\[
\frac{\partial (b)\mathcal{R}_-}{\partial r} - \frac{i}{r} \frac{\partial (b)\mathcal{R}_-}{\partial \phi} + \frac{5}{2r} (b)\mathcal{R}_- + (b)A_0 \cdot (b)\mathcal{R}_+ \\
e^{-2i\phi} \left\{ \frac{1}{r} \frac{\partial (b)\mathcal{S}_-}{\partial \vartheta} - \frac{\cot \vartheta}{r} \cdot \left[ \frac{1}{2} (b)\mathcal{S}_- + i \frac{\partial (b)\mathcal{S}_-}{\partial \phi} \right] \right\} = \frac{M - M_*}{\hbar} c \cdot (b)\mathcal{R}_+
\]

\[
\frac{\partial (b)\mathcal{S}_-}{\partial r} + \frac{i}{r} \frac{\partial (b)\mathcal{S}_-}{\partial \phi} + \frac{5}{2r} (b)\mathcal{S}_- - (b)A_0 \cdot (b)\mathcal{S}_+ \\
e^{2i\phi} \left\{ \frac{1}{r} \frac{\partial (b)\mathcal{R}_-}{\partial \vartheta} - \frac{\cot \vartheta}{r} \cdot \left[ \frac{1}{2} (b)\mathcal{R}_- - i \frac{\partial (b)\mathcal{R}_-}{\partial \phi} \right] \right\} = \frac{M - M_*}{\hbar} c \cdot (b)\mathcal{S}_+ .
\]

This may appear as a relatively complicated system but it can be simplified by imposing some plausible requirements on the desired solutions. Naturally, these requirements will refer to angular momentum, which usually serves to classify the solutions of the energy eigenvalue problems for the few-particle systems. Thus it is surely reasonable to demand that the eigensolutions of the present ortho-system \(\text{(IV.1a)--(IV.1d)}\) be classifiable by means of the associated eigenvalues \((b)j_z \text{(III.45)}\) of \(\hat{J}_z (\doteq \hat{j}_z^{(+) \oplus \hat{j}_z^{(-)})}\). Recall here our hypothesis that the total spin of a bound system agrees with the individual spins of both Pauli two-spinors which build up the common basis for each of the Dirac four-spinors (in the present case \(s_O = s_1 + s_2 = 1\), see the discussion below \(\text{(III.53)}\)).
In this sense, we try now to obtain solutions for the present ortho-system \([IV.1a]–[IV.1d]\) which are of the following form:

\[
(b)R_\pm (r, \vartheta, \phi) = \frac{e^{i\ell_\pm \phi}}{\sin \vartheta \sqrt{r \sin \vartheta}} \cdot (b)\tilde{R}_\pm (r, \vartheta) \tag{IV.2a}
\]

\[
(b)S_\pm (r, \vartheta, \phi) = \sqrt{\frac{\sin \vartheta}{r}} e^{i(\ell_\pm + 1)\phi} \cdot (b)\tilde{S}_\pm (r, \vartheta) \tag{IV.2b}
\]

Indeed, by this ansatz the eigenvalue equations \([III.43a]–[III.45]\) for angular momentum are actually satisfied; and furthermore the original mass eigenvalue system \([IV.1a]–[IV.1d]\) becomes transcribed to the new amplitude fields \((b)\tilde{R}_\pm (r, \vartheta), (b)\tilde{S}_\pm (r, \vartheta)\) and thus reappears now as follows:

\[
\begin{align*}
\frac{\partial (b)\tilde{R}_+ (r, \vartheta)}{\partial r} &- \frac{(b)j_z}{r} \cdot (b)\tilde{R}_+ (r, \vartheta) - (b)A_0 (r, \vartheta) \cdot (b)\tilde{R}_- (r, \vartheta) \\
&+ \frac{\sin^2 \vartheta}{r} \cdot \frac{\partial (b)\tilde{S}_+ (r, \vartheta)}{\partial \vartheta} + \frac{(b)j_z + 1}{r} \sin \vartheta \cos \vartheta \cdot (b)\tilde{S}_+ (r, \vartheta) = \frac{M + M^*}{\hbar} c \cdot (b)\tilde{R}_- (r, \vartheta) 
\end{align*}
\tag{IV.3a}
\]

\[
\begin{align*}
\frac{\partial (b)\tilde{S}_+ (r, \vartheta)}{\partial r} + \frac{(b)j_z}{r} \cdot (b)\tilde{S}_+ (r, \vartheta) - (b)A_0 (r, \vartheta) \cdot (b)\tilde{S}_- (r, \vartheta) \\
- \frac{1}{r \sin^2 \vartheta} \cdot \frac{\partial (b)\tilde{R}_+ (r, \vartheta)}{\partial \vartheta} + \frac{(b)j_z + 1}{r \sin^2 \vartheta} \cot \vartheta \cdot (b)\tilde{R}_+ (r, \vartheta) = \frac{M + M^*}{\hbar} c \cdot (b)\tilde{S}_- (r, \vartheta) 
\end{align*}
\tag{IV.3b}
\]

\[
\begin{align*}
\frac{\partial (b)\tilde{R}_- (r, \vartheta)}{\partial r} + \frac{(b)j_z + 1}{r} \cdot (b)\tilde{R}_- (r, \vartheta) + (b)A_0 (r, \vartheta) \cdot (b)\tilde{R}_+ (r, \vartheta) \\
- \frac{\sin^2 \vartheta}{r} \cdot \frac{\partial (b)\tilde{S}_- (r, \vartheta)}{\partial \vartheta} - \frac{\sin \vartheta \cos \vartheta}{r} \cdot (b)j_z + 1 \cdot (b)\tilde{S}_- (r, \vartheta) = \frac{M - M^*}{\hbar} c \cdot (b)\tilde{R}_+ (r, \vartheta) 
\end{align*}
\tag{IV.3c}
\]

\[
\begin{align*}
\frac{\partial (b)\tilde{S}_- (r, \vartheta)}{\partial r} - \frac{(b)j_z - 1}{r} \cdot (b)\tilde{S}_- (r, \vartheta) + (b)A_0 (r, \vartheta) \cdot (b)\tilde{S}_+ (r, \vartheta) \\
+ \frac{1}{r \sin^2 \vartheta} \cdot \frac{\partial (b)\tilde{R}_- (r, \vartheta)}{\partial \vartheta} - \frac{(b)j_z + 1}{r \sin^2 \vartheta} \cot \vartheta \cdot (b)\tilde{R}_- (r, \vartheta) = \frac{M - M^*}{\hbar} c \cdot (b)\tilde{S}_+ (r, \vartheta) .
\end{align*}
\tag{IV.3d}
\]

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This is still a system too complicated in order that there could be hope to find exact solutions, even if one could consider the ortho-potential \((b)A_0(r, \vartheta)\) being prescribed from the outside. However, this potential does actually couple back to the ortho-wave function \(\psi_b(\vec{r})\), via the Poisson equation (III.21), i.e. in terms of the new amplitude fields \((b)\tilde{R}_\pm(r, \vartheta)\) and \((b)\tilde{S}_\pm(r, \vartheta)\) (IV.2a)–(IV.2b)

\[
\Delta (b)A_0(r, \vartheta) = -\alpha_s \left\{ \frac{\left[(b)\tilde{R}_+(r, \vartheta)\right]^2 + \left[(b)\tilde{R}_-(r, \vartheta)\right]^2}{r \sin^3 \vartheta} \right. \\
+ \left. \frac{\sin \vartheta}{r} \left( \left[(b)\tilde{S}_+(r, \vartheta)\right]^2 + \left[(b)\tilde{S}_-(r, \vartheta)\right]^2 \right) \right\}.
\]

**Product Ansatz**

In view of these complications it should be obvious that it is necessary to resort to some approximative procedure in order to extract the physically relevant solutions of that intricately coupled system (IV.3a)–(IV.4). For this purpose, the *spherically symmetric approximation* suggests itself where the angular dependence of the gauge potential \((b)A_0(r, \vartheta)\) is neglected, i.e. we replace \((b)A_0(r, \vartheta)\) by its spherically symmetric approximation \([b]A_0(r)\). But observe here that this approximation assumption does *not* entail the spherical symmetry of the new wave amplitudes \((b)\tilde{R}_\pm(r, \vartheta)\) and \((b)\tilde{S}_\pm(r, \vartheta)\) (IV.2a)–(IV.2b)! However, the angular dependence of the wave amplitudes becomes now manageable, namely by applying the following product ansatz:

\[
(b)\tilde{R}_\pm(r, \vartheta) = g_R(\vartheta) \cdot \upnu\tilde{R}_\pm(r) \quad \text{(IV.5a)} \\
(b)\tilde{S}_\pm(r, \vartheta) = g_S(\vartheta) \cdot \upnu\tilde{S}_\pm(r). \quad \text{(IV.5b)}
\]

Indeed, substituting this ansatz into the eigenvalue system (IV.3a)–(IV.3d) enables us
to separate this system into two first-order subsystems, namely the angular system

\[
\begin{align}
\frac{dg_R(\vartheta)}{d\vartheta} - (b' j_z + 1) \cot \vartheta \cdot g_R(\vartheta) &= \ell_\vartheta^\ast \sin^2 \vartheta \cdot g_S(\vartheta) \\
\frac{dg_S(\vartheta)}{d\vartheta} + (b' j_z + 1) \cot \vartheta \cdot g_S(\vartheta) &= \ell_\vartheta \sin^2 \vartheta \cdot g_R(\vartheta)
\end{align}
\] (IV.6a)

and the radial system

\[
\begin{align}
\frac{d^2 R_+}{dr^2} - \frac{(b) j_z}{r} \cdot \frac{R_+}{r} - [b] A_0(r) \cdot \frac{R_-}{r} + \frac{\ell_\vartheta}{r} \cdot \frac{S_+}{r} &= \frac{M + M_\ast}{h} \cdot c \cdot R_-(r) \\
\frac{d^2 S_+}{dr^2} + \frac{(b) j_z}{r} \cdot \frac{S_+}{r} - [b] A_0(r) \cdot \frac{S_-}{r} - \frac{\ell_\vartheta}{r} \cdot \frac{R_+}{r} &= \frac{M + M_\ast}{h} \cdot c \cdot S_-(r) \\
\frac{d^2 R_-}{dr^2} + \frac{(b) j_z + 1}{r} \cdot \frac{R_-}{r} + [b] A_0(r) \cdot \frac{R_+}{r} - \frac{\ell_\vartheta}{r} \cdot \frac{S_-}{r} &= \frac{M - M_\ast}{h} \cdot c \cdot R_+(r) \\
\frac{d^2 S_-}{dr^2} - \frac{(b) j_z - 1}{r} \cdot \frac{S_-}{r} + [b] A_0(r) \cdot \frac{S_+}{r} + \frac{\ell_\vartheta}{r} \cdot \frac{R_-}{r} &= \frac{M - M_\ast}{h} \cdot c \cdot S_+(r)
\end{align}
\] (IV.7a–d)

The meaning of the newly introduced constants \( \ell_\vartheta \) and \( \ell_\vartheta^\ast \) will readily be clarified, but first we will perform a further simplification of the present ortho-system (IV.7a–d). Indeed, it may appear somewhat strange that all four equations (IV.7a–d) for the four variables \( ^\ast R_\pm, S_\pm \) are necessary in order to determine the one single mass eigenvalue \( M_\ast \). Such a system surely appears to be overdetermined; and therefore the overdetermination must be eliminated, namely by identifying the amplitude fields in such a way that there remain two independent amplitude fields (\( \tilde{\Omega}_\pm(r) \), say) which satisfy a coupled
first-order system of only two equations. The wanted identification of the amplitude fields is the following:

\[ ^{II}R_+(r) \equiv ^{II}S_+(r) \equiv \tilde{\Omega}_+(r) \]  
\[ ^{II}R_-(r) \equiv ^{II}S_-(r) \equiv \tilde{\Omega}_-(r) \]  

(IV.8a)

(IV.8b)

By this identification requirement, the four equations (IV.7a)–(IV.7d) become concentrated to only two equations, namely

\[ \frac{d \tilde{\Omega}_+(r)}{dr} + \left( \frac{\ell_O - \ell'_O}{2r} \right) \cdot \tilde{\Omega}_+(r) - [b]A_0(r) \cdot \tilde{\Omega}_-(r) = \frac{M + M_s}{h} c \cdot \tilde{\Omega}_+(r) \]  
\[ \frac{d \tilde{\Omega}_-(r)}{dr} + \left( \frac{2 - (\ell_O - \ell'_O)}{2r} \right) \cdot \tilde{\Omega}_-(r) + [b]A_0(r) \cdot \tilde{\Omega}_+(r) = \frac{M - M_s}{h} c \cdot \tilde{\Omega}_-(r) \]  

(IV.9a)

(IV.9b)

Moreover, the identification requirement (IV.8a)–(IV.8b) yields also the constraint

\[ ^{(b)}j_z = \frac{1}{2} \left( \ell_O + \ell'_O \right) \]  

(IV.10)

Of course, it is self-suggesting that those newly introduced constants \( \ell_O \) and \( \ell'_O \) (IV.6a)–(IV.6b) must have to do something with the quantum number \( j_O \), say) of the total angular momentum of the ortho-states. In order to preliminarily reveal that supposed interrelationship we pass over to the non-relativistic approximation of the latter eigenvalue system (IV.9a)–(IV.9b) for the amplitude fields \( \tilde{\Omega}_\pm(r) \). This non-relativistic limit may be attained by approximately solving the first-equation (IV.9a) for \( \tilde{\Omega}_-(r) \), yielding

\[ \tilde{\Omega}_-(r) \approx \frac{\hbar}{2Mc} \left\{ \frac{d \tilde{\Omega}_+(r)}{dr} + \left( \frac{\ell_O - \ell'_O}{2r} \right) \cdot \tilde{\Omega}_+(r) \right\} , \]  

(IV.11)

and substituting this into the second equation (IV.9b). The result is a decoupled second-order equation for \( \tilde{\Omega}_+(r) \) (being simply denoted by \( \tilde{\Omega}(r) \)) which then looks as follows:

\[ -\frac{\hbar^2}{2M} \left( \frac{d^2 \tilde{\Omega}(r)}{dr^2} + \frac{1}{r} \frac{d \tilde{\Omega}(r)}{dr} \right) + \frac{\hbar^2}{2Mr^2} \left( \frac{\ell_O - \ell'_O}{2} \right)^2 \cdot \tilde{\Omega}(r) \]  
\[ - \hbar c [b]A_0(r) \cdot \tilde{\Omega}(r) = (M_s - M) c^2 \cdot \tilde{\Omega}(r) . \]  

(IV.12)

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Obviously this looks like a Schrödinger-like eigenvalue equation for the determination of the (non-relativistic) energy eigenvalue $E_*$

$$E_* \doteq (M_* - M) c^2 , \quad \text{(IV.13)}$$

where the effect of angular momentum is expressed by the term containing $\ell_O$ and $\ell_{\ddot{O}}$. In view of this strong analogy it seems reasonable to define the quantum number ($j_O$) of the total (i.e. spin plus orbital) angular momentum for the solution of the Schrödinger equation (IV.12) by

$$j_O \doteq \left| \frac{\ell_O - \ell_{\ddot{O}}}{2} \right| . \quad \text{(IV.14)}$$

Thus we have now two equations, namely (IV.10) and (IV.14), which relate the quantum numbers of angular momentum ($^{(b)}j_z$ and $j_O$) to the constants $\ell_O$ and $\ell_{\ddot{O}}$; and this then admits to express the latter in terms of the first ones (although in an ambiguous way) as

$$\ell_O = (^{(b)}j_z \pm j_O) \quad \text{(IV.15a)}$$

$$\ell_{\ddot{O}} = (^{(b)}j_z \mp j_O) . \quad \text{(IV.15b)}$$

But obviously, the product of both constants is unambiguous:

$$\ell_O \cdot \ell_{\ddot{O}} = (^{(b)}j_z^2 - j_O^2) . \quad \text{(IV.16)}$$

Anticipating here the fact that the magnitude $j_O$ of angular momentum is never smaller than its $z$-component ($^{(b)}j_z$ i.e. $j_O \geq \left| ^{(b)}j_z \right|$), we infer that both constants $\ell_O$ and $\ell_{\ddot{O}}$ must always be of opposite sign ($\ell_O \cdot \ell_{\ddot{O}} \leq 0$).

Thus, one formally obtains from (IV.12) a true Schrödinger equation

$$-\frac{\hbar^2}{2M} \left( \frac{d^2 \tilde{\Omega}(r)}{dr^2} + \frac{1}{r} \frac{d \tilde{\Omega}(r)}{dr} \right) + \frac{\hbar^2}{2Mr^2} j_O^2 \cdot \tilde{\Omega}(r) - \hbar c \left| ^{(b)}A_0(r) \cdot \tilde{\Omega}(r) \right| = E_* \cdot \tilde{\Omega}(r) . \quad \text{(IV.17)}$$
However, one should keep in mind that the potential \( [b]A_0(r) \) is not fixed from the outside (as in the conventional Schrödinger theory) but must be considered the solution of the non-relativistic Poisson equation (IV.4), i.e.

\[
\Delta [b]A_0(r) = -\alpha_s \frac{\tilde{\Omega}^2(r)}{r} .
\] (IV.18)

One guesses from this fact that the interaction potential \( [b]A_0(r) \) will depend on the ortho-state \( \tilde{\Omega}(r) \) itself so that the eigenvalue problem appears highly intricate. Different states \( \tilde{\Omega}(r) \) will generate different potentials \( [b]A_0(r) \) according to (IV.18) so that the energy eigenvalues \( E_* \) due to different states will be found to be different, too (\( \Rightarrow \) elimination of the conventional degeneracy (I.18)); and thus the RST energy spectrum of positronium must be expected to be much more intricate than predicted by the conventional theory (I.18); already in the non-relativistic domain and in the electrostatic approximation.

2. Angular Momentum Quantization in RST

It is rather evident that the off-separated angular system (IV.6a)–(IV.6b) represents an extra problem which may be tackled independently of the proper energy eigenvalue problem (IV.17)–(IV.18). On the other hand, the eigenvalues \( E_* \) of the latter problem will clearly be influenced by the solutions of the angular problem (IV.6a)–(IV.6b), namely via the quantum number \( j_0 \) of angular momentum (IV.14) and in general also via the interaction potential \( [b]A_0(r) \) since this potential “feels” the angular behaviour of the amplitude fields via the Poisson equation (IV.4).

Anisotropy of the Gauge Potential

This anisotropic influence can be expressed even more distinctly by observing our product ansatz (IV.5a)–(IV.5b) together with the identifications (IV.8a)–(IV.8b) which then recasts that former Poisson equation (IV.4) to the more concise form

\[
\Delta^{(b)}A_0(r, \vartheta) = -4\pi\alpha_s \, (^{(b)}k_0(r, \vartheta) = -4\pi\alpha_s \, (^{(b)}k_0(\vartheta) \cdot (^{(b)}k_0(r) ,
\] (IV.19)
i.e. the charge density \((b)k_0(\vec{r})\) becomes now also factorized \((b)k_0(r, \vartheta)\) with the angular factor \((b)k_0(\vartheta)\) being specified by

\[
(b)k_0(\vartheta) = \frac{1}{4\pi} \left\{ \frac{g_R^2(\vartheta)}{\sin^2 \vartheta} + \sin \vartheta \cdot g_S^2(\vartheta) \right\} \tag{IV.20}
\]

and the radial factor \((b)k_0(r)\) by

\[
(b)k_0(r) = \frac{\tilde{\Omega}_+^2(r) + \tilde{\Omega}_-^2(r)}{r} \tag{IV.21}
\]

This factorization effect will subsequently allow us to develop a suitable approximation procedure in order to manage the anisotropy of the interaction potential \((b)A_0(r, \vartheta)\). Namely, the formal solution of the Poisson equation \((IV.19)\) reads

\[
(b)A_0(r, \vartheta) = \alpha_s \int d^3\vec{r}' \frac{(b)k_0(r', \vartheta')}{||\vec{r} - \vec{r}'||} \tag{IV.22}
\]

\[
= \alpha_s \int \frac{d \Omega'}{4\pi} \left\{ \frac{g_R^2(\vartheta')}{\sin^2 \vartheta'} + \sin \vartheta' \cdot g_S^2(\vartheta') \right\} \int dr' \frac{\tilde{\Omega}_+^2(r') + \tilde{\Omega}_-^2(r')}{||\vec{r} - \vec{r}'||},
\]

where the charge normalization condition

\[
\int d^3\vec{r}(b)k_0(r, \vartheta) = 1 \tag{IV.23}
\]

allows now also a factorized form:

\[
\int d\Omega (b)k_0(\vartheta) = \int d\Omega \left\{ \frac{g_R^2(\vartheta)}{\sin^2 \vartheta} + \sin \vartheta \cdot g_S^2(\vartheta) \right\} = 1 \tag{IV.24a}
\]

\[
\int dr r^2 (b)k_0(r) = \int dr r \left\{ \tilde{\Omega}_+^2(r) + \tilde{\Omega}_-^2(r) \right\} = 1 . \tag{IV.24b}
\]

This, however, helps us now to get approximate results for the gauge potential \((b)A_0(r, \vartheta)\) from its integral representation \((IV.22)\). For instance, the roughest approximation consists in neglecting completely the angular dependence of the radial integral in \((IV.22)\) (by replacing it through its angular average) so that the angular normalization condition \((IV.24a)\) can be immediately applied which then yields

\[
(b)A_0(r, \vartheta) \Rightarrow [b]A_0(r) = \frac{\alpha_s}{4\pi} \int_0^\infty \frac{d^3\vec{r}' \tilde{\Omega}_+^2(r') + \tilde{\Omega}_-^2(r')}{r' ||\vec{r} - \vec{r}'||} \tag{IV.25}
\]

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whose non-relativistic approximation reads

\[ [b]A_0(r) = \frac{\alpha_s}{4\pi} \int \frac{d^3 \vec{r}'}{r'} \frac{\hat{\Omega}^2(r')}{||\vec{r}' - \vec{r}||} \]  

(IV.26)

and thus is the solution of the “spherically symmetric” Poisson equation (IV.18). Consequently, if we wish to go beyond this spherically symmetric approximation for the interaction potential \([b]A_0(r, \vartheta)\) (IV.22) we are forced to first work out the solutions \(g_R(\vartheta)\) and \(g_S(\vartheta)\) of the original angular eigenvalue problem (IV.6a)–(IV.6b).

### Solving the Eigenvalue Problem of Angular Momentum

The close interrelationship between angular momentum of both particles and anisotropy of their interaction potential \([b]A_0(r, \vartheta)\) (IV.22) necessitates now to explicitly solve the coupled angular system (IV.6a)–(IV.6b). For this purpose, one first decouples that system by differentiating once more which yields

\[
\frac{d^2 g_R(\vartheta)}{d\vartheta^2} - 2 \cot \vartheta \cdot \frac{dg_R(\vartheta)}{d\vartheta} + \left\{ \left( j_O^2 - 1 \right) + \frac{\left( \frac{3}{2} \right)^2 - \left( (b)j_z - \frac{1}{2} \right)^2}{\sin^2 \vartheta} \right\} \cdot g_R(\vartheta) = 0  
\]  

(IV.27a)

\[
\frac{d^2 g_S(\vartheta)}{d\vartheta^2} + 2 \cot \vartheta \cdot \frac{dg_S(\vartheta)}{d\vartheta} + \left\{ \left( j_O^2 - 1 \right) + \frac{\left( \frac{1}{2} \right)^2 - \left( (b)j_z + \frac{1}{2} \right)^2}{\sin^2 \vartheta} \right\} \cdot g_S(\vartheta) = 0  
\]  

(IV.27b)

where \((b)j_z\) is defined by equation (III.45) and \(j_O\) by (IV.14).

Once we have arrived at two decoupled equations one can try to separately solve each of both by some transformation of variables which renders the problem more manageable. Thus, putting

\[
x = \sin \vartheta  
\]  

(IV.28a)

\[ g_R(\vartheta) \Rightarrow G_R(x) \]  

(IV.28b)

\[ g_S(\vartheta) \Rightarrow G_S(x) \]  

(IV.28c)
the decoupled second-order equations (IV.27a)–(IV.27b) adopt the following form

\[
\begin{align*}
(1 - x^2) \frac{d^2 G_R(x)}{dx^2} &+ \left( x - \frac{2}{x} \right) \frac{d G_R(x)}{dx} + \\
&\quad + \left\{ (j \frac{x}{2})^2 - \left( \frac{b}{2} \frac{j_z - \frac{1}{2}}{x^2} \right)^2 \right\} \cdot G_R(x) = 0
\end{align*}
\]

(IV.29a)

\[
\begin{align*}
(1 - x^2) \frac{d^2 G_S(x)}{dx^2} &+ \left( \frac{2}{x} - 3x \right) \frac{d G_S(x)}{dx} + \\
&\quad + \left\{ (j \frac{x}{2})^2 - \left( \frac{b}{2} \frac{j_z + \frac{1}{2}}{x^2} \right)^2 \right\} \cdot G_S(x) = 0.
\end{align*}
\]

(IV.29b)

It is true, the coupled first-order system (IV.6a)–(IV.6b) does not allow that both angular functions \(g_R(\vartheta)\) and \(g_S(\vartheta)\) can simultaneously be written in the form claimed by equations (IV.28a)–(IV.28c); but the fact, that each one of these two equations (IV.6a) and (IV.6b) can emerge in the form (IV.29a)–(IV.29b), means that always one of both equations (IV.29a) or (IV.29b) may be realized. Thus, our strategy of elaborating the desired solutions works as follows: first, select one of both equations (IV.29a)–(IV.29b) and determine its solution as a function of \(x\) (IV.28a). Then determine the associated angular function \(g_R(\vartheta)\), or \(g_S(\vartheta)\), resp., according to the relations (IV.28b)–(IV.28c); and finally determine the residual angular function \(g_S(\vartheta)\), or \(g_R(\vartheta)\), resp., from the corresponding other angular equation (IV.6a), or (IV.6b), resp.

The very form of the second-order equations (IV.29a)–(IV.29b) suggests to try a power series

\[
G_R(x) = \sum_n \rho_n \cdot x^n \quad \text{and} \quad G_S(x) = \sum_n \sigma_n \cdot x^n.
\]

(IV.30a)

(IV.30b)

If this is substituted in the second-order equations (IV.29a)–(IV.29b), one gets by the
standard methods the following recurrence formulae
\begin{align}
\rho_{n+2} &= \frac{(n-1)^2 - j_z^2}{(n+2)(n-1) - ((b)j_z + 1)((b)j_z - 2)} \cdot \rho_n \\  
\sigma_{n+2} &= \frac{n(n+2) - (j_0 + 1)(j_0 - 1)}{(n+2)(n+3) - (b)j_z((b)j_z + 1)} \cdot \sigma_n .
\end{align}
(IV.31a, b)

In order that these solutions be unique, we next have to fix the lowest order coefficients of both series. For the first series (IV.30a) we obtain for the lowest power \(n_{\text{min}}\)
\[n_{\text{min}} = \begin{cases} (b)j_z + 1, & (b)j_z \geq 0 \\ -(b)j_z - 2, & (b)j_z < 0 \end{cases}
\] (IV.32)

and for the second series (IV.30b)
\[n_{\text{min}} = \begin{cases} (b)j_z, & (b)j_z \geq 0 \\ -(b)j_z + 1, & (b)j_z < 0 \end{cases}
\] (IV.33)

On the other hand, for \(n \to \infty\) the coefficients \(\rho_{n+2}\) and \(\sigma_{n+2}\) would tend to \(\rho_n\) and \(\sigma_n\), resp.; and therefore both sums (IV.30a)–(IV.30b) cannot adopt definite values if they do not stop at some finite \(n_{\text{max}}\). However, such a maximal value \(n_{\text{max}}\) of the power \(n\) can immediately be read off from the recurrence formulae (IV.31a)–(IV.31b)
\[n_{\text{max}} = \begin{cases} j_0 + 1, & (IV.31a) \\ j_0 - 1, & (IV.31b) \end{cases}.
\] (IV.34)

These results enable us to closer specify now our original ansätze (IV.30a)–(IV.30b); namely
\[G_R(x) = \begin{cases} \sum_{n=(b)j_z+1}^{j_0+1} \rho_n \cdot x^n, & (b)j_z \geq 0 \\ \sum_{n=-(b)j_z-2}^{j_0+1} \rho_n \cdot x^n, & (b)j_z < 0 \end{cases}
\] (IV.35)
and

\[
G_S(x) = \begin{cases} 
\sum_{n=(b)j_z}^{j_O-1} \sigma_n \cdot x^n, & (b)j_z \geq 0 \\
\sum_{n=-(b)j_z+1}^{j_O-1} \sigma_n \cdot x^n, & (b)j_z < 0 
\end{cases} 
\] (IV.36)

From these results one concludes that the range of quantum numbers \(j_O\) and \((b)j_z\) is the following:

\[-(j_O - 1) \leq (b)j_z \leq j_O \quad \text{for } G_R(x) \quad \text{(IV.35)}\]

\[-j_O \leq (b)j_z \leq (j_O - 1) \quad \text{for } G_S(x) \quad \text{(IV.36)}\]

with \(j_O\) being an integer \((j_O = 0, 1, 2, 3, \ldots)\).

As a brief concrete demonstration of the general method, we consider the situation with \(j_O = 2 \Rightarrow -2 \leq (b)j_z \leq +2\). Starting here with \((b)j_z = 0\), we first conclude from the arrangements (IV.35)–(IV.36) that the first case (IV.35) does apply where the function \(G_R(x)\) must then look as follows

\[G_R(x) = \sum_{n=1}^{3} \rho_n \cdot x^n = \rho_1 x + \rho_3 x^3,\] (IV.37)

or by means of the recurrence formula (IV.31a)

\[G_R(x) = \rho_1 (x - 2x^3)\] (IV.38)

with the constraint \(\rho_1\) to be fixed (below) by the normalization condition. Next, since the counterpart \(G_S(x)\) of \(G_R(x)\) cannot exist for \(j_O = 2, (b)j_z = 0\) we have to determine the second angular function \(g_S(\vartheta)\) directly from the first-order equation (IV.6a) with \(g_R(\vartheta)\) being deduced from \(G_R(x)\) (IV.38) as

\[g_R(\vartheta) = \rho_1 \sin \vartheta \left(1 - 2 \sin^2 \vartheta\right).\] (IV.39)

This yields

\[g_S(\vartheta) = -\frac{4\rho_1}{\ell_O} \cos \vartheta.\] (IV.40)
Now that both angular functions are fixed up to the normalization constant $\rho_1$, we can pin the latter down by the normalization condition (IV.24a) which adopts the following form for the present situation

$$1 = \int \frac{d\Omega}{4\pi} \left\{ \frac{g_R^2(\vartheta)}{\sin^2 \vartheta} + \sin \vartheta \cdot g_S^2(\vartheta) \right\} \tag{IV.41}$$

$$= \frac{1}{2} \rho_1^2 \int_0^\pi d\vartheta \left\{ [1 - 2\sin^2 \vartheta]^2 + \left( \frac{4}{\tilde{\ell}_O} \right)^2 \sin^2 \vartheta \cos^2 \vartheta \right\}.$$  

This ascribes to $\rho_1$ the value

$$\rho_1^2 = \frac{4}{\pi \left( 1 + \frac{4}{\tilde{\ell}_O} \right)}. \tag{IV.42}$$

Here, one wishes to express the constant $\tilde{\ell}_O$ through $j_O$ and $(b)j_z$, see equation (IV.15b), which, however, offers two possibilities, namely either

$$\dot{\ell}_O = (b)j_z + j_O \Rightarrow +2 \tag{IV.43a}$$

$$\ddot{\ell}_O = (b)j_z - j_O \Rightarrow -2 \tag{IV.43b}$$

or

$$\dot{\ell}_O = (b)j_z - j_O \Rightarrow -2 \tag{IV.44a}$$

$$\ddot{\ell}_O = (b)j_z + j_O \Rightarrow +2. \tag{IV.44b}$$

But these two possibilities differ merely in sign and therefore do not generate essentially different solutions of the eigenvalue problem under consideration (in contrast to the other cases with $j_z \neq 0$, see the table below). Indeed, both situations (IV.43a)–(IV.43b) and (IV.44a)–(IV.44b) yield the same normalization constant $\rho_1$ (IV.42), i.e.

$$\rho_1 = \pm \sqrt{\frac{2}{\pi}}, \tag{IV.45}$$

where the ambiguity in sign is immaterial. Thus the solutions $g_R(\vartheta)$ (IV.39) and $g_S(\vartheta)$
The peculiar point with this result is that the *essentially* ambiguous situation (IV.15a)–(IV.15b) does not entail the existence of two essentially different solutions for *all* allowed values of \( (b) j_z \) but only for *some* \( (b) j_z \neq 0 \) (see the table below). Indeed, that essential ambiguity of some solutions of the angular eigenvalue problem (IV.6a)–(IV.6b) is just the core of the *ortho-dimorphism*, i.e. the dimorphism of the ortho-positronium configurations. Naturally, the most urgent question arising in this context must refer to the energy difference of such a dimorphic pair, which will readily be worked out.

\[
\begin{align*}
\dot{j}_O &= 2 \\
\begin{array}{|c|c|c|c|c|c|}
\hline
(b) j_z & \ell_O & \ell_O' & G_R(x) & G_S(x) & g_R(\vartheta) & g_S(\vartheta) \\
\hline
2 & 0 & 4 & \rho_3 \cdot x^3 & - & \frac{4}{\sqrt{3\pi}} \sin^3 \vartheta & 0 \\
1 & 3 & -1 & - & \sigma_1 \cdot x & \frac{2}{\sqrt{3\pi}} \sin^2 \vartheta \cos \vartheta & \frac{2}{\sqrt{3\pi}} \sin \vartheta \\
& -1 & 3 & - & - & - \frac{6}{\sqrt{3\pi}} \sin^2 \vartheta \cos \vartheta & \frac{2}{\sqrt{3\pi}} \sin \vartheta \\
0 & 2 & -2 & \rho_1 (x - 2x^3) & - & \sqrt{\frac{2}{3\pi}} \sin \vartheta \left(1 - 2 \sin^2 \vartheta\right) & -2 \sqrt{\frac{2}{3\pi}} \cos \vartheta \\
& -2 & 2 & - & - & - & - \\
-1 & 1 & -3 & \rho_3 \cdot x^3 & - & \frac{2}{\sqrt{3\pi}} \sin^3 \vartheta & -\frac{2}{\sqrt{3\pi}} \cos \vartheta \\
& -3 & 1 & - & - & - & - \\
-2 & -4 & 0 & - & \sigma_1 \cdot x & 0 & \frac{4}{\sqrt{3\pi}} \sin \vartheta \\
\hline
\end{array}
\end{align*}
\]
Ortho-Dimorphism for $j_\mathcal{O} = 2$

The table (precedent page) displays the possible configurations of the pair $\ell_\mathcal{O}, \ell_\mathcal{O}$ corresponding to the quantum numbers $(b)j_z = -2, -1, 0, 1, 2$ due to $j_\mathcal{O} = 2$. The associated angular functions $g_R(\vartheta), g_S(\vartheta)$ as solutions of the first-order system (IV.6a)–(IV.6b) emerge ambiguously for $(b)j_z = \pm 1$ but are unique for $(b)j_z = 0, \pm 2$. The case with $(b)j_z = -1$ is the simplest one and has already been treated in ref. [34] (in that paper the present quantum number $j_\mathcal{O}$ has there been denoted by $\ell_\mathcal{O}$).

The table of angular functions $g_R(\vartheta), g_S(\vartheta)$ (for $j_\mathcal{O} = 2$) obviously displays some regularities (or symmetries, resp.) as far as the permutation of both functions $g_R(\vartheta)$ and $g_S(\vartheta)$ is concerned. Surely, this must have to do something with the isotropy of three-space, especially with respect to the replacement $(b)j_z \leftrightarrow -(b)j_z$. Indeed, if this replacement is associated with the following replacements (irrespective of an irrelevant change of sign)

\[ g_R(\vartheta) \Rightarrow g_S(\vartheta) \cdot \sin^2 \vartheta \quad (IV.47a) \]
\[ g_S(\vartheta) \Rightarrow -\frac{g_R(\vartheta)}{\sin^2(\vartheta)} \quad (IV.47b) \]
\[ \ell_\mathcal{O} \Rightarrow -\ell_\mathcal{O} , \quad \ell_\mathcal{O} \Rightarrow -\ell_\mathcal{O} \quad (IV.47c) \]

then both eigenvalue equations (IV.6a)–(IV.6b) become merely interchanged and the angular density $(b)k_0(\vartheta)$ is left invariant.

