Reply to
“Extended Rejoinder to
“Extended Comment on
“One-Range Addition Theorems for Coulomb Interaction Potential and Its Derivatives”
by I. I. Guseinov
(Chem. Phys. Vol. 309 (2005), pp. 209 - 211)”, arXiv:0706.0975v2”

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Abstract
In the years from 2001 to 2006, Guseinov and his coworkers published 40 articles on the derivation and application of one-range addition theorems. In E. J. Weniger, Extended Comment on “One-Range Addition Theorems for Coulomb Interaction Potential and Its Derivatives” by I. I. Guseinov (Chem. Phys. Vol. 309 (2005), pp. 209 - 213), arXiv:0704.1088v2 [math-ph], it was argued that Guseinov’s treatment of one-range addition theorems is at best questionable and in some cases fundamentally flawed. In I. I. Guseinov, Extended Rejoinder to “Extended Comment on “One-Range Addition Theorems for Coulomb Interaction Potential and Its Derivatives” by I. I. Guseinov (Chem. Phys. and Vol. 309 (2005)”, pp. 209-213), arXiv:0706.0975v2 [physics.chem-ph], these claims were disputed. To clarify the situation, the most serious mathematical flaws in Guseinov’s treatment of one-range addition theorems are discussed in more depth.
1 Introduction

The efficient and reliable evaluation of multicenter integrals is among the oldest mathematical and computational problems of molecular electronic structure theory. In spite of heroic efforts, the mathematical and computational problems, that occur in this context, are not yet solved in a completely satisfactory way, and there is still a considerable amount of research going on. Particularly difficult are multicenter integrals of the physically better motivated exponentially decaying functions, whose efficient and reliable evaluation is – in spite of all the mathematical and computational advances of recent years – still very difficult.

From a methodological point of view, research on multicenter integrals is essentially mathematical in nature, although relatively few mathematicians have been involved in this research. In my opinion, this is quite deplorable. But within mathematics, research on multicenter integrals is highly interdisciplinary. Absolutely essential is a good knowledge of special function theory and of classical analysis: The derivation of explicit expressions for multicenter integrals is to a large extent some kind of 19th century mathematics. However, in order to succeed we also need modern mathematical concepts as for example Hilbert spaces, approximation theory, generalized functions, and angular momentum theory.

It is the ultimate goal of research on multicenter integrals to produce computer code that permits an efficient and reliable evaluation of these integrals. Accordingly, a good knowledge of sophisticated numerical techniques is absolutely indispensable.

Research on multicenter integrals is difficult, and there are many chances of making errors. Firstly, there are errors that violate basic mathematical principles, which could be called first-order errors. Secondly, there are mathematically correct manipulations and/or deductions, which lead to computer code that is either hopelessly inefficient or unreliable and which could be called second-order errors.

Multicenter integrals are difficult to evaluate because the integration variables occur in unseparated form. Principal mathematical tools, that can accomplish such a separation of variables, are so-called addition theorems. These are expansions of a given function \( f(r \pm r') \) with \( r, r' \in \mathbb{R}^3 \) in products of other functions that only depend on either \( r \) or \( r' \).

In the articles \([1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40]\), Guseinov and coworkers derived so-called one-range addition theorems for a variety of different functions and applied them for the evaluation of multicenter integrals.

In my Comment \([41]\), I presented a very detailed criticism of Guseinov’s work on one-range addition theorems and showed that both first- and second-order errors occur quite abundantly. I also criticized in \([41]\) that Guseinov’s articles are often remarkably similar and that they do not always give due credit to the previous work of others. Moreover, I made several suggestions how Guseinov’s flawed approach could be improved: In \([41\text{ Section 7}]\) I suggested to employ advanced mathematical concepts from the theory of generalized functions in order to give a meaning to divergent one-range addition theorems, or to use nonlinear sequence transformations (see for example \([42, 43]\ and references therein), either to sum divergent series, whose occur-
rence was apparently either overlooked or ignored, or to accelerate the convergence of series expansions for multicenter integrals, whose convergence need not be rapid.