In order to get a broader basis for our inductive reasoning, we extend the calculations to $j_\mathcal{O} = 3$, see the table below. Combining both tables for $j_\mathcal{O} = 2$ and $j_\mathcal{O} = 3$ we conclude that the angular functions $g_R(\vartheta)$ and $g_S(\vartheta)$ are always unique for $(b)j_z = 0$ and for $(b)j_z = \pm j_\mathcal{O}$ for arbitrary $j_\mathcal{O} (= 1, 2, 3, 4 \ldots)$. This is proven quite generally in App.A. For the other values of $(b)j_z$ (i.e. $0 < |(b)j_z| < j_\mathcal{O}$) the angular functions $g_R(\vartheta), g_S(\vartheta)$ are generally expected to be ambiguous. However, the extent of this ambiguity deserves an extra discussion where perhaps the energy difference of the ambiguous configurations may be taken as a quantitative measure of just that ambiguity.
| $^{(b)}j_z$ | $\ell_O$ | $\bar{\ell}_O$ | $G_R(x)$ | $G_S(x)$ | $g_R(\vartheta)$ | $g_S(\vartheta)$ |
|---|---|---|---|---|---|---|
| 3 | 0 | 6 | $\rho_4 x^4$ | $-$ | $\sqrt{\frac{2}{3\pi}} \sin^4 \vartheta$ | 0 |
| 2 | 5 | -1 | $-$ | $\sigma_2 x^2$ | $\sqrt{\frac{16}{3\pi}} \sin^3 \vartheta \cos \vartheta$ | $\sqrt{\frac{16}{3\pi}} \sin^2 \vartheta$ |
| | -1 | 5 | $-$ | $-$ | $-5 \sqrt{\frac{16}{3\pi}} \sin^3 \vartheta \cos \vartheta$ | $\sqrt{\frac{16}{3\pi}} \sin^2 \vartheta$ |
| 1 | 4 | -2 | $\rho_2 (x^2 - \frac{4}{3} x^4)$ | $-$ | $\sqrt{\frac{12}{\pi}} \sin^2 \vartheta (1 - \frac{4}{3} \sin^2 \vartheta)$ | $\sqrt{\frac{12}{\pi}} \sin \vartheta \cos \vartheta$ |
| | -2 | 4 | $-$ | $-$ | $\sqrt{\frac{24}{\pi}} \sin^2 \vartheta (1 - \frac{4}{3} \sin^2 \vartheta)$ | $-\frac{2}{3} \sqrt{\frac{24}{\pi}} \sin \vartheta \cos \vartheta$ |
| 0 | 3 | -3 | $-$ | $\sigma_0 (1 - \frac{4}{3} x^2)$ | $\sqrt{\frac{2}{\pi}} \sin \vartheta \cos \vartheta (1 - 4 \sin^2 \vartheta)$ | $\sqrt{\frac{18}{\pi}} (1 - \frac{4}{3} \sin^2 \vartheta)$ |
| -1 | 2 | -4 | $-$ | $\sigma_0 (1 - \frac{4}{3} x^2)$ | $-\frac{4}{3} \sqrt{\frac{12}{\pi}} \sin^3 \vartheta \cos \vartheta$ | $\sqrt{\frac{12}{\pi}} (1 - \frac{4}{3} \sin^2 \vartheta)$ |
| | -4 | 2 | $-$ | $-$ | $\frac{2}{3} \sqrt{\frac{24}{\pi}} \sin^3 \vartheta \cos \vartheta$ | $\sqrt{\frac{24}{\pi}} (1 - \frac{4}{3} \sin^2 \vartheta)$ |
| -2 | 1 | -5 | $\rho_4 x^4$ | $-$ | $\sqrt{\frac{16}{3\pi}} \sin^4 \vartheta$ | $-\sqrt{\frac{16}{3\pi}} \sin \vartheta \cos \vartheta$ |
| | -5 | 1 | $-$ | $-$ | $\sqrt{\frac{16}{3\pi}} \sin^4 \vartheta$ | $5 \sqrt{\frac{16}{3\pi}} \sin \vartheta \cos \vartheta$ |
| -3 | -6 | 0 | $-$ | $\sigma_2 x^2$ | $-$ | $0$ |

**Ortho-Dimorphism for $j_O = 3$**

The possible configurations due to $j_O = 3$ are $^{(b)}j_z = 0, \pm 1, \pm 2, \pm 3$ and display again the corresponding ambiguities (for $^{(b)}j_z = \pm 1, \pm 2$) and uniqueness (for $^{(b)}j_z = 0$ and $^{(b)}j_z = \pm j_O$). Thus, one concludes that for general $j_O$ ($= 1, 2, 3, 4, \ldots$) one always has $2j_O + 1 - 3 = 2(j_O - 1)$ dimorphic pairs and 3 solitary angular distributions.
The somewhat hidden symmetries of the pair of functions $g_R(\vartheta)$ and $g_S(\vartheta)$ due to the interchange of the positive and negative $z$-direction ($\vartheta = 0 \Leftrightarrow \vartheta = \pi$) becomes now more obvious by looking at the angular densities $^{(b)}k_0(\vartheta)$ \textbf{[IV.20]}. The subsequent table presents a collection of all these angular objects due to $j_\varphi = 1, 2, 3$. From here it becomes immediately obvious that the ambiguous pair $g_R(\vartheta), g_S(\vartheta)$ due to a given $^{(b)}j_z$ (with $0 < |^{(b)}j_z| < j_\varphi$) does generate the same couple of angular densities $^{(b)}k_0(\vartheta)$ as does the pair $g_R(\vartheta), g_S(\vartheta)$ due to $^{(b)}j_z$. Consequently, the \textit{electric} charge density $^{(b)}k_0(\vec{r})$ does not single out a preferential direction on the $z$-axis (contrary to the \textit{current} density $\vec{k}_b(\vec{r})$).

| $j_\varphi$ | $^{(b)}j_z$ | $^{(b)}k_0(\vartheta)$ \textbf{[IV.20]} |
|------------|-------------|--------------------------------|
| 1          | 0           | $\frac{1}{2\pi^2} \cdot \frac{1}{\sin \vartheta}$ |
| 1          | ±1          | $\sin \vartheta$ |
| 2          | 0           | $\frac{1}{2\pi^2} \cdot \frac{1}{\sin \vartheta}$ |
| 2          | ±1          | $\frac{1}{3\pi^2} \{9 \sin \vartheta - 8 \sin^3 \vartheta\}$ |
| 2          | ±2          | $\frac{4}{3\pi^2} \sin^3 \vartheta$ |
| 3          | 0           | $\frac{1}{2\pi^2} \cdot \frac{1}{\sin \vartheta}$ |
| 3          | ±1          | $\frac{3}{\pi^2} \{\sin \vartheta - \frac{8}{9} \sin^3 \vartheta\}$ |
| 3          | ±2          | $\frac{4}{3\pi^2} \sin^3 \vartheta$ |
| 3          | ±3          | $\frac{8}{5\pi^2} \sin^5 \vartheta$ |

\textit{Angular Density $^{(b)}k_0(\vartheta)$ \textbf{[IV.20]} for the States Due to $j_\varphi = 1, 2, 3$}
Quite intuitively, one would suppose that the shape of the charge density \( b^{(b)}k_0(\vartheta) \) is influenced by both the azimuthal quantum number \( b^{(b)}j_z \) and the total number \( j_O \). However, the above table says that the angular densities \( b^{(b)}k_0(\vartheta) \) are the same for \( j_O = 2 \), \( b^{(b)}j_z = 0 \) and \( j_O = 3 \), \( b^{(b)}j_z = 0 \) and also for \( j_O = 1 \), \( b^{(b)}j_z = 0 \). Indeed, one can show that the angular charge density \( b^{(b)}k_0(\vartheta) \) for \( b^{(b)}j_z = 0 \) is the same for all values of \( j_O \), see equation (A.3) of App.A. Thus one becomes tempted to attribute the deformations of the angular charge distributions \( b^{(b)}k_0(\vartheta) \) to the action of “centrifugal forces”, which are linked to the azimuthal quantum number \( b^{(b)}j_z \) rather than to the total number \( j_O \)! In this sense, one expects that for \( b^{(b)}j_z = 0 \) the charge distribution is concentrated in the vicinity of the rotational axis \( (\vartheta = 0, \pi) \); whereas for maximal \( b^{(b)}j_z = \pm j_O \) the charge distribution \( b^{(b)}k_0 \) becomes rolled out to a disc-like shape. Indeed, the occurrence of this effect is demonstrated by the Fig.IV.A below. Moreover it should be considered a matter of course that such a deformation of the charge clouds will entail some change of the electrostatic interaction which then implies that the \( j_z \)-degeneracy becomes eliminated (see below). This elimination of degeneracy, however, has nothing to do with the ortho-dimorphism which occurs for dimorphic partners belonging to the same pair of quantum numbers \( j_O, b^{(b)}j_z \); see Fig.IV.B below for a simple demonstration.
For small rotational quantum number \((b)j_z\) (solid curve: \((b)j_z = 0\)) the charge density 
\[(b)k_0(r, \vartheta) = (b)k_0(\vartheta) \cdot (b)k_0(r)\] 
is concentrated close to the rotation axis (i.e. z-axis; \(\vartheta = 0\)). The angular pre-factor 
\((b)k_0(\vartheta)\) due to \((b)j_z = 0\) is the same for all values of \(j_\sigma (= 0, 1, 2, 3, \ldots)\), i.e.
\[
\sin \vartheta \cdot (b)k_0(\vartheta) = \frac{1}{2\pi^2} \quad \text{(solid line)}
\]
see App.A, equation (A.5). However, for extremal value of \((b)j_z\) (i.e. \((b)j_z = \pm j_\sigma\)) the charge cloud becomes rolled out to a disc-like shape through the centrifugal forces; dotted curve: \((b)j_z = j_\sigma = 3\) with
\[
\sin \vartheta \cdot (b)k_0(\vartheta) = \frac{8}{5\pi^2} \cdot \sin^6 \vartheta ,
\]
see the table on p. 71. Such an inertial deformation of the rotating charge clouds is to be considered the origin of the elimination of the $j_z$-degeneracy which itself occurs only in the spherically symmetric approximation.
Fig. IV.B  **Dimorphism of Angular Density** \((b)k_0(\vartheta)\)

for \(j_O = 3, (b)j_z = \pm 2\)

Even for the *same* rotational quantum numbers \(j_O\) and \((b)j_z\) the angular density \((b)k_0(\vartheta)\) occurs in two different forms, provided the quantum number \((b)j_z\) is restricted by the condition \(0 < |(b)j_z| < j_O\), see App.A. For the present situation \((j_O = 3, (b)j_z = \pm 2)\), the two forms of angular density are given by (see table on p. 71)

\[
(b)k_0(\vartheta) = \begin{cases} 
\frac{4}{3\pi} \sin^3 \vartheta , & \text{solid curve} \\
\frac{4}{\pi^2} \left( \frac{5}{3} \sin^3 \vartheta - \frac{8}{5} \sin^5 \vartheta \right) , & \text{dotted curve} 
\end{cases}
\]

The different shape of the electric charge clouds entails different electrostatic energy and therefore also different binding energies (\(\sim\) "ortho-dimorphism").

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V  Anisotropy of the Gauge Potential \( (b)A_0(\vec{r}) \)

Besides the matter fields, the second basic building block of RST is constituted by the gauge fields. Since the latter fields are coupled to the matter fields via the Poisson equations, the anisotropy of the matter fields is transferred to the gauge fields just by these Poisson equations. For the present electrostatic approximation, the gauge fields enter the theory only in form of their time component \( (b)A_0(\vec{r}) \) due to the corresponding four-potential \( (b)A_{\mu} \). The field equations for the gauge fields are the (generally non-Abelian) Maxwell equations, which however for the present electrostatic situation reduce to the ordinary Poisson equation (IV.4). Here, the charge density \( (b)k_0(\vec{r}) \) factorizes as shown by equation (IV.19); two examples of this dimorphism of the angular factor \( (b)k_0(\vartheta) \) are given by the above tables at the end of Subsect.IV.2. Thus it should be evident that exact solutions of the Poisson equation (IV.19) can not easily be found. However, this should not be considered a bad situation since there are approximation procedures at hand which are able to mediate a rough picture of how the exact solution \( (b)A_0(\vec{r}) \) will look like. The point of departure for this picture is the “spherically symmetric approximation”, which has already been briefly mentioned in connection with the equations (IV.18) and (IV.25)–(IV.26).

1. Spherical Symmetry as a First Approximation

The spherically symmetric approximation of the gauge potential has been based upon the assumption that this potential is SO(3) symmetric, i.e. we put

\[
(b)A_0(\vec{r}) \Rightarrow [b]A_0(r) \quad \text{(V.1)}
\]

\[
(r = ||\vec{r}||)
\]

The corresponding Poisson equation (IV.18) for the approximative potential \([b]A_0(r)\) is obtained through extremalizing the electro-static part \(\langle e\bar{E}_{[\Omega]} \rangle\) of the full energy functional.
\( \mathcal{E}_{[\Omega]} \) which of course must consist of both the gauge field part \((G)\mathcal{E}_{[\Omega]}\) and the (Dirac) matter part \((D)\mathcal{E}_{[\Omega]}\), see ref. [2]

\[
\mathcal{E}_{[\Omega]} = (D)\mathcal{E}_{[\Omega]} + (G)\mathcal{E}_{[\Omega]} .
\] (V.2)

Here, the matter part \((D)\mathcal{E}_{[\Omega]}\) will be readily specified and discussed, but in the present context we are rather interested in the electric contribution \((e)\mathcal{E}_{[\Omega]}\) to the gauge part \((G)\mathcal{E}_{[\Omega]}\) because the extremalization of the latter part already yields the desired electrostatic field equations.

Indeed, the wanted electrostatic part \((e)\mathcal{E}_{[\Omega]}\) is composed of two contributions

\[
(e)\mathcal{E}_{[\Omega]} = E^{(e)}_R + \lambda^{(e)}_G \cdot \tilde{N}^{(e)}_G .
\] (V.3)

The Lagrangean multiplier adopts the value \(\lambda^{(e)}_G = -2\) and the first contribution \((E^{(e)}_R)\) is the electrostatic gauge field energy

\[
E^{(e)}_R = - \frac{\hbar c}{4\pi \alpha_s} \int d^3 \vec{r} \left( \vec{E}_b(\vec{r}) \cdot \vec{E}_b(\vec{r}) \right)
\] (V.4)

where the electrostatic field strength \(\vec{E}_b(\vec{r})\) of the ortho-configurations is given as usual by

\[
\vec{E}_b(\vec{r}) = -\vec{\nabla} \ [b] A_0(\vec{r})
\] (V.5)

(this simple form of \(\vec{E}_b(\vec{r})\) does exclusively apply to non-identical particles, see ref. [34]).

For our presently considered spherical symmetric approximation \((\text{V.1})\), the general form \(\vec{E}_b(\vec{r})\) \(\text{(V.5)}\) does reduce to

\[
\vec{E}_b(\vec{r}) \Rightarrow -\vec{\nabla} \ [b] A_0(r) = - \vec{e}_r \frac{d \ [b] A_0(r)}{dr} ,
\] (V.6)

and consequently the electrostatic energy \(E^{(e)}_R\) \(\text{(V.4)}\) becomes simplified to

\[
E^{(e)}_R \Rightarrow E^{(e)}_R = - \frac{\hbar c}{\alpha_s} \int dr \ r^2 \left( \frac{d \ [b] A_0(r)}{dr} \right)^2 .
\] (V.7)
A similar conclusion does also hold for the “Poisson constraint” $\tilde{N}^{(e)}_G$ which generally is defined as the difference of the gauge field energy $E^{(e)}_R$ and its “mass equivalent” $M^{(e)} c^2$ [2]:

$$N^{(e)}_G = E^{(e)}_R - M^{(e)} c^2,$$  \hspace{1cm} (V.8)

where the mass equivalent itself is defined through [Zitat]

$$M^{(e)} c^2 \overset{\Delta}{=} -\hbar c \int d^3 \vec{r} \left( b^{(b)} k_0(\vec{r}) \right) \cdot \left( b^{(b)} k_0(\vec{r}) \right).$$ \hspace{1cm} (V.9)

For the spherically symmetric approximation, the gauge potential is assumed to be SO(3) symmetric, cf. (V.1), and the charge density $(b^{(b)} k_0(\vec{r}))$ is of the product form described by (IV.19)–(IV.21). Therefore the mass equivalent (V.9) factorizes as follows

$$M^{(e)} c^2 \Rightarrow -\hbar c \int d\Omega \left( b^{(b)} k_0(\vartheta) \right) \int_0^\infty dr r^2 \left( b^{(b)} A_0(r) \right) \cdot \left( b^{(b)} k_0(r) \right).$$ \hspace{1cm} (V.10)

But here we can resort to the angular normalization condition (IV.24) for $(b^{(b)} k_0(\vartheta))$ and also to the non-relativistic version of the radial charge density $(b^{(b)} k_0(r))$ (IV.21)

$$(b^{(b)} k_0(r)) = \frac{\tilde{\Omega}^2(r)}{r}$$ \hspace{1cm} (V.11)

so that we end up with the final form of the (“isotropic”) mass equivalent

$$M^{(e)} c^2 \Rightarrow \tilde{M}^{[e]} c^2 = -\hbar c \int_0^\infty dr r \left( b^{(b)} A_0(r) \right) \cdot \tilde{\Omega}^2(r).$$ \hspace{1cm} (V.12)

With all these arrangements, the “spherically symmetric” form of the electrostatic gauge field functional $^{(e)}\tilde{E}_{[\Omega]}$ is of the shape

$$^{(e)}\tilde{E}_{[\Omega]} \Rightarrow [^{(e)}\tilde{E}_{[\Omega]}] = E^{(e)}_R + \lambda^{(e)}_G \cdot \tilde{N}^{[e]}_G$$ \hspace{1cm} (V.13)

with $E^{(e)}_R$ being given by (V.7) and

$$\tilde{N}^{[e]}_G = E^{[e]}_R - \tilde{M}^{[e]} c^2.$$ \hspace{1cm} (V.14)
Now that the specific SO(3) symmetric form of all individual contributions is clarified, one can carry through the variational process for $\tilde{E}_\Omega (V.13)$ and thereby obtains the well-known Poisson equation (IV.18) for $[b]A_0(r)$. The standard formal solution is here given by equation (IV.26) which we will readily exploit for the study of the corresponding anisotropy corrections.

2. Anisotropy Corrections

If one disregards for the moment the spherically symmetric approximation (V.1), the general Poisson equation is found as the extremal equation due to the general gauge field functional $(e)\tilde{E}_\Omega$. Furthermore, the use of the product ansatz (IV.5a)–(IV.5b) recast the general Poisson equation (IV.4) to the more specific form (IV.19) with the formal solution

$$\{b\}A_0(r, \vartheta) = \alpha_s \int d^3r' \{b\}k_0(\vartheta') \cdot \{b\}k_0(r') \left|\frac{\vec{r} - \vec{r}'}{|\vec{r} - \vec{r}'|}\right| .$$  

Clearly, this is the anisotropic generalization (up to a factor of $4\pi$) of the former result (IV.26) for the spherically symmetric approximation.

It is true, the latter approximation disregards completely the anisotropic features of the exact solution of the eigenvalue problem, but nevertheless it plays a certain role when considering now the anisotropic potential $\{b\}A_0(r, \vartheta)$ (V.15). Namely, since it appears rather difficult to exactly calculate the integral of that formal solution (V.15) we are forced to think about some approximative evaluation. For this purpose, one may resort to an expansion of the anisotropic potential $\{b\}A_0(r, \vartheta)$ around the spherically symmetric potential $[b]A_0(r)$ (IV.26), i.e. an expansion with respect to the magnitude of anisotropy. In this sense, one may look upon the spherically symmetric approximation $[b]A_0(r)$ as the leading term of such an expansion, namely such that it appears as the angular average of the more general anisotropic solution $\{b\}A_0(r, \vartheta)$ (V.15), i.e. explicitly

$$[b]A_0(r) = \int \frac{d\Omega}{4\pi} \{b\}A_0(r, \vartheta)$$  

$$(d\Omega \doteq d\vartheta d\phi \sin \vartheta) .$$
In order to build up now such an expansion with respect to the magnitude of anisotropy, one starts with the following expansion of the denominator in the integral representation (V.15) of \( b_A^0(r, \vartheta) \) \[^2\]

\[
\frac{1}{||\vec{r} - \vec{r}'||} = \frac{1}{(r^2 + r'^2)^{1/2}} + \frac{r r'}{(r^2 + r'^2)^{3/2}} (\hat{\vec{r}} \cdot \hat{\vec{r}}') + \frac{3}{2} \frac{r^2 r'^2}{(r^2 + r'^2)^{5/2}} (\hat{\vec{r}} \cdot \hat{\vec{r}}')^2 + \ldots
\]

(V.17)

\[
+ \frac{5}{2} \frac{r^3 r'^3}{(r^2 + r'^2)^{7/2}} (\hat{\vec{r}} \cdot \hat{\vec{r}}')^3 + \frac{35}{8} \frac{r^4 r'^4}{(r^2 + r'^2)^{7/2}} (\hat{\vec{r}} \cdot \hat{\vec{r}}')^4 + \ldots
\]

\[
(\vec{r}' = \frac{\vec{r}}{||\vec{r}||}, \hat{\vec{r}}' = \frac{\vec{r}}{||\vec{r}'||} \Rightarrow ||\hat{\vec{r}}|| = ||\hat{\vec{r}}'|| = 1).
\]

However, this expansion is not directly introduced in the integral of equation (V.15) but we first define the properly anisotropic part \( b_A^{an}(r, \vartheta) \) of \( b_A^0(r, \vartheta) \) (V.15) through

\[
b_A^{an}(r, \vartheta) \equiv b_A^0(r, \vartheta) - [b] A_0(r),
\]

(V.18)

so that the spherically symmetric approximation \([b] A_0(r)\) actually appears as the expected leading term of the proposed expansion:

\[
b_A^0(r, \vartheta) = [b] A_0(r) + b_A^{an}(r, \vartheta).
\]

(V.19)

As a consistency requirement, the former averaging postulate (V.16) entails now that the average value of the anisotropic part \( b_A^{an}(r, \vartheta) \) must vanish

\[
\frac{d\Omega}{4\pi} b_A^{an}(r, \vartheta) = 0.
\]

(V.20)

But once the anisotropic part of the gauge potential is precisely defined now, its power series expansion can be easily carried through. Here, the point of departure is the corresponding integral representation of \( b_A^{an}(r, \vartheta) \), which is obtained by substituting both integral representations (IV.26) and (V.15) into (V.18) yielding

\[
b_A^{an}(r, \vartheta) = \alpha s \int d^3r' \frac{1}{||\vec{r}' - \vec{r}||} \left( b_A^{0}(\vartheta') - \frac{1}{4\pi} \right) \cdot b_A^{0}(r')
\]

(V.21)
and if the expansion (V.17) is inserted herein one finds emerging a series expansion of the following product form:

\[
\{b\} A^m(r, \vartheta) = \{b\} A^0(\vartheta) \cdot \{b\} A^0(r) + \{b\} A^1(\vartheta) \cdot \{b\} A^1(r) + \{b\} A^2(\vartheta) \cdot \{b\} A^2(r) + \{b\} A^3(\vartheta) \cdot \{b\} A^3(r) + \{b\} A^4(\vartheta) \cdot \{b\} A^4(r) + \ldots
\]

(V.22)

Here, the angular factors appear first in integral form, and the lowest orders may easily be calculated exactly:

\[
\{b\} A^1(\vartheta) \doteq \int d\vartheta' \left( \{b\} k_0(\vartheta') - \frac{1}{4\pi} \right) = 0
\]

(V.23a)

\[
\{b\} A^2(\vartheta) \doteq \int d\vartheta' \left( \{b\} k_0(\vartheta') - \frac{1}{4\pi} \right) \left( \hat{r} \cdot \hat{r}' \right) = 0
\]

(V.23b)

\[
(d\vartheta' \doteq d\vartheta' d\varphi' \sin \vartheta').
\]

The importance of these lowest-order results lies in the circumstance that they are valid for any angular distribution \(\{b\} k_0(\vartheta)\); namely the first result (V.23a) is a consequence of the separate angular normalization condition (IV.24a) and the second result (V.23b) is an implication of the skew symmetry of the integrand with respect to the reflection of the two-sphere at the equatorial two-plane \((\vartheta = \frac{\pi}{2})\). Moreover by the latter argument, all the angular factors of odd order are trivial, i.e.

\[
\int d\vartheta' \left( \{b\} k_0(\vartheta') - \frac{1}{4\pi} \right) \left( \hat{r} \cdot \hat{r}' \right)^{2n+1} = 0
\]

(V.24)

\((n = 0, 1, 2, 3, \ldots)\).

Consequently, the first non-trivial angular factor is \(\{b\} A^3(\vartheta)\), followed by \(\{b\} A^5(\vartheta)\):

\[
\{b\} A^3(\vartheta) \doteq \frac{3}{2} \int d\vartheta' \left( \{b\} k_0(\vartheta') - \frac{1}{4\pi} \right) \left( \hat{r} \cdot \hat{r}' \right)^2, \quad \text{quadrupole}
\]

(V.25a)

\[
\{b\} A^5(\vartheta) \doteq \frac{35}{8} \int d\vartheta' \left( \{b\} k_0(\vartheta') - \frac{1}{4\pi} \right) \left( \hat{r} \cdot \hat{r}' \right)^4, \quad \text{octupole}
\]

(V.25b)

However, it should be evident that the precise value of these integrals will depend on the actual density \(\{b\} k_0(\vartheta)\); for instance, any member of a dichotomic pair of ortho-states
(due to the same quantum number $j_0$) may have its own angular factor $^{(b)}A_{III}(\vartheta)$ etc. being different from that one due to its $j_0$-partner. But a common property of all angular factors $^{(b)}A_{III}(\vartheta)$ etc. is that their average on the two-sphere is zero

$$\int \frac{d\Omega}{4\pi} \, ^{(b)}A_{III}(\vartheta) = \int \frac{d\Omega}{4\pi} \, ^{(b)}A^V(\vartheta) = \ldots = 0 \, ,$$

which in turn implies that the anisotropic correction $^{(b)}A_{an}(r, \vartheta)$ (V.21) has also zero average over the two-sphere, cf. (V.20).

For the sake of brevity, we are satisfied for the moment with a treatment of only the lowest-order case (V.25a) for $j_0 = 2, 3, 4$ and $^{(b)}j_z = \pm 1$. But even for this restriction to only a few values of $j_0$ we can observe the ortho-dimorphism, see the subsequent table which transcribes the densities $^{(b)}k_0(\vartheta)$ to the corresponding angular factors $^{(b)}A_{III}(\vartheta)$ according to the prescription (V.25a).

| $j_0$ | $^{(b)}j_z$ | $^{(b)}k_0(\vartheta)$ | (V.20) | $^{(b)}A_{III}(\vartheta)$ | (V.25a) |
|-------|-------------|------------------------|--------|-----------------------------|--------|
| 2     | $\pm 1$     | $\frac{\sin \vartheta}{2\pi^2} \cdot (9 - 8 \sin^2 \vartheta)$ | $-\frac{3}{16} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{3}{16} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ |
| 3     | $\pm 1$     | $\frac{3}{2\pi} \sin \vartheta \left( 1 - \frac{8}{3} \sin^2 \vartheta \right)$ | $\frac{3}{16} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{9}{32} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ |
| 4     | $\pm 1$     | $\frac{10}{2\pi} \sin \vartheta \left( \frac{5}{3} - 4 \sin^2 \vartheta + \frac{12}{5} \sin^4 \vartheta \right)$ | $\frac{3}{16} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{9}{32} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ |
|       |             | $\frac{10}{2\pi} \sin \vartheta \left( 1 - 4 \sin^2 \vartheta + \frac{28}{5} \sin^4 \vartheta - \frac{64}{25} \sin^6 \vartheta \right)$ | $\frac{51}{160} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ |

This table demonstrates some striking features of the quadrupole correction term $^{(b)}A_{III}(\vartheta)$. First, the quadrupole corrections $^{(b)}A_{III}(\vartheta)$ (V.25a) for both ortho-densities $^{(b)}k_0(\vartheta)$ due to $j_0 = 2$ differ merely in sign. This circumstance has its consequences as far as the energy (being concentrated in the anisotropic field configuration) is concerned, see below for the discussion of the corresponding degeneracy. But in order to see here somewhat more clearly the origin of this strange effect, which partly (i.e. from the energetic point of view) suppresses the ortho-dimorphism just elaborated, one reconsiders the orig-
inal definition (V.25a) of \( A_{III}(\vartheta) \) and observes also the separate angular normalization (IV.24a) of the density \( \{b\}k_0(\vartheta) \), together with the specific angular structure of the scalar product of unit vectors \( \hat{r}, \hat{r}' \):

\[
(\hat{r} \cdot \hat{r}')^2 = \sin^2 \vartheta \sin^2 \vartheta' \cos^2(\phi - \phi') + \cos^2 \vartheta \cos^2 \vartheta' + 2 \sin \vartheta \sin \vartheta' \cos \vartheta \cos \vartheta' \cos(\phi - \phi').
\]

(V.27)

Indeed, these simple mathematical elements are sufficient in order to deduce, with a little bit algebra, the following general form of \( \{b\}A_{III}(\vartheta) \):

\[
\{b\}A_{III}(\vartheta) = \frac{-3}{4} \left( 1 - 3 \cdot K_{III}(\{b\}) \right) \left[ \cos^2 \vartheta - \frac{1}{3} \right],
\]

(V.28)

where the integral \( K_{III}(\{b\}) \) is defined by

\[
K_{III}(\{b\}) = \int d\Omega' \cos^2 \vartheta' \{b\}k_0(\vartheta') = 2\pi \int d\vartheta' \sin \vartheta' \cos^2 \vartheta' \{b\}k_0(\vartheta').
\]

(V.29)

This result (V.28) explains why both ortho-configurations due to \( j_O = 2 \) and \( (b)j_z = \pm 1 \) share the same angular dependence, apart from sign. The value of this integral \( K_{III}(\{b\}) \) on both densities \( \{b\}k_0(\vartheta) \) due to \( j_O = 2 \) (see the table of densities \( \{b\}k_0(\vartheta) \) on p. 82) yields now

\[
K_{III}(\{b\}) = \begin{cases} 
\frac{1}{4} & \text{first density, } \{b\}k_0(\vartheta) = \frac{1}{2\pi} \sin \vartheta \\
\frac{5}{12} & \text{second density, } \{b\}k_0(\vartheta) = \frac{1}{3\pi} \sin \vartheta \cdot (9 - 8 \sin^2 \vartheta). 
\end{cases}
\]

(V.30)

Inserting now these two possible values of the integral \( K_{III}(\{b\}) \) into the general relation (V.28) yields just the two quadrupole corrections \( \{b\}A_{III}(\vartheta) \) for \( j_O = 2 \) with their different signs, as displayed by the table on p. 82. As we shall readily see, this difference in sign of both versions \( \{b\}A_{III}(\vartheta) \) is not sufficient in order to equip both corresponding solutions of the eigenvalue problem with different energies \( E_{O}^{(3)} \). Thus the result will be that the lowest approximation order (with respect to the anisotropy corrections) cannot induce an electrostatic energy difference for the dimorphic pair of states due to \( n_O = 3, j_O = 2, (b)j_z = \pm 1 \). (See also some further comments on this in App.D.)
However, as is clearly demonstrated by the lower half of that table on p. 82, this result does hold only for the non-relativistic state due to \( J_\sigma = 2 \) of ortho-positronium. For the excited ortho-states \( (J_\sigma = 3 \text{ and } J_\sigma = 4) \), the angular densities \( \{^b k_0(\vartheta)\} \) and therefore also the quadrupole corrections \( \{^b A^\text{III}(\vartheta)\} \) of both dimorphic partners are seen to be distinctly different from each other (App.D) which then will entail also different electrostatic interaction energies. Of course, this energetic degeneracy of the dimorphic ortho-states \( (J_\sigma = 2, \ (b) j_z = \pm 1) \) does refer exclusively to the first anisotropy correction as expressed by \( \{^b A^\text{III}(\vartheta)\} \) (V.25a)! The next higher approximation order \( \{^b A^\text{V}(\vartheta)\} \) (V.25b) will surely eliminate this first-order degeneracy. Indeed, this expectation can easily be verified by inserting both ortho-densities \( \{^b k_0(\vartheta)\} \) due to \( J_\sigma = 2 \) (see table on p. 82) into the general prescription (V.25b) for the quadrupole correction \( \{^b A^\text{V}(\vartheta)\} \) in order to yield the following results:

\[
\begin{align*}
\{^b k_0(\vartheta)\} &= \frac{\sin \vartheta}{\pi^2} \Rightarrow \{^b A^\text{V}(\vartheta)\} = \frac{35}{256} \left\{ \frac{11}{10} - 3 \cos^2 \vartheta - \frac{1}{2} \sin^2 \vartheta \right\} \quad (V.31a) \\
\{^b k_0(\vartheta)\} &= \frac{\sin \vartheta}{3\pi^2} \cdot \left( \sin^2 \vartheta + 9 \cos^2 \vartheta \right) \Rightarrow \{^b A^\text{V}(\vartheta)\} = \frac{7}{256} \left\{ -7 + 30 \cos^2 \vartheta - 15 \cos^4 \vartheta \right\} \quad (V.31b)
\end{align*}
\]

\( (J_\sigma = 2, \ (b) j_z = \pm 1) \).

Obviously, this second approximation order \( \{^b A^\text{V}(\vartheta)\} \) displays no common angular dependence for the dimorphic pair as is the case with the first approximation order \( \{^b A^\text{III}(\vartheta)\} \) (V.28)–(V.30), but nevertheless the average of all multipole corrections \( \{^b A^\text{III}(\vartheta)\}, \{^b A^\text{V}(\vartheta)\} \) over the two-sphere is zero, as required by equation (V.26). However, in contrast to their trivial mean values, the contribution of these anisotropy corrections to the binding energy is readily seen to be non-trivial.
VI Energy of Matter and Gauge Fields

It should be a matter of course that different interaction potentials \( \{ b \} A_0(\mathbf{r}, \vartheta) \) for both positronium constituents will entail different binding energies \( \mathbb{E}_{O}^{(j)} \). This is surely a reasonable assumption and may be expected to hold also for the approximate solutions of the eigenvalue problem to be discussed subsequently. The corresponding approximation method is the same as has been applied in the precedent paper [2], where the RST energy functional \( \tilde{\mathbb{E}}_{[\Omega]} \) is extremalized on a suitably selected set of trial configurations.

The trial amplitudes \( \tilde{\Omega}(r) \) are postulated to be of adequate form and include some variational parameters (here \( \beta, \nu \)):

\[
\tilde{\Omega}(r) = \Omega_e r^\nu e^{-\beta r} \quad \text{(VI.1a)}
\]

\[
\Omega^2 = \frac{(2\beta)^{2\nu+2}}{\Gamma(2\nu+2)} \quad \text{(VI.1b)}
\]

Obviously, after separating off the angular dependence (see (IV.5a)–(IV.5b)), the selected class of trial amplitudes \( \tilde{\Omega}(r) \) is here of the spherically symmetric form which itself is surely an approximation to the exact solutions; but for the purposes of the present paper we will be satisfied with such a spherically symmetric form of the wave amplitudes \( \tilde{\Omega}(r) \).

In contrast to this, the interaction potential \( \{ b \} A_0(\mathbf{r}) \) is admitted to be anisotropic; however, it is assumed to be the sum of a spherically symmetric part \( \{ b \} A_0(r) \) plus an anisotropic perturbation \( \{ b \} A_{an}(r, \vartheta) \), see equation (V.19). Furthermore, these two constituents of the interaction potential \( \{ b \} A_0(r, \vartheta) \) are assumed now to be kinematically independent, where this independence of the anisotropic part \( \{ b \} A_{an}(r, \vartheta) \) refers exclusively to the radial auxiliary potentials \( \{ b \} A_{III}(r) \), \( \{ b \} A_{V}(r) \) etc., cf. the series expansion (V.22); whereas their angular counterparts \( \{ b \} A_{III}(\vartheta) \), \( \{ b \} A_{V}(\vartheta) \) etc. are fixed through the integral relations (V.25a), (V.25b) etc. Thus our selected trial configurations consist of a set of spherically symmetric fields \( \{ \tilde{\Omega}(r); \{ b \} A_0(r), \{ b \} A_{III}(r), \{ b \} A_{V}(r), \ldots \} \) where only the trial amplitudes \( \tilde{\Omega}(r) \) are of a pre-specified form (cf. (VI.1a)–(VI.1b)) with undetermined variational parameters \( \beta \) and \( \nu \). In contrast to this, the spherically symmetric potential \( \{ b \} A_0(r) \)
and the radial auxiliary potentials $\{b\}A_0(r), \{b\}A_{III}(r)$ etc. are first left unspecified and must afterwards be determined from their extremal equations, i.e. from extremalization of the energy functional $\tilde{E}_{[Ω]}$ to be understood as the anisotropic generalization of the spherically symmetric version (V.2). The extremalization of $\tilde{E}_{[Ω]}$ with respect to the trial amplitude $\tilde{Ω}(r)$ occurs then through extremalization with respect to the variational parameters $β$ and $ν$ which themselves are entering also the potentials $\{b\}A_0(r), \{b\}A_{III}(r), \{b\}A_{V}(r)$ etc., namely via the solutions of the extremal equations for those potentials whose source is determined by just the square of the amplitude $\tilde{Ω}(r)$.

Thus, summarizing the approximation procedure, we will end up with a certain energy function $E^{IV}(β, ν)$ of the two variational parameters $β$ and $ν$; and the stationary points of this function, being determined by the requirements

\[
\frac{∂E^{IV}(β, ν)}{∂β} = 0, \quad \frac{∂E^{IV}(β, ν)}{∂ν} = 0,
\]

yield the equilibrium values $β_*, ν_*$ so that the wanted energies appear as the values $E^{IV}(β_*, ν_*)$ of that energy function $E^{IV}(β, ν)$ on these special values $β_*, ν_*$. According to the sum structure of the ortho-functional $\tilde{E}_{[Ω]} (V.2)$, its value $E_{Ω}(β, ν)$ on our selected trial configurations will appear as the sum of the matter energy $E_{kin}(β, ν)$ and the anisotropic gauge field energy $E^{eR}_G(β, ν)$ plus the constraint terms:

\[
E_{Ω}(β, ν) = 2E_{kin}(β, ν) + E^{eR}_G(β, ν) + 2λ_s \cdot \tilde{N}_{Ω}(β, ν) + λ_G^{(e)} \cdot \tilde{N}^{e}_G(β, ν)
\]

\[\equiv E^{IV}(β, ν) + 2λ_s \cdot \tilde{N}_{Ω}(β, ν) + λ_G^{(e)} \cdot \tilde{N}^{e}_G(β, ν).
\]

Whether or not the Poisson constraint term $\tilde{N}^{(e)}_G (V.8)$ in its anisotropic form $\tilde{N}^{e}_G$, i.e.

\[
\tilde{N}^{e}_G \equiv E^{eR}_G - \tilde{M}^{(e)}_G c^2,
\]

will contribute in a non-trivial way must be discussed separately (see below). In contrast to this, the other constraint term refers to the normalization condition for the non-relativistic
amplitude $\tilde{\Omega}(r)$

$$\tilde{N}_\Omega \doteq \int_0^\infty dr \, \tilde{\Omega}^2(r) - 1 \quad \text{(VI.5)}$$

and can always be put to zero by simply admitting only those trial amplitudes $\tilde{\Omega}(r)$ which are normalized to unity ($\sim \tilde{N}_\Omega = 0$). However, from formal reasons it is necessary to first include the constraint terms in the energy functional $\tilde{E}[\Omega]$ so that both the matter equation [IV.17] and the gauge field equation [IV.18] do appear as the extremal equations due to that ortho-functional $\tilde{E}[\Omega]$ (V.2) whose matter part appears now as

$$(P)\tilde{E}[\Omega] = 2E_{\text{kin}} + 2\lambda_s \cdot \tilde{N}_\Omega \quad \text{(VI.6)}$$

and similarly its gauge field part as

$$(G)\tilde{E}[\Omega] \Rightarrow (e)\tilde{E}[\Omega] = E_R^{(e)} + \lambda_G^{(e)} \cdot \tilde{N}_G^{(e)} \quad \text{(VI.7)}$$

1. Energy of the Matter Fields

First, we may turn to the kinetic energy which for the two-particle system is twice the one-particle energy $E_{\text{kin}}$ [34]

$$E_{\text{kin}} = \frac{\hbar^2}{2M} \int_0^\infty dr \, r \left\{ \left( \frac{d\tilde{\Omega}(r)}{dr} \right)^2 + \frac{j_\tilde{\Omega}^2}{r^2} \cdot \tilde{\Omega}^2(r) \right\} \quad \text{(VI.8)}$$

Here, the centrifugal term ($\sim j_\tilde{\Omega}^2$) is induced by the former product ansatz [IV.5a]–[IV.5b] and evidently does account for the total angular momentum of the considered ortho-state. Substituting herein the selected form (VI.1a)–(VI.1b) of the trial amplitude $\tilde{\Omega}(r)$ yields for the one-particle kinetic energy $E_{\text{kin}}$ (VI.8)

$$E_{\text{kin}}(\beta, \nu) = \frac{e^2}{2a_B} (2a_B \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) \quad \text{(VI.9a)}$$

$$\varepsilon_{\text{kin}}(\nu) \doteq \frac{1}{2\nu + 1} \left( \frac{1}{4} + \frac{j_\tilde{\Theta}^2}{2\nu} \right) \quad \text{(VI.9b)}$$

see equation (VI.154b) of ref. [34]. This is formally the same kinetic energy function as was used for para-positronium with merely the quantum number $l_\nu (= j_\nu)$ for para-positronium being replaced now by $j_\tilde{\Theta}$ for ortho-positronium.
2. Energy of the Gauge Fields

Next, the gauge field part \( \tilde{G} \) is to be specified in terms of the three gauge field constituents \( [b] A_0(r), [b] A_{III}(r), [b] A^V(r) \) which we treat as independent constituents of the gauge field subsystem. Since, on account of the specific form of the Poisson constraint \( \tilde{N}_G \) (VI.4), the desired gauge field part \( \tilde{E}^{(e)}[\Omega] \) (VI.7) consists essentially of the gauge field energy \( E^{(e)}_R \) and its mass equivalent \( \tilde{M}^{(e)} c^2 \) it is sufficient to explicitly display these two objects in terms of the newly introduced gauge fields \( [b] A_0(r), [b] A_{III}(r), [b] A^V(r) \).

Turning here first to the electrostatic gauge field energy \( E^{(e)}_R \), the spherically symmetric relation (V.7) is to be generalized for the presently considered anisotropic situation to

\[
\vec{E}_b(\vec{r}) = -\vec{\nabla} \ {\langle b \rangle} A_0(r, \vartheta) = -\vec{e}_r \frac{\partial \ {\langle b \rangle} A_0(r, \vartheta)}{\partial r} - \vec{e}_\vartheta \frac{1}{r} \frac{\partial \ {\langle b \rangle} A_0(r, \vartheta)}{\partial \vartheta},
\]

so that the gauge field energy (V.4) reappears as

\[
E^{(e)}_R = -\frac{\hbar c}{4\pi \alpha_s} \int d^3\vec{r} \left\{ \left( \frac{\partial \ {\langle b \rangle} A_0(r, \vartheta)}{\partial r} \right)^2 + \frac{1}{r^2} \left( \frac{\partial \ {\langle b \rangle} A_0(r, \vartheta)}{\partial \vartheta} \right)^2 \right\}.
\]

But here we have to observe the splitting of the anisotropic potential \( \{b\} A_0(r, \vartheta) \) into the sum of the isotropic part \( [b] A_0(r) \) and the anisotropic perturbation \( \{b\} A_{an}(r, \vartheta) \), cf. equation (V.19); and this must then induce a similar splitting of the gauge field energy \( E^{(e)}_R \) (VI.11) into two parts, i.e. we put

\[
E^{(e)}_R = E^{(e)}_R + E^{(e)}_{an}.
\]

Here, the “isotropic” part \( E^{(e)}_R \) has already been specified in terms of \( [b] A_0(r) \) by equation (V.7) and the “anisotropic” energy \( E^{(e)}_{an} \) is found to be of the following form

\[
E^{(e)}_{an} = -\frac{\hbar c}{4\pi \alpha_s} \int d^3\vec{r} \left\{ \left( \frac{\partial \{b\} A_{an}(r, \vartheta)}{\partial r} \right)^2 + \frac{1}{r^2} \left( \frac{\partial \{b\} A_{an}(r, \vartheta)}{\partial \vartheta} \right)^2 \right\}.
\]

(See the precedent paper [1] for the reason why there is no mixed term involving both parts \( [b] A_0(r) \) and \( \{b\} A_{an}(r, \vartheta) \)).

For further specifying down this anisotropic part \( E^{(e)}_{an} \) (VI.13) one observes the decomposition (V.22) of the anisotropic correction \( \{b\} A_{an}(r, \vartheta) \) into the sum of products of
an angular and radial auxiliary potential; here we retain only the first two terms of the
series expansion (VI.22):

\[
\{b\} A_0(r, \vartheta) = \{b\} A_{III}(r) \cdot \{b\} A_{III}(\vartheta) + \{b\} A^V(\vartheta) \cdot \{b\} A^V(r). 
\]  

(VI.14)

This arrangement lets then reappear the “anisotropic” gauge field energy \(E_{\text{an}}^{(e)}\) in
the following final form

\[
E_{\text{an}}^{(e)} = -\frac{\hbar c}{\alpha_s} \int_0^\infty dr \, r^2 \left\{ (b) e_{\text{III}} \cdot \left( \frac{d \{b\} A_{III}(r)}{dr} \right)^2 + (b) f_{\text{III}} \cdot \left( \frac{\{b\} A_{III}(r)}{r} \right)^2 \right\} 
+ \left\{ (b) e_{\text{V}} \cdot \left( \frac{d \{b\} A^V(r)}{dr} \right)^2 + (b) f_{\text{V}} \cdot \left( \frac{\{b\} A^V(r)}{r} \right)^2 \right\} 
+ 2 \left\{ (b) e_{\text{IV}} \frac{d \{b\} A_{III}(r)}{dr} \cdot \frac{d \{b\} A^V(r)}{dr} + (b) f_{\text{IV}} \frac{\{b\} A_{III}(r)}{r} \cdot \frac{\{b\} A^V(r)}{r} \right\} . 
\]  

(VI.15)

The angular coefficients \(e_N, f_N\) \((N = \text{III, IV, V})\) do arise here by carrying out the corre-
sponding angular integrations in the original energy integral (VI.13) which yields

\[
(b) e_{\text{III}} = \int \frac{d\Omega}{4\pi} \left( \{b\} A_{III}(\vartheta) \right)^2, \quad (b) f_{\text{III}} = \int \frac{d\Omega}{4\pi} \left( \frac{d \{b\} A_{III}(\vartheta)}{d\vartheta} \right)^2 \]  

(VI.16a)

\[
(b) e_{\text{IV}} = \int \frac{d\Omega}{4\pi} \{b\} A_{III}(\vartheta) \cdot \{b\} A^V(\vartheta), \quad (b) f_{\text{IV}} = \int \frac{d\Omega}{4\pi} \left( \frac{d \{b\} A_{III}(\vartheta)}{d\vartheta} \right) \cdot \left( \frac{d \{b\} A^V(\vartheta)}{d\vartheta} \right) \]  

(VI.16b)

\[
(b) e_{\text{V}} = \int \frac{d\Omega}{4\pi} \left( \{b\} A^V(\vartheta) \right)^2, \quad (b) f_{\text{V}} = \int \frac{d\Omega}{4\pi} \left( \frac{d \{b\} A^V(\vartheta)}{d\vartheta} \right)^2 . \]  

(VI.16c)

displaySince the angular functions \(\{b\} A_{III}(\vartheta), \{b\} A^V(\vartheta)\) are known and depend on both quantum
numbers \(j_\varphi\) and \((b) j_z\) but depend also on the dimorphic type, the angular coefficients
\(e_N, f_N\) \((N = \text{III, IV, V})\) are functionals of the considered ambiguous quantum state \((j_\varphi, (b) j_z)\)
but are otherwise to be treated as fixed numerical constants. We will readily see that
through this arrangement the principle of minimal energy becomes reduced to a purely
radial variational problem. The numerical values of the constants are displayed by the
subsequent table for the quadrupole approximation \((\sim \{b\} A_{III}(\vartheta))\).
The striking feature of these numerical values refers to the fact that the ratios $\frac{f_3}{e_3}$ and $\frac{m_3}{e_3}$ are all the same (see App.A)

$$\frac{(b) f_{III}}{(b) e_{III}} = 6 \quad (VI.17a)$$

$$\frac{(b) m_{III}}{(b) e_{III}} = 5 \quad (VI.17b)$$

The meaning of this will readily become obvious when considering below the quadrupole equation for the radial potential correction $(b)A_{III}(r)$.

3. Mass Equivalent

Similar arguments as for the anisotropy energy $E_{an}^{(e)}$ (VI.15) do also apply to the mass equivalent $M^{(e)}c^2$ (V.3). Indeed, inserting therein the series expansion (V.22) (up to the $V$-th order) in combination with the factorized density $(b)k_0 (\hat{r})$ (IV.20)–(IV.21) and the separate angular normalization (IV.24a) lets emerge the (non-relativistic) mass equivalent in a form analogous to the “anisotropic” gauge field energy $E_{R}^{(e)}$ (VI.12):

$$M^{(e)}c^2 \Rightarrow \tilde{M}^{(e)}c^2 = \tilde{M}_{an}^{(e)}c^2 + \tilde{M}_{an}^{(e)}c^2 . \quad (VI.18)$$

This says that the general mass equivalent splits up into the sum of the spherically symmetric part $\tilde{M}_{an}^{(e)}c^2$ (V.12) and the anisotropic correction $\tilde{M}_{an}^{(e)}c^2$, where the latter part
appears as the sum of the \( \text{III} \)-rd and \( \text{V} \)-th order, i.e.

\[
\tilde{M}^{(e)c^2}_{\text{an}} = \tilde{M}^{(e)c^2}_{\text{III}} + \tilde{M}^{(e)c^2}_{\text{V}} .
\]  
(VI.19)

This yields finally the following decomposition

\[
\tilde{M}^{(e)c^2}_{\text{an}} = \tilde{M}^{(e)c^2}_{\text{an}} + \tilde{M}^{(e)c^2}_{\text{III}} + \tilde{M}^{(e)c^2}_{\text{V}}
\]  
(VI.20)

where the spherically symmetric part \( \tilde{M}^{(e)c^2}_{\text{an}} \) has already been specified by equation (V.12) and the anisotropy corrections are given by

\[
\tilde{M}^{(e)c^2}_{\text{III}} = -\hbar c \,(^{(b)m_{\text{III}}} \int_0^\infty dr \, r \,(^{(b)A^{\text{III}}(r)} \cdot \tilde{\Omega}^2(r) )
\]  
(VI.21a)

\[
\tilde{M}^{(e)c^2}_{\text{V}} = -\hbar c \,(^{(b)m_{\text{V}}} \int_0^\infty dr \, r \,(^{(b)A^{\text{V}}(r)} \cdot \tilde{\Omega}^2(r) )
\]  
(VI.21b)

with the angular constants \( ^{(b)m_{\text{III}}} \) and \( ^{(b)m_{\text{V}}} \) being defined through

\[
^{(b)m_{\text{III}}} \equiv \int d\Omega \,(^{(b)A^{\text{III}}(\vartheta)} \cdot ^{(b)k_0(\vartheta)}
\]  
(VI.22a)

\[
^{(b)m_{\text{V}}} \equiv \int d\Omega \,(^{(b)A^{\text{V}}(\vartheta)} \cdot ^{(b)k_0(\vartheta)}
\]  
(VI.22b)

The angular coefficient \( ^{(b)m_{\text{III}}} \) (VI.22a) is obviously due to the formerly considered quadrupole approximation and some values have already been displayed in the table on p. 90.

The last point concerning the gauge field subsystem refers to the “anisotropic” Poisson constraint \( \tilde{N}^{(e)}_G \) (VI.13). Since both constituents \( E^{(e)}_R \) and \( \tilde{M}^{(e)c^2} \) have been split up into sums of the isotropic and anisotropic parts, cf. (VI.12) and (VI.18), the constraint itself must undergo a similar splitting:

\[
\tilde{N}^{(e)}_G = \tilde{N}^{(e)}_G + \tilde{N}^{(e)}_{\text{an}}
\]  
(VI.23)

where the isotropic part \( \tilde{N}^{(e)}_G \) is of course built up by the isotropic parts of the gauge field energy and its mass equivalent, cf. (V.14), and analogously for the anisotropic part \( \tilde{N}^{(e)}_{\text{an}} \)

\[
\tilde{N}^{(e)}_{\text{an}} = E^{(e)}_{\text{an}} - \tilde{M}^{(e)c^2}_{\text{an}}
\]  
(VI.24)
Summarizing, we ultimately arrive at a splitting of the whole energy functional $\tilde{E}_{\Omega}$ not only in two but rather three constituents which correspond in a self-evident way to the matter part and the isotropic and anisotropic gauge field parts:

$$\tilde{E}_{\Omega} = 2E_{\text{kin}} + 2\lambda_s \cdot \tilde{N}_\Omega + \left[E^{(e)}_R + \lambda_G^{(e)} \cdot \tilde{N}^{(e)}_G\right] + \left[E^{(e)}_{\text{an}} + \lambda_G^{(e)} \cdot \tilde{N}^{(e)}_{\text{an}}\right]$$  \hspace{1cm} (VI.25)

These three subsystems will now be adopted as three kinematically independent (but coupled) degrees of freedom so that we can deduce the corresponding field equations by extremalization of this functional $\tilde{E}_{\Omega}$ (VI.25) on the space of selected trial configurations \{\hat{\Omega}(r), [^b]A_0(r), [^b]A_{\text{III}}(r), [^b]A_{\text{V}}(r)\}.

### 4. Principle of Minimal Energy

Once the energy functional for the RST configurations has been set up, cf. (VI.25), one can now look for the corresponding extremal equations. For this purpose, one may derive benefit from the fact that the various terms of $\tilde{E}_{\Omega}$ do not contain all four independent quantities \{\hat{\Omega}; [^b]A_0, [^b]A_{\text{III}}, [^b]A_{\text{V}}\}. Therefore the variational process for any of these field quantities does comprehend only a certain subset of all those terms constituting $\tilde{E}_{\Omega}$.

For instance, the extremalization of $\tilde{E}_{\Omega}$ with respect to the amplitude field $\tilde{\Omega}(r)$ disregards the electrostatic gauge field energy $E^{(e)}_R$ (VI.11) and thus takes into account only the matter part $(D)\tilde{E}_{\Omega}$ (VI.6) and the mass equivalent $\tilde{M}^{(e)}_G c^2$ (VI.20). Thus the extremalization ($\delta_{\tilde{\Omega}}$, say) with respect to the amplitude $\tilde{\Omega}(r)$ looks as follows:

$$0 \equiv \delta_{\tilde{\Omega}} \tilde{E}_{\Omega} = \delta_{\tilde{\Omega}} (D)\tilde{E}_{\Omega} - \lambda_G^{(e)} \cdot \delta_{\tilde{\Omega}} \left\{\tilde{M}^{(e)}_G c^2 + \tilde{M}^{(e)}_{\text{III}} c^2 + \tilde{M}^{(e)}_{\text{V}} c^2\right\},$$  \hspace{1cm} (VI.26)

and this yields for $\tilde{\Omega}(r)$ the Schrödinger-like equation (provided we put $\lambda_G^{(e)} = -2$):

$$-\frac{\hbar^2}{2M} \left\{\frac{d^2 \tilde{\Omega}(r)}{dr^2} + \frac{1}{r} \frac{d \tilde{\Omega}(r)}{dr}\right\} + \frac{\hbar^2}{2Mr^2} j^2 \cdot \tilde{\Omega}(r)$$

$$-\hbar c \left\{[^b]A_0(r) + [^b]m_{\text{III}} \cdot [^b]A_{\text{III}}(r) + [^b]m_{\text{V}} \cdot [^b]A_{\text{V}}(r)\right\} \cdot \tilde{\Omega}(r) = E^*_\epsilon \cdot \tilde{\Omega}(r).$$  \hspace{1cm} (VI.27)
Obviously, this is the anisotropic generalization of the former eigenvalue equation (IV.17) which thus is seen to refer exclusively to the spherically symmetric approximation (V.1). If the anisotropic corrections \([b]A^0(r, \vartheta)\) and \([b]A^V(r, \vartheta)\) are taken into account, their radial parts \([b]A^0(r)\), \([b]A^V(r)\) do obviously also couple to the spherically symmetric trial amplitude \(\hat{\Omega}(r)\), where \([b]m^0_{\mathrm{III}}\) and \([b]m^0_{\mathrm{V}}\) (VI.22a)–(VI.22b) play the role of coupling constants.

Clearly, we are not able to solve the amplitude equation (VI.27) exactly, but instead we will resort to the previously used trial functions \(\hat{\Omega}(r)\) (VI.1a)–(VI.1b). Thus, denoting the value of the matter functional \(D\hat{\mathcal{E}}_{[\Omega]}\) (VI.25) on this normalized trial amplitude by \(2E_{\mathrm{kin}}(\beta, \nu)\), one readily is led back to the former results (VI.9a)–(VI.9b).

**Isotropic Energy Function** \(\mathcal{E}^\mathrm{IV}(\beta, \nu)\)

Next, concerning the extremal equation for the spherically symmetric approximation \([b]A_0(r)\), one observes that this isotropic potential does enter the functional \(\hat{\mathcal{E}}_{[\Omega]}\) (VI.25) only via its second constituent \(\epsilon\hat{\mathcal{E}}_{[\Omega]}\) (V.13). Therefore the “isotropic” extremalization process \(\delta_0\), say) becomes active only on this “isotropic” constituent \(\epsilon\hat{\mathcal{E}}_{[\Omega]}\)

\[
\delta_0 \hat{\mathcal{E}}_{[\Omega]} = \delta_0 \epsilon \hat{\mathcal{E}}_{[\Omega]} \overset{1}{=} 0 \quad (\text{VI.28})
\]

so that of course the “isotropic” Poisson equation (IV.18) is recovered here. But the point with our present approximation procedure is now that we do not try some (more or less reasonable) potential \([b]A_0(r)\), but rather we prefer to solve *exactly* that isotropic Poisson equation, albeit for the situation where the amplitude \(\hat{\Omega}(r)\) is given by our trial ansatz (VI.1a)–(VI.1b). For this purpose, one recasts the Poisson equation (IV.18) in dimensionless form

\[
\Delta_y \hat{a}_\nu(y) = -\frac{y^{2\nu-1} \cdot e^{-y}}{\Gamma(2\nu + 2)} \equiv -\frac{1}{\Gamma(2\nu + 2)} \frac{\hat{\Omega}_\nu^2(y)}{y}, \quad (\text{VI.29})
\]
see equation (A.1) of the precedent paper [1]; here the solution can easily be found for integer $2\nu$ as
\[
\tilde{a}_\nu(y) = \frac{1}{y} \left(1 - e^{-y} \cdot \sum_{n=0}^{2\nu} \frac{2\nu + 1 - n}{2\nu + 1} \cdot \frac{y^n}{n!}\right).
\] (VI.30)

This can be shown to be a special case of the general situation with arbitrary real values of the variational parameter $\nu \geq -\frac{1}{2}$ where the desired solution then adopts the following form:
\[
\tilde{a}_\nu(y) = \frac{1}{2\nu + 1} \left(1 - e^{-y} \cdot \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu + 2 + n)} y^{2\nu+n}\right).
\] (VI.31)

But once the isotropic potential $[b] A_0(r)$ (or $\tilde{a}_\nu(y)$, resp.) is known, one can readily calculate the associated “isotropic” energy $E^e_R$ (V.7) and its mass equivalent $\tilde{M}^e c^2$ (V.12). In the dimensionless form, both objects appear as [2, 33]
\[
E^e_R = -e^2 (2\beta) \int_0^\infty dy \ y^2 \left(\frac{d\tilde{a}_\nu(y)}{dy}\right)^2 = -\frac{e^2}{a_B} (2a_B \beta) \cdot \varepsilon_{pot}(\nu)
\] (VI.32a)
\[
\tilde{M}^e c^2 = -e^2 (2\beta) \frac{1}{\Gamma(2\nu + 2)} \int_0^\infty dy \ y \ \tilde{a}_\nu(y) \ \tilde{\Omega}^2_\nu(y) = -\frac{e^2}{a_B} (2a_B \beta) \cdot \varepsilon_{pot}(\nu)
\] (VI.32b)

with the “isotropic” potential function $\varepsilon_{pot}(\nu)$ being given by [1, 33]
\[
\varepsilon_{pot}(\nu) = \frac{1}{2\nu + 1} \left(1 - 2^{4\nu+2} \cdot \sum_{n=0}^{\infty} \frac{n}{\Gamma(2\nu + 2 + n)} \cdot \frac{\Gamma(4\nu + 2 + n)}{\Gamma(2\nu + 2) \cdot \Gamma(2\nu + 2 + n)}\right).
\] (VI.33)

Observe here the fact that the electrostatic gauge field energy $E^e_R$ (VI.32a) equals its mass equivalent $\tilde{M}^e c^2$ (VI.32b) so that the “isotropic” Poisson constraint (V.14) is zero
\[
\tilde{N}^e_G(\beta, \nu) \equiv 0,
\] (VI.34)

and thus this constraint term disappears from the energy function $\tilde{E}_\Omega(\beta, \nu)$ due to (VI.25).

The reason for this is that for the isotropic potential $[b] A_0(r)$ (or $\tilde{a}_\nu(y)$, resp.) we use an exact solution of the corresponding Poisson equation, e.g. in the dimensionless form (VI.30) and (VI.31); and for this situation it can easily be shown through integration by
parts and use of the Poisson equation (VI.29) that both integrals in (VI.32a)–(VI.32b)
are actually identical:

\[ \varepsilon_{\text{pot}}(\nu) \overset{\text{d}}{=} \int_{0}^{\infty} dy \, y^2 \left( \frac{d\tilde{a}_\nu(y)}{dy} \right)^2 = \frac{1}{\Gamma(2\nu + 2)} \int_{0}^{\infty} dy \, \tilde{a}_\nu(y) \tilde{\Omega}_\nu^2(y) . \quad (VI.35) \]

At this point of the discussion it may be instructive to discontinue for a moment in
order to get some survey of what has been attained up to now. Evidently, with both
the matter part \((D\tilde{E}_[\Omega])\) and the “isotropic” gauge field part \(e\tilde{E}_[\Omega]\) being at hand now,
one has at one’s disposal the isotropic part of the energy functional \(\tilde{E}_[\Omega]\) (VI.25). Indeed,
with the results (VI.9a)–(VI.9b) for the kinetic energy \(E_{\text{kin}}\) and with the “isotropic” gauge
field energy \(E_{\text{R}}^{[\epsilon]}\) (VI.32a) one possesses knowledge of the corresponding “isotropic” energy
function \(E^{[IV]}(\beta, \nu)\), i.e.

\[ E^{[IV]}(\beta, \nu) = 2E_{\text{kin}}(\beta, \nu) + E_{\text{R}}^{[\epsilon]}(\beta, \nu) \]

\[ = \frac{e^2}{aB} \left\{ (2aB \beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) - (aB \beta) \cdot \varepsilon_{\text{pot}}(\nu) \right\} . \quad (VI.36) \]

This result may now be exploited in order to obtain the (non-relativistic) energy spec-
trum of ortho-positronium in the isotropic approximation. To this end, one subjects
this “isotropic” function \(E^{[IV]}(\beta, \nu)\) (VI.36) to the first one (VI.2a) of both extremalizing
conditions in order to find the corresponding equilibrium value \(\beta_\ast\) as

\[ 2\alpha_s \beta_\ast = \frac{\varepsilon_{\text{pot}}(\nu)}{2\varepsilon_{\text{kin}}(\nu)} . \quad (VI.37) \]

Substituting this back into the original energy function \(E^{[IV]}(\beta, \nu)\) yields its reduced form
as

\[ E^{[IV]}(\beta, \nu) \Rightarrow E_T(\nu) = -\frac{e^2}{4aB} \cdot S_\text{O}(\nu) , \quad (VI.38) \]

with the “isotropic” spectral function \(S_\text{O}(\nu)\) being given by

\[ S_\text{O}(\nu) = \frac{\varepsilon_{\text{pot}}^2(\nu)}{\varepsilon_{\text{kin}}(\nu)} . \quad (VI.39) \]
Finally in the last step, one looks for the extremal points of this function
\[\frac{dS_0(\nu)}{d\nu} = 0\] (VI.40)
in order to find the equilibrium value \((\nu_*)\) of the second variational parameter \((\nu)\).

In this way, one gets the energy spectrum \(\{E_T^{(\nu)}(\nu_*)\} \div \{E_0^{[n]}\}\) of ortho-positronium in the spherically symmetric (i.e. “isotropic”) approximation. Of course, this spectrum is numerically the same as for para-positronium, if calculated on the same level of approximation, see the table on p. 163. Observe however that there is an important difference between both energy spectra. Namely, the presently considered ortho-levels are dimorphic doublets, due to the occurrence of different charge distributions \(\{^{(b)k}_0(r, \vartheta)\}\) for the same quantum numbers \(j_z, j_0 = n_0 - 1\). This dimorphism of the ortho-states will induce a certain energy difference between the members of such a doublet which is readily to be discussed now in greater detail (the degree of degeneracy of the ortho-levels will be studied in an other paper).

### Anisotropic Energy Function \(\tilde{E}^{[IV]}(\beta, \nu)\)

Naturally, the “isotropic” energy function \(E^{[IV]}(\beta, \nu)\) (VI.36) must undergo certain corrections if the “anisotropic” constituent \((\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tilde{\tile
Carrying here through both extremalization processes yields the following coupled Poisson-like equations for the anisotropy corrections \( \{ b \} A^\text{III}(r) \), \( \{ b \} A^\text{V}(r) \):

\[
\begin{align*}
(b) \epsilon_\text{III} \cdot \Delta_r \{ b \} A^\text{III}(r) + (b) \epsilon_\text{IV} \cdot \Delta_r \{ b \} A^\text{V}(r) - (b) f_\text{III} \cdot \frac{\{ b \} A^\text{III}(r)}{r^2} - (b) f_\text{IV} \cdot \frac{\{ b \} A^\text{V}(r)}{r^2} = -(b) m_\text{III} \alpha_s \cdot \tilde{\Omega}^2(r) \quad \text{(VI.43a)} \\
(b) \epsilon_\text{IV} \cdot \Delta_r \{ b \} A^\text{V}(r) + (b) \epsilon_\text{III} \cdot \Delta_r \{ b \} A^\text{III}(r) - (b) f_\text{IV} \cdot \frac{\{ b \} A^\text{V}(r)}{r^2} - (b) f_\text{III} \cdot \frac{\{ b \} A^\text{III}(r)}{r^2} = -(b) m_\text{IV} \alpha_s \cdot \tilde{\Omega}^2(r). \quad \text{(VI.43b)}
\end{align*}
\]

If it were possible to find \textit{exact} solutions of the present coupled system (VI.27) plus (VI.43a)–(VI.43b), then the “anisotropic” Poisson constraint term (VI.24) would be zero

\[
\tilde{N}^{(e)}_{\text{an}} \equiv 0 \quad \text{(VI.44)}.
\]

But clearly, it is very hard to get these (surely existing) exact solutions; but even if we manage to get exact solutions only of both coupled Poisson equations (VI.43a)–(VI.43b) alone (i.e. for arbitrary source \( \tilde{\Omega}(r) \), e.g. (VI.1a)–(VI.1b)), then the “anisotropic” Poisson identity (VI.44) will nevertheless hold. This may easily be verified by multiplying through the coupled equations (VI.43a)–(VI.43b) with \( \{ b \} A^\text{III}(r) \) and \( \{ b \} A^\text{V}(r) \), resp., and integrating over whole three-space under regard of \( E_{\text{an}}^{(e)} \) (VI.15) and its mass equivalent \( \tilde{M}_{\text{an}}^{(e)} c^2 \) (VI.19). For such a situation where both Poisson identities (VI.34) and (VI.44) are valid, the anisotropic part \( (\text{an}) \tilde{E}^{[g]} \) (VI.41) gets rid of its constraint and thus becomes reduced to its proper physical part \( E_{\text{an}}^{(e)} \), i.e.

\[
(\text{an}) \tilde{E}^{[g]} \Rightarrow E_{\text{an}}^{(e)} \quad \text{(VI.45)}.
\]

But the same conclusion does hold also for the isotropic part, i.e. the “isotropic” Poisson constraint term \( \tilde{N}^{(e)}_{\text{G}} \) (VI.17) vanishes whenever an exact solution of the “isotropic” Poisson equation (IV.18) is used, see equation (VI.34). Taking this altogether we get rid
of all the constraint terms in the original energy functional \( \tilde{E}_{[\Omega]} \) (VI.25) which then also becomes reduced to its proper physical part \( E^{(IV)} \):

\[
\tilde{E}_{[\Omega]} \Rightarrow E^{(IV)} = 2E_{\text{kin}} + E_{\text{R}}^{[e]} + E_{\text{an}}^{[e]} .
\] (VI.46)

The value of this reduced functional on the set of our trial configurations, parametrized by the variational parameters \( \{\beta, \nu\} \), yields again some energy function \( E^{(IV)}(\beta, \nu) \) whose stationary points according to (VI.2a)–(VI.2b) determine the energy spectrum of ortho-positronium in the next higher orders beyond the spherically symmetric approximation. Naturally, one expects that there will emerge some energy difference between the corresponding ortho- and para-states and also between the dimorphic partners of ortho-positronium. With the precedent preparations, these questions will now be discussed in some numerical detail.
VII Energy Difference of Dimorphic Partners

The Poisson-like equations (VI.43a)–(VI.43b) provide us now with the possibility to study the energy difference of both dimorphic partners. In order to keep our demonstration of this effect as simple as possible it may be sufficient here to study only the case \((b)j_z = \pm 1\) for \(j_0 = 2, 3, 4\). Indeed the results, obtained so far, say that the dimorphism cannot occur for \((b)j_z = 0\) and \((b)j_z = \pm j_0, \forall j_0\); and this excludes a priori its occurrence for \(j_0 = 0, 1\).

It should be evident that such an energy difference is in the first line due to the corresponding anisotropy corrections \({}^{(b)}A^{III}(r)\) and \({}^{(b)}A^{V}(r)\) which stand for the first and second order of our anisotropy approximation, cf. the perturbation expansion (V.22). In contrast to this, the kinetic energy \(E_{\text{kin}}\) is assumed to be still of the simple form (VI.9a)–(VI.9b). Thus one may raise the question whether perhaps the expected energy difference emerges already in the first approximation order \((\sim {}^{(b)}A^{III}(r))\)? If yes, is then the magnitude of the second order-correction \((\sim {}^{(b)}A^{V}(r))\) considerably smaller than the first-order correction \((\sim {}^{(b)}A^{III}(r))\)? Obviously, these questions can now be settled by first solving one (or both) of those Poisson-like equations (VI.43a)–(VI.43b) for given source \(\tilde{\Omega}(r)\) (e.g. (VI.1a)–(VI.1b)) and then minimalizing the resulting energy function \(E^{(IV)}(\beta, \nu)\) with respect to both variational parameters \(\beta\) and \(\nu\). This will yield the binding energy of ortho-positronium for \((b)j_z = \pm 1\) due to \(j_0 = 2, 3, 4\), quite similarly to the discussion of the isotropic situation (cf. (VI.36)–(VI.40)). The result will be that, for \(j_0 = 2, (b)j_z = \pm 1\), the energetic degeneracy of both dimorphic configurations survives the first anisotropy correction \((\sim {}^{(b)}A^{III}(r))\); but in the second approximation order \((\sim {}^{(b)}A^{V}(r))\) the degeneracy becomes eliminated, albeit only by 0.04 [eV] (i.e. 0.6 % of the binding energy), see the table on p. 145.
1. Quadrupole Corrections \(( \sim (b)^{A^{III}}(r)) ; \quad j_O = 2, 3, 4; (b)^{j}_z = \pm 1\)

For a first estimate of the anisotropy corrections one may accept for the moment the hypothesis that the second-order corrections \(( \sim (b)^{A^{V}}(r))\) will turn out as being much smaller than their first-order counterparts \(( \sim (b)^{A^{III}}(r))\) so that in the lowest-order approximation we can neglect \((b)^{A^{V}}(r)\) altogether and thus arrive at the following truncated form of equation (VI.43a):

\[
(b)^{e}_{III} \cdot \Delta_r (b)^{A^{III}}(r) - (b)^{f}_{III} \cdot \frac{(b)^{A^{III}}(r)}{r^2} = -\alpha_s (b)^{m}_{III} \cdot \frac{\tilde{\Omega}^2(r)}{r}.
\]  

(VII.1)

Here, the constants \((b)^{e}_{III}, (b)^{f}_{III}, (b)^{m}_{III}\) are defined by the equations (VI.16a) and (VI.22a); and this clearly demonstrates their dependency on the angular density \((b)^{k}_0(\vartheta)\). However, since the latter object is of dimorphic nature, see the two possibilities for \((b)^{k}_0(\vartheta)\) and the associated \((b)^{A^{III}}(\vartheta)\) in the table on p. 82, one expects to get two different sets of constants \((b)^{e}_{III}, (b)^{f}_{III}, (b)^{m}_{III}\) \{\}, which then would entail two different equations of the present form (VII.1). But such a dimorphic equation (VII.1) would imply the occurrence of two different solutions for the anisotropy correction \((b)^{A^{III}}(r)\); and this, in turn, would yield two different anisotropy energies \(E^{(e)}_{an}\) (VII.5)

\[
E^{(e)}_{an} \Rightarrow E^{(e)}_{III} = \frac{\hbar c}{\alpha_s} (b)^{e}_{III} \int_0^{\infty} r^2 \left\{ \left( \frac{d(b)^{A^{III}}(r)}{dr} \right)^2 + \frac{(b)^{f}_{III}}{(b)^{e}_{III}} \left( \frac{(b)^{A^{III}}(r)}{r} \right)^2 \right\} .
\]  

(VII.2)

Furthermore, since the anisotropy energy is an essential part of the total energy \(E^{(IV)}\), cf. (VI.46), one would also end up with two different energy functions \(E^{(IV)}(\beta, \nu)\), namely as the values of that functional \(E^{(IV)}\) (VII.46) on both trial configurations \{\(\tilde{\Omega}(r), (b)^{A_0}(r), (b)^{A^{III}}(r)\}\}. But these two energy functions would immediately include the existence of a certain energy difference between both dimorphic partners!

Actually, in the considered quadrupole approximation there is no energy difference between both dimorphic states due to \(j_O = 2, (b)^{j}_z = \pm 1\)! The crucial point here is that, despite the dimorphic nature of \((b)^{k}_0(\vartheta)\) and \((b)^{A^{III}}(\vartheta)\), all three constants \((b)^{e}_{III}, (b)^{f}_{III}, (b)^{m}_{III}\)
turn out to be identical, no matter whether they are calculated by means of the first trial configuration (↔ first line of the table on p. 82) or the second one (↔ second line of that table). For both cases one finds the same result:

\[(b) \varepsilon_{III} = \int \frac{d\Omega}{4\pi} \left( (b)A_{III}(\vartheta) \right)^2 = \frac{1}{320}, \quad \text{(VII.3a)}\]

\[(b) f_{III} = \int \frac{d\Omega}{4\pi} \left( \frac{d(b)A_{III}(\vartheta)}{d\vartheta} \right)^2 = \frac{3}{160}, \quad \text{(VII.3b)}\]

\[(b) m_{III} = \int d\Omega \ (b)A_{III}(\vartheta) \cdot (b)k_0(\vartheta) = \frac{1}{64}. \quad \text{(VII.3c)}\]

Of course, this identity of \((b) \varepsilon_{III}\) and \((b) f_{III}\) for both dimorphic configurations due to \(j_0 = 2\) comes not as a surprise, because the quadrupole correction \((b)A_{III}(\vartheta)\) differs only in sign for both dimorphic partners; but on the other hand, the equality of \((b) m_{III}\) (VII.3c) for both dimorphic partners is surely somewhat amazing since the angular density \((b)k_0(\vartheta)\) is distinctly different for both cases (recall the table on p. 82). However, the situation is different for \(j_0 = 3\) since in this case all three constants \((b) \varepsilon_{III}, (b) f_{III}, (b) m_{III}\) are different for both dimorphic partners; and thus it is merely the ratio (VI.17a)-(VI.17b) what remains identical. Therefore one expects that the dimorphic partners will have different binding energy exclusively from \(j_0 = 3\) on (in the quadrupole approximation).