Apparently, my Comment \[41\] did not impress Guseinov too much, who recently wrote a Rejoinder \[44\] to my Comment \[41\]. In his Abstract, Guseinov stated

*The concrete criticism raised in Weniger’s comment against our papers actually touches a very minor aspect of the works that are not relevant at all for the conclusions, which are made.*

and

*All claims of inconsistencies and flaws in the theoretical framework are rejected as unfounded. This rejoinder paper contains all of the answers to Weniger’s comments.*

This is wrong. In \[44\], Guseinov did not address at all the most serious and consequential first-order errors, which I had criticized in my Comment \[41\] and which raise serious doubts on the mathematical soundness of Guseinov’s treatment of one-range addition theorems. Guseinov’s questionable attitude towards mathematical rigor becomes also evident in his even more recent preprints \[45, 46\], in which he proceeds in the same style and spirit as in his previous articles on one-range addition theorems mentioned above, completely ignoring my criticism.

In this Replay to Guseinov’s Rejoinder \[44\], I discuss once more and in more depth the most important mathematical flaws of Guseinov’s work. In contrast to my earlier and longer Comment \[41\], I concentrate entirely on first-order errors.

In \[1, 3\], Guseinov had derived one-range addition theorems for Slater-type functions $\chi^M_{\nu,L}(\beta,r) = (\beta r)^{-L-1} e^{-\beta r} Y^M_L(\beta r), \quad \beta > 0$, \hspace{1cm} (1.1)

with in general nonintegral principal quantum numbers $N \in \mathbb{R} \setminus \mathbb{N}$ by expanding them in terms his functions $\Psi_{\nu,k}^n(\beta,r)$ defined by \[1.1\], which are complete and orthonormal in the weighted Hilbert spaces $L^2_{\nu,k}(\mathbb{R}^3)$ defined by \[D.5\] (for details, see \[41\] Sections 4 - 6). Here, $Y^M_L(\beta r)$ is a regular solid harmonic (compare \[41\] Eq. (A.2)).

As long as the principal quantum numbers $N$ are not too negative, Slater-type functions $\chi^M_{\nu,L}$ belong for $k = -1, 0, 1, 2, \ldots$ to the weighted Hilbert spaces $L^2_{\nu,k}(\mathbb{R}^3)$ defined by \[D.5\], which was implicitly used by Guseinov. In this case, the one-range addition theorems derived in \[1, 3\] exist and converge in the mean with respect to the norms \[D.4\] of these Hilbert spaces.

Guseinov’s addition theorems for Slater-type functions $\chi^M_{\nu,L}$ yield for $N = L = M = 0$ the corresponding addition theorems for the Yukawa potential $\exp(-\beta r)/r$. Guseinov \[17\] derived his one-range addition theorems for the Coulomb potential by exploiting the obvious relationship $1/r = \lim_{\beta \to 0} \exp(-\beta r)/r$ in his one-range addition theorems for the Yukawa potential.

At first sight, it may look like a good idea to derive one-range addition theorems for the Coulomb potential by performing the comparatively simple limit $\beta \to 0$ in the one-range addition theorems for the Yukawa potential. This pragmatic approach
seems to permit an efficient utilization of the available information and of previous work. Unfortunately, the situation is much more complicated.

As shown in Section 2, the limit $\beta \to 0$ in mathematically well defined integrals containing the Yukawa potential is not necessarily continuous and does not always lead to a finite result. So, whenever we try to find an expression for an integral containing the Coulomb potential as the limiting case of the expression for an analogous integral containing the Yukawa potential, we have to be cautious and be prepared for complications. As discussed in Sections 3 and 4, similar complications can occur also in orthogonal expansions of the Yukawa potential.

A very serious weakness of Guseinov’s earlier work on one-range addition theorems is that he completely ignored the obvious fact that orthogonal expansions can diverge, and he still does this in his recent Rejoinder [44] and in his even more recent preprints [45, 46]. On p. 3 of his Rejoinder [44], Guseinov states:

\begin{quote}
The essential facts of Hilbert space and approximation theory as well as all questions of convergence and existence have been taken into account by Guseinov and his coworkers in the context of one-range addition theorems and multicenter integrals. Thus, the Guseinov’s treatment of one-range addition theorems is not questionable, and is fundamentally flawless from a mathematical point of view.
\end{quote}

Again, this is wrong. Let us assume that $\mathcal{H}$ is a Hilbert space, and that $\{\phi_n\}_{n=0}^\infty$ is a function set that is complete and orthonormal in $\mathcal{H}$. If $f \in \mathcal{H}$, then standard Hilbert space theory tells us that the expansion $\sum_{n=0}^\infty (\phi_n | f) \phi_n$ converges to $f$ in the mean with respect to the norm of $\mathcal{H}$. If, however, $f \notin \mathcal{H}$, then it follows – as shown in Section 3 – from the Riesz-Fischer Theorem (see for example [47, Theorem 7.43 on p. 191]) that the formal orthogonal expansion $f = \sum_{n=0}^\infty (\phi_n | f) \phi_n$ diverges in the mean with respect to the norm of $\mathcal{H}$.

Since Guseinov ignores the fact that orthogonal expansions can diverge, he fails to take into account that divergent orthogonal expansions cannot be treated like convergent orthogonal expansions (obviously, the divergence of an orthogonal series can do a lot of harm in integrals). So, Guseinov never wonders whether and under which conditions divergent expansions can safely be used in multicenter integrals, although this is by no means obvious.

As shown in Section 3, it is nevertheless possible to use divergent orthogonal expansions in inner products or other functionals – in our case usually multicenter integrals – in a mathematically meaningful way. The key is that the functionals, in which these expansions are to be used, have to satisfy additional and possibly very restrictive regularity conditions. This follows from the Riesz Representation Theorem (see for example [47, Theorem 7.60 on p. 199]). Accordingly, divergent orthogonal expansions are essentially generalized functions in the sense of Schwartz [48] that can – in spite of their divergence – converge weakly when used in suitably restricted functionals.

When Guseinov derived in [17] one-range addition theorems for the Coulomb potential by considering the limit $\beta \to 0$ in one-range addition theorems for the Yukawa potential $\exp(-\beta r)/r$, he overlooked some very consequential facts.
The Yukawa potential belongs for $k = 0, 1, 2, \ldots$, to the weighted Hilbert space $L^2_{\omega_k}(\mathbb{R}^3)$ defined by (D.5), but not for $k = -1$ (this obvious fact was apparently overlooked by Guseinov). Accordingly, Guseinov’s one-range addition theorems for the Yukawa potential converge for $k = 0, 1, 2, \ldots$ in the mean with respect to the norm (D.4) of $L^2_{\omega_k}(\mathbb{R}^3)$, but not for $k = -1$ (see also Appendix E where the convergence of the one-center limit of these addition theorems is analyzed).

As discussed in Section 4, the Coulomb potential does not belong to any of the Hilbert spaces $L^2_{\omega_k}(\mathbb{R}^3)$ which Guseinov had implicitly used. This is quite consequential: Guseinov’s one-range addition theorems for the Coulomb potential diverge for all $k = -1, 0, 1, 2, \ldots$ in the mean with respect to the norm (D.4) of $L^2_{\omega_k}(\mathbb{R}^3)$, although they were derived by a limiting procedure from the corresponding addition theorems of the Yukawa potential, which converge at least for $k = 0, 1, 2, \ldots$ in the mean. This is another example that the limit $\beta \to 0$ in expressions involving the Yukawa potential $\exp(-\beta r)/r$ need not be continuous and does not necessarily produce something finite.