Quadrupole Equation

But in any case, with the first-order coefficients (VII.3a)-(VII.3c) being fixed in such a way, the equation (VII.1) becomes specified (for all cases due to \(j_0 = 2, 3, 4\)) to the same “quadrupole equation” (recall the ratios (VI.17a)-(VI.17b)

\[\Delta_r (b)A_{III}(r) - 6 \frac{(b)A_{III}(r)}{r^2} = -5a_s \frac{\hat{\Omega}^2(r)}{r}, \quad \text{(VII.4)}\]

where an example for the trial amplitude \(\hat{\Omega}(r)\) has already been specified by equations (VI.1a)-(VI.1b). This equation has been studied extensively in connection with parapositronium in the precedent paper (see ref. [2]). It is possible to find the exact solution
of this quadrupole equation (VII.4) for the case where the trial amplitude $\tilde{\Omega}(r)$ is given by equations (VI.1a)–(VI.1b). For integer values of the variational parameter $2\nu$ the appropriate solutions read in dimensionless units ($y \equiv 2\beta r$; $\{^b\}A_{\nu}^{\text{III}}(y) \equiv (2\beta \alpha_s)^{-1}.\{^b\}A_{\nu}^{\text{III}}(r)$)

$$\{^b\}A_{\nu}^{\text{III}}(y) = (2\nu + 3)(\nu + 1) \left\{ \frac{1}{10} \{^b\}A_{\nu}^{\text{III}}(y) - 10y^2 e^{-y} \sum_{n=6}^{2\nu+3} \frac{1}{n!} \sum_{m=0}^{n-6} \frac{d^m}{dy^m}(y^{n-6}) \right\}$$ (VII.5)

where for $\nu = 1$ the second term (in the bracket) must be put to zero; and the solution $\{^b\}A_{1}^{\text{III}}(y)$ for $\nu = 1$ is given by

$$\{^b\}A_{1}^{\text{III}}(y) = \frac{20}{y^3} \left\{ 1 - e^{-y} \sum_{n=0}^{4} \frac{y^n}{n!} \right\}.$$ (VII.6)

Indeed, the case for $\nu = 1$ plays an important part for this set of solutions because it fixes the boundary conditions. Namely, observe that the homogeneous (dimensionless) form of the quadrupole equation (VII.4)

$$\left( \Delta_y - \frac{6}{y^2} \right) \{^b\}A_{\nu}^{\text{III}}(y) = 0$$ (VII.7)

admits two simple solutions

$$\{^b\}A_{\nu}^{\text{III}}(y) \Rightarrow y^2 \text{ or } y^{-3}$$ (VII.8)

from which we conclude the limit behaviour

$$\lim_{y \to 0} \{^b\}A_{\nu}^{\text{III}}(y) = \text{const} \cdot y^2$$ (VII.9a)

$$\lim_{y \to \infty} \{^b\}A_{\nu}^{\text{III}}(y) = \frac{(2\nu + 3)(2\nu + 2)}{y^3}.$$ (VII.9b)

The second limit ($y \to \infty$) is immediately obvious from the combination of both equations (VII.5) and (VII.6); and for verifying the first limit ($y \to 0$) it may suffice to look at the
lowest-order cases $\nu = 1, \frac{3}{2}, 2, \frac{5}{2}$:

\[
{\nu}^{\text{III}} A_{1}(y) \Rightarrow \frac{1}{6} \left( y^2 - \frac{5}{6} y^3 + \frac{5}{14} y^4 - \frac{5}{48} y^5 \ldots \right) \tag{VII.10a}
\]

\[
{\nu}^{\text{III}} A_{3/2}(y) = \frac{3}{2} \cdot {\nu}^{\text{III}} A_{1}(y) - \frac{5}{24} y^2 e^{-y} \Rightarrow \frac{1}{24} \left( y^2 - \frac{5}{14} y^4 \ldots \right) \tag{VII.10b}
\]

\[
{\nu}^{\text{III}} A_{2}(y) = \frac{21}{10} \cdot {\nu}^{\text{III}} A_{1}(y) - \frac{1}{24} y^2 e^{-y} (8 + y) \Rightarrow \frac{1}{60} \left( y^2 - \frac{5}{48} y^5 \ldots \right) \tag{VII.10c}
\]

\[
{\nu}^{\text{III}} A_{5/2}(y) = \frac{14}{5} \cdot {\nu}^{\text{III}} A_{1}(y) - \frac{1}{144} y^2 e^{-y} (y^2 + 10 y + 66) \Rightarrow \frac{1}{120} \left( y^2 + o(y^6) \right) . \tag{VII.10d}
\]

Once the quadrupole solutions are exactly known one may substitute them into the first-order form of the anisotropy energy $E_{\text{III}}^{(e)}$ (VII.2) which then must equal its mass equivalent $\tilde{M}_{\text{III}}^{(e)} c^2$ (VI.21a), i.e. the value of the Poisson constraint $\tilde{N}_{\text{an}}^{(e)}$ (VI.24) on our selected trial configuration $\left\{ \tilde{\Omega}(r), {\nu}^{\text{III}} A_{\nu}(r) \right\}$ is again zero

\[
\tilde{N}_{\text{an}}^{(e)}(\beta, \nu) \Rightarrow \tilde{N}_{\text{III}}^{(e)} \equiv E_{\text{III}}^{(e)} - \tilde{M}_{\text{III}}^{(e)} c^2 \equiv 0 . \tag{VII.11}
\]

Here, the anisotropy energy $E_{\text{III}}^{(e)}$ (VII.2) adopts the following form

\[
E_{\text{III}}^{(e)} = \frac{\hbar c}{\alpha_s} \int_0^\infty dr r^2 \left\{ \left( \frac{d}{dr} A_{\nu}(r) \right)^2 + 6 \left( \frac{A_{\nu}(r)}{r} \right)^2 \right\} \tag{VII.12}
\]

\[
\begin{align*}
\equiv (\nu^{\text{III}} A_{\nu}(y))^2 \int_0^\infty dy y^2 \left\{ \left( \frac{d}{dy} A_{\nu}(y) \right)^2 + 6 \left( \frac{A_{\nu}(y)}{y} \right)^2 \right\} 
\end{align*}
\]

and equals its mass equivalent $\tilde{M}_{\text{III}}^{(e)} c^2$ (VI.21a) which may be rewritten as

\[
\tilde{M}_{\text{III}}^{(e)} c^2 = \frac{\hbar c}{\alpha_B} \int_0^\infty dr \cdot \tilde{M}_{\text{III}}^{(e)}(r) \cdot \tilde{\Omega}^2(r) \tag{VII.13}
\]

\[
\begin{align*}
\equiv (\nu^{\text{III}} A_{\nu}(y))^2 \int_0^\infty dy y^2 \left\{ \left( \frac{d}{dy} A_{\nu}(y) \right)^2 + 6 \left( \frac{A_{\nu}(y)}{y} \right)^2 \right\} 
\end{align*}
\]

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so that the claimed Poisson identity (VII.11) can here explicitly be validated by reference to the solution (VII.5) of the quadrupole equation (VII.4) in the form

\[(b) \epsilon_{\text{III}} \cdot \epsilon_{\text{pot}}^{\text{III}}(\nu) = (b) m_{\text{III}} \cdot \mu_{\text{III}}^{(e)}(\nu) . \quad (VII.14)\]

Properly speaking, the present final form of the energy functional $\tilde{E}_{[\Omega]}$, i.e. $E^{(IV)} (VI.46)$, would require now the use of the anisotropy energy $E^{(e)}_{\text{III}} (VII.12)$; but since the calculation of this object is somewhat tedious one may resort to its mass equivalent $\tilde{M}_{\text{III}}^{(e)} c^2 (VII.13)$ which is known to be numerically identical to the desired $E^{(e)}_{\text{III}}$ because of the vanishing of the Poisson constraint $\tilde{N}_{\text{III}}^{(e)} (VII.11)$. A closer inspection of the mass equivalent (VII.13) reveals the following structure for the involved mass-equivalent function $\mu_{\text{III}}^{(e)}(\nu)$ [2]:

\[
\mu_{\text{III}}^{(e)}(\nu) = \frac{1}{\Gamma(2\nu + 2)} \int_{0}^{\infty} dy y^{2\nu+1} e^{-y} \{b\} A_{\nu}^{\text{III}}(y) = \frac{\Gamma(2\nu + 4) \cdot \Gamma(2\nu - 1)}{\Gamma(2\nu + 2)^2} + \frac{1}{\Gamma(2\nu + 2)^2} \cdot \sum_{n=0}^{\infty} p_n(\nu) \frac{\Gamma(4\nu + 3 + n)}{2^{4\nu+3+n}} ,
\]

where the coefficients $p_n(\nu)$ are given by

\[
p_n(\nu) = \frac{\Gamma(2\nu + 4)}{\Gamma(2\nu + 5 + n)} - \frac{\Gamma(2\nu - 1)}{\Gamma(2\nu + n)} . \quad (VII.16)\]

2. Energy Function of the Anisotropic Configurations

Since the total gauge field energy $E_{R}^{(e)} (VI.12)$ appears as the sum of the isotropic and the anisotropic parts, with the isotropic part $E_{R}^{(e)}$ being given by equations (VI.32a)–(VI.33) and the anisotropic part $E_{an}^{(e)}$ by equation (VII.12), one ultimately obtains the gauge field energy in the following form:

\[
E_{R}^{(e)} = -\frac{e^2}{a_B} (2a_B\beta) \left\{ \epsilon_{\text{pot}}(\nu) + (b) m_{\text{III}} \cdot \mu_{\text{III}}^{(e)}(\nu) \right\} \approx -\frac{e^2}{a_B} (2a_B\beta) \cdot \epsilon_{\text{tot}}^{(e)}(\nu) . \quad (VII.17)
\]

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Obviously, the dimorphism enters the total gauge field energy $E_R^{(e)}$ via the mass-equivalent parameter $(b)m_{III}$ which in general has been shown to adopt different values for the dimorphic partners, see the table on p. 90. The important point with this result is that, also after the inclusion of the anisotropy correction, the total gauge field energy $E_R^{(e)}$ still persists in form of a linear function of the first variational parameter $\beta$. On the other hand, the kinetic energy $E_{\text{kin}}$ has already been found to be a quadratic term of $\beta$, cf. (VI.9a)–(VI.9b); and therefore the total energy function $E^{(IV)}(\beta, \nu)$ emerges as the sum of a linear and a quadratic term of $\beta$, i.e.

$$E^{(IV)}(\beta, \nu) = \frac{\varepsilon^2}{a_B} \left\{ (2a_B\beta)^2 \cdot \varepsilon_{\text{kin}}(\nu) - (2a_B\beta) \cdot \varepsilon_{\text{tot}}^{(e)}(\nu) \right\}.$$  

(VII.18)

This “anisotropic” energy function is of the same form as its “isotropic” precursor $E^{(IV)}(\beta, \nu)$ (VI.36) and therefore the extremalization process runs in a quite similar way, cf. equations (VI.36)–(VI.40), i.e. we ultimately have to look for the minimal values of the spectral function $S_{O}(\nu)$ being defined through

$$S^{(j)}_{O}(\nu) = \frac{\left( \varepsilon^{(e)}_{\text{tot}}(\nu) \right)^2}{\varepsilon_{\text{kin}}(\nu)},$$  

(VII.19)

where \{j\} symbolizes the pair configuration of quantum numbers \{j_O, (b)j_z\}. Here $\varepsilon_{\text{tot}}^{(e)}(\nu)$ is to be taken over from equation (VII.17)

$$\varepsilon_{\text{tot}}^{(e)}(\nu) = \varepsilon_{\text{pot}}(\nu) + (b)m_{III} \cdot \mu_{III}^{(e)}(\nu),$$  

(VII.20)

and $\varepsilon_{\text{kin}}(\nu)$ is specified by equation (VI.9b). Denoting the maximalizing parameter for the spectral function $S^{(j)}_{O}(\nu)$ (VII.19) by $\nu_*$

$$\left. \frac{dS^{(j)}_{O}(\nu)}{d\nu} \right|_{\nu = \nu_*} = 0,$$  

(VII.21)

the corresponding energy spectrum $E^{(j)}_{O}$ is then obtained again from the local maxima of
\( S_{n}^{(j)}(\nu) \)

\[
E^{(j)} = -\frac{e^{2}}{4a_{B}} \cdot S_{n}^{(j)}_{\max} \quad (VII.22)
\]

\[
\left( \frac{e^{2}}{4a_{B}} \simeq 6,8029 \ldots [eV] \right).
\]

The results for \( \text{^b}j_{z} = \pm 1, j_{\nu} = 1, 2, 3, 4 \) are collected in the following table:

| \( j_{\nu} \Rightarrow \) | 0 | 1 | 2 | 3 | 4 |
|---|---|---|---|---|---|
| \( \text{^b}j_{z} \Rightarrow \) | 0 | ±1 | ±1 | ±1 | ±1 |
| \( \text{^b} m_{\text{III}} \Rightarrow \) | \( \frac{1}{16} \) | \( \frac{1}{64} \) | \( \frac{1}{64} \) | \( \frac{1}{64} \) | \( \frac{9}{256} \) |
| \( \text{^E}^{(j)}_{\nu} \Rightarrow \) | \( -7.5378 \ldots \) | \( -1,575 \ldots \) | \( -0.6811 \ldots \) | \( -0.3808 \ldots \) | \( -0.2501 \ldots \) |
| [eV] | \( -0.3900 \ldots \) | \( -0.2533 \ldots \) | \( -0.3808 \ldots \) | \( -0.2501 \ldots \) | \( -0.2533 \ldots \) |

As expected, the ortho-dimorphism does not occur for quantum-numbers \( j_{\nu} = 0 \) and \( j_{\nu} = 1 \). The lowest-order possibility for its occurrence is \( j_{\nu} = 2, \text{^b}j_{z} = \pm 1 \). But now the important point with this result is that the calculated energy \( E_{\nu}^{(j,1)} \) (VII.22) (in this first-order approximation to anisotropy) numerically the same for both dimorphic configurations with their rather different charge distributions \( \{^b k_{0}(\vartheta) \} \), see the upper half \( (j_{\nu} = 2) \) of the table on p. 82. Clearly, such an amazing result calls for an explanation. But here the first observation is that both angular anisotropy corrections \( \text{^b}A_{\text{III}}(\vartheta) \) differ only in sign, cf. the table on p. 82; and therefore the coefficients \( \text{^b} m_{\text{III}} \) (VII.3a) and \( \text{^b} f_{\text{III}} \) (VII.3b) must be numerically identical for the dimorphic pair with \( j_{\nu} = 2 \). Furthermore, the coefficient \( \text{^b} m_{\text{III}} \) (VII.3c) turns also out to be the same for both configurations. This, however, entails that the first-order equation (VII.1) must be identical for both dimorphic configurations, see its common form equation (VII.4). But for this situation it is clear that the corresponding solution \( \text{^b}A_{\text{III}}(\vartheta) \) of that “quadrupole equation” is also the same, since for both cases one takes the same trial amplitude \( \tilde{\Omega}(r) \) (VII.1a)–(VII.1b). Furthermore, the latter argument does also apply to the spherically symmetric approximation \( \text{^b}A_{0}(r) \) (V.16).
so that now all three fields \( \{ \tilde{\Omega}(r), [b]A_0(r), [b]A^\text{III}(r) \} \) are identical for both dimorphic configurations \( (j_O = 2) \), albeit only in the lowest order of the anisotropy approximation.

But this is sufficient in order that all three energy contributions to \( E^{(IV)} \) (VI.46) are also identical; and thus both configurations \{2, \pm 1\} carry the same energy \( E^{(2,1)}_O \) (VII.22). In physical terms, this says that the degeneracy of the dimorphic partners (occurring in the spherically symmetric approximation) is not eliminated by the present first-order anisotropy corrections (see Fig.VII.A below)! See also App.D for entering into particulars.

3. Comparison of Ortho- and Para-Levels

The reference basis of the comparison of the various RST levels is the conventional level system \( E^{(n)}_C \) \([1,18]\), solid line. The various RST approximations are the spherically symmetric approximation \( E^{[n]}_T \) (■ ■ ■ ) and the quadrupole approximations for para-positronium \( E^{(j)}_o \) (xxx) and ortho-positronium \( E^{(j)}_O \) (● ● ●).

All three RST approximations \( E^{[n]}_T, E^{(j)}_O, E^{(j)}_O \) are based on the partial-extremalization process which relies on the maximalization of the spectral function \( S^{(j)}_{O,p} \), cf. (VII.22)

\[
S^{(j)}_{O,p}(\nu) = \frac{[\varepsilon_{\text{pot}}(\nu) + (b,p)m_{\text{III}} \cdot \mu^{[e]}_{\text{III}}(\nu)]^2}{\frac{1}{2\nu+1} \left( \frac{1}{4} + \frac{j_O \nu^2}{2\nu} \right)}.
\] (VII.23)

For the spherically symmetric approximation \( E^{[n]}_T \) \([1]\), one puts \( j_O,p = 0 \); and concerning \( (b,p)m_{\text{III}} \) for the quadrupole approximation of para-positronium one reads off the mass-equivalent parameter \( (p)m_{\text{III}} \) from the table on p.163; and finally for ortho-positronium one takes \( (b)m_{\text{III}} \) from that table on p. 163 The conclusions of these numerical results for the spherically symmetric and quadrupole approximations are now the following (Fig.VII.A):
Fig. VII.A  Comparison of Ortho- and Para-Levels for Principal Quantum Numbers $n = 4$ and $n = 5$
i) RST and Conventional Predictions

All three RST approximations $E_T^{[n]}(\bullet \bullet \bullet)$, $E_p^{\{j\}}(\ldots\ldots)$, $E_\Omega^{\{j\}}((\ldots\ldots)$ yield numerical predictions above the conventional $E_{[C]}^{(n)}(\ldots\ldots)$! This may be understood as a consequence of the fact that the RST energy functional $\tilde{E}_{[\Omega]}$ (VI.25) has a lower bound which is in the immediate neighborhood of the conventional levels $E_{[C]}^{(n)}$. Therefore the value of this RST functional $\tilde{E}_{[\Omega]}$ on a (non-optimal) trial amplitude $\hat{\Omega}(r)$, such as our variational ansatz (VI.1a)-(VI.1b), will yield predictions which always surmount the corresponding conventional prediction $E_{C}^{(n)}$ (i.e. $E_T^{[n]},E_p^{\{j\}},E_\Omega^{\{j\}}>E_{[C]}^{(n)}$). Thus one may expect that a more clever selection of the trial amplitude $\hat{\Omega}(r)$ will shift all three kinds of RST predictions further towards the conventional $E_{C}^{(n)}$. Of course, one would like to know how close to $E_{[C]}^{(n)}$ the RST predictions will turn out for the (hitherto unknown) exact solution of the RST eigenvalue problem.

However, one qualitative feature of the RST spectrum should be mentioned in this context: namely, a closer inspection of the larger principal quantum numbers ($n \gtrsim 10$, say) yields the result that the RST predictions $E_p^{\{j\}}$ become smaller than their conventional counterparts $E_{C}^{(n)}$ (i.e. $E_p^{\{j\}} < E_{C}^{(n)}$ for $n \gtrsim 10$) even for the non-optimal trial amplitude $\hat{\Omega}(r)$ (VI.1). Therefore the true RST energy eigenvalues should also be smaller than their conventional counterparts $E_{C}^{(n)}$ for sufficiently large principal number $n$ (or $n_\sigma, n_\rho$ resp.).

ii) Elimination of the $j_z$-Degeneracy

The second observation concerns the elimination of the $j_z$-degeneracy which has been discussed in great detail in the precedent paper [2]. This means that the $(2j_{\sigma,\rho}+1)$-fold degeneracy of the conventional and the spherically symmetric RST levels (due to any fixed $j_{\sigma,\rho}$) becomes eliminated by the anisotropy of the elec-
trostatic interaction potential. This anisotropy may be thought to come about by the action of the centrifugal forces on the rotating charge clouds \((b,p)_{j_z} \neq 0\). We assume that this degeneracy elimination for para-positronium \[2\] does occur in an analogous way also for ortho-positronium, but we do not study this phenomenon in the present paper which is rather concerned with the effect of dimorphism (see also App.D).

iii) Dimorphism of Ortho-Positronium

The effect of dimorphism acts physically in a similar way as do the centrifugal forces in the case of the \(j_z\)-degeneracy; namely by anisotropic deformation of the electric charge distributions, see Fig.IV.A. However the difference between both deforming mechanisms is that the ortho-dimorphism is an intrinsic geometric feature of the eigenvalue problem (IV.6a)-(IV.6b) itself; i.e. an indirect consequence of the presence of spin. If there is no angular momentum \((b)_{j_z} = 0\), App.A), then there is no dimorphism (see the tables on p. 145 and p. 152), as one may expect also intuitively. But a somewhat counter-intuitive effect occurs for maximal angular momentum \((b)_{j_z} = \pm j_O\), where there is also no dimorphism (see App.A). A hint at the possibility that the present quadrupole approximation may not display the true occurrence of the ortho-dimorphism comes from the quantum number \(j_O = 2\). Here it is possible to satisfy the condition \(0 < |(b)_{j_z}| < j_O\) for the occurrence of dimorphism, i.e. by choosing \((b)_{j_z} = \pm 1\); but nevertheless the dimorphism does not exist (see the table on p. 145), at least within the framework of the quadrupole approximation. Therefore the next step must consist in inspecting the octupole approximation (Sect.VIII), especially with respect to the dimorphism.

iv) Ortho- and Para-Levels

Finally, it is also interesting to notice the specific way in which the para-levels \(E_{\text{pq}}^{(j)}\) become splitted into the ortho-levels \(E_{\text{o}}^{(j)}\) and \(E_{\text{oc}}^{(j)}\) by the dimorphism.
The first observation is here (see table on p. 145 and App.D) that the ortho-levels do agree with the para-levels for those states which are not subjected to the dimorphism: \( E_{O}^{(j)} = E_{P}^{(j)} \). This is exemplified here for \( j_{O} = 0 \) and \( j_{O} = 1 \) (see the table on p. 163), but presumably it holds for all values of \( j_{O} \). But even if the dimorphic splitting is active (here: \( j_{O} = 3, 4 \); \( j_{z} = \pm 1 \)), one of the two split levels (i.e. \( \tilde{E}_{O}^{(j)} \)) does furthermore agree with the corresponding para-level \( E_{P}^{(j)} \) (Fig.VII.A on p. 108).

The other split level of the ortho-configuration (i.e. \( \tilde{E}_{O}^{(j)} \)) is shifted upwards off from the residual ortho/para-level. This enhances the deviation from the corresponding conventional prediction \( E_{C}^{(n)} \). It remains to be checked whether this result survives the consideration of the next higher (i.e. octupole) approximation.
VIII Multipole Solutions

Naturally, one cannot be quite sure that all the essential features of the ortho-spectrum are already accounted for by the quadrupole approximation. The uncertainty refers here mainly to three questions:

i) is the elimination of the \((b)j_z\)-degeneracy a true effect or an artefact of the quadrupole approximation,

ii) if it is a true effect, is then the order of magnitude of the level splitting width correctly accounted for already by the quadrupole approximation, or do the higher-order multipole results exceed/reduce the magnitude of the quadrupole predictions,

iii) is the “incidental” missing of the ortho-dimorphism for \(j_0 = 2; (b)j_z = \pm 1\) an artefact of the quadrupole approximation and thus disappears again when passing over to the multipole approximations of higher order?

Subsequently, we will try to answer these questions by a first preliminary inspection of the multipole solutions of higher order.

1. Alternative Multipole Expansion

The perturbation expansion (V.22) of the anisotropic part \({^b}A^{an} (r, \vartheta)\) of the original gauge potential \({^b}A_0 (r, \vartheta)\) (V.19) may be further elaborated by observing the specific form of the two lowest-order contributions \({^b}A^{\text{III}} (\vartheta)\) (table on p. 82) and \({^b}A^{\text{V}} (\vartheta)\) (V.31a)–(V.31b). Indeed, the latter two pertubations (V.31a)–(V.31b) can be recast to
the following form

\[ (V.31a): \quad \{b\}k_0(\vartheta) = \frac{\sin \vartheta}{\pi^2} \]  

\[ \Rightarrow \{b\}A^V(\vartheta) = -\frac{105}{256} \left[ \cos^2 \vartheta - \frac{1}{3} \right] - \frac{35}{512} \left[ \cos^4 \vartheta - \frac{1}{5} \right] \]  

\[ (V.31b): \quad \{b\}k_0(\vartheta) = \frac{\sin \vartheta}{3\pi^2} (\sin^2 \vartheta + 9 \cos^2 \vartheta) \]  

\[ \Rightarrow \{b\}A^V(\vartheta) = \frac{105}{128} \left[ \cos^2 \vartheta - \frac{1}{3} \right] - \frac{105}{256} \left[ \cos^4 \vartheta - \frac{1}{5} \right]. \]

Thus, one is lead to suppose here that the original anisotropic expansion \((V.22)\) yields an angular expansion in terms of the specific functions \(C^{(2l)}(\vartheta)\) being defined by \((l = 1, 2, 3, 4, \ldots)\)

\[ \mathcal{C}^{(2l)}(\vartheta) \doteq \cos^{2l} \vartheta - \frac{1}{2l + 1}, \]  

i.e. the original anisotropy expansion \((V.22)\) would then look as follows

\[ \{b\}A^a_n(r, \vartheta) = \sum_{l=1}^{\infty} \mathcal{C}^{(2l)}(\vartheta) \cdot \{b\}A_{2l}(r). \]  

**Properties of the New Basis Functions**

The new basis functions \(\mathcal{C}^{(2l)}(\vartheta)\) have some interesting properties which we will later on exploit for our purposes of attaining better approximations for the wanted ortho-spectrum. First, observe here that the angular average of all the basis functions is zero:

\[ \int \frac{d\Omega}{4\pi} \mathcal{C}^{(2l)}(\vartheta) = 0, \]  

so that the anisotropic part \(\{b\}A^a_n(r, \vartheta)\) \((VIII.3)\) of the gauge potential actually does obey the requirement \((V.20)\) of vanishing angular average. Next, split up the Laplacean \(\Delta_{r,\vartheta,\phi}\) into the three contributions due to the spherical polar coodinates \(r, \vartheta, \phi\)

\[ \Delta_{r,\vartheta,\phi} = \Delta_r + \frac{1}{r^2} \Delta_{\vartheta} + \frac{1}{r^2 \sin^2 \vartheta} \Delta_{\phi}. \]  

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with

\[ \Delta_r = \frac{\partial^2}{\partial r^2} + \frac{2}{r} \frac{\partial}{\partial r} \]  
\( \text{(VIII.6a)} \)

\[ \Delta_\vartheta = \frac{\partial^2}{\partial \vartheta^2} + \cot \vartheta \frac{\partial}{\partial \vartheta} \]  
\( \text{(VIII.6b)} \)

\[ \Delta_\phi = \frac{\partial^2}{\partial \phi^2} \]  
\( \text{(VIII.6c)} \)

and then find that the longitudinal part \( \Delta_\vartheta \) \( \text{(VIII.6b)} \) of the Laplacean \( \Delta_r,\vartheta,\phi \) acting on the basis functions \( C^{(2l)}(\vartheta) \) as follows

\[ \Delta_\vartheta C^{(2l)}(\vartheta) = 2l (2l - 1) \cdot C^{(2l-2)}(\vartheta) - 2l (2l + 1) \cdot C^{(2l)}(\vartheta) , \]  
\( \text{(VIII.7)} \)

i.e. the set of basis functions is closed under the action of the longitudinal Laplacean \( \Delta_\vartheta \).

From this we conclude that the Poisson equation for the anisotropic part \( (b)A^{an}(r, \vartheta) \)

\[ \Delta (b)A^{an}(r, \vartheta) = -4\pi \alpha_s \left[ (b)k_0(r, \vartheta) - \frac{(b)k_0(r)}{4\pi} \right] \]  
\( \text{(VIII.8)} \)

will transcribe to a system of coupled Poisson-like equations for the radial potential corrections \( (b)A_2(r) \) \( \text{(VIII.3)} \), see below. In order to deduce that system by means of the principle of minimal energy it is necessary to define a scalar product \( \{C_{l,m}\} \) for the vector space spanned by the basis functions. A nearby choice for this is:

\[ C_{l,m} \approx \frac{1}{2} \int_0^\pi d\vartheta \sin \vartheta \cdot C^{(2l)}(\vartheta) \cdot C^{(2m)}(\vartheta) \]  
\( \text{(VIII.9)} \)

\[ = \frac{1}{2m + 2n + 1} - \frac{1}{(2m + 1)(2n + 1)} . \]

For instance, for a treatment including terms up to the octupole approximation \( (b)A^V(\vartheta) \) \( \text{(VIII.1a)–(VIII.1b)} \) one has to work with the following (symmetric) coefficient matrix

\[ \{C_{l,m}\} \Rightarrow \begin{pmatrix} 4 & 105 \\ 105 & 4 \end{pmatrix} , \quad \{C_{l,m}^{-1}\} = \frac{1}{16} \begin{pmatrix} 49 & -105 \\ -105 & 24 \end{pmatrix} . \]  
\( \text{(VIII.10)} \)
The quadrupole approximation (∼ \{b\}^A_{III}(\vartheta)) is a subcase hereof where only one single matrix element \(C_{1,1} = \frac{1}{\sqrt{3}}\) is needed. For the higher-multipole approximations one correspondingly extends the dimension of the matrix \(\{C_{l,m}\}\) according to (VIII.9).

We will readily see the relevancy of these coefficient matrices \(\{C_{l,m}\}\) which obviously do represent a generalization of the former coefficients \((b)_e^{III}, (b)_e^{IV}, (b)_e^{V}, \ldots\) (VI.16a)–(VI.16c) occurring in connection with the original perturbation expansion (V.22). The analogous generalization of the former coefficients \((b)_f^{III}, (b)_f^{IV}, (b)_f^{V}, \ldots\) (VI.16a)–(VI.16c) would now obviously be a certain matrix \(\{F_{l,m}\}\) which is to be introduced by means of the derivatives of the new basis functions \(C^{(2l)}(\vartheta)\), i.e. we define:

\[
F_{l,m} \doteq \frac{1}{2} \int_{0}^{\pi} d\vartheta \sin \vartheta \left( \frac{dC^{(2l)}(\vartheta)}{d\vartheta} \right) \cdot \left( \frac{dC^{(2m)}(\vartheta)}{d\vartheta} \right) = \frac{8ml}{(2l + 2m)^2 - 1}. \tag{VIII.11}
\]

The two-dimensional case \((l \leq 2, m \leq 2)\) is again needed for the octupole approximation and is found to look as follows:

\[
\{F_{l,m}\} \Rightarrow \begin{pmatrix}
\frac{8}{15} & \frac{16}{35} \\
\frac{16}{35} & \frac{32}{63}
\end{pmatrix}. \tag{VIII.12}
\]

The case of the higher-multipole approximations should be self-evident now.

Finally, one has to inquire after the higher-multipole generalization of the mass-equivalent parameters \((b)_m^{III}, (b)_m^{IV}, \ldots\) (VI.22a)–(VI.22b). For this purpose, one restarts from the general definition of the mass equivalent \(M(e)c^2\) (V.9) and inserts therein the new anisotropy expansion (VIII.3), i.e. we then obtain the “anisotropic” mass equivalent \(\tilde{M}^{(e)}_{an}c^2\) in the following form

\[
\tilde{M}^{(e)}_{an}c^2 = -\hbar c \sum_{l=1}^{\infty} (b)_m^{l} \int_{0}^{\infty} dr \, r \tilde{\Omega}^2(r) \,(b)_A^{2l}(r) = \sum_{l=1}^{\infty} \tilde{M}^{(e)}_{2l}c^2 \tag{VIII.13}
\]

where the new mass-equivalent parameters \((b)_m^{l}\) are given by

\[
(b)_m^{l} \doteq \int d\Omega \,(b)_k^{0}(\vartheta) C^{(2l)}(\vartheta). \tag{VIII.14}
\]
In contrast to the precedent matrices $C_{l,m}$ and $F_{l,m}$ the new parameters $(b)_{m_{l}}$ depend now on the angular distribution $(b)_{k_{0}}(\vartheta)$ and are thus not merely numerical objects of general character.

The new definition (VIII.14) of the mass-equivalent parameters looks very similar to the old one (VI.22a)–(VI.22b); and indeed, both definitions are almost (but not really) identical. Indeed, there is a certain (albeit technical) difference between the original perturbation formalism (V.22) and the new one (VIII.3) if one stops at a finite perturbation order; although both formalisms would yield the same result if the infinite number of perturbation contributions could be taken into account. In order to see this technical difference somewhat more clearly, consider (e.g.) the peculiar situation with $j_{O} = 2$, $(b)_{j_{z}} = \pm 1$ (see the table on p. 82). Here, the new prescription (VIII.14) yields for both dimorphic densities $(b)_{k_{0}}(\vartheta)$ the following results for the mass-equivalent parameter $(b)_{m_{l}}$ up to the octupole approximation

\[
(b)_{k_{0}}(\vartheta) = \frac{\sin \vartheta}{\pi^2} \Rightarrow \begin{cases} 
(b)_{m_{1}} = -\frac{1}{12}, & \text{quadrupole} \\
(b)_{m_{2}} = -\frac{3}{40}, & \text{octupole}
\end{cases} \quad \text{(VIII.15a)}
\]

\[
(b)_{k_{0}}(\vartheta) = 3 \frac{\sin \vartheta}{\pi^2} \left(1 - \frac{8}{9} \sin^2 \vartheta\right) \Rightarrow \begin{cases}
(b)_{m_{1}} = \frac{1}{12}, & \text{quadrupole} \\
(b)_{m_{2}} = \frac{1}{20}, & \text{octupole}
\end{cases} \quad \text{(VIII.15b)}
\]

Thus the new quadrupole parameters are found to differ in sign $(b)_{m_{1}} = \pm \frac{1}{12}$ and are some three times larger than their counterpart $(b)_{m_{III}}$ of the original formalism

\[
(b)_{m_{1}} = \mp \frac{16}{3}, (b)_{m_{III}} = \mp \frac{16}{3} \cdot \frac{1}{64} = \mp \frac{1}{12}, \quad \text{(VIII.16)}
\]

see the table on p. 163. Thus, on the level of the quadrupole approximation there is actually no essential difference of both formalisms because the objects are of the same order of perturbation and differ merely by some unsubstantial numerical factor. It remains to be
shown (see below) that such a difference of the intermediate objects of both approaches does not generate any difference of the final predictions of physical relevance.

\textit{Comparison of the Expansion Coefficients}

However, the analogous comparison of the \textit{octupole} contribution of both formalisms reveals now some (albeit purely formal) distinctions. For the sake of simplicity, we restrict ourselves again to the specific state in question \((j_o = 2, \ (b)_j = \pm 1)\) and observe that the octupole potential term \(^{(b)}A^V(\vartheta)\) (VIII.1a)–(VIII.1b) emerges as a decomposition with respect to the new basis \(C^{(2)}(\vartheta)\) (VIII.2):

\[
^{(b)}A^V(\vartheta) = \sum_{l=1}^{2} a_l^{(V)} C^{(2)}(\vartheta). \tag{VIII.17}
\]

Such a finite series expansion of the original angular modes \(^{(b)}A^{\text{III}}(\vartheta), \ ^{(b)}A^V(\vartheta), \ ^{(b)}A^{\text{VII}}(\vartheta), \ldots\) in terms of the new modes \(C^{(2)}(\vartheta)\) seems to occur for any perturbation order. The expansion coefficients \(a_l^{(\text{III})}, a_l^{(V)}, a_l^{(\text{VII})}, \ldots\) are functionals of the angular density \(^{(b)}k_0(\vartheta)\), for instance for the present octupole cases (VIII.1a)–(VIII.1b)

\[
a_1^{(V)} = \begin{cases} 
\frac{105}{256}, & \text{first density (VIII.1a)} \\
\frac{105}{128}, & \text{second density (VIII.1b)}
\end{cases} \tag{VIII.18a}
\]

\[
a_2^{(V)} = \begin{cases} 
-\frac{35}{512}, & \text{first density (VIII.1a)} \\
-\frac{105}{256}, & \text{second density (VIII.1b)}
\end{cases} \tag{VIII.18b}
\]

Naturally, in view of the definitions of both mass-equivalent parameters \(^{(b)}m_V\) (VI.22b) and \(^{b}m_l\) (VIII.14) the expansion (VIII.17) can now be transcribed also to these parameters:

\[
^{(b)}m_V = \sum_{l=1}^{2} a_l^{(V)} \ ^{(b)}m_l, \tag{VIII.19}
\]

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i.e. concretely for the present demonstration \((\text{VIII.15a})-(\text{VIII.15b})\)

\[
\begin{align*}
(j_0 = 2, \quad (b)_z = \pm 1)
(b)_{m_{V}} &= \begin{cases}
-105/256 \cdot \left(-\frac{1}{12}\right) \\
105/128 \cdot \frac{1}{12}
\end{cases} + \begin{cases}
-35/512 \cdot \left(-\frac{3}{40}\right) \\
-105/256 \cdot \frac{1}{20}
\end{cases} = \begin{cases}
\frac{161}{4096}, \quad \text{first density} \\
\frac{49}{1024}, \quad \text{second density}
\end{cases} \quad \text{(VIII.20)}
\end{align*}
\]

It should become now obvious from the numerical comparison of both approaches \((b)_{m_{III}} \lnot \lnot (b)_{m_{1}}, \quad (b)_{m_{V}} \lnot \lnot (b)_{m_{2}}\) that their corresponding perturbation orders are of equivalent numerical magnitude \((\sim 10^{-2})\), at least concerning the present lowest orders \((l = 1, 2)\). This suggests that none of both competitors is numerically more advantageous, as far as the rapid convergence of their series expansion is concerned. However, the basis elements \(\mathbb{C}^{(2)}(\vartheta) \quad \text{(VIII.2)}\) of the second expansion \((\text{VIII.3})\) are more favourable from the purely technical viewpoint because, in contrast to their counterparts \(\{b\}A^{\text{III}}(\vartheta) \quad \text{(V.25a)}\) etc. due to the original expansion \((\text{V.22})\), they are independent of the angular density \(\{b\}k_{0}(\vartheta)\) and therefore the second approach appears to be more manageable for dealing with the higher orders of the multipole expansion (see below).

### 2. Multipole Equations

Once a new basis system of some promise is at hand now, one would like to see how the former quadrupole and octupole equations \((\text{VI.43a})-(\text{VI.43b})\) transcribe to the corresponding new radial potentials \(\{b\}A_{2}(r) \quad \text{(VIII.3)}\). The desired Poisson-like equations for \(\{b\}A_{2}(r)\) may be deduced by inserting the new expansion \((\text{VIII.3})\) of the anisotropic part \(\{b\}A_{\text{an}}(r, \vartheta)\) of the gauge potential \(\{b\}A_{0}(r, \vartheta) \quad \text{(V.19)}\) in the “anisotropic” gauge-field energy \(E_{\text{an}}^{(e)} \quad \text{(VI.13)}\) and also in the “anisotropic” Poisson constraint \(\tilde{N}_{\text{an}}^{(e)} \quad \text{(VI.24)}\). Since the latter two contribute to the energy functional \(\tilde{E}_{[\varrho]} \quad \text{(VI.25)}\) are the sole ones which contain the anisotropic part \(\{b\}A_{\text{an}}(r, \vartheta)\) it is sufficient to consider the anisotropic part \(\{\text{an}\}\tilde{E}_{[\varrho]} \quad \text{of the energy functional alone, i.e.}\n\]

\[
\{\text{an}\}\tilde{E}_{[\varrho]} = E_{\text{an}}^{(e)} + \lambda_{G}^{(e)} \cdot \tilde{N}_{\text{an}}^{(e)}, \quad \text{(VIII.21)}
\]
namely in order to deduce hereof the Poisson-like equations for the new radial potentials \( b_{A_2}(r) \) by means of the principle of minimal energy

\[
\delta l_{\text{an}} \tilde{E}_{\text{an}} = 0.
\]  

(VIII.22)

Here, \( \delta l \) is the functional derivative with respect to any potential \( b_{A_2}(r) \) \( (l = 1, 2, 3, 4, \ldots) \)

where the derivative of the mass-equivalent \( \tilde{M}_{\text{an}} \) \((\text{VIII.13})\) is immediately evident:

\[
\delta l_{\text{an}} \tilde{M}_{\text{an}} = \int_0^\infty dr \ r^2 \left( \delta b_{A_2}(r) \right) \cdot \left\{ -\hbar c \frac{\partial b_{A_2}}{\partial r} \frac{\Omega^2(r)}{r} \right\}.
\]  

(VIII.23)

**Anisotropy Energy**

The case of the anisotropy energy \( E_{\text{an}} \) \((\text{VI.13})\) is a little bit more complicated. It is the sum of a radial derivative term \( E_{\text{an}}^{(r)} \) and a longitudinal term \( E_{\text{an}}^{(\vartheta)} \), i.e.

\[
E_{\text{an}} = E_{\text{an}}^{(r)} + E_{\text{an}}^{(\vartheta)},
\]  

(VIII.24)

with the radial contribution being given by

\[
E_{\text{an}}^{(r)} = -\frac{\hbar c}{4\pi\alpha_s} \int d^3r \cdot \left( \frac{\partial b_{A_2}(r, \vartheta)}{\partial r} \right)^2.
\]  

(VIII.25)

and its longitudinal counterpart by

\[
E_{\text{an}}^{(\vartheta)} = -\frac{\hbar c}{4\pi\alpha_s} \int d^3r \cdot \left( \frac{1}{r} \frac{\partial b_{A_2}(r, \vartheta)}{\partial \vartheta} \right)^2.
\]  

(VIII.26)

Inserting herein the new series expansion \((\text{VIII.3})\) of the anisotropic part \( b_{A_2}(r, \vartheta) \) yields for the radial energy \( E_{\text{an}}^{(r)} \) \((\text{VIII.25})\)

\[
E_{\text{an}}^{(r)} = -\frac{\hbar c}{\alpha_s} \sum_{l,m=1}^{\infty} C_{l,m} \int_0^\infty dr \ r^2 \frac{d b_{A_2}(r)}{dr} \cdot \frac{d b_{A_2}(r)}{dr}.
\]  

(VIII.27)

and analogously for the longitudinal part \( E_{\text{an}}^{(\vartheta)} \) \((\text{VIII.26})\)

\[
E_{\text{an}}^{(\vartheta)} = -\frac{\hbar c}{\alpha_s} \sum_{l,m=1}^{\infty} F_{l,m} \int dr \ r^2 \frac{b_{A_2}(r)}{r^2} \cdot \frac{b_{A_2}(r)}{r^2}.
\]  

(VIII.28)
The functional derivatives of both energy contributions are easily seen to look as follows

\[
\delta I E_{an}(r) = \int dr \ r^2 \left( \delta \{b\} A_{2l}(r) \right) \cdot \left\{ 2 \frac{\hbar c}{\alpha_s} \sum_k C_{l,k} \Delta_r \{b\} A_{2m}(r) \right\} \quad (VIII.29a)
\]

\[
\delta I E_{an}(\vartheta) = \int dr \ r^2 \left( \delta \{b\} A_{2l}(r) \right) \cdot \left\{ -2 \frac{\hbar c}{\alpha_s} \sum_k F_{l,k} \frac{\{b\} A_{2k}(r)}{r^2} \right\} \quad (VIII.29b)
\]

But with all three functional derivatives being at hand now, one can substitute them in the anisotropic part of the *principle of minimal energy* (VIII.22) which then reads explicitly

\[
\delta I \{an\} E[\Omega] \equiv \left( 1 + \lambda_G^{(e)} \right) \cdot \delta I E^{(e)}_{an} - \lambda_G^{(e)} \cdot \delta I \left( \tilde{M}_{an}^{(e)} \right)^2 \quad (VIII.30)
\]

with the Lagrangean multiplier \( \lambda_G^{(e)} = -2 \).

**General Multipole Equation**

This then yields the following Poisson-like equations for the radial correction potentials \( \{b\} A_{2l}(r) \) (“multipole equations”)

\[
\Delta_r \{b\} A_{2l}(r) - \sum_{k=1}^{\infty} F'_{l,k} \cdot \frac{\{b\} A_{2k}(r)}{r^2} = -\alpha_s \{b\} m'_l \cdot \frac{\tilde{\Omega}^2(r)}{r} , \quad (VIII.31)
\]

where the transformed mass-equivalent parameter \( \{b\} m'_l \) is given by

\[
\{b\} m'_l = \sum_{k=1}^{\infty} C^{-1}_{l,k} \cdot \{b\} m_k \quad (VIII.32)
\]

and the transformed matrix \( \{F'_{l,k}\} \) by

\[
F'_{l,k} = \sum_{j=1}^{\infty} C^{-1}_{l,j} \cdot F_{j,k} \quad . \quad (VIII.33)
\]

For instance, for the octupole approximation where the matrix \( \{C^{-1}_{l,m}\} \) is given by equation (VIII.10) and \( \{F_{l,m}\} \) by (VIII.12) one finds for \( \{F'_{l,k}\} \) (VIII.33)

\[
\{F'_{l,k}\} = \begin{pmatrix} 6 & -12 \\ 0 & 20 \end{pmatrix} . \quad (VIII.34)
\]

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Observe also that all the higher-order multipole potentials \( (b)A_2(r) \) become coupled by equation (VIII.31) to the spherically-symmetric amplitude \( \tilde{\Omega}(r) \)!

**Quadrupole Approximation**

As a brief demonstration of the alternative perturbation expansion (VIII.3) one may resort again to the quadrupole approximation. Here, some results have already been worked out within the framework of the original perturbation expansion (V.22), see Sect.VII; and it may be instructive now to see how the same results can be obtained also by use of the alternative expansion (VIII.3). Once we thus have gained some confidence in this alternative approach, one may then tackle the octupole approximation (or even the higher-multipole approximations) which will then appear in a more pleasant shape than in the original perturbation formalism.

The quadrupole approximation is the lowest order of perturbation for which the system of multipole equations (VIII.31) becomes reduced to one single equation \( (l = m = 1) \). Thus the multipole matrices \( \{C_{l,m}\} \) (VIII.10) and \( \{F_{l,m}\} \) (VIII.12) become reduced to their components \( C_{1,1} = \frac{4}{45} \) and \( F_{1,1} = \frac{8}{15} \), hence the transformed matrix simplifies to

\[
F'_{1,1} \Rightarrow C^{-1}_{1,1} \cdot F_{1,1} = \frac{45}{4} \cdot \frac{8}{15} = 6.
\]

Furthermore, the mass-equivalent parameter \( (b)m'_1 \) (VIII.32) becomes

\[
(b)m'_1 = C^{-1}_{1,1} \cdot (b)m_1 = \frac{45}{4} \cdot \left( \mp \frac{1}{12} \right) = \mp \frac{15}{16},
\]

cf. (VIII.15a)–(VIII.15b). As a result of all these quadrupole specifications, the general multipole equation (VIII.31) becomes cut down to the quadrupole equation:

\[
\Delta_r (b)A_2(r) - 6 \frac{(b)A_2(r)}{r^2} = \pm \frac{15}{16} \alpha_s \frac{\tilde{\Omega}^2(r)}{r},
\]

where the upper/lower sign refers to the first/second density \( (b)k_0(\vartheta) \) (VIII.15a)/(VIII.15b). Already from this form of the quadrupole equation it is possible to conclude that both
quadrupole correction potentials \( {^{(b)} A_2}(r) \) (for \( j_0 = 2, \ (^{(b)} j_z = \pm 1 \)) due to both densities (VIII.15a) and (VIII.15b) will differ only in sign, just as was the case for the corresponding quadrupole potentials \( {^{(b)} A_III}(r) \), see the table on p. 82. This difference in sign has already been shown to represent the origin of the missing of the dimorphism for the states with \( j_0 = 2, \ (^{(b)} j_z = \pm 1, \) so that this effect must occur also in the quadrupole approximation of the present alternative approach. Furthermore, the quadrupole equations of both approaches, cf. (VII.4) vs. (VIII.37), are almost of the same shape and differ merely in the coupling parameters, cf. (VI.17b) and (VIII.36):

\[
\begin{align*}
\text{(VI.17b):} & \quad \frac{\nu_{III}^{(b) m}}{\nu_{III}^{(b) e}} = 5 \quad \text{v.} \quad \text{(VIII.36):} & \quad {^{(b)} m}_1' = \begin{cases} 
-\frac{15}{16}, & \text{first density (VIII.15a)} \\
+\frac{15}{16}, & \text{second density (VIII.15b)}
\end{cases} 
\end{align*}
\]

This similarity of both quadrupole equations then entails that their solutions must be proportional, i.e.

\[
{^{(b)} A_2}(r) = \frac{\nu_{III}^{(b) m}}{\nu_{III}^{(b) e}} \cdot {^{(b)} A_III}(r) = \mp \frac{3}{16} \cdot {^{(b)} A_III}(r).
\]

Concerning now the energy being stored in this quadrupole mode, one specialises the general mass equivalent \( \tilde{M}^{(e)}_c c^2 \) (VIII.13) of the alternative approach down to the quadrupole approximation (\( l = 1 \)), i.e.

\[
\tilde{M}^{(e)}_c c^2 \quad \text{v.} \quad \tilde{M}^{(e)}_2 c^2 = -\hbar c \cdot {^{(b)} m}_1 \cdot {^{(b)} m}_1' \int_0^{\infty} dr \ r^2 \ {^{(b)} A_2}(r) \frac{\tilde{\Omega}^2(r)}{r},
\]

or by use of the link (VIII.39) to the original quadrupole potential \( {^{(b)} A_III}(r) \)

\[
\tilde{M}^{(e)}_2 c^2 = -\hbar c \cdot {^{(b)} m}_1 \cdot {^{(b)} m}_1' \int_0^{\infty} dr \ r^2 \ {^{(b)} A_III}(r) \frac{\tilde{\Omega}^2(r)}{r}.
\]

Here, the pre-factor is found by means of (VIII.36) and (VI.17b)

\[
\frac{\nu_{III}^{(b) m}}{\nu_{III}^{(b) e}} = \frac{45}{5} \cdot (\pm \frac{1}{17})^2 = \frac{1}{64},
\]

(VIII.42)
so that the quadrupole mass equivalent in the alternative approach \( \tilde{M}_2^{(e)} c^2 \) \(^{(VIII.41)}\) actually equals the original form \( \tilde{M}_3^{(e)} c^2 \); cf. \(^{(VI.22a)}\):

\[
\tilde{M}_3^{(e)} c^2 \equiv \tilde{M}_2^{(e)} c^2 .
\] \(^{(VIII.43)}\)

For the specific form of \( M_3^{(e)} c^2 \) see equation \(^{(VII.13)}\).

Of course, this identity of the mass equivalents must have its counterpart for the quadrupole energies, i.e. one concludes

\[
E_3^{(e)} \equiv E_2^{(e)} ,
\] \(^{(VIII.44)}\)

where the original form of \( E_3^{(e)} \) is given by equation \(^{(VII.12)}\), with \( ^{(b)l}_{\text{III}} = \frac{1}{320} \) (table on p. 90), and its alternative form \( E_2^{(e)} \) is the specialization of \( E_{an}^{(e)} \) \(^{(VIII.24)}\) to the quadrupole case \( (l = 1) \), i.e.

\[
E_{an}^{(e)} \Rightarrow E_{2l}^{(e)} \bigg|_{l=1} \equiv E_2^{(e)} = -\frac{\hbar c}{\alpha_s} \int_0^\infty dr \ r^2 \ \left\{ C_{1,1} \left( \frac{d^{(b)}A_2(r)}{dr} \right)^2 + F_{1,1} \left( \frac{^{(b)}A_2(r)}{r} \right)^2 \right\} .
\] \(^{(VIII.45)}\)

Inserting here again the required matrix elements from the matrices \( C_{l,m} \) \(^{(VIII.10)}\) and \( F_{l,m} \) \(^{(VIII.12)}\) in combination with the transformation of the quadrupole potentials \(^{(VIII.39)}\) does actually validate the claimed equality \(^{(VIII.44)}\). For the precise form of \( E_3^{(e)} \) see equation \(^{(VII.12)}\).

This complete equivalence of the original and the alternative perturbation approach (within the framework of the quadrupole approximation) should provide now sufficient confidence for tackling the next higher order of the perturbation expansion, i.e. the octupole approximation, just by means of the alternative technique.
3. Octupole Approximation

Surely, it is reasonable to suppose that a certain improvement of the quadrupole results (Fig.VII.A) can be attained by taking into account also the octupole character of the charge distribution \( b^k_0(r, \vartheta) \), i.e. we consider now the multipole equations (VIII.31) with restriction of the multipole order to \( l, m \leq 2 \). The required octupole matrices \( \{ C_{l,m} \} \), \( \{ C^{-1}_{l,m} \} \), \( \{ F_{l,m} \} \) and \( \{ F'_{l,m} \} \) have already been specified by equations (VIII.10), (VIII.12) and (VIII.34). Thus, we obtain from the general multipole system (VIII.31) for \( l = 1 \) the modified quadrupole equation

\[
\Delta_r \{ b \}_2^2(r) - 6 \frac{\{ b \}_2^4(r)}{r^2} + 12 \frac{\{ b \}_4^4(r)}{r^2} = -\alpha_s \{ b \}_1^1 \cdot \tilde{\Omega}^2(r) \tag{VIII.46}
\]

and for \( l = 2 \) the pure octupole equation

\[
\Delta_r \{ b \}_4^4(r) - 20 \frac{\{ b \}_4^4(r)}{r^2} = -\alpha_s \{ b \}_2^2 \cdot \tilde{\Omega}^2(r) \tag{VIII.47}
\]

Any individual multipole equation of order \( l \) owns its specific coupling constant \( \{ b \}_l^m \) (VIII.32); especially for the present octupole approximation (\( l \leq 2 \)) we have for the quadrupole coupling constant in equation (VIII.46)

\[
\{ b \}_1^1 = C_{1,1}^{-1} \cdot \{ b \}_1^1 \quad \text{first density (VIII.15a)}
\]

\[
\{ b \}_2^2 = C_{1,2}^{-1} \cdot \{ b \}_1^1 + C_{2,2}^{-1} \cdot \{ b \}_2^2
\]

\[
\begin{cases}
-\frac{105}{256}, & \text{first density (VIII.15a)} \\
\frac{525}{128}, & \text{second density (VIII.15b)}
\end{cases}
\]  

and similarly for the octupole coupling constant in equation (VIII.47)

\[
\{ b \}_2^2 = C_{2,1}^{-1} \cdot \{ b \}_1^1 \quad \text{first density (VIII.15a)}
\]

\[
\{ b \}_2^2 = C_{2,2}^{-1} \cdot \{ b \}_1^1 + C_{2,2}^{-1} \cdot \{ b \}_2^2
\]

\[
\begin{cases}
-\frac{315}{512}, & \text{first density (VIII.15a)} \\
-\frac{945}{256}, & \text{second density (VIII.15b)}
\end{cases}
\]

Observe here that, on account of the particular form of the matrix \( \{ F'_{l,m} \} \) (VIII.34), the octupole equation (VIII.47) expresses the decoupling from the quadrupole influence whereas the quadrupole equation (VIII.46) still contains the octupole potential \( \{ b \}_4^4(r) \). Surely, it would be more aesthetic if one could deduce also a pure quadrupole equation which formally does contain only the proper quadrupole terms (see below).
Octupole Energy

Concerning the energy being stored in the quadrupole and octupole modes, one may first turn to the mass equivalent $\tilde{M}_{\text{an}}^{(e)} c^2$ \text{(VIII.13)} which is the sum of the individual multipole contributions, without any interference term:

$$\tilde{M}_{\text{an}}^{(e)} c^2 \Rightarrow \tilde{M}_{2+4}^{(e)} c^2 = \tilde{M}_2^{(e)} c^2 + \tilde{M}_4^{(e)} c^2,$$

(VIII.50)

with the quadrupole contribution being given by

$$\tilde{M}_2^{(e)} c^2 = -\hbar c \{^b m_1 \cdot \int_0^\infty dr r^2 \{^b A_2(r) \frac{\tilde{\Omega}^2(r)}{r} \}$$

(VIII.51)

and analogously for the octupole contribution

$$\tilde{M}_4^{(e)} c^2 = -\hbar c \{^b m_2 \cdot \int_0^\infty dr r^2 \{^b A_4(r) \frac{\tilde{\Omega}^2(r)}{r} \}$$

(VIII.52)

(For the mass-equivalent parameters $^b m_1$ and $^b m_2$ see equations \text{(VIII.15a)--(VIII.15b)}).

Unfortunately, such a pleasant separation of the various multipole contributions does not occur for the anisotropy energy $E_{\text{an}}^{(e)}$ \text{(VII.13)}. For its radial part $E_{\text{an}}^{(r)}$ \text{(VIII.27)} one finds

$$E_{\text{an}}^{(r)} \Rightarrow E_{2+4}^{(r)} = - \left( \frac{4}{15} \right)^2 \frac{\hbar c}{\alpha_s} \int_0^\infty dr r^2 \left\{ \frac{5}{4} \left( \frac{d \{^b A_2(r) \}}{dr} \right)^2 + \frac{15}{r} \cdot \frac{d \{^b A_2(r) \}}{dr} \frac{d \{^b A_4(r) \}}{dr} + \left( \frac{d \{^b A_4(r) \}}{dr} \right)^2 \right\},$$

(VIII.53)

and similarly for the longitudinal part $E_{\text{an}}^{(q)}$ \text{(VIII.28)}

$$E_{\text{an}}^{(q)} \Rightarrow E_{2+4}^{(q)} = -8 \frac{\hbar c}{\alpha_s} \int_0^\infty dr \left\{ \frac{1}{15} \left( \{^b A_2(r) \}^2 + \frac{4}{35} \{^b A_2(r) \} \cdot \{^b A_4(r) \} \right) + \frac{4}{63} \left( \{^b A_4(r) \}^2 \right) \right\}.$$
But now that all contributions to the “anisotropic” energy are explicitly known one can of course carry through the variational principle of minimal energy (VIII.22) for \( l = 1, 2 \) and would then regain the quadrupole-octupole system (VIII.46)–(VIII.47). Though this result provides sufficient confidence in the consistency of the general multipole approach (VIII.31) it is nevertheless very instructive to consider also a slight modification thereof.

\textit{Conjugate Potentials}

Reconsidering for a moment the radial anisotropy energy \( E_{2n}^{(r)} \) (VIII.27), one is tempted to introduce the conjugate potentials \( \{ b \} A'_{2l}(r) \) through

\[
\{ b \} A'_{2l}(r) = \sum_{m=1}^{\infty} C_{l,m} \{ b \} A_{2m}(r), \tag{VIII.55}
\]

or conversely

\[
\{ b \} A_{2l}(r) = \sum_{m=1}^{\infty} C_{l,m}^{-1} \{ b \} A'_{2m}(r). \tag{VIII.56}
\]

In terms of these conjugate potentials, the former multipole equation (VIII.31) reappears now in the following form

\[
\Delta_r \{ b \} A'_{2l}(r) - \sum_{k=1}^{\infty} F''_{l,k} \{ b \} A'_{2k}(r) = \frac{-\alpha_s}{r^2} \{ b \} \tilde{\Omega}^2(r). \tag{VIII.57}
\]

The matrix \( \{ F'_{l,k} \} \) emerging here is in general asymmetric and is defined through

\[
F''_{l,k} = \sum_{m=1}^{\infty} F_{l,m} \cdot C_{m,k}^{-1}. \tag{VIII.58}
\]

For instance, for the octupole approximation (i.e. \( m, l, k \mid 1, 2 \)) this matrix looks as follows

\[
\{ F''_{l,k} \} = \begin{pmatrix} 6 & 0 \\ -12 & 20 \end{pmatrix}. \tag{VIII.59}
\]

and thus is the transpose of the former matrix \( \{ F'_{l,k} \} \) (VIII.34). Furthermore, the octupole approximation \( (l, k \mid \leq 2) \) of the general multipole system (VIII.57) consists now of a pure
quadrupole equation \((l = 1)\)

\[
\Delta r \frac{\langle b \rangle A_2'(r)}{r^2} - 6 \frac{\langle b \rangle A_2'(r)}{r^2} = -\alpha_s \frac{\langle b \rangle m_1}{r} \cdot \frac{\tilde{\Omega}^2}{r},
\]  

(VIII.60)

and a modified octupole equation \((l = 2)\)

\[
\Delta \frac{\langle b \rangle A_4'(r)}{r^2} - 20 \frac{\langle b \rangle A_4'(r)}{r^2} + 12 \frac{\langle b \rangle A_2'(r)}{r^2} = -\alpha_s \frac{\langle b \rangle m_2}{r} \cdot \frac{\tilde{\Omega}^2}{r},
\]  

(VIII.61)

which is just the other way round if compared to the original case (VIII.46)–(VIII.47).

Of course, the conjugate multipole system (VIII.57) can also be deduced from the principle of minimal energy

\[
\delta'_l \left\{ \langle \text{an} \rangle \tilde{E}'_{\langle \Omega \rangle} \right\} = 0
\]  

(VIII.62)

where \(\delta'_l\) denotes the functional derivative of \(\left\{ \langle \text{an} \rangle \tilde{E}'_{\langle \Omega \rangle} \right\}\) with respect to the conjugate potentials \(\langle b \rangle A_2'(r)\) (VIII.55); and \(\langle \text{an} \rangle \tilde{E}'_{\langle \Omega \rangle}\) is the former functional \(\left\{ \langle \text{an} \rangle \tilde{E}_{\langle \Omega \rangle} \right\}\) expressed in terms of the conjugate potentials \(\langle b \rangle A_2'(r)\), cf. (VII.23). In order to validate this claim, one first transcribes the mass equivalent \(\tilde{M}^{(e)}_{\text{an}} c^2\) (VIII.13) to its conjugate form:

\[
\tilde{M}^{(e)}_{\text{an}} c^2 \Rightarrow \tilde{M}^{(e)}_{\text{an}} c^2 = -\hbar c \sum_{l=1}^{\infty} \langle b \rangle m'_l \cdot \int_0^{\infty} dr \ r^2 \frac{\langle b \rangle A_2'(r)}{r} \frac{\tilde{\Omega}^2}{r}. \]  

(VIII.63)

Next, the radial energy \(E^{(r)}_{\text{an}}\) (VIII.27) reappears as

\[
E^{(r)}_{\text{an}} \Rightarrow E^{(r)}_{\text{an}} = -\frac{\hbar c}{\alpha_s} \sum_{l,k=1}^{\infty} C_{l,k}^{-1} \int_0^{\infty} dr \ r^2 \frac{d\langle b \rangle A_2'(r)}{dr} \cdot \frac{d\langle b \rangle A_2'(r)}{dr} \cdot \frac{\tilde{\Omega}^2}{r}. \]  

(VIII.64)

and finally the longitudinal energy \(E^{(\vartheta)}_{\text{an}}\) (VIII.28) adopts the following shape

\[
E^{(\vartheta)}_{\text{an}} \Rightarrow E^{(\vartheta)}_{\text{an}} = -\frac{\hbar c}{\alpha_s} \sum_{l,k=1}^{\infty} F^{m}_{l,k} \int_0^{\infty} dr \ r^2 \frac{\langle b \rangle A_2'(r)}{r^2} \cdot \frac{\langle b \rangle A_2'(r)}{r^2} \cdot \frac{\tilde{\Omega}^2}{r}. \]  

(VIII.65)

with the symmetric matrix \(\left\{ F^{m}_{l,k} \right\}\) being given by

\[
F^{m}_{l,k} = \sum_{m,n=1}^{\infty} C_{m,k}^{-1} F_{m,n} C_{n,l}^{-1}. \]  

(VIII.66)
Now one can carry through again the variational principle (VIII.62) (see (VIII.30) for a more explicit form of this) in order to find the corresponding extremal equations just coinciding with the result (VIII.57), as expected.

For a concrete demonstration of the conjugate formalism, one resorts again to the octupole approximation \((j, k, l, m | \leq 2)\). Here, the mass equivalent \(\tilde{\mathcal{M}}_{(e)} c^2\) \(\text{VIII.63}\) appears again as the sum of the quadrupole and the octupole contributions

\[
\tilde{\mathcal{M}}_{(e)} c^2 \Rightarrow \tilde{\mathcal{M}}_{2+4} c^2 = \tilde{\mathcal{M}}_{2} c^2 + \tilde{\mathcal{M}}_{4} c^2 .
\]  
\((\text{VIII.67})\)

The conjugate quadrupole part is given here by

\[
\tilde{\mathcal{M}}_{2} c^2 = -\hbar c \{b\} m_1 \int_0^\infty dr \ r^2 \{b\} A_2'(r) \cdot \frac{\hat{\Omega}^2(r)}{r} 
\]  
\((\text{VIII.68})\)

and the corresponding octupole part by

\[
\tilde{\mathcal{M}}_{4} c^2 = -\hbar c \{b\} m_2 \int_0^\infty dr \ r^2 \{b\} A_4'(r) \cdot \frac{\hat{\Omega}^2(r)}{r} .
\]  
\((\text{VIII.69})\)

Next, the radial energy \(\tilde{E}_{\text{an}}^{(r)}\) \(\text{VIII.64}\) becomes specified down to

\[
\tilde{E}_{\text{an}}^{(r)} \Rightarrow E_{2+4}^{(r)} = -\frac{45}{16} \frac{hc}{\alpha_s} \int_0^\infty dr \ r^2 \left\{ 49 \left( \frac{d \{b\} A_2'(r)}{dr} \right)^2 - 105 \frac{d \{b\} A_2'(r)}{dr} \cdot \frac{d \{b\} A_4'(r)}{dr} + 245 \left( \frac{d \{b\} A_4'(r)}{dr} \right)^2 \right\} .
\]  
\((\text{VIII.70})\)

And finally, the longitudinal energy \(\tilde{E}_{\text{an}}^{(\vartheta)}\) \(\text{VIII.65}\) is found as

\[
\tilde{E}_{\text{an}}^{(\vartheta)} \Rightarrow E_{2+4}^{(\vartheta)} =
-\frac{45}{16} \frac{hc}{\alpha_s} \int_0^\infty dr \ r^2 \left( \{b\} A_2'(r) \right)^2 - 2100 \{b\} A_2'(r) \cdot \{b\} A_4'(r) + 1225 \left( \{b\} A_4'(r) \right)^2
\]  
\((\text{VIII.71})\)

For the desired deduction of the octupole system \((\text{VIII.60})-\text{VIII.61}\) by the extremalization of the “anisotropic” energy functional \(\text{an} \tilde{E}[\varpi]\) \(\text{VI.25}\) we have to write down now
that functional in the octupole approximation again in terms of the conjugate potentials \( \{ b \} A_{2l}^\prime (r) \), i.e.

\[
\{ an \} \hat{E}_\Omega \Rightarrow \{ 2+4 \} \hat{E}_\Omega^{\prime} \equiv \delta E^{(r)}_{2+4} + \lambda_G^{(e)} \cdot \hat{M}^{(e)}_{2+4} \quad (VIII.72)
\]

\[
= E^{(r)}_{2+4} + E^{(\vartheta)}_{2+4} + \lambda^{(e)} \cdot \left\{ E^{(r)}_{2+4} + E^{(\vartheta)}_{2+4} - \hat{M}^{(e)}_{2} - \hat{M}^{(e)}_{4} \right\}
\]

\[
= \left( 1 + \lambda^{(e)} \right) \cdot \left\{ E^{(r)}_{2+4} + E^{(\vartheta)}_{2+4} \right\} - \lambda^{(e)} \cdot \left\{ \hat{M}^{(e)}_{2} + \hat{M}^{(e)}_{4} \right\}.
\]

By means of the standard variational technique, it is then easy to see that both extremal equations

\[
\delta_2 \{ 2+4 \} \hat{E}_\Omega^{\prime} = 0 \quad (VIII.73a)
\]

\[
\delta_4 \{ 2+4 \} \hat{E}_\Omega^{\prime} = 0 \quad (VIII.73b)
\]

actually do lead us back to just the claimed octupole system (VIII.60)–(VIII.61)!

**Hybrid Method**

There exists also a kind of hybrid formulation of the octupole system which then contains both kinds of potentials \( \{ b \} A_{2l}^\prime (r) \) and \( \{ b \} A_{2l}^\prime (r) \). Indeed, it is easy to see that the radial energy \( E^{\{ r \}}_{an} \) (VIII.27) can also be written in the following form

\[
E^{\{ r \}}_{an} \Rightarrow E^{\{ r \}}_{hy} \equiv -\frac{\hbar c}{\alpha_s} \sum_{l=1}^{\infty} \int_0^\infty dr \, r^2 \frac{d \{ b \} A_{2l}(r)}{dr} \cdot \frac{d \{ b \} A_{2l}^\prime (r)}{dr}, \quad (VIII.74)
\]

and similarly for the longitudinal contribution \( E^{\{ \vartheta \}}_{an} \) (VIII.28)

\[
E^{\{ \vartheta \}}_{an} \Rightarrow E^{\{ \vartheta \}}_{hy} \equiv -\frac{\hbar c}{\alpha_s} \sum_{k,l=1}^{\infty} \int_0^\infty dr \, r^2 \frac{\{ b \} A_{2l}(r)}{r^2} \cdot \frac{\{ b \} A_{2k}^\prime (r)}{r^2}, \quad (VIII.75)
\]

where the matrix \( \{ F_{l,k}^{\prime} \} \) has already been specified by equation (VIII.58). Concerning the mass equivalent, one takes half the sum of its two forms given by (VIII.13) and (VIII.63),

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The corresponding hybrid form of the energy functional \( \{\text{an}\} \tilde{E}[\Omega] \) (VI.25) is

\[
\{\text{an}\} \tilde{E}[\Omega] \Rightarrow \{\text{hy}\} \tilde{E}[\Omega] = - \left( E^{(r)}_{hy} + E^{(\theta)}_{hy} \right) + 2 \tilde{M}_{\text{hy}} c^2 \quad \text{(VIII.77)}
\]

and its extremalization, cf. (VIII.30) and (VIII.73a)-(VIII.73b), with respect to both potentials \( \{b\} A_2(r) \) and \( \{b\} A'_2(r) \) leads us again back to both former multipole systems (VIII.46)-(VIII.47) and (VIII.60)-(VIII.61).

* * *

At this point, it seems worth while to pause for a moment in order to briefly survey the results of the octupole approximation obtained so far. Perhaps the most interesting feature is that one can work with two alternative formalisms, namely the one being based upon the alternative multipole potentials \( \{b\} A_2(r) \), which were introduced in connection with the new basis system, cf. (VIII.3), or one may work with the conjugate potentials \( \{b\} A'_2(r) \) (VIII.55). Clearly, both formalisms are completely equivalent and one may prefer the first or the second one. Indeed, both approaches lead us to an octupole system of equations, i.e. in the first case (VIII.46)-(VIII.47) and in the second case (VIII.60)-(VIII.61). Each one of both systems consists of a quadrupole equation, i.e. (VIII.46) and (VIII.60), and of an octupole equation, i.e. (VIII.47) and (VIII.61). Furthermore, both approaches admit the existence of a variational principle and thus are equipped with an energy functional,
\{2+4\} \tilde{E}_0[\Omega] \text{ and } \{2+4\} \tilde{E}_0'[\Omega] \text{ (VIII.72)}, whose extremalization yields just the corresponding octupole systems.

But a difference (albeit only in a technical respect) exists concerning the specific shape of the multipole equations: whereas in the first case (VIII.46)-(VIII.47) the second equation (VIII.47) for the octupole potential \(b^0A_4(r)\) appears decoupled from the quadrupole potential \(b^0A_2(r)\), the first equation (VIII.46) for the quadrupole potential \(b^0A_2(r)\) contains a coupling to the octupole potential \(b^0A_4(r)\), i.e. the octupole potential \(b^0A_4(r)\) appears to be independent of the quadrupole potential, but the converse is not true. This quadrupole-octupole interrelationship is just the opposite of the second case (VIII.60)-(VIII.61); here the quadrupole potential \(b^0A'_2(r)\) seems to be independent of its octupole counterpart \(b^0A'_4(r)\), whereas the latter is coupled back to the quadrupole potential \(b^0A'_2(r)\), cf. (VIII.61).

**Separative Method**

This coupling between the quadrupole \((b^0A_2(r), b^0A'_2(r))\) and octupole \((b^0A_4(r), b^0A'_4(r))\) potentials cannot be removed by resorting to the hybrid method since the latter does embrace both coupled octupole systems, i.e. (VIII.46)-(VIII.47) and (VIII.60)-(VIII.61). However, it would be very desirable to have a completely decoupled system because in this case it would become possible to associate well-defined anisotropy energies to both the quadrupole mode \((l = 1)\) and to the octupole mode \((l = 2)\). Indeed, only for such a situation it would be legitimate to talk about a “quadrupole energy” and an “octupole energy”. But such a mode separation of the anisotropy energy is not possible up to now because the anisotropy energy \(E^{(e)}_{an} = E^{(r)}_{2+4} + E^{(θ)}_{2+4}\) of all three methods do contain a mixed term consisting of both the quadrupole potential \(b^0A_2(r)/b^0A'_2(r)\) and the octupole potential \(b^0A_4(r)/b^0A'_4(r)\), cf. equations (VIII.33)-(VIII.54), (VIII.70)-(VIII.71), and (VIII.74)-(VIII.75).

Fortunately, there exists a possibility for the complete separation of the quadrupole
and octupole modes, namely by introducing suitable new potentials \( (b)A''_2(r) \) and \( (b)A''_4(r) \):

\[
(b)A''_2(r) \equiv (b)A'_2(r) \quad \text{(VIII.78a)} \\
(b)A''_4(r) \equiv (b)A'_4(r) \quad \text{(VIII.78b)}
\]

This says that the new (separative) quadrupole potential \( (b)A''_2(r) \) is identified with the conjugate potential \( (b)A'_2(r) \) (VIII.55) and the new (separative) octupole potential \( (b)A''_4(r) \) is identified with the alternative octupole potential \( (b)A'_4(r) \) being formerly introduced by the transition (VIII.3) to the new basis system \( \{c(2l)_{(2)}\} \). Since the new separative potentials are composed of both the alternative and the conjugate potentials, the present separative method is obviously the true hybrid method. Clearly, the separative potentials may be expressed also solely in terms of the alternative potentials \( (b)A_{2l}(r) \)

\[
(b)A''_2(r) = \frac{4}{45} \cdot (b)A_2(r) + \frac{8}{105} \cdot (b)A_4(r) \quad \text{(VIII.79a)} \\
(b)A''_4(r) = (b)A_4(r) \quad \text{(VIII.79b)}
\]

or solely in terms of the conjugate potentials \( (b)A'_{2l}(r) \):

\[
(b)A''_2(r) = (b)A'_2(r) \quad \text{(VIII.80a)} \\
(b)A''_4(r) = -\frac{4725}{32} \cdot (b)A'_2(r) + \frac{11025}{64} \cdot (b)A'_4(r) \quad \text{(VIII.80b)}
\]

Conversely, the alternative potentials \( (b)A_{2l}(r) \) read in terms of the separative potentials \( (b)A''_{2l}(r) \) as

\[
(b)A_2(r) = \frac{45}{4} \cdot (b)A''_2(r) - \frac{6}{7} (b)A''_4(r) \quad \text{(VIII.81a)} \\
(b)A_4(r) = (b)A''_4(r) \quad \text{(VIII.81b)}
\]

or similarly, the conjugate potentials \( (b)A'_{2l}(r) \) do reappear in terms of the separative potentials \( (b)A''_{2l}(r) \) as

\[
(b)A'_2(r) = (b)A''_2(r) \quad \text{(VIII.82a)} \\
(b)A'_4(r) = \frac{6}{7} \cdot (b)A''_2(r) + \frac{64}{11025} \cdot (b)A''_4(r) \quad \text{(VIII.82b)}
\]

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By means of these results, one can now eliminate the alternative (or conjugate) potentials in favour of the separative potentials so that the corresponding systems, i.e. the “alternative” system (VIII.46)-(VIII.47) or the “conjugate” system (VIII.60)-(VIII.61), are both recast, in terms of the separative potentials $^{(b)A''_2}(r)$ and $^{(b)A''_4}(r)$ to the following form:

$$
\Delta_r^{(b)A''_2}(r) - 6 \frac{^{(b)A''_2}(r)}{r^2} = -^{(b)m_1} \cdot \alpha_s \tilde{\Omega}^2(r) \quad \text{(VIII.83a)}
$$

$$
\Delta_r^{(b)A''_4}(r) - 20 \frac{^{(b)A''_4}(r)}{r^2} = -^{(b)m'_2} \cdot \alpha_s \tilde{\Omega}^2(r) . \quad \text{(VIII.83b)}
$$

For the values of the mass-equivalent parameters $^{(b)m_1}$ and $^{(b)m'_2}$ see equations (VIII.16) and (VIII.49), and observe also their relationship

$$
^{(b)m'_2} = \frac{11025}{64} \left( ^{(b)m_2} - \frac{6}{7} ^{(b)m_1} \right) . \quad \text{(VIII.84)}
$$

Thus the separative method takes over both the pure quadrupole equation (VIII.60) and the pure octupole equation (VIII.47), inclusive the corresponding mass-equivalent parameters. Evidently, our attempt (VIII.78a)-(VIII.78b) of decoupling the octupole systems has thus been successful; and consequently we can now look for the separative form of the energy functional so that the present octupole system (VIII.83a)-(VIII.83b) represents just the corresponding extremal equations thereof.

**Separative Energy Functional**

From the purely formal viewpoint, the desired “separative” energy functional $^{(24)\tilde{E}''_{[\Omega]}}$, say) must of course be of the same shape as its “conjugate” and “hybrid” predecessors $^{(2+4)\tilde{E}''_{[\Omega]}}$ (VIII.72) and $^{(hy)\tilde{E}''_{[\Omega]}}$ (VIII.77); i.e. one expects again the splitting of the anisotropy energy in a radial and a longitudinal part:

$$
^{\mu E_{an}} \Rightarrow ^{\mu E_{2,4}} = ^{\mu E_{2,4}}^{(r)} + ^{\mu E_{2,4}}^{(\vartheta)} , \quad \text{(VIII.85)}
$$

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just as was the case with all the predecessors, e.g. (VIII.24) for the alternative choice of basis system. Thus the “separative” functional \( \{2,4\} \tilde{E}_{\Omega}'' \) will appear again as (cf. \( \{2+4\} \tilde{E}_{\Omega}'' \) (VIII.72) and \( \{hy\} \tilde{E}_{\Omega}'' \) (VIII.77))

\[
\{2,4\} \tilde{E}_{\Omega}'' = -''E^{(r)}_{2,4} - ''E^{(\varphi)}_{2,4} + 2''\tilde{M}^{(e)}_{2,4}.
\] (VIII.86)

But the pleasant property of this functional is now that it decays in a sum of subfunctionals, i.e. the quadrupole and octupole contributions:

\[
\{2,4\} \tilde{E}_{\Omega}'' = \{2\} \tilde{E}_{\Omega}'' + \{4\} \tilde{E}_{\Omega}''
\] (VIII.87)

where the quadrupole contribution is given by

\[
\{2\} \tilde{E}_{\Omega}'' = -''E^{(r)}_{2} - ''E^{(\varphi)}_{2} + 2''\tilde{M}^{(e)}_{2}
\] (VIII.88)

and the octupole contribution by

\[
\{4\} \tilde{E}_{\Omega}'' = -''E^{(r)}_{4} - ''E^{(\varphi)}_{4} + 2''\tilde{M}^{(e)}_{4}.
\] (VIII.89)

Here, the individual energy contributions are obtained by simply inserting those inverse transformation relations (VIII.81a)–(VIII.81b) or (VIII.82a)–(VIII.82b) in the corresponding “conjugated” or “separative” results; this yields for the quadrupole contributions (VIII.88)

\[
''E^{(r)}_{2} = -\frac{45}{4} \cdot \frac{\hbar c}{\alpha_s} \int_0^\infty dr \, r^2 \left( \frac{d (b) A''_2(r)}{dr} \right)^2
\] (VIII.90a)

\[
''E^{(\varphi)}_{2} = -\frac{45}{4} \cdot \frac{\hbar c}{\alpha_s} \int_0^\infty dr \, \left( (b) A''_2(r) \right)^2
\] (VIII.90b)

\[
''\tilde{M}^{(e)}_{2} c^2 = -\frac{45}{4} (b) m_1 \cdot \hbar c \int_0^\infty dr \, r^2 (b) A''_2(r) \frac{\tilde{\gamma}^2(r)}{r},
\] (VIII.90c)
and similarly for the octupole contributions (VIII.89)

\[ \tilde{M}_4^{(e)} c^2 = - \frac{64}{11025} \cdot \frac{\hbar c}{\alpha_s} \cdot \int_0^\infty dr r^2 \frac{A''_4(r)}{r} \tilde{\Omega}^2(r) \]  

(VIII.91c)

Such a pleasant decay of the energy functional (as being given by equation (VIII.87)) into pure quadrupole and octupole contributions \{\tilde{E}''_{4}^{(r)}\} \text{(VIII.88)} and \{\tilde{E}''_{4}^{(q)}\}, cf. (VIII.88)–(VIII.89), does not occur for the other approaches, i.e. “alternative”, “conjugate”, and “hybrid”. And the consequence is that any subfunctional is sufficient in order to deduce the corresponding multipole equation. Indeed, it is easy to see that the extremalization of the quadrupole subfunctional \{\tilde{E}''_{4}^{(r)}\} (VIII.88) yields just the quadrupole equation (VIII.83a), and analogously the extremalization of the octupole subfunctional \{\tilde{E}''_{4}^{(q)}\} (VIII.89) yields the octupole equation (VIII.83b). This neat separation of the quadrupole and octupole effects can now be used in order to clarify the question of octupole dimorphism for those states with quantum numbers \( n_O = j_O + 1 = 3, \quad (b)j_z = \pm 1 \) which in the quadrupole approximation misses this effect of dimorphism (see the discussion of this effect on p. 82).

4. Magnitude of Octupole Splitting

For a closer inspection of the critical energy level \{\( n_O = 3, j_O = 2, (b)j_z = \pm 1 \)\) it is very instructive to first consider the quadrupole part (VIII.83a) of the octupole approximation (VIII.83a)-(VIII.83b)
Quadrupole Part

Observe here, that this is not identical to the former quadrupole approximation (VIII.37), being due to the “alternative” approach, since the coupling constant is now \( \{b\}_{m_1} \) (VIII.15a)–(VIII.15b) in place of \( \{b\}_{m_1}' \) (VIII.36). But a common property is the fact that the quadrupole ambiguity shows here up again in form of the sign ambiguity of the mass-equivalent parameter \( \{b\}_{m_1} \) (VIII.15a)–(VIII.15b), just as is the case with \( \{b\}_{m_1}' \) (VIII.36); and this ambiguity transcribes then also quite correspondingly to both solutions \( \{b\}_A^2(r) \) and \( \{b\}_A'^2(r) \). The consequence of this is that, also within the framework of the separative method, there can occur no dimorphic energy splitting of those states specified by the quantum numbers \( \{n_O = 3, j_O = 2, \{b\}_j = \pm 1\} \). The reason is again that the corresponding anisotropy energy \( \{\nu E_2^{(e)}\} \left( = \{\nu E_2^{(r)} + \nu E_2^{(q)}\}\right) \) (VIII.90a)-(VIII.90b) is quadratic with respect to the quadrupole potential \( \{b\}_A^2(r) \), and is therefore insensitive with respect to a change of sign of \( \{b\}_A'^2(r) \)!

A further common property of the former quadrupole approximation (VIII.37) and the present quadrupole part (VIII.83a) is the fact that both approaches do yield the same quadrupole energy, i.e. we have not only the energy identity (VIII.44) but also

\[
E^{(e)}_{III} = \nu E_2^{(e)}
\]  

(VIII.92)

where \( E^{(e)}_{III} \) has been defined in terms of the original potential correction \( \{b\}_A^{III}(r) \) by equation (VII.12) and the present energy \( \nu E_2^{(e)} \left( = \nu E_2^{(r)} + \nu E_2^{(q)}\right) \) by the equations (VIII.90a)-(VIII.90b). In order to validate this claim, simply observe that when \( \{b\}_A^{III}(r) \) is the solution of the former original quadrupole equation (VII.4) then the solution of the present quadrupole part (VIII.83a) is

\[
\{b\}_A'^2(r) = \frac{1}{5} \{b\}_{m_1} \cdot \{b\}_A^{III}(r).
\]  

(VIII.93)

On the other hand, the quadrupole part (VIII.83a) of the octupole approximation is uniquely linked to the quadrupole energy \( \nu E_2^{(e)} \left( = \nu E_2^{(r)} + \nu E_2^{(q)}\right) \) (VIII.90a)-(VIII.90b)
so that we merely need to substitute therein the solution \(^{(b)}A_2''(r)\) (VIII.93) in order to validate the claimed identification (VIII.92).

**Octupole Energy**

Finally, let us mention also the fact that the decoupling of the quadrupole and octupole potentials \(^{(b)}A_2''(r)\) and \(^{(b)}A_4''(r)\) by the separative method, as expressed by (VIII.83a)-(VIII.83b) entails the separate validity of the octupole identity

\[ n_{E_4^{(e)}} = n_{\tilde{M}_4^{(e)}} c^2, \]  

(VIII.94)

where the octupole energy \(n_{E_4^{(e)}} \left( = n_{E_4^{(r)}} + n_{E_4^{(v)}} \right) \) is given by equations (VIII.91a)-(VIII.91b) and the corresponding mass equivalent \(n_{\tilde{M}_4^{(e)}} c^2\) by (VIII.91c). If we are satisfied here again with the former trial amplitude \(\tilde{\Omega}(r)\) (VI.1a)-(VI.1b), both objects (VIII.94) become functions of the trial parameters \(\beta\) and \(\nu\), i.e.

\[ n_{E_4^{(e)}} = -\frac{e^2}{a_B} (2\beta a_B) \left( \{^\{b\}m_2' \}^2 \right) \cdot \varepsilon_4^{(e)}(\nu) \]  

(VIII.95a)

\[ n_{\tilde{M}_4^{(e)}} c^2 = -\frac{e^2}{a_B} (2\beta a_B) \left( \{^\{b\}m_2' \}^2 \right) \cdot \mu_4^{(e)}(\nu) \]  

(VIII.95b)

where both functions \(\varepsilon_4^{(e)}(\nu)\) and \(\mu_4^{(e)}(\nu)\) are explicitly determined in App.E. Thus, the octupole identity (VIII.94) reads in coefficient form

\[ \varepsilon_4^{(e)}(\nu) \equiv \mu_4^{(e)}(\nu). \]  

(VIII.96)

The latter results (VIII.95a)-(VIII.95b) can now be used in order to convince oneself that the absence of the energy splitting becomes eliminated by the octupole approximation: namely, the mass-equivalent \(n_{\tilde{M}_4^{(e)}} c^2\) (VIII.95b) shows that this object is **quadratic** with respect to the mass-equivalent parameter \(\{^\{b\}m_2' \}\), i.e.

\[ n_{\tilde{M}_4^{(e)}} c^2 \sim \left( \{^\{b\}m_2' \} \right)^2, \]  

(VIII.97)
because \( \mu_4^e(\nu) \) is independent of \( ^{(b)}m'_2 \), see equation (E.27) of App.E. On the other hand, it has already been shown through the equations (VIII.49) that \( ^{(b)}m'_2 \) must adopt two different values which differ by a factor of six due to the existence of two different angular densities \( ^{(b)}k_0(\vartheta) \), see equations (VIII.15a)–(VIII.15b). Therefore the octupole correction energy (VIII.95a)-(VIII.95b) must lower the gauge field energy of the considered ortho-state (with \( n_0 = j_O + 1 = 3, ^{(b)}j_z = \pm 1 \)) in two ways and thus creates the dimorphic energy splitting for this state! The corresponding two (energy lowering) octupole-corrections will differ by a factor of six, see below.

\[ \text{Schrödinger Equation with Octupole Interaction} \]

Properly speaking, the Schrödinger-like equation for the amplitude field \( \tilde{\Omega}(r) \) has already been deduced from the energy functional \( \tilde{\mathcal{E}}_{[\Omega]} \) (VI.25) and yielded the equation (VI.27). However, that deduction had been based on the original decomposition (V.22) of the anisotropic gauge field \( ^{(b)}A^\text{an}(r, \vartheta) \) so that the corresponding Schrödinger equation (VI.27) refers to the potential corrections \( ^{(b)}A^\text{III}(r) \) and \( ^{(b)}A^\text{V}(r) \), etc. However, in the meantime it has turned out to be more advantageous to decompose the anisotropic gauge field \( ^{(b)}A^\text{an}(r, \vartheta) \) as shown by equation (VIII.3) where the alternative potentials \( ^{(b)}A_{2l}(r) \) have been further transcribed to the conjugated gauge fields \( ^{(b)}A'_{2l}(r) \) and ultimately to the separative potentials \( ^{(b)}A''_{2l}(r) \) and \( ^{(b)}A''_{4l}(r) \) (VIII.78a)–(VIII.78b). But since the separative method provided us with a clear decoupling of the quadrupole and octupole interactions, it will surely be helpful to write down the Schrödinger equation for the amplitude field also in terms of the separative potentials \( ^{(b)}A''_{2l}(r) \) and \( ^{(b)}A''_{4l}(r) \).

For this purpose, we have to go back to the original energy functional \( \tilde{\mathcal{E}}_{[\Omega]} \) (VI.25) and have to recast the anisotropic gauge field part \( ^{(an)}\tilde{\mathcal{E}}_{[\Omega]} \) in terms of the separative potentials \( ^{(b)}A''_{2l}(r) \) and \( ^{(b)}A''_{4l}(r) \), whereas the matter part \( ^{(D)}\tilde{\mathcal{E}}_{[\Omega]} \) and the “isotropic” gauge field part \( ^{(i)}\tilde{\mathcal{E}}_{[\Omega]} \) remains unchanged. The latter fact then implies also that the Poisson equation (IV.18) for the isotropic potential \( ^{(b)}A_0(r) \) remains unchanged. Thus, it is only
the Schrödinger equation (VI.27) which must get a new shape.

The latter is to be deduced from the energy functional (VI.25) by extremalization with respect to the amplitude field $\tilde{\Omega}(r)$, which is contained only in the matter part $(D)\tilde{E}[\tilde{\Omega}] \equiv 2E_{\text{kin}} + 2\lambda_s \cdot \tilde{N}_{\Omega}$ and in all the mass equivalents $\tilde{M}^{[e]}c^2$ (V.12), $''\tilde{M}_2^{[e]}c^2$ (VIII.90c), and $''\tilde{M}_4^{[e]}$ (VIII.91c). Consequently, denoting the functional derivative with respect to the amplitude field $\tilde{\Omega}(r)$ by $\delta_{\tilde{\Omega}}$, the corresponding extremal equation reads in abstract form

$$0 = \delta_{\tilde{\Omega}}''\tilde{E}[\tilde{\Omega}] = \delta_{\tilde{\Omega}}((D)\tilde{E}[\tilde{\Omega}]) - \lambda^{(e)}_{\tilde{G}} \delta_{\tilde{\Omega}}''\tilde{M}^{[e]}c^2 \,,$$

or concretely

$$-\frac{\hbar^2}{2M} \left( \frac{d^2}{dr^2} + \frac{1}{r} \frac{d}{dr} \right) \tilde{\Omega}(r) + \frac{\hbar^2}{2Mr^2} \cdot j^3 \tilde{\Omega}(r)$$

$$-\hbar c \left\{ [b]A_0(r) + \frac{45}{4} [b]m_1 \cdot [b]A_2''(r) + \frac{64}{11025} [b]m_2 \cdot [b]A_4''(r) \right\} \tilde{\Omega}(r)$$

$$= -\lambda_s \cdot \tilde{\Omega}(r) \,,$$

where the Lagrangean parameter $\lambda_s$ plays the part of the Schrödinger energy eigenvalue $E_s (\equiv -\lambda_s)$. Neglecting the octupole interactions ($'^{[b]}A_4''(r) \Rightarrow 0$) and observing

$$\frac{45}{4} [b]m_1 \cdot [b]A_2''(r) \Rightarrow [b]m_{\text{III}} \cdot [b]A_4''(r)$$

lets the present octupole Schrödinger equation (VIII.99) becoming identical to the former quadrupole Schrödinger equation (VI.27).

**Variational Procedure**

Unfortunately, we are not smart enough in order to find the exact solution of the eigenvalue problem (VIII.99) which must be complemented by the monopole equation (IV.18) for the spherically symmetric approximation $^[b]A_0(r)$, by the quadrupole equation (VIII.83a) for $^[b]A_2''(r)$ and finally by the octupole equation (VIII.83b) for $^[b]A_4''(r)$. 

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Therefore we must be satisfied here with the extremalization of the energy functional
\[ \hat{\mathcal{E}}_{\{\Omega\}} \] (VI.25) on the subspace of the trial amplitudes \( \hat{\Omega}(r) \) (VI.1a)–(VI.1b) and its descendants \( \{b\} \hat{A}_0(r) \Rightarrow \{b\} \hat{a}_\nu(y) \) (VI.30), \( \{b\} \hat{A}_2^\nu(r) \Rightarrow \{b\} \hat{A}_{II}^\nu(y) \) (VII.5), and \( \{b\} \hat{A}_4^\nu(r) \Rightarrow \{b\} \hat{P}_4(y) \) (E.26). Each of these spherically-symmetric multipole potentials carries its own energy content, i.e.

\[ \{b\} \hat{A}_0(r) \Rightarrow E_R^{[e]} = -\frac{e^2}{a_B} (2\beta a_B) \cdot \varepsilon_{pot}(\nu) \] (VIII.101a)

\[ \{b\} \hat{A}_2^\nu(r) \Rightarrow E_{\{e\}}^\nu = -\frac{e^2}{a_B} (2\beta a_B) \cdot \{b\} \hat{m}_{III} \cdot \mu_{\{e\}}^\nu(\nu) \] (VIII.101b)

\[ \{b\} \hat{A}_4^\nu(r) \Rightarrow \varepsilon_{\{e\}}^\nu = -\frac{e^2}{a_B} (2\beta a_B) \left( \{b\} \hat{m}_2^2 \right)^2 \cdot \mu_{\{e\}}^\nu(\nu) \] (VIII.101c)

(Observe here that the quadrupole energy \( E_{\{e\}}^{III} = \varepsilon_{\{e\}}^\nu \) (VIII.101b) appears to be proportional to the mass-equivalent parameter \( \{b\} \hat{m}_{III} \) whereas the octupole energy \( \varepsilon_{\{e\}}^\nu \) (VIII.101c) is quadratic with respect to the corresponding parameter \( \{b\} \hat{m}_2^2 \). The reason is that the universality of the ratio \( \frac{\{b\} \hat{m}_{III}}{\{b\} \hat{m}_2^2} = 5 \) (VI.17b) admits to absorb this into the quadrupole potential \( \{b\} \hat{A}^{III}(r) \), cf. the quadrupole equation (VII.4); see also the discussion in Appendix A.

The total gauge field energy \( E_R^{[e]} \) (VI.12) in the octupole approximation is now due to the sum of all three multipole components (VIII.101a)–(VIII.101c), i.e.

\[ E_R^{[e]} = -\frac{e^2}{a_B} (2\beta a_B) \cdot \varepsilon_{tot}^{[e]}(\nu) \] (VIII.102)

with the total potential function \( \varepsilon_{tot}^{[e]}(\nu) \) being defined through

\[ \varepsilon_{tot}^{[e]}(\nu) = \varepsilon_{pot}(\nu) + \{b\} \hat{m}_{III} \cdot \mu_{\{e\}}^\nu(\nu) + \left( \{b\} \hat{m}_2^2 \right)^2 \cdot \mu_{\{e\}}^\nu(\nu) \] (VIII.103)

Recall here also that the functions \( \varepsilon_{pot}(\nu) \) (VI.33), \( \mu_{\{e\}}^\nu(\nu) \) (VII.13), and \( \mu_{\{e\}}^\nu(\nu) \) (E.27) are independent of the quantum numbers \( n_O, j_O, \{b\} j_z \). Furthermore, the kinetic energy \( E_{kin} \) (VI.8) is still given by (VI.9a)–(VI.9b); and the three poisson identities (VI.34), (VII.11), and (VIII.94) are satisfied since we always use the exact solutions of the corresponding...
multipole equations. Therefore these constraints can be omitted in the energy functional \( \tilde{E}_{[\Omega]} \) (VI.25) together with the normalization condition (VI.5): \( \tilde{N}_{\Omega} = 0 \), provided that we restrict ourselves to the use of normalized trial amplitudes \( \tilde{\Omega}(r) \). This cuts down the energy functional \( \tilde{E}_{[\Omega]} \) (VI.25) to its physical part \( \tilde{E}_{[IV]} \):

\[
\tilde{E}_{[\Omega]} \Rightarrow \tilde{E}_{[IV]} = 2E_{\text{kin}} + E_{R}^{[e]} + E_{\text{III}}^{[e]} + "E_{4}^{[e]} \),
\]

(VIII.104)

and the value of this reduced functional on the subspace of RST fields \( \{\tilde{\Omega}(r); [b]A_{0}(r), [b]A_{u}(r), [b]A_{1}(r)\} \) due to our trial ansatz (VI.1a)-(VI.1b) yields then an energy function \( \tilde{E}_{[IV]}(\beta, \nu) \) which depends on the trial parameters \( \beta \) and \( \nu \):

\[
\tilde{E}_{[IV]}(\beta, \nu) = \frac{e^2}{a_B} (2\beta a_B)^2 \cdot \varepsilon_{\text{kin}}(\nu) - \frac{e^2}{a_B} (2\beta a_B) \cdot \varepsilon_{\text{tot}}^{[e]}(\nu),
\]

(VIII.105)

where \( \varepsilon_{\text{kin}}(\nu) \) is given by (VI.91) and \( \varepsilon_{\text{tot}}^{[e]}(\nu) \) by (VIII.103).

The quantum number \( j_{\text{O}} (= n_{\text{O}} - 1) \) is contained explicitly in the kinetic function \( \varepsilon_{\text{kin}}(\nu) \) (VI.91) and implicitly in \( \varepsilon_{\text{tot}}^{[e]}(\nu) \) (VIII.103) via \( (b)_{\text{III}} \) and \( (b)_{4} \), whereas the azimuthal quantum number \( (b)_{jz} \) is (implicitly) contained only in the potential function \( \varepsilon_{\text{tot}}^{[e]}(\nu) \) (VIII.103). But after having fixed both quantum numbers \( j_{\text{O}} (= n_{\text{O}} - 1) \) and \( (b)_{jz} \) with \( -j_{\text{O}} \leq (b)_{jz} \leq j_{\text{O}} \), we can obtain the non-relativistic energy spectrum of orthopositronium by simply looking for the minimal values of the energy function \( \tilde{E}_{[IV]}(\beta, \nu) \) (VIII.105) with respect to both trial parameters \( \beta \) and \( \nu \). By means of partial extremalization (i.e. with respect to \( \beta \)), there remains to minimize the reduced energy function \( \tilde{E}_{[\text{O}]}^{(j)}(\nu) \) with respect to the residual parameter \( \nu \)

\[
\tilde{E}_{[\text{O}]}^{(j)}(\nu) = -\frac{e^2}{4a_B} \cdot S_{\text{O}}^{(j)}(\nu),
\]

(VIII.106)

i.e. the desired energy value \( \tilde{E}_{[\text{O}]}^{(j)} \), associated to the quantum numbers \( \{j\} \equiv \{j_{\text{O}}, (b)_{jz}\} \), is given by the maximal value of the spectral function \( S_{\text{O}}^{(j)}(\nu) \):

\[
\tilde{E}_{[\text{O}]}^{(j)} = -\frac{e^2}{4a_B} S_{\text{O}, \text{max}}^{(j)}.
\]

(VIII.107)
Here, the spectral function \( S^{(j)}_O(\nu) \) contains the relevant quantum numbers \( \{j_O, (b)j_z\} \) in the following way

\[
S^{(j)}_O(\nu) = \frac{\left[ \frac{\varepsilon_{\text{tot}}^{(e)}(\nu)}{\varepsilon_{\text{kin}}(\nu)} \right]^2}{\frac{1}{2\nu+1} \left( \frac{1}{4} + \frac{\beta^2}{2\nu} \right)} \left[ \varepsilon_{\text{pot}}(\nu) + \left( (b)m_1 \right)^2 \cdot \mu_2^{(e)}(\nu) + \left( (b)m_2' \right)^2 \cdot \mu_4^{(e)}(\nu) \right]^2. \tag{VIII.108}
\]

The simple potential function \( \varepsilon_{\text{pot}}(\nu) \) due to the spherically symmetric approximation is given by equation (VI.33); its octupole analogue \( \varepsilon^{(e)}_4(\nu) \left( \equiv \mu_4^{(e)}(\nu) \right) \) is also explicitly prepared in App.E, cf. (E.27); and thus it is only the quadrupole mass-equivalent function \( \mu_2^{(e)}(\nu) \) which necessitates a brief comment. However, the quadrupole approximation has already been studied thoroughly in the preceding sections; and if we identify the corresponding mass equivalent \( \tilde{M}^{(e)}_3 c^2 \) (VIII.13) with its separative counterpart \( n\tilde{M}^{(e)}_2 c^2 \) (VIII.90c) one is immediately led to the identification of the mass-equivalent functions:

\[
(b)m_3 \cdot \mu_3^{(e)}(\nu) = \left( (b)m_1 \right)^2 \cdot \mu_2^{(e)}(\nu). \tag{VIII.109}
\]

But from here it is a simple exercise to find the direct link of both mass-equivalent functions: inserting the general form (A.1) of the quadrupole potential \( (b)A_3(\nu) \) in the definition (VI.22a) of the mass equivalent \( (b)m_3 \) yields

\[
(b)m_3 = a_3 \cdot (b)m_1. \tag{VIII.110}
\]

Next, observe equation (A.4) and conclude from this

\[
\{b\}m_1 = \frac{4}{9} a_3 \tag{VIII.111}
\]

which then finally yields

\[
(b)m_3 = \frac{9}{4} \left( (b)m_1 \right)^2 \tag{VIII.112}
\]

and thus

\[
\mu_2^{(e)}(\nu) = \frac{9}{4} \mu_3^{(e)}(\nu). \tag{VIII.113}
\]

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So we can ultimately express the spectral function $S^{(j)}_{\mathcal{O}}(\nu)$ in terms of the three known-functions $\varepsilon_{\text{pot}}(\nu)$ (VI.33), $\mu_{\text{III}}^{(e)}(\nu)$ (VII.15), and $\mu_{4}^{(e)}(\nu)$ (E.27):

$$S^{(j)}_{\mathcal{O}}(\nu) = \left[ \varepsilon_{\text{pot}}(\nu) + \left( \frac{3}{2} (b)m_{1} \right)^{2} \cdot \mu_{\text{III}}^{(e)}(\nu) + \left( \frac{3}{2}m_{2} \right)^{2} \cdot \mu_{4}^{(e)}(\nu) \right]^{2} \cdot \frac{1}{2\nu+1} \left( \frac{1}{4} + \frac{j_{\mathcal{O}}^{2}}{2\nu} \right).$$

(VIII.114)

If desired, the three functions $\varepsilon_{\text{pot}}(\nu), \mu_{\text{III}}^{(e)}(\nu), \mu_{4}^{(e)}(\nu)$ may be alternatively used here in their closed analytic form, cf. (D.3a)-(D.3b) and (E.49). The subsequent table (see p. 145) represents a collection of the numerical results:

i) The groundstate ($j_{\mathcal{O}} = 0$, first line) is not doubled (App.s A and B) and receives a relatively bad numerical prediction. The conventional value, cf. (I.18), is $E_{\mathcal{C}}^{(1)} \simeq -6,8029 \text{[eV]}$ whereas the present RST octupole approximation yields $-7,5957 \text{[eV]}$ which is a deviation of $-11,6\%$. Why the groundstate has such a large negative deviation in contrast to the positive deviations of the excited states ($j_{\mathcal{O}} = 1, 2, 3, \ldots$) must be clarified elsewhere. For instance, the first excited state $j_{\mathcal{O}} = 1, (b)j_{z} = \pm 1$ (second line) has a deviation of $+7,4\%$.

ii) The exceptional case $\{n_{\mathcal{O}} = 3, j_{\mathcal{O}} = 2, (b)j_{z} = \pm 1\}$, which misses the level doubling in the quadrupole approximation (see the discussion of the table below equation VII.22 and App.D), is found to undergo now also the level doubling in the octupole approximation (third line). The energy difference of the emerging dimorphic pair is found as $0,68566 - 0,68124 \simeq 0,00442 \text{[eV]}$ which amounts to (roughly) $0,65\%$ of the binding energy of the dimorphic partners. The corresponding energy difference for the other two dimorphic pairs, i.e. $j_{\mathcal{O}} = 3$ and $j_{\mathcal{O}} = 4$, show up in the same order of magnitude ($1,65\%$).

iii) It is also interesting to see how the predictions change when one passes beyond the quadrupole approximation (fourth column) to the octupole approximation (sixth column). As a convenient measure of this change one may introduce the relative
quadrupole-octupole deviation through

\[ \Delta^{(j)} = \frac{E^{(j)}_O|_{qu} - E^{(j)}_O|_{oc}}{E^{(j)}_O|_{oc}}, \]  

(VIII.115)

see the seventh column of the subsequent table. Here it is interesting to note that the quadrupole predictions (fourth column) become corrected at most by (roughly) 0.5\% or less. This may be understood as a signal that our separative perturbation method can be expected to converge very rapidly. In any case, the level splitting due to the ortho- dimorphism seems to be at least twice the present octupole corrections; and therefore the doubling of the ortho-levels can hardly be interpreted as an artefact occurring only in the low perturbation orders (i.e. quadrupole and octupole). Of course, this question should be studied in greater detail by an extra treatment.
| $J\sigma = (n\sigma - 1)$ | $^{(b)}j_z$ | $^{(b)}m_{III} = \left(\frac{1}{2}^{(b)}m_1\right)^2$ | $^{(b)}E_\sigma^{(j)}$ [eV] | Quadrupole, [VII.22] | $^{(b)}m'_2$ | $^{(b)}E_\sigma^{(j)}$ [eV] | Octupole, [VIII.84] | $\Delta^{(j)}$ % | $E^{(n)}_C$ |
|-----------------------------|-------------|---------------------------------|-----------------|-------------------|-------------|-----------------|-----------------|----------|----------------|
| 0                           | 0           | $\frac{1}{16} = 0.0625$        | $-7.53786$      | Quadrupole, [VII.22] | $\left(\frac{19845}{3584}\right)^2 \approx 30.6595$ | $-7.59507$      | $-0.75\%$       | $-6.8029\ldots$ |
| 1                           | $\pm1$      | $\frac{1}{64} = 0.015625$      | $-1.57527$      | Quadrupole, [VII.22] | $\left(\frac{315}{512}\right)^2 \approx 0.3785$  | $-1.57551$      | $-0.015\%$      | $-1.7007\ldots$ |
| 2                           | $\pm1$      | $\frac{1}{64} = 0.015625$      | $-0.68112$      | Quadrupole, [VII.22] | $\left(\frac{315}{512}\right)^2 \approx 0.3785$  | $-0.68124$      | $-0.017\%$      | $-0.7558\ldots$ |
| 3                           | $\pm1$      | $\frac{9}{256} \approx 0.03515$| $-0.38089$      | Quadrupole, [VII.22] | $\left(\frac{945}{256}\right)^2 \approx 13.6264$ | $-0.38374$      | $-0.74\%$       | $-0.4251\ldots$ |
| 4                           | $\pm1$      | $\frac{9}{256} \approx 0.03515$| $-0.25010$      | Quadrupole, [VII.22] | $\left(\frac{945}{1024}\right)^2 \approx 0.8516$ | $-0.25023$      | $-0.051\%$      | $-0.2721\ldots$ |
Appendix A

General Properties of the Quadrupole Approximation

For getting some survey of all properties of the quadrupole approximation it is most instructive to consider also a further example, i.e. the case $j_0 = 4$. The subsequent table (at the end of this appendix) presents a collection of the corresponding relevant data for $j_0 = 4$ and thus complements the precedent tables as our basis of inductive reasoning.

General Validity of the Ratios $(VI.17a)$–$(VI.17b)$

The first and most striking observation refers to the fact that the ratios $(VI.17a)$–$(VI.17b)$ are valid for all considered cases ranging from $j_0 = 1$ up to $j_0 = 4$. Thus the self-suggesting conclusion from this limited number of cases is that these ratios could perhaps be valid for all $j_0$ (i.e. $j_0 = 1, 2, 3, 4, \ldots$). If this conclusion could be shown to be true, the quadrupole equation $(VII.4)$ for the potential correction $^{(b)}A_{III}(r)$ would be generally valid, as well as the general form of the quadrupole energy $E_{III}^{(e)}$ $(VII.12)$.

Indeed, it is a rather simple matter to validate the first one of these ratios, i.e. $(VI.17a)$. For this purpose, observe first that the general form of the angular potential factor $^{(b)}A_{III}(\vartheta)$ $(V.25a)$ is

\[ ^{(b)}A_{III}(\vartheta) = a_{III} \cdot \left( \cos^2 \vartheta - \frac{1}{3} \right) \] (A.1)

with the constant $a_{III}$ being given by

\[ a_{III} = -\frac{3}{4} \left( 1 - 3 K_{I(4)} \right) , \] (A.2)

see equation $(V.28)$. Next, calculate both constants $^{(b)}e_{III}$ and $^{(b)}f_{III}$ $(VI.16a)$ by use of
the present form of \( \{b\} A^{\text{III}}(\vartheta) \) (A.1) and find

\[
\begin{align*}
\{b\} e_{\text{III}} &= \frac{4}{45} \cdot a_{\text{III}}^2, \quad \text{(A.3a)} \\
\{b\} f_{\text{III}} &= \frac{8}{15} \cdot a_{\text{III}}^2. \quad \text{(A.3b)}
\end{align*}
\]

Consequently, this verifies the first ratio (VI.17a). Observe here that this ratio is a purely geometric relation, independent of the specific angular density \( \{b\} k_0(\vartheta) \).

A quite similar (albeit somewhat more complicated) reasoning yields for the constant \( \{b\} m_{\text{III}} \) (VI.22a)

\[
\{b\} m_{\text{III}} = \left( \frac{2}{3} a_{\text{III}} \right)^2 \quad \text{(A.4)}
\]

which then validates the second ratio (VI.17b). Thus both ratios (VI.17a), (VI.17b) are found to represent quite general features of the quadrupole approximation and thus turn out to be independent of the chosen trial amplitude \( \tilde{\Omega}(r) \) (VI.1a). It is also a rather easy exercise to verify that all states with \( j_{\mathcal{O}} = 4 \) (see end of this appendix) actually do satisfy the claimed relations (VI.17a)–(VI.17b). Especially, these relations must hold also for the exact (unknown) solution of the eigenvalue problem in the quadrupole approximation.

**No Dimorphism for \( \{b\} j_z = 0 \)**

The subsequent table for \( j_{\mathcal{O}} = 4 \), p. 152 suggests in combination with the precedent table on p. 70 that for \( \{b\} j_z = 0 \) and all values of \( j_{\mathcal{O}} \) (i.e. \( j_{\mathcal{O}} = 0, 1, 2, 3, 4, \ldots \) ) there does occur *no* dimorphism; and furthermore the angular density \( \{b\} k_0(\vartheta) \) (IV.20) is always given by

\[
\{b\} k_0(\vartheta) = \frac{1}{2\pi^2} \cdot \frac{1}{\sin \vartheta}, \quad \text{(A.5)}
\]

so that the angular potential factor \( \{b\} A^{\text{III}}(\vartheta) \) (V.25a) must always appear for \( \{b\} j_z = 0 \) as

\[
\{b\} A^{\text{III}}(\vartheta) = \frac{3}{8} \left[ \cos^2 \vartheta - \frac{1}{3} \right]. \quad \text{(A.6)}
\]

Clearly, once the claim (A.5) for the angular density \( \{b\} k_0(\vartheta) \) is verified, then the result (A.6) for the angular factor \( \{b\} A^{\text{III}}(\vartheta) \) is an inevitable consequence thereof, see equations
Therefore, we merely have to show that the claim (A.5) for \((b)j_z = 0\) is correct.

However, the desired proof is very simple: First, specify the original angular system (IV.6a)–(IV.6b) down to \((b)j_z = 0\) in order to find

\[
\frac{d g_R(\vartheta)}{d\vartheta} - \cot \vartheta \cdot g_R(\vartheta) = \mp j_O \sin^2 \vartheta \cdot g_S(\vartheta) \tag{A.7a}
\]

\[
\frac{d g_S(\vartheta)}{d\vartheta} + \cot \vartheta \cdot g_S(\vartheta) = \pm j_O \frac{g_R(\vartheta)}{\sin^2 \vartheta}. \tag{A.7b}
\]

This system is to be understood as actually representing two different coupled systems according to whether one takes the upper (u) or lower (l) signs. Let the solution of the upper case be denoted by \((u)g_R(\vartheta), (u)g_S(\vartheta)\) and the solutions of the lower case by \((l)g_R(\vartheta), (l)g_S(\vartheta)\). Then it is found that the only difference between both sets of solutions refers to a change of the signs, i.e.

\[
(l)g_R(\vartheta) = -(u)g_R(\vartheta) \tag{A.8a}
\]

\[
(l)g_S(\vartheta) = (u)g_S(\vartheta). \tag{A.8b}
\]

However, as the very definition of angular density \({}^b k_0(\vartheta)\) (IV.20) says, such a difference in sign does not imply a difference in the angular density itself; and this then entails also that the angular potential \({}^b A_{III}(\vartheta)\) is invariant under that change of sign (A.8a)–(A.8b). Such a change may be brought about also in the first-order system (A.7a)–(A.7b) by simply putting \(j_O \Rightarrow -j_O\). Finally, the Schrödinger-like equation (IV.17) remains unchanged by the latter replacement \((j_O \Rightarrow -j_O)\); and thus the solution \(\hat{\Omega}(r)\) cannot react to it either, nor the solution \((b)A_0(r, \vartheta)\) of the Poisson equation (IV.18). The result is that the physically relevant objects are insensitive to the change of sign (A.8a)–(A.8b) and thus all the quantum states due to \((b)j_z = 0\) are physically unique (\(\Rightarrow\) no dimorphism).

Finally, it remains to explain why all these states (with \((b)j_z = 0\)) share the same angular density \((b)k_0(\vartheta)\) (A.5), independently of the quantum number \(j_O\). To this end, reconsider the definition of angular density \((b)k_0(\vartheta)\) (IV.20) and find by use of the present
first-order system (A.7a)–(A.7b) the differential equation
\[
\frac{d}{d\vartheta} \{b\}_{0}(\vartheta) + \cot \vartheta \cdot \{b\}_{0}(\vartheta) = 0 .
\] (A.9)

Of course, the solution hereof (being normalized to unity according to the prescription (IV.24a)) is just identical to our claim (A.5).

No Dimorphism for \((b)_{j} z = \pm j_{O}\)

As suggested by the tabulated cases for \(j_{O} = 2, 3, 4\) p. 70 there is also sufficient motivation to suppose that no dimorphism can occur quite generally for \((b)_{j} z = \pm j_{O}\). This supposition can easily be validated by writing down the eigenvalue equations for angular momentum (IV.6a)–(IV.6b) in terms of the eigenvalues \((b)_{j} z\) and \(j_{O}\):
\[
\frac{d}{d\vartheta} g_{R}(\vartheta) - ((b)_{j} z + 1) \cot \vartheta \cdot g_{R}(\vartheta) = ((b)_{j} z \mp j_{O}) \sin^{2} \vartheta \cdot g_{S}(\vartheta) \] (A.10a)
\[
\frac{d}{d\vartheta} g_{S}(\vartheta) + ((b)_{j} z + 1) \cot \vartheta \cdot g_{S}(\vartheta) = ((b)_{j} z \pm j_{O}) \cdot \frac{g_{R}(\vartheta)}{\sin^{2} \vartheta} . \] (A.10b)

Now for \((b)_{j} z = j_{O}\) this reduces to either
\[
\frac{d}{d\vartheta} g_{R}(\vartheta) - (j_{O} + 1) \cot \vartheta \cdot g_{R}(\vartheta) = 0 \] (A.11a)
\[
\frac{d}{d\vartheta} g_{S}(\vartheta) + (j_{O} + 1) \cot \vartheta \cdot g_{S}(\vartheta) = 2j_{O} \cdot \frac{g_{R}(\vartheta)}{\sin^{2} \vartheta} \] (A.11b)
or to
\[
\frac{d}{d\vartheta} g_{R}(\vartheta) - (j_{O} + 1) \cot \vartheta \cdot g_{R}(\vartheta) = 2j_{O} \cdot \sin^{2} \vartheta \cdot g_{S}(\vartheta) \] (A.12a)
\[
\frac{d}{d\vartheta} g_{S}(\vartheta) + (j_{O} + 1) \cot \vartheta \cdot g_{S}(\vartheta) = 0 , \] (A.12b)
according to whether we take the upper or the lower signs in (A.10a)–(A.10b). The dimorphism under consideration can occur if both systems (A.11a)–(A.11b) and (A.12a)–(A.12b) do admit normalizable solutions. This, however, can not be true.

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Obviously, the critical equations are here (A.11a) and (A.11b) because these equations cannot admit simultaneously the required non-singular and normalizable solution. Indeed, the general solution of (A.11a) is found as

\[
g_R(\vartheta) = g_* (\sin \vartheta)^{j_\sigma+1} \text{ .} \tag{A.13}
\]

\((g_* = \text{const.})\)

It is true, this is an absolutely reasonable solution, but if this is inserted on the right-hand side of the second equation (A.11b) we get

\[
\frac{d}{d\vartheta} \left[ (\sin \vartheta)^{j_\sigma+1} \cdot g_S(\vartheta) \right] = 2j_\sigma (\sin \vartheta)^{j_\sigma-1} \cdot g_R(\vartheta)
\]

\[
= 2g_* j_\sigma (\sin \vartheta)^{2j_\sigma} , \tag{A.14}
\]

with the obvious solution being given by

\[
g_S(\vartheta) = 2j_\sigma g_* \frac{1}{(\sin \vartheta)^{j_\sigma+1}} \int_0^\vartheta (\sin \vartheta')^{2j_\sigma} . \tag{A.15}
\]

But this solution for the second angular function \(g_S(\vartheta)\) is obviously singular for \(\vartheta \Rightarrow \pi\) which thus spoils the required normalization condition for the angular density \((^{(b)}k_0(\vartheta))\) [IV.24a]! Consequently, we have to reject the first system (A.11a)–(A.11b); and a regular solution can be expected exclusively from the second set of equations (A.12a)–(A.12b).

However, the rejected system (A.11a)–(A.11b) admits also an exceptional case, i.e. \(j_\sigma = (^{(b)}j_z = 0\). For this case, the second equation (A.11b) becomes homogeneous

\[
\frac{d}{d\vartheta} g_S(\vartheta) + \cot \vartheta \cdot g_S(\vartheta) = 0 , \tag{A.16}
\]

and thus admits the trivial solution \(g_S(\vartheta) \equiv 0\). Furthermore, the solution \(g_R(\vartheta)\) (A.13) becomes specified to

\[
g_R(\vartheta) = g_* \cdot \sin \vartheta , \tag{A.17}
\]

and we end up with the angular density

\[
(^{(b)}k_0(\vartheta) = \frac{1}{4\pi} \cdot \frac{g_R^2(\vartheta)}{\sin^3 \vartheta} = \frac{g_*^2}{4\pi} \cdot \frac{1}{\sin \vartheta} , \tag{A.18}
\]

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or in normalized form, resp.

\[ \{^b\}k_0(\vartheta) = \frac{1}{2\pi^2} \cdot \frac{1}{\sin \vartheta} . \]  \hspace{1cm} (A.19)

This is just the one single solution listed at the end of the subsequent table for \( j_O = 4 \), whose general emergence for all values of \( j_O \) has been proven by the above arguments below equation (A.5).

Thus, there remains to be considered the second system (A.12a)–(A.12b). Here, the second equation (A.12b) admits only the trivial solution \( g_S(\vartheta) \equiv 0 \), and this leaves (A.12a) for \( g_R(\vartheta) \) also as a homogeneous equation, namely just the precedent case (A.11a) whose solution has already been specified by equation (A.13). Combining now both solutions \( g_S(\vartheta) \equiv 0 \) and (A.13) yields the angular density \( \{^b\}k_0(\vartheta) \) as

\[ \{^b\}k_0(\vartheta) = \frac{1}{4\pi} \frac{g^2_R(\vartheta)}{\sin^3 \vartheta} = \frac{1}{4\pi} g_*^2 (\sin \vartheta)^{2j_O - 1} , \]  \hspace{1cm} (A.20)

i.e. in normalized form

\[ \{^b\}k_0(\vartheta) = \frac{1}{2\pi^2} \frac{(2j_O)!!}{(2j_O - 1)!!} (\sin \vartheta)^{2j_O - 1} . \]  \hspace{1cm} (A.21)

Special cases (\( j_O = 2, 3 \)) of this result are found in the table on p. 71 for \( j_O = 4 \) see the table below.
| $j_0$ | $(b)j_z$ | $(b)k_0(\vartheta)$ | $(b)A_{III}(\vartheta)$ | $(b)\epsilon_{III}$ | $(b)f_{III}$ | $(b)m_{III}$ |
|-------|----------|----------------------|-------------------------|-------------------|--------------|-------------|
| 4     | ±4       | $\frac{64}{35\pi^7} \sin^7 \vartheta$ | $-\frac{21}{40} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{49}{10000}$ | $147$ | $49$ | $400$ |
| 4     | ±3       | $\frac{8}{5\pi^7} \sin^5 \vartheta$ | $-\frac{15}{32} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{5}{128}$ | $15$ | $25$ | $256$ |
| 4     | ±2       | $\frac{6}{3\pi^7} \sin^3 \vartheta \left( 1 - \frac{24}{25} \sin^2 \vartheta \right)$ | $\frac{3}{20} \left[ \cos^2 \vartheta - 1 \right]$ | $\frac{1}{5000}$ | $3$ | $1$ | $100$ |
| 4     | ±1       | $\frac{6}{7\pi^7} \sin \vartheta \left( 1 - \frac{20}{21} \sin^2 \theta + \frac{4}{3} \sin^4 \vartheta \right)$ | $\frac{9}{32} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{9}{12800}$ | $27$ | $9$ | $256$ |
| 4     | 0        | $\frac{1}{2\pi^7} \cdot \frac{1}{\sin \vartheta}$ | $\frac{3}{8} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$ | $\frac{1}{800}$ | $3$ | $1$ | $16$ |

*Angular Density $(b)k_0(\vartheta)$ (IV.20)*

*and Angular Potential $(b)A_{III}(\nu)$ (V.25a) for $j_0 = 4$*
Appendix B

**Groundstate** \( (n_\mathcal{O} = 1 \Rightarrow j_\mathcal{O} = 0; \ (b)j_z = 0) \)

The absence of the ortho-dimorphism for both \( (b)j_z = 0 \) and \( (b)j_z = \pm j_\mathcal{O} \) implies now that this effect of dimorphism can not occur especially for \( j_\mathcal{O} = 0 \) and \( j_\mathcal{O} = 1 \). For the first case \( (j_\mathcal{O} = 0) \), the quantum number \( (b)j_z \) can assume exclusively the value \( (b)j_z = 0 \) (because of \( -j_\mathcal{O} \leq (b)j_z \leq j_\mathcal{O} \)), and for \( (b)j_z = 0 \) we already have proven that the dimorphism cannot occur (see App.A). Nevertheless, this case \( j_\mathcal{O} = 0 \) owns some peculiarities so that it may appear worthwhile to reconsider it in some detail.

First, observe here that the angular eigenvalue system \((\text{IV.6a})–(\text{IV.6b})\) becomes decoupled because both constants \( \dot{j}_\mathcal{O} \) and \( \ddot{j}_\mathcal{O} \) \((\text{IV.15a})–(\text{IV.15b})\) must vanish together with \( (b)j_z \) and \( j_\mathcal{O} \). Thus, we are left with the following decoupled system

\[
\frac{dg_R(\vartheta)}{d\vartheta} - \cot \vartheta \cdot g_R(\vartheta) = 0 \quad \text{(B.1a)}
\]

\[
\frac{dg_S(\vartheta)}{d\vartheta} + \cot \vartheta \cdot g_S(\vartheta) = 0 \quad \text{(B.1b)}
\]

The solution of the first equation \((\text{B.1a})\) is

\[
g_R(\vartheta) = g_{R,*} \cdot \sin \vartheta, \quad \text{(B.2)}
\]

and similarly, the solution of the second equation \((\text{B.1b})\) is obtained as

\[
g_S(\vartheta) = g_{S,*} \cdot \frac{1}{\sin \vartheta} \quad \text{(B.3)}
\]

where \( g_{R,*} \) and \( g_{S,*} \) are the integration constants. But actually, the coupling of these eigenvalue equations \((\text{IV.6a})–(\text{IV.6b})\) does enforce the presence of only one integration constant. However, for the present exceptional situation (i.e. \( j_\mathcal{O} = (b)j_z = 0 \)) we have to admit the existence of two independent integration constants \( g_{R,*} \) and \( g_{S,*} \) which become restricted by the normalization condition \((\text{IV.24a})\) to the constraint

\[
g_{R,*}^2 + g_{S,*}^2 = \frac{2}{\pi} \quad \text{(B.4)}
\]

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This restriction admits the parametrization by only one constant $\gamma_*$, say

$$g_R = \sqrt{\frac{2}{\pi}} \cdot \cos \gamma_*$$  \hspace{1cm} (B.5a)

$$g_S = \sqrt{\frac{2}{\pi}} \cdot \sin \gamma_*$$  \hspace{1cm} (B.5b)

so that the solution (B.2)-(B.3) becomes

$$g_R(\vartheta) = \sqrt{\frac{2}{\pi}} \cdot \cos \gamma_* \cdot \sin \vartheta$$  \hspace{1cm} (B.6a)

$$g_S(\vartheta) = \sqrt{\frac{2}{\pi}} \cdot \frac{\sin \gamma_*}{\sin \vartheta}$$  \hspace{1cm} (B.6b)

with the angular density $\{b\}k_0(\vartheta)$ being found in agreement with the former claim (A.19).

As a special case, one recovers here the former solution (A.17) for $\gamma_* = 0$.

Concerning now the energy of the groundstate of ortho-positronium ($n_O = 1, j_O = 0, (b)j_z = 0$), one first observes that the angular density $\{b\}k_0(\vartheta)$ (A.19) is the same as for the groundstate of para-positronium [2]; and therefore both the first angular potential correction $\{b\}A^{III}(\vartheta)$ (VI.25a) and the constants $\{b\}e^{III}$, $\{b\}f^{III}$ (VI.16a), $\{b\}m^{III}$ (VI.22a) must then also be the same, i.e.

$$\{b\}A^{III}(\vartheta) = \frac{3}{8} \left[ \cos^2 \vartheta - \frac{1}{3} \right]$$  \hspace{1cm} (B.7a)

$$\{b,p\}e^{III} = \frac{1}{80}$$  \hspace{1cm} (B.7b)

$$\{b,p\}f^{III} = \frac{3}{40}$$  \hspace{1cm} (B.7c)

$$\{b,p\}m^{III} = \frac{1}{16}.$$  \hspace{1cm} (B.7d)

Furthermore, these numerical results ensure again the validity of the quadrupole equation (VII.4) which then leads us to the gauge field energy $E_R^{(e)}$ (VII.17). This is to be added to the kinetic energy $E_{kin}$ (VII.9a)-(VII.9b) for the groundstate ($j_O = 0$)

$$E_{kin} \Rightarrow \varepsilon_{kin}^2 \left( \frac{e^2}{2a_B} \right)^2 \cdot \frac{1}{4(2\nu + 1)} \cdot \frac{1}{4(2\nu + 1)}$$  \hspace{1cm} (B.8)
in order to obtain for the reduced form of the groundstate energy function, cf. (VII.22)

$$E_{O}^{(0,0)}(\nu) = -\frac{e^2}{a_B} (2\nu + 1) \left[ \varepsilon_{\text{pot}}(\nu) + \frac{1}{16} \mu_{\text{III}}(\nu) \right]^2$$

(B.9)

According to the principle of minimal energy, the (approximate) groundstate energy $E_{O}^{(0,0)}$ of ortho-positronium is now given by the minimal value of the energy function $E_{O}^{(0,0)}(\nu)$ (B.9) and is found as

$$E_{O}^{(0,0)} \simeq -7,5378 \; [\text{eV}] .$$

(B.10)

This groundstate energy is unique because the corresponding angular density $^b k_0(\vartheta)$ turned out to be unique despite of the continuous set of solutions (B.6a)-(B.6b). This confirms the former assertion that the ortho-dimorphism cannot occur for angular states due to $^b j_z = 0$, i.e. especially for $j_O = 0$.

Furthermore, it happens that the ortho-groundstate energy $E_{O}^{(0,0)}$ (B.10) is (in the quadrupole approximation) the same as the groundstate energy $E_{P}^{(0,0)}$ of para-positronium [2]. The reason for this is the simple fact that all ingredients of the groundstate energy function $E^{(IV)}(\beta, \nu)$ are the same for ortho- and para-positronium, i.e. especially the angular-dependent functions $^b k_0(\vartheta) \equiv [^p]k_0(\vartheta), [^b]A_{\text{III}}(\vartheta) \equiv [^p]A_{\text{III}}(\vartheta), [^b]A_0(r) \equiv [^p]A_0(r)$. The equality of these angular functions ensures then also the equality of the coefficients

$$^p c_{\text{III}} = [^b]c_{\text{III}} = \frac{1}{80}$$

(B.11a)

$$^p f_{\text{III}} = [^b]f_{\text{III}} = \frac{3}{40}$$

(B.11b)

$$^p m_{\text{III}} = [^b]m_{\text{III}} = \frac{1}{16} .$$

(B.11c)

And finally, the equality of the angular functions plus that of the associated coefficients admits then also the equality of the corresponding groundstate energies, i.e.

$$E_{O}^{(0,0)} \equiv E_{P}^{(0,0)} = -7,5378 \; [\text{eV}] ,$$

(B.12)

cf. the process of partial extremalization (VII.18)–(VII.22). Indeed by means of the above mentioned equalities, both spectral functions $S^{(0,0)}(\nu)$ become identified for the
groundstate \( n_O = n_P \equiv \ell_P + 1 = 1, \) \( \langle b \rangle_jz = \langle p \rangle_jz \equiv \ell_z = 0 \) 

\[
S_O^{(0,0)}(\nu) = S_P^{(0,0)}(\nu) = 4(2\nu + 1) \left[ \varepsilon_{\text{pot}}(\nu) + \frac{1}{16} \cdot \mu_{\text{iii}}^{(e)}(\nu) \right]^2 ,
\]

(B.13)

see the precedent paper [2] for the corresponding treatment of para-positronium.
Appendix C

No Dimorphism for the first Excited State \((n_\sigma = 2)\)

Since the ortho-dimorphism can occur only if the quantum number \((b)j_z\) is in the range \(0 < |(b)j_z| < j_\sigma\), that phenomenon of dimorphism can surely not emerge for the first excited state \(n_\sigma = 2\) \((\Rightarrow j_\sigma = 0, 1; (b)j_z = 0, \pm 1)\). However, the mathematical mechanism for the exclusion is quite different. Whereas for \((b)j_z = 0\) both configurations \(\{1, -1\}\) and \(\{-1, 1\}\) of \(\{\ell_\sigma, \bar{\ell}_\sigma\}\) are allowed but yield one and the same physical state, in the case \((b)j_z = 1\) one has to reject the configuration \(\{2, 0\}\) and to resort to \(\{0, 2\}\); and analogously for \((b)j_z = -1\) one can conversely admit only the configuration \(\{2, 0\}\) and has to reject \(\{0, 2\}\).

\(j_\sigma = 1, (b)j_z = 0\)

For \(\{j_\sigma, (b)j_z\} = \{1, 0\}\) one first deduces from equation (IV.36) that \(G_S(x)\) must be constant

\[G_S(x) = \sigma_0 = \text{const.} \quad (C.1)\]

Indeed, the second-order equation (IV.29b) is satisfied for this conclusion (C.1). The corresponding angular function \(g_S(\vartheta)\) (IV.28c) must then also be a constant

\[g_S(\vartheta) = \sigma_0, \quad (C.2)\]

and for the associated angular function \(g_R(\vartheta)\) one deduces from the second first-order equation (IV.6b)

\[g_R(\vartheta) = \frac{\sigma_0}{\ell_\sigma} \sin \vartheta \cos \vartheta. \quad (C.3)\]

But both possibilities \(\ell_\sigma = \pm 1\) (IV.15a) yield here merely a change of sign which may be compensated for by the integration constant \(\sigma_0\). Thus, one obtains for the (normalized) angular density \((b)k_0(\vartheta)\) (IV.20) just the unambiguous result (A.19), as claimed above.
\[ \dot{J}_\mathcal{O} = 1, \ (b)j_z = 1 \]

The question of unambiguity is somewhat different for \((b)j_z = \pm 1\) (and still \(J_\mathcal{O} = 1\)). First, one concludes again from equation (IV.35) that the angular eigenfunction \(g_R(\vartheta)\) must look as follows

\[ g_R(\vartheta) = \rho_2 \cdot \sin^2 \vartheta . \]  

(C.4)

If this solution is substituted in the first eigenvalue equation (IV.6a), one finds

\[ \ddot{\ell}_\mathcal{O} \cdot g_S(\vartheta) \equiv 0 \]  

(C.5)

so that either \(\ddot{\ell}_\mathcal{O}\) or \(g_S(\vartheta)\) must vanish. Furthermore, the solution (C.4) for \(g_R(\vartheta)\) recasts the second eigenvalue equation (IV.6b) to the following form

\[ \frac{dg_S(\vartheta)}{d\vartheta} + 2 \cot \vartheta \cdot g_S(\vartheta) = \dot{\ell}_\mathcal{O} \cdot \rho_2 \]  

(C.6)

whose solution is

\[ g_S(\vartheta) = \rho_2 \left\{ \frac{\vartheta}{\sin^2 \vartheta} - \frac{\sin(2\vartheta)}{2 \sin^2 \vartheta} \right\} . \]  

(C.7)

However, this solution must be rejected because it is singular at \(\vartheta = \pi\). As a consequence, we have to demand \(\dot{\ell}_\mathcal{O} = 0\), so that the equation (C.6) for \(g_S(\vartheta)\) admits the trivial solution in place of the former \(g_S(\vartheta)\) (C.7):

\[ g_S(\vartheta) \equiv 0 . \]  

(C.8)

This result says that the configuration \(\dot{\ell}_\mathcal{O} = 2, \ddot{\ell}_\mathcal{O} = 0\) must be rejected which leaves us with \(\dot{\ell}_\mathcal{O} = 0, \ddot{\ell}_\mathcal{O} = 2\). Thus, both angular eigenfunctions do generate the unambiguous (normalized) density \((b)k_0(\vartheta)\) in the form

\[ \{b\}k_0(\vartheta) = \frac{\sin \vartheta}{\pi^2} \]  

(C.9)

which validates again the above mentioned claim of unambiguity.
\( j_O = 1, \quad (b)j_z = -1 \)

The remaining case \((b)j_z = -1\) (and \(j_O = 1\)) can be settled now by a very brief argument; namely by simply evoking the symmetry replacements (IV.47a)-(IV.47b). This transcribes the present solution for \((b)j_z = 1\) to the corresponding *unambiguous* solution for \((b)j_z = -1:\)

\[
\begin{align*}
\dot{\ell}_O &= 2 \quad \text{(C.10a)} \\
\ddot{\ell}_O &= 0 \quad \text{(C.10b)} \\
g_R(\vartheta) &\equiv 0 \quad \text{(C.10c)} \\
g_S(\vartheta) &= \sqrt{\frac{4}{\pi}} = \text{const.} \quad \text{(C.10d)}
\end{align*}
\]

Indeed it is easy to see that this is a solution of both eigenvalue equations (IV.6a)-(IV.6b) with the angular density \((b)k_0(\vartheta)\) (IV.20) coinciding just with the former result (C.9) for \((b)j_z = 1\). Thus, both cases \((b)j_z = 0\) and \((b)j_z = \pm 1\) for \(j_O = 1\) are actually not subjected to the ortho-dimorphism!

Concerning now the energy \(E^{(1,\pm 1)}_{j_O}\) of the excited states due to \(n_O = 2, \quad j_O = 1, \quad (b)j_z = \pm 1\), one can apply again the method of partial extremalization which is based upon the spectral function \(S^{(j)}_{j_O}(\nu)\) (VII.19). For the present case \((j_O = 1, \quad (b)j_z = \pm 1, \quad n_O = 2\) the spectral function adopts the following form

\[
S^{(1,\pm 1)}_{j_O}(\nu) = \frac{\left[\varepsilon_{\text{pot}}(\nu) + \frac{1}{4\pi} \mu_{\text{III}}^{(e)}(\nu)\right]^2}{\frac{1}{2\nu+1} \left(\frac{1}{4} + \frac{1}{2\nu}\right)}.
\]  

(C.11)

This is the same spectral function as was found for the corresponding first excited state of para-positronium \((\ell_z = \ell_P = 1)\), see ref. [2], equation (IV.161). Therefore the present *unambiguous* (!) ortho-state with quantum numbers \(\{n_O = 2, \quad j_O = 1, \quad (b)j_z = \pm 1\}\) has the same RST binding energy as the para-state \(\{n_P = 2, \quad j_P \equiv \ell_P = 1, \quad (p)j_z \equiv \ell_z = \pm 1\}\), namely [2]

\[
E^{(1,\pm 1)}_{j_O} = -1,57527 \ldots [\text{eV}].
\]  

(C.12)
Appendix D

**Dimorphism vs. Elimination of $j_z$-Degeneracy**

It is important to observe that the occurrence of the ortho-dimorphism and the effect of degeneracy elimination are two separate things which are independent of each other and have different origins. Nevertheless, they may occur in a combined way. For such a combined situation, there naturally arises the question of magnitude of those energy differences being induced by both kinds of level splitting (i.e. degeneracy elimination vs. dimorphism).

In order to elucidate this question a little bit more, it may be instructive to consider a somewhat larger value of the quantum number $j_O$ ($j_O = 4$, say) where both effects can occur simultaneously. Here, the quantum number $(^b)j_z$ can adopt nine values (i.e. $-4 \leq (^b)j_z \leq 4$) which, at first glance, would have to be linked to five different angular densities $(^b)k_0(\theta)$, namely any one density being associated with any one value of $|(^b)j_z|$ ($= 0, 1, 2, 3, 4$); and therefore one expects the occurrence of five different energy levels due to $j_O = 4$ (yielding the electrostatic fine structure). But the effect of dimorphism consists now in the additional splitting of three of these five energy levels (i.e. $|(^b)j_z| = 1, 2, 3$) so that two of them (i.e. those due to $|(^b)j_z| = 0, 4$) remain unsplit! Thus, the splitting effect says that there should ultimately be left over *eight* different energy levels for the quantum number $j_O = 4$ (i.e. *one* level for any $|(^b)j_z| = 0, 4$ and *two* levels for any $|(^b)j_z| = 1, 2, 3$). The subsequent table presents a collection of the actual results.
\[ j_0 = 4 \]

| \( b j_x \) | \( g_n(\vartheta) \) | \( g_s(\vartheta) \) | \( (b)k_0(\vartheta) \) |
|-----------------|------------------|------------------|------------------|
| 4               | \[ \frac{16}{\sqrt{35\pi}} \cdot \sin^5 \vartheta \] | 0                | \[ \frac{64}{35\pi^2} \cdot \sin^7 \vartheta \] |
| 3               | \[ \sqrt{\frac{32}{35\pi}} \cdot \sin^4 \vartheta \cos \vartheta \] | \[ \sqrt{\frac{32}{35\pi}} \cdot \sin^3 \vartheta \] | \[ \frac{8}{5\pi^2} \cdot \sin^5 \vartheta \] |
|                 | \[ -7 \sqrt{\frac{32}{35\pi}} \cdot \sin^4 \vartheta \cos \vartheta \] | \[ \sqrt{\frac{32}{35\pi}} \cdot \sin^3 \vartheta \] | \[ \frac{56}{5\pi^2} \cdot \sin^5 \vartheta (1 - \frac{48}{49} \sin^2 \vartheta) \] |
| 2               | \[ \sqrt{\frac{80}{3\pi}} \cdot \sin^3 \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ \frac{6}{5} \sqrt{\frac{80}{3\pi}} \cdot \sin^2 \vartheta \cos \vartheta \] | \[ \frac{4}{\pi^2} \cdot \sin^3 \vartheta \left( \frac{5}{3} - \frac{8}{5} \sin^2 \vartheta \right) \] |
|                 | \[ \sqrt{\frac{80}{3\pi}} \cdot \sin^3 \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ -\frac{8}{\sqrt{5\pi}} \cdot \sin^2 \vartheta \cos \vartheta \] | \[ \frac{20}{\pi^2} \sin^3 \vartheta \left(1 - \frac{56}{25} \sin^2 \vartheta + \frac{32}{25} \sin^4 \vartheta \right) \] |
| 1               | \[ 6 \sqrt{\frac{2}{3\pi}} \cdot \sin^2 \vartheta \cos \vartheta (1 - 2 \sin^2 \vartheta) \] | \[ 10 \sqrt{\frac{2}{3\pi}} \sin \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ \frac{6}{\pi^2} \cdot \sin \vartheta \left(1 - \frac{4}{5} \sin^2 \vartheta + \frac{3}{5} \sin^4 \vartheta \right) \] |
|                 | \[ -2 \sqrt{\frac{10}{\pi}} \cdot \sin^2 \vartheta \cos \vartheta (1 - 2 \sin^2 \vartheta) \] | \[ 2 \sqrt{\frac{10}{\pi}} \sin \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ \frac{10}{\pi^2} \cdot \sin \vartheta \left(1 - 4 \sin^2 \vartheta + \frac{28}{5} \sin^4 \vartheta - \frac{64}{25} \sin^6 \vartheta \right) \] |
| 0               | \[ \sqrt{\frac{2}{\pi}} \cdot \sin \vartheta (1 - 8 \sin^2 \vartheta + 8 \sin^4 \vartheta) \] | \[ \sqrt{\frac{32}{\pi}} \cdot \cos \vartheta (1 - 2 \sin^2 \vartheta) \] | \[ \frac{1}{2\pi^2} \cdot \frac{1}{\sin \vartheta} \] |
| -1              | \[ -10 \sqrt{\frac{2}{3\pi}} \cdot \sin^3 \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ 6 \sqrt{\frac{2}{3\pi}} \cos \vartheta (1 - 2 \sin^2 \vartheta) \] | \[ \frac{6}{\pi^2} \cdot \sin \vartheta \left(1 - \frac{20}{9} \sin^2 \vartheta + \frac{4}{3} \sin^4 \vartheta \right) \] |
|                 | \[ -2 \sqrt{\frac{10}{\pi}} \cdot \sin^3 \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ -2 \sqrt{\frac{10}{\pi}} \cdot \cos \vartheta (1 - 2 \sin^2 \vartheta) \] | \[ \frac{10}{\pi^2} \cdot \sin \vartheta \left(1 - 4 \sin^2 \vartheta + \frac{28}{5} \sin^4 \vartheta - \frac{64}{25} \sin^6 \vartheta \right) \] |
| -2              | \[ -\frac{6}{\pi} \sqrt{\frac{80}{3\pi}} \cdot \sin^4 \vartheta \cos \vartheta \] | \[ \sqrt{\frac{80}{3\pi}} \sin \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ \frac{4}{\pi^2} \cdot \sin^3 \vartheta \left( \frac{5}{3} - 8 \sin^2 \vartheta \right) \] |
|                 | \[ \frac{2}{\pi} \sqrt{\frac{80}{\pi}} \cdot \sin^4 \vartheta \cos \vartheta \] | \[ \sqrt{\frac{80}{\pi}} \sin \vartheta (1 - \frac{6}{5} \sin^2 \vartheta) \] | \[ \frac{20}{\pi^2} \cdot \sin^3 \vartheta \left( 1 - \frac{56}{25} \sin^2 \vartheta + \frac{32}{25} \sin^4 \vartheta \right) \] |
| -3              | \[ \sqrt{\frac{32}{5\pi}} \cdot \sin^5 \vartheta \] | \[ -\sqrt{\frac{32}{5\pi}} \cdot \sin^2 \vartheta \cos \vartheta \] | \[ \frac{8}{5\pi^2} \cdot \sin^5 \vartheta \] |
|                 | \[ \sqrt{\frac{32}{35\pi}} \cdot \sin^5 \vartheta \] | \[ 7 \sqrt{\frac{32}{35\pi}} \cdot \sin^2 \vartheta \cos \vartheta \] | \[ \frac{56}{5\pi^2} \cdot \sin^5 \vartheta \left( 1 - \frac{48}{49} \sin^2 \vartheta \right) \] |
| -4              | 0                | \[ \frac{16}{\sqrt{35\pi}} \cdot \sin^3 \vartheta \] | \[ \frac{64}{35\pi^2} \cdot \sin^7 \vartheta \] |
This table demonstrates clearly the symmetries of the ortho-spectrum:

(i) the transition from $(b)j_z$ to $-(b)j_z$ leaves invariant the angular density $(b)k_0(\vartheta)$ \[IV.20\], but not the angular functions $g_R(\vartheta)$ and $g_S(\vartheta)$

(ii) concerning the angular functions $g_R(\vartheta)$ and $g_S(\vartheta)$ themselves, the transition from $(b)j_z$ to $-(b)j_z$ rearranges them according to the recipe \[IV.47a\]-\[IV.47b\], apart eventually from an overall change of sign (i.e. $g_R(\vartheta) \Rightarrow -g_R(\vartheta)$; $g_S(\vartheta) \Rightarrow -g_S(\vartheta)$). Observe that the latter is admitted by the eigenvalue system \[IV.6a\]-\[IV.6b\]

(iii) observe also that the symmetry rearrangement \[IV.47a\]-\[IV.47b\] generates a second solution for $(b)j_z = 0$, namely

\[
g_R(\vartheta) = \sqrt{\frac{32}{\pi}} \cdot \sin^2 \vartheta \cos \vartheta \left(1 - 2 \sin^2 \vartheta\right) \tag{D.1a}
\]

\[
g_S(\vartheta) = -\sqrt{\frac{2}{\pi}} \cdot \frac{1}{\sin \vartheta} \left(1 - 8 \sin^2 \vartheta + 8 \sin^4 \vartheta\right) \tag{D.1b}
\]

but this leads us to the same angular density $(b)k_0(\vartheta)$ and therefore yields no further level splitting.

For a preliminary synopsis of those cooperative effects of degeneracy elimination plus dimorphism it is instructive to collect the results for the lowest energy levels (i.e. for principal quantum number $n \leq 5$) in a further table, see below. Here it is especially interesting to compare the RST results of the spherically symmetric approximation, the results of the para/ortho dichotomy, and those of the dimorphism to the conventional results $E_C^{(n)} \[I.18\]$. Concerning the effect of degeneracy, the RST spherically symmetric approximation $E_T^{[n]}$ \textit{(fourth column)} respects the conventional degree of degeneracy \[I.18\] but yields numerically only a moderate approximation to those conventional results $E_C^{(n)}$ \textit{(third column)}. 

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All RST predictions in the quadrupole approximation are based upon the method of partial extremalizing, i.e. maximalization of the spectral function \( S_{O,P}^{(j)}(\nu) \)

\[
S_{O,P}^{(j)}(\nu) = \left[ \varepsilon_{\text{pot}}(\nu) + (b,p)_{\text{III}} \cdot \mu_{\text{III}}^{(e)}(\nu) \right]^2 \cdot \frac{1}{2 \nu + 1} \left( \frac{1}{4} + \frac{\nu + 1}{2 \nu} \right).
\]

Whenever both quantum numbers of para- and ortho-positronium do agree (i.e. \( j_O = j_P; (b)j_z = (p)j_z \iff (b)m_{\text{III}} = (p)m_{\text{III}} \)), the corresponding energies are identical (\( E_O^{(j)} = E_P^{(j)} \)). The ortho-dimorphism arises because for the same quantum numbers \( j_O = j_P \) and \( (b)j_z = (p)j_z \) there can sometimes exist two values for \( (b)m_{\text{III}} \) (but not for \( (p)m_{\text{III}} \)), see the last two lines of the table, \( n = 4, 5 \).
The functions $\varepsilon_{\text{pot}}(\nu)$ (VI.33) and $\mu_{\text{III}}^{[e]}$ (VII.15), which enter the numerator of the spectral function (D.2), may also be written down in a closed analytic form:

$$\varepsilon_{\text{pot}}(\nu) = \left(1 - \frac{\Gamma(4\nu + 3)}{2^{4\nu+2}[\Gamma(2\nu + 2)]^2}\right) \cdot (2\nu + 1)^{-1}.$$  \hspace{1cm} (D.3a)

$$\mu_{\text{III}}^{[e]}(\nu) = \frac{2\nu^2 + 5\nu + 3}{\nu(4\nu^2 - 1)} - \frac{10\nu^2 + 15\nu + 6}{\nu(4\nu^2 - 1)} \cdot \frac{\Gamma(2\nu + 3/2)}{\sqrt{\pi} \cdot \Gamma(2\nu + 2)}. \hspace{1cm} (D.3b)$$

**Lowering of Groundstate Energy**

There is some curious effect with the groundstate ($n = 1$): whereas all the RST predictions $E_{\text{T}}^{[n]}$, $E_{\text{P}}^{[j]}$, $E_{\text{O}}^{[j]}$ for the groundstate energy ($n = n_{\text{P}} = n_{\text{O}} = 1$) are lower than their conventional counterpart $E_{\text{conv}}^{(1)}$ (third column), the excited states ($n > 1$) are equipped by RST with higher energy. For instance, for $j_{\text{O}} = j_{\text{P}} = 2$, $^{(b)}j_z = ^{(p)}j_z = \pm 1$ the conventional prediction is $E_{\text{conv}}^{(3)} = -0,75588\ldots$ [eV] whereas the RST prediction is $E_{\text{O}}^{(2,1)} = E_{\text{P}}^{(2,1)} = -0,68113$ [eV]. Thus one may expect that better trial configurations will further lower the RST energy of the excited states and thus shift it towards the conventional predictions. Of course, it is highly desirable to know the exact RST solutions in order to see more clearly how close the RST predictions do approach the conventional results. But those “better” trial configurations will then rather lower the groundstate prediction then raise it, quite in agreement with the true spirit of the principle of minimal energy!

**No Dimorphism for $j_{\text{O}} = 2$**

The next effect to be discussed concerns the unexpected missing of the dimorphism for the level being specified by the quantum numbers $n_{\text{O}} = 3$, $j_{\text{O}} = 2$, $^{(p)}j_z = ^{(b)}j_z = \pm 1$. Indeed for this value ($n = 3$) of the principal quantum number $n_{\text{O}}$, the ortho-number
\( j_\Box \) can adopt the values \( j_\Box = 0, 1, 2 \) where it is clear that for the possibilities \( j_\Box = 0 \) \((\Rightarrow (b)_z = 0)\), \( j_\Box = 1 \), and \( j_\Box = |(b)_z| = 2 \) the ortho-dimorphism cannot occur (see App.A+B). But for \( j_\Box = 2 \) and \(|(b)_z| = 1 \) the dimorphism could principally occur; nevertheless it “incidentally” does not occur in the present quadrupole approximation! What is the reason for this? It seems near at hand that this is the very logical structure of the quadrupole approximation itself.

In order to see this more clearly, reconsider the spectral function \( S^{(j)}_{\Omega,P}(\nu) \) (D.2) whose general form does apply to both ortho-\((\Box)\) and para-\((P)\) positronium. Since the RST energy predictions are obtained by extremalizing that spectral function \( S^{(j)}_{\Omega,P}(\nu) \) with respect to the continuous variable \( \nu \), the quantum numbers \( j_\Box \) and \((b)_z \) \((\Rightarrow (b,p)m_{III})\) being held fixed, the corresponding energy predictions can be different not only if at least one of the two quantum numbers \( j_\Box \) and \((b)_z \) is different, but also if for the same pair \( j_\Box, (b)_z \) the parameter \((b)m_{III} \) (VI.22a) can adopt more than one definite value. Recalling here the route back from \((b)m_{III} \) to the angular density \((b)k_0(\vartheta) \) via the relations (A.4), (A.2) and (V.29):

\[
(b)m_{III} = \left[ 1 - 3 \int d\Omega \cos^2 \vartheta \, (b)k_0(\vartheta) \right] \frac{2}{2}, \quad (D.4)
\]

the two possible values for \((b)m_{III} \) are seen to become induced by the two possible angular densities \((b)k_0(\vartheta) \) due to the same pair \( j_\Box, (b)_z \). But the latter two possibilities for \((b)k_0(\vartheta) \) are of course induced by the two possibilities for \( g_R(\vartheta) \) and \( g_S(\vartheta) \) (table on p. 70) according to the prescription (IV.20). Especially for the present case \( j_\Box = 2, (b)_z = \pm 1 \) we find the following two angular densities

\[
(b)k_0(\vartheta) = \begin{cases} 
\frac{1}{\pi^2} \cdot \sin \vartheta, & \text{(D.5a)} \\
\frac{3}{\pi^2} \cdot \sin \vartheta \left( 1 - \frac{8}{9} \sin^2 \vartheta \right), & \text{(D.5b)}
\end{cases}
\]

see the tables on p. 71 and 82. And the crucial point with these two densities (D.5a)-(D.5b) is now that their substitution in the prescription (D.4) for \((b,p)m_{III} \) yields “incidentally”
one and the same mass-equivalent parameter \((b)m_{III}\):

\[
(b)m_{III} = \frac{1}{64}. \tag{D.6}
\]

But clearly, when there is only one parameter \((b)m_{III}\) at hand for given values of \(j_O\) and \((b)j_z\) the associated spectral function \(S^{(j)}_O(\nu)\) is unique and provides us with one unique maximum, i.e. we end up with one single energy level. This is the reason why there is only one energy level associated with the quantum numbers \(j_O = 2, (b)j_z = \pm 1\).

**Equality of Ortho- and Para-Levels**

Even when the ortho-dimorphism can occur (e.g. for the combinations \(j_O = 3, 4\) and \((b)j_z = \pm 1\), see the table on p. 163), then the ortho- and para-levels are not necessarily different in the quadrupole approximation. For instance, take \(j_O = j_P = 3\) together with \((b)j_z = \pm 1\) and read from the table on p. 163 that one of the two ortho-parameters \((b)m_{III}\) of a dimorphic pair does agree with the corresponding para-parameter \((p)m_{III}\), e.g. for \(j_O = j_P = 3\):

\[
j_O = 3, (b)j_z = \pm 1 \implies \begin{cases} (b)m_{III} = \frac{1}{64} \\ (b)m_{III} = \frac{9}{256} \end{cases} \tag{D.7a}
\]

\[
j_P = 3, (p)j_z = \pm 1 \implies (p)m_{III} = \frac{9}{256}, \tag{D.7b}
\]

or similarly for \(j_O = j_P = 4\):

\[
j_O = 4, (b)j_z = \pm 1 \implies \begin{cases} (b)m_{III} = \frac{9}{256} \\ (b)m_{III} = \frac{289}{6400} \end{cases} \tag{D.8a}
\]

\[
j_P = 4, (p)j_z = \pm 1 \implies (p)m_{III} = \frac{289}{6400}. \tag{D.8b}
\]

Consequently, one of the two spectral ortho-functions \(S^{(j)}_O(\nu)\) must agree with the corresponding para-function \(S^{(j)}_P(\nu)\) and therefore the corresponding ortho- and para-levels
must also agree, i.e. for $j_O = j_P = 3, (n_O = n_P = 4)$:

$$E^{(3,1)}_{O} \Rightarrow \begin{cases} 
\bar{E}^{(3,1)}_O = -0.3808 \ldots [eV] \\
\check{E}^{(3,1)}_O = -0.3900 \ldots [eV] = E^{(3,1)}_P,
\end{cases}$$

(D.9)

and analogously for $j_O = j_P = 4, (n_O = n_P = 5)$:

$$E^{(4,1)}_{O} \Rightarrow \begin{cases} 
\bar{E}^{(4,1)}_O = -0.2501 \ldots [eV] \\
\check{E}^{(4,1)}_O = -0.2533 \ldots [eV] = E^{(4,1)}_P,
\end{cases}$$

(D.10)

see Fig.VII.A. Thus, the result of this ortho-splitting is that the lower one of the two ortho-levels does agree with the corresponding para-level whereas the solitary ortho-level being left over is higher and therefore farer away from to the conventional prediction $E^{(n)}_c$. However, the width of this ortho-splitting is clearly smaller than the deviation of the ortho- and para-levels from their conventional counterpart: in (D.9) the dimorphic splitting width is $(0.3900 - 0.3808) = 0.0092 [eV]$ whereas the average deviation of the ortho/para-levels from their corresponding conventional level is $(0.425 \ldots - 0.385 \ldots) [eV] \simeq 0.04 [eV]$, which is (roughly) four times larger than the dimorphic splitting width! See also Fig.VII.A. This result says that the dimorphic splitting effect is of the same order of magnitude as the degeneracy-elimination effect which for para-positronium has been estimated by $0.42003 [eV] - 0.37369 [eV] \simeq 0.046 \ldots [eV]$, see the table on p. 96 of ref. [2].

Thus, the difference of ortho- and para-energies comes about (in the quadrupole approximation) solely through the dimorphic effect!
Appendix E

Octupole Solution

For the calculation of the octupole energy \(\varepsilon_4^{(e)}\) and its mass equivalent \(\mu_4^{(e)}\) we obviously have first to determine the octupole potential \(A''_A(r)\) as the solution of the octupole equation (VIII.83b), whereas for the amplitude field \(\tilde{\Omega}(r)\) we will resort to our variational ansatz (VI.1a)–(VI.1b). For these purposes, it is very helpful to pass over to dimensionless variables; i.e. we put again

\[ y \doteq 2\beta r \quad \text{(E.1a)} \]
\[ \{b\}P_4(y) \doteq \frac{\Gamma(2\nu + 2)}{m'_2} \cdot \frac{\{b\}A''_A(r)}{2\beta a_s} \quad \text{(E.1b)} \]

so that the octupole equation (VIII.83b) adopts its dimensionless form as follows:

\[ \Delta_y \{b\}P_4(y) - 20 \frac{\{b\}P_4(y)}{y^2} = -y^{2\nu - 1} e^{-y} \quad . \quad \text{(E.2)} \]

Furthermore, the octupole energy \(\varepsilon_4^{(e)}\) reappears in terms of the dimensionless variables as

\[ \varepsilon_4^{(e)} = -\frac{e^2}{a_B} (2\beta a_B) \cdot \frac{64}{11025} \left( \frac{\{b\}m'_2}{\Gamma(2\nu + 2)} \right)^2 \int_0^\infty dy \, y^2 \left\{ \left( \frac{d\{b\}P_4(y)}{dy} \right)^2 \right. \]
\[ \left. + 20 \left( \frac{\{b\}P_4(y)}{y} \right)^2 \right\} . \quad \text{(E.3)} \]

Comparing now this result to the more concise one (VIII.95a) one deduces thereof the “anisotropic” potential function \(\varepsilon_4^{(e)}(\nu)\) as

\[ \varepsilon_4^{(e)}(\nu) = \frac{64}{11025} \frac{1}{\Gamma(2\nu + 2)^2} \int_0^\infty dy \, y^2 \left\{ \left( \frac{d\{b\}P_4(y)}{dy} \right)^2 + 20 \left( \frac{\{b\}P_4(y)}{y} \right)^2 \right\} . \quad \text{(E.4)} \]

By a similar calculation one finds the mass-equivalent function \(\mu_4^{(e)}(\nu)\) of equation (VIII.95b) as

\[ \mu_4^{(e)}(\nu) = \frac{64}{11025} \frac{1}{\Gamma(2\nu + 2)^2} \int_0^\infty dy \, y^{2\nu + 1} e^{-y} \cdot \{b\}P_4(y) . \quad \text{(E.5)} \]

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The claimed octupole identity in coefficient form \((\text{VIII.96})\) is now easily verified by partial integration in \((\text{E.4})-(\text{E.5})\) and use of the octupole equation \((\text{E.2})\).

**Boundary Conditions**

Before turning to the elaboration of the desired exact solution \({}^{(b)}P_4(y)\) of the octupole equation \((\text{VIII.83b})\), or \((\text{E.2})\), resp., it is necessary to regard the right boundary conditions. The right-hand side of this octupole equation is the “octupole source” and does vanish very fast at infinity \((r \to \infty, \text{ or } y \to \infty, \text{ resp.})\), because we adopt the exponential trial function \(\Omega(r) (\text{VI.1a)–(VI.1b)}\). In contrast to this exponential decay at infinity, our octupole solution may be assumed to decay much slower (via some power law \(y^{-w}, w > 0\)). But also for sufficiently large value of the trial parameter \(\nu\), the trial amplitude \(\tilde{\Omega}(r)\) may be assumed to be much smaller near the origin \((y = 0)\) than the octupole solution \({}^{(b)}P_4(y)\). Thus we have two regions of three-space where the solution \({}^{(b)}P_4(y)\) is to be expected to obey the homogeneous octupole equation:

\[
\Delta_y {}^{(b)}P_4(y) - 20 \frac{{}^{(b)}P_4(y)}{y^2} = 0 .
\]

(E.6)

From here it is easy to deduce the following limiting behaviour in these asymptotic regions

\[
\lim_{y \to \infty} {}^{(b)}P_4(y) = \frac{B^{(4)}_\infty}{y^5}, \quad (E.7a)
\]

\[
\lim_{y \to 0} {}^{(b)}P_4(y) = B^{(4)}_0 \cdot y^4, \quad (E.7b)
\]

where both \(B^{(4)}_\infty\) and \(B^{(4)}_0\) are constants.

The constant \(B^{(4)}_\infty\) characterizes the behaviour at infinity \((y \to \infty)\) and may be determined by a first integration of the octupole equation \((\text{E.2})\). This can be realized as follows: First, rewrite the octupole equation \((\text{E.2})\) in the following form

\[
\frac{1}{y^6} \frac{d}{dy} \left[ y^{10} \cdot \frac{d}{dy} \left( \frac{{}^{(b)}P_4(y)}{y^4} \right) \right] = -y^{2w-1} e^{-y} . \quad (E.8)
\]
Next, integrate here from $y$ to $\infty$ with observation of the boundary conditions (E.7a)-(E.7b) and find

$$y^{10} \frac{d}{dy} \left( \frac{\{b\} P_4(y)}{y^4} \right) = \int_y^\infty dy' y'^{2\nu+5} \cdot e^{-y'} - \int_0^\infty dy' y'^{2\nu+5} e^{-y'} . \quad (E.9)$$

Now take this equation at infinity ($y \to \infty$) and observe also the boundary condition (E.7a) which then yields

$$\lim_{y \to \infty} \left\{ y^{10} \frac{d}{dy} \left( \frac{\{b\} P_4(y)}{y^4} \right) \right\} = -9 B_4^{(4)} = -\Gamma(2\nu + 6) . \quad (E.10)$$

Thus, the asymptotic constant $B_4^{(4)}$ (E.7a) becomes hereby fixed to

$$B_4^{(4)} = \frac{1}{9} \cdot \Gamma(2\nu + 6) . \quad (E.11)$$

In order to try out whether perhaps the first integration step (E.9) contains also some information about the second boundary condition (E.7b) one further carries out the integral on the right-hand side of that equation, i.e.

$$\int_y^\infty dy' y'^{2\nu+5} e^{-y'} = \left( \int_0^\infty dy' y'^{2\nu+5} e^{-y'} \right) \cdot \left\{ 1 - e^{-y} \sum_{n=0}^{\infty} \frac{y^{2\nu+6+n}}{\Gamma(2\nu + 7 + n)} \right\} . \quad (E.12)$$

By use of this result, the first step of integration (E.9) adopts the following shape

$$\frac{d}{dy} \left( \frac{\{b\} P_4(y)}{y^4} \right) = -\Gamma(2\nu + 6) e^{-y} \sum_{n=0}^{\infty} \frac{y^{2\nu-4+n}}{\Gamma(2\nu + 7 + n)} . \quad (E.13)$$

The conclusion from this result is that we must demand $\nu > 2$ in order to have the boundary condition (E.7b) satisfied! But more detailed conclusions, concerning that boundary condition, cannot be drawn from the present result (E.13).
Exact Octupole Solution

In order to finally get the solution \( \{b\}P_4(y) \) of the first-order equation (E.13) it suggests itself to try a power series of the following form:

\[
\frac{\{b\}P_4(y)}{y^4} = \Gamma(2\nu + 6) e^{-y} \sum_{n=0}^{\infty} p_n \cdot y^{2\nu - 3 + n} .
\]  

(E.14)

This ansatz satisfies the equation (E.13) provided the coefficients \( p_n \) do obey the following recurrence formula

\[
p_{n+1} = \frac{p_n}{2\nu - 2 + n} - \frac{1}{(2\nu - 2 + n) \cdot \Gamma(2\nu + 8 + n)} ,
\]  

(E.15)

with the lowest-order coefficient being given by

\[
p_0 = -\frac{1}{(2\nu - 3) \cdot \Gamma(2\nu + 7)} .
\]

(E.16)

The solution of (E.15) is \((n = 1, 2, 3, 4, \ldots)\)

\[
p_n = \frac{1}{9} \left\{ \frac{1}{\Gamma(2\nu + 7 + n)} - \frac{\Gamma(2\nu - 3)}{\Gamma(2\nu + 6)} \cdot \frac{1}{\Gamma(2\nu - 2 + n)} \right\} .
\]

(E.17)

Thus, the (preliminary) solution appears ultimately as

\[
\{b\}P_4(y) = \Gamma(2\nu + 6) e^{-y} \sum_{n=0}^{\infty} p_n \cdot y^{2\nu + 1 + n}
\]  

(E.18)

with the coefficients \( p_n \) (E.16)–(E.17). However, observe now that this solution behaves in the vicinity of the origin \((y = 0)\) like

\[
\lim_{y \to 0} \{b\}P_4(y) = \Gamma(2\nu + 6) p_0 y^{2\nu + 1},
\]

(E.19)

in contrast to the second boundary condition (E.7D) (recall here the former demand \( \nu > 2 \)). But it is possible to add some fourth-order term \((\sim y^4)\) to the solution (E.18) because the latter is a solution of the homogeneous version (E.6) of the octupole equation (E.2)! 

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For the determination of the correct fourth-order term, to be added to the preliminary solution (E.18), we simplify for a moment the problem by resorting to integer values of the variational parameter $2\nu$, i.e. $2\nu = 5, 6, 7, 8, \ldots$. For this simplified situation, the preliminary solution (E.18) can be transcribed to the following form:

$$
\{b\}P_4(y) \Rightarrow \frac{1}{9} \left[ \Gamma(2\nu + 6) \left\{ 1 - e^{-y} \sum_{n=0}^{2\nu+5} \frac{y^n}{n!} \right\} - \Gamma(2\nu - 3) \cdot y^4 \left\{ 1 - e^{-y} \sum_{n=0}^{2\nu-4} \frac{y^n}{n!} \right\} \right].
$$

(E.20)

But in this form the deficiency of the preliminary solution (E.18) becomes now evident: for approaching infinity ($y \Rightarrow \infty$) we have for integer $2\nu$ in (E.20)

$$
\lim_{y \to \infty} \{b\}P_4(y) = -\frac{1}{9} \Gamma(2\nu - 3) \cdot y^4,
$$

(E.21)

which says that the preliminary solution (E.20) does not obey the required boundary condition (E.7a) at infinity! We can now easily remedy this deficiency of the preliminary solution by simply adding to it the negative of the false limit term (E.21) which itself is a solution of the homogeneous form (E.6) of the octupole equation (E.2). Thus, the correct octupole solution for integer $2\nu$ can be read off from equation (E.20) as

$$
\{b\}P_4(y) = \frac{1}{9} \left[ \frac{(2\nu + 5)!}{y^5} \left\{ 1 - e^{-y} \sum_{n=0}^{2\nu+5} \frac{y^n}{n!} \right\} + (2\nu - 4)! y^4 e^{-y} \sum_{n=0}^{2\nu-4} \frac{y^n}{n!} \right].
$$

(E.22)

Obviously, this “integer-valued” solution $\{b\}P_4(y)$ consists of two parts:

$$
\{b\}P_4(y) = \{b\}P_4^{(\infty)}(y) + \{b\}P_4^{(0)}(y),
$$

(E.23)

with

$$
\{b\}P_4^{(\infty)}(y) = \frac{1}{9} \left( \frac{2\nu + 5)!}{y^5} \left\{ 1 - e^{-y} \sum_{n=0}^{2\nu+5} \frac{y^n}{n!} \right\} \right) = \frac{(2\nu + 5)!}{9 y^5} e^{-y} \sum_{n=2\nu+6}^{\infty} \frac{y^n}{n!},
$$

(E.24a)

$$
\{b\}P_4^{(0)}(y) = \frac{1}{9} (2\nu - 4)! y^4 e^{-y} \sum_{n=0}^{2\nu-4} \frac{y^n}{n!} = \frac{(2\nu - 4)!}{9} y^4 \left( 1 - e^{-y} \sum_{n=2\nu-3}^{\infty} \frac{y^n}{n!} \right),
$$

(E.24b)

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such that the first part \( \{^b\mathcal{P}_4^{(\infty)}(y) \} \) (E.24a) is responsible for satisfying the boundary condition (E.7a) at infinity; and the second part \( \{^b\mathcal{P}_4^{(0)}(y) \} \) (E.24b) is responsible for satisfying the other boundary condition (E.7b) near the origin. Both parts \( \{^b\mathcal{P}_4^{(\infty)}(y) \} \) and \( \{^b\mathcal{P}_4^{(0)}(y) \} \) do cooperate in order that their sum \( \{^b\mathcal{P}_4(y) \} \) (E.23) can actually satisfy the octupole equation (E.2), namely via the following differential relations:

\[
\left( \Delta_y - \frac{20}{y^2} \right) \{^b\mathcal{P}_4^{(\infty)}(y) \} = \frac{1}{9} \left\{ (2\nu - 3) e^{-y} \cdot y^{2\nu - 1} - e^{-y} \cdot y^{2\nu} \right\} \tag{E.25a}
\]

\[
\left( \Delta_y - \frac{20}{y^2} \right) \{^b\mathcal{P}_4^{(0)}(y) \} = -\frac{1}{9} \left\{ (2\nu + 6) e^{-y} \cdot y^{2\nu - 1} - e^{-y} \cdot y^{2\nu} \right\} . \tag{E.25b}
\]

Finally, it remains to recast that “integer-valued” solution (E.22) to the general case of arbitrary (but real) values of the variational parameter \( \nu \). This may simply be done by adding the negative of the false limit term (E.21) to the more general (but preliminary) solution (E.18) which then ultimately yields the correct solution as

\[
\{^b\mathcal{P}_4(y) \} = \frac{1}{9} \Gamma(2\nu - 3) \cdot y^4 + \Gamma(2\nu + 6) e^{-y} \sum_{n=0}^{\infty} p_n(\nu) y^{2\nu+1+n} . \tag{E.26}
\]

**Mass-Equivalent Function \( \mu_4^{(e)}(\nu) \)**

Once the exact octupole solution \( \{^b\mathcal{P}_4(y) \} \) for arbitrary value of the variational parameter \( \nu \) is now at hand, cf. (E.26), one can go the last step and insert this solution in the former result (E.5) for the mass-equivalent function \( \mu_4^{(e)}(\nu) \). This then fixes the latter object definitely as follows:

\[
\mu_4^{(e)}(\nu) = \frac{64}{11025} \cdot \frac{\Gamma(2\nu + 6)}{\Gamma(2\nu + 2)^2} \left\{ \frac{\Gamma(2\nu - 3)}{9} + \frac{1}{2^{4\nu+3}} \sum_{n=0}^{\infty} \frac{p_n(\nu)}{2^n} \Gamma(4\nu + 3 + n) \right\} \tag{E.27}
\]

where the coefficients \( p_n(\nu) \) have already been specified by equations (E.16)-(E.17). For integer values of \( 2\nu \), one substitutes the solution \( \{^b\mathcal{P}_4(y) \} \) (E.22) into the right-hand side of equation (E.5) and thus finds the “integer-valued” version of (E.27) as

\[
\mu_4^{(e)}(\nu) = \{^{(\infty)}\mu_4^{(e)}(\nu) + \{^{(0)}\mu_4^{(e)}(\nu) \} (E.28)
\]

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with the first part \((\infty \mu_4^{(e)}(\nu))\), being due to \(^{(b)}\mathcal{P}_4^{(\infty)}(y)\) \((E.24a)\), being given by

\[
(\infty \mu_4^{(e)}(\nu)) = \frac{64}{99225} \frac{(2\nu + 5)!}{[(2\nu + 1)!]^2} \left( (2\nu - 4)! - \sum_{n=0}^{2\nu+5} \frac{(2\nu - 4 + n)!}{n! 2^{2\nu-3+n}} \right) \equiv \frac{64}{99225} \frac{(2\nu + 5)!}{[(2\nu + 1)!]^2} \sum_{n=2\nu+6}^{\infty} \frac{(2\nu - 4 + n)!}{n! 2^{2\nu-3+n}} .
\]

(E.29)

and, analogously, the second part \((0) \mu_4^{(e)}(\nu))\), being due to \(^{(b)}\mathcal{P}_4^{(0)}(y)\) \((E.24b)\), by

\[
(0) \mu_4^{(e)}(\nu)) = \frac{1}{99225} \frac{(2\nu - 4)!}{[(2\nu + 1)!]^2} \sum_{n=0}^{2\nu-4} \frac{(2\nu + 5 + n)!}{n! 2^{2\nu+n}}
\]

\[
\equiv \frac{64}{99225} \frac{(2\nu - 4)!}{[(2\nu + 1)!]^2} \left( (2\nu + 5)! - \sum_{n=2\nu-3}^{\infty} \frac{(2\nu + 5 + n)!}{n! 2^{2\nu+6+n}} \right) .
\]

(E.30)

The identities emerging in both equations \((E.29)\) and \((E.30)\) may easily be validated by tracing them back to the following identity, needed here for \(z = 2\nu - 4\) and \(z = 2\nu + 5\):

\[
2^{z+1} \cdot \Gamma(z + 1) = \sum_{n=0}^{\infty} \frac{\Gamma(z + n + 1)}{2^n \cdot n!} .
\]

(E.31)

**Relative Magnitude of Quadrupole and Octupole Corrections**

In order to better understand the numerical differences between the quadrupole and octupole corrections (see the table on p. 163) it is helpful to oppose both perturbation orders \(l = 1\) and \(l = 2\) to each other on the same notational footing. In this sense, we recast the quadrupole potential \(^{(b)}A_2''(r)\) to its dimensionless form \(^{(b)}\mathcal{P}_2(y)\) by putting:

\[
^{(b)}A_2''(r) \doteq \frac{\{b\} m_1}{\Gamma(2\nu + 2)} (2\beta \alpha_s) \cdot ^{(b)}\mathcal{P}_2(y) ,
\]

(E.32)

in close analogy to the octupole case \((E.1a)-(E.1b)\). By this rescaling, the quadrupole equation \((VII.4)\) or \((VIII.83a)\), resp., becomes simplified to

\[
\left( \Delta_y - \frac{6}{y^2} \right) ^{(b)}\mathcal{P}_2(y) = -y^{2\nu-1} \cdot e^{-y}
\]

(E.33)

which says that the dimensionless quadrupole potential \(^{(b)}\mathcal{P}_2(y)\) feels the same source (\(\sim\) right-hand side) as does its octupole counter-part \(^{(b)}\mathcal{P}_4(y)\), cf. \((E.2)\).
Indeed, there are many similarities between the former octupole and present quadrupole modes (presumably these similarities can be generalized to arbitrary \(l = 1, 2, 3, 4, \ldots\)). For instance, the former octupole boundary conditions (E.7a)–(E.7b) transcribe to the present quadrupole case as

\[
\lim_{y \to \infty} \{b\}P_2(y) = \frac{B_\infty^{(2)}}{y^2}, \tag{E.34a}
\]

\[
\lim_{y \to 0} \{b\}P_2(y) = B_0^{(2)} \cdot y^2. \tag{E.34b}
\]

The constant \(B_\infty^{(2)}\) may again be determined by a first integration step for the quadrupole equation (E.32), quite analogously to the octupole situation (E.9):

\[
y^6 \frac{d}{dy} \left[ \frac{\{b\}P_2(y)}{y^2} \right] = \int_y^\infty dy' y'^{2\nu+3} \cdot e^{-y'} - \int_0^y dy' y'^{2\nu+3} \cdot e^{-y'}.
\tag{E.35}
\]

From this result, one concludes for the quadrupole limit at infinity (E.34a)

\[
B_\infty^{(2)} = \frac{1}{5} \cdot \Gamma(2
\nu + 4), \tag{E.36}
\]

quite analogously to the octupole limit (E.11).

The exact solution of the quadrupole equation (E.32) can also be determined in form of a power-series expansion which is found to look as follows [2]

\[
\{b\}P_2(y) = \frac{1}{5} \cdot \Gamma(2\nu - 1) \cdot y^2 + \frac{1}{5} \cdot e^{-y} \sum_{n=0}^\infty b_n(\nu) \cdot y^{2\nu+1+n},
\tag{E.37}
\]

with the coefficients \(b_n(\nu)\) being given by

\[
b_n(\nu) = \frac{\Gamma(2\nu + 4)}{\Gamma(2\nu + 5 + n)} - \frac{\Gamma(2\nu - 1)}{\Gamma(2\nu + n)}.
\tag{E.38}
\]

Thus, the constant \(B_0^{(2)}\) (E.34b) is deduced hereof as

\[
B_0^{(2)} = \frac{1}{5} \cdot \Gamma(2\nu - 1), \tag{E.39}
\]

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which thus turns out as the quadrupole analogue of the octupole limit (E.7b). And finally, the “integer-valued” \((2\nu = 2, 3, 4, \ldots)\) version of the general result (E.36) reads

\[
\{^{(b)}P_2\}(y) = \frac{(2\nu + 3)!}{5} \cdot \frac{1 - e^{-y} \sum_{n=0}^{2\nu+3} \frac{y^n}{n!}}{y^3} + \frac{(2\nu - 2)!}{5} \cdot y^2 e^{-y} \sum_{n=0}^{2\nu-2} \frac{y^n}{n!}. \tag{E.40}
\]

This is obviously the quadrupole analogue of the former octupole result (E.22) and consists again of two parts

\[
\{^{(b)}P_2\}(y) = \{^{(b)}P_2^{(\infty)}\}(y) + \{^{(b)}P_2^{(0)}\}(y) \tag{E.41}
\]

with the first part \(\{^{(b)}P_2^{(\infty)}\}(y)\) being again responsible for the behaviour (E.34b) at infinity

\[
\{^{(b)}P_2^{(\infty)}\}(y) = \frac{(2\nu + 3)!}{5} \cdot \frac{1 - e^{-y} \sum_{n=0}^{2\nu+3} \frac{y^n}{n!}}{y^3}, \tag{E.42}
\]

and the second part \(\{^{(b)}P_2^{(0)}\}(y)\) near the origin \((y = 0)\):

\[
\{^{(b)}P_2^{(0)}\}(y) = \frac{(2\nu - 2)!}{5} y^2 e^{-y} \sum_{n=0}^{2\nu-2} \frac{y^n}{n!}. \tag{E.43}
\]

Clearly, the sum \(\{^{(b)}P_2\}(y)\) (E.40) must again obey the quadrupole equation (E.32) which, however, is ensured just by the separate differential relations for the long-range part \(\{^{(b)}P_2^{(\infty)}\}(y)\) (E.42)

\[
\left(\Delta_y - \frac{6}{y^2}\right) \{^{(b)}P_2^{(\infty)}\}(y) = \frac{2\nu - 1}{5} e^{-y} \cdot y^{2\nu-1} - \frac{1}{5} e^{-y} \cdot y^{2\nu} \tag{E.44}
\]

and the short-range part \(\{^{(b)}P_2^{(0)}\}(y)\) (E.42)

\[
\left(\Delta_y - \frac{6}{y^2}\right) \{^{(b)}P_2^{(0)}\}(y) = -\frac{2\nu + 4}{5} e^{-y} \cdot y^{2\nu-1} + \frac{1}{5} e^{-y} \cdot y^{2\nu}. \tag{E.45}
\]

cf. the octupole case (E.25a)–(E.25b).

The quadrupole energy \(\nu^E_2 = \nu^{(r)}_2 + \nu^{(q)}_2\) (VIII.90a)–(VIII.90b) and also its mass-equivalent \(\nu^M_2\) may now be re-expressed in terms of the dimensionless
quadrupole potential $\{^b\mathcal{P}_2(y)\}$ and thus read as follows

$$\eta_{E_2}^{(e)} = -\frac{e^2}{a_B} (2\beta a_B) \left(\{^b\mathcal{P}_1\}\right)^2 \cdot \varepsilon_2^{(e)}(\nu)$$  \hspace{1cm} (E.46a)

$$\eta_{M_2}^{(e)} e^2 = -\frac{e^2}{a_B} (2\beta a_B) \left(\{^b\mathcal{P}_1\}\right)^2 \cdot \mu_2^{(e)}(\nu),$$  \hspace{1cm} (E.46b)

with the electrostatic function $\varepsilon_2^{(e)}(\nu)$ being given by

$$\varepsilon_2^{(e)}(\nu) \equiv \frac{45}{4} \frac{1}{\Gamma(2\nu + 2)^2} \int_0^\infty dy \ y^2 \left\{ \left( \frac{d \{^b\mathcal{P}_2(y)\}}{dy} \right)^2 + 6 \left( \frac{\{^b\mathcal{P}_2(y)\}}{y} \right)^2 \right\}$$  \hspace{1cm} (E.47)

and the corresponding mass-equivalent function $\mu_2^{(e)}(\nu)$ by

$$\mu_2^{(e)}(\nu) = \frac{45}{4} \frac{1}{\Gamma(2\nu + 2)^2} \int_0^\infty dy \ y^{2\nu + 1} e^{-y} \cdot \{^b\mathcal{P}_2(y)\}.$$  \hspace{1cm} (E.48)

Just as in the octupole case \textit{[VIII.96]}, there is here also a corresponding quadrupole identity

$$\varepsilon_2^{(e)} \equiv \mu_2^{(e)}$$  \hspace{1cm} (E.49)

which may easily be verified by integrating by parts in (E.47) and using the quadrupole equation (E.33). Observe here that these separate identities (VIII.96) and (E.47) can occur only because the separative method admitted us to decouple completely the quadrupole and octupole modes!

Now that both modes are elaborated in great detail, one can proceed to the intended study of their numerical relationships.

The qualitative features of these multipole solutions $\{^b\mathcal{P}_2(y)\}$ and $\{^b\mathcal{P}_4(y)\}$ may perhaps be best seen from their sketch, cf. \textbf{Fig.E.I} below. For $y \gtrsim 20$ one actually observes the asymptotic behaviour (E.34a) and (E.7a) for $\{^b\mathcal{P}_{2/4}(y)\}$. In a similar way, the behavior (E.7b) and (E.34b) near the origin ($y = 0$) is also neatly displayed by \textbf{Fig.E.I}. Furthermore, one expects that any multipole solution $\{^b\mathcal{P}_{2l}(y)\}$ of higher order $l'$ is smaller (for fixed value of $\nu$) than its counterpart $\{^b\mathcal{P}_{2l}(y)\}$ due to a lower multipole order $l (< l')$.  \hspace{1cm} 177
For \( l' = 2, l = 1 \) this expectation is also clearly expressed by Fig.E.1 below. Observe, however, that the magnitudes of the multipole solutions \( \{b\}P_{2,4}(y) \) are not directly responsible for the magnitudes of the corresponding multipole energy corrections.
Fig.E.I  Quadrupole Solution $^{(b)}\mathcal{P}_2(y) \ (E.36)$ and Octupole Solution $^{(b)}\mathcal{P}_4(y) \ (E.26)$ for $\nu = 3$
Both multipole energy corrections \( \tilde{M}^2(e) c^2 \) (E.46b) and \( \tilde{M}^4(e) c^2 \) (VIII.95b) do essentially appear as the product of some reference energy \( \mu^2(e)(\nu) \) and \( \mu^4(e)(\nu) \) times the mass-equivalent parameter \( (b m_1)^2 \) or \( (b m'_2)^2 \), resp. Here, the reference energies \( \mu^2(e)(\nu) \) (E.5) and \( \mu^4(e)(\nu) \) (E.47) do not depend on the quantum number \( (b j_z) \) of angular momentum but are determined solely by the spherically symmetric trial density \( \tilde{\Phi}^2(r) \) (VI.1a)-(VI.1b). Thus the “anisotropic” energy corrections are composed of two different effects, one of “radial” and the other of “angular” type. The latter one is measured by the mass-equivalent parameters \( (b m_1) \) and \( (b m'_2) \) which then play the part of quadrupole and octupole “strengths” and are displayed by the table on p. 145. From the entries of that table it becomes clear that the octupole strength \( (b m'_2) \) is larger than its quadrupole counterpart \( (b m_1) \) (i.e. \( (b m'_2) > (b m_1) \)) which is of course due to the specific anisotropy of the charge distributions, see Fig.IV.A. But this does not yet admit the conclusion that the octupole corrections are larger than their quadrupole counterparts.

Indeed, it is necessary to take into account also the second influence on the “anisotropic” energy corrections, i.e. the reference energies \( \mu^4(e)(\nu) \). The subsequent Fig.E.II presents a plot of both functions \( \mu^2(e)(\nu) = \frac{9}{4} \mu^4(e)(\nu) \) (VII.15) and \( \mu^4(e)(\nu) \) (E.27). Observe here that, just as for \( \mu^4(e)(\nu) \) (D.3b), there does exist also a closed analytic form for \( \mu^4(e)(\nu) \) (E.50):

\[
\mu^4(e)(\nu) = \frac{64}{99225} \frac{4\nu^4 + 28\nu^3 + 71\nu^2 + 77\nu + 30}{\nu (2\nu - 3) (\nu - 1)} \frac{1}{(4\nu^2 - 1)} - \frac{64}{33075} \frac{(12\nu^4 + 44\nu^3 + 81\nu^2 + 67\nu + 20)}{\sqrt{\pi}\nu (2\nu - 3) (\nu - 1)} \frac{1}{(4\nu^2 - 1) \Gamma(2\nu + 2)}.
\]

(E.50)
Quadrupole Function \( \mu_{2}^{(e)}(\nu) = \frac{9}{4} \mu_{III}^{(e)}(\nu) \) (VII.15) and Octupole Function \( \mu_{4}^{(e)}(\nu) \) (E.27)
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