Section 4 shows conclusively that it is impossible to construct one-range addition theorems for the Coulomb potential that converge in the mean with respect to the norms of the weighted Hilbert spaces $L^2_{\omega_k}(\mathbb{R}^3)$. More advanced mathematical concepts such as the theory of generalized functions or possibly also powerful numerical techniques for the summation of divergent series (see for example [42, 43] and references therein) are needed to give divergent orthogonal expansions of that kind any meaning beyond purely formal expansions. None of these things are discussed in Guseinov’s articles on one-range addition theorems [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40] or in his recent Rejoinder [44].

Unfortunately, this is not yet the end of Guseinov’s grave first-order errors in his treatment of one-range addition theorems. As discussed in Section 5, Guseinov preferred to replace the complete and orthonormal expansion functions $k \Psi_{m, n, \ell}^m(\beta, r)$ of his one-range addition theorems for Slater-type functions by nonorthogonal Slater-type functions with integral principal quantum numbers and to rearrange the order of summations of the resulting expansions. In this way, Guseinov obtained expansions of Slater-type functions $\chi_{N, L}^M(\beta, r \pm r')$ with in general nonintegral principal quantum numbers $N \in \mathbb{R} \setminus \mathbb{N}$ in terms of Slater-type functions $\chi_{n, \ell}^m(\beta, r)$ with integral principal quantum numbers $n \in \mathbb{N}$ located at a different center.

As is well known, Slater-type functions are complete in the Hilbert spaces implicitly used by Guseinov, but not orthogonal. This is very consequential. It is extensively documented both in the mathematical literature (see for example [49, Theorem 10 on p. 54] or [50, Section 1.4]) as well as in the literature on electronic structure calculations [51, 52, 53, 54, 55, 56]) that the existence of expansions in terms of nonorthogonal function sets is not guaranteed in the case of essentially arbitrary functions. Such an expansions may or may not exist. Thus, as already emphasized in [41, Section 6]), Guseinov’s approach is dangerous and potentially disastrous and the validity of his rearranged addition theorems has to be checked explicitly.

As discussed in Section 5, Guseinov disagreed in his Rejoinder [44, p. 7] with my conclusions, and claimed instead that the validity of his approach follows from Eq.
(3.11) of his Rejoinder. It is easy to show that Guseinov’s reasoning is superficial and that it is indeed necessary to analyze whether Guseinov’s rearranged addition theorems exist or not.

There is the practical problem that one-range additions theorems for exponentially decaying functions are fairly complicated mathematical objects. Accordingly, explicit proofs of their convergence or divergence are very difficult and would most likely require a considerable amount of time and effort. Fortunately, at least some insight can be gained by analyzing instead the much simpler one-center limits of Guseinov’s one-range addition theorems, although this approach does not answer all questions of interest.

In Section 5 and also in [41, Section 6], it is shown that it is impossible to rearrange the one-center limits of Guseinov’s one-range addition theorems for Slater-type functions if the principal quantum number \( N \) is nonintegral, \( N \in \mathbb{R} \setminus \mathbb{N} \). Guseinov’s rearrangements do not lead to divergent series in the usual sense, but to power series with series coefficients that are for all but a finite number of indices \( \infty \). While I can probably claim with some confidence that I have a lot of experience with the summation of divergent series (see for example [42, 43, 57] and references therein), I nevertheless must admit that I have not the slightest idea what to do with power series with an infinite number of infinite terms.

This article is concluded by a Summary in Section 6. For the convenience of the readers, the most important conventions and definitions of this Reply are listed in Appendices A - D. Finally, there is Appendix E analyzing the convergence of the one-center limit of Guseinov’s one-range addition theorems for the Yukawa potential in the weighted Hilbert space \( L^2_{r^k}(\mathbb{R}^3) \).

2 On the Continuity of Limits in Integrals

Because of its exponential decay, the Yukawa potential \( \exp(-\beta r)/r \) is in many respects a much more convenient mathematical object than the closely related Coulomb potential \( 1/r \). This is particularly true for integrals over the whole three-dimensional space \( \mathbb{R}^3 \) as they occur in atomic or molecular electronic structure calculations.

Consequently, it is an obvious idea to derive explicit expressions for integrals involving the Coulomb potential by performing the limit \( \beta \to 0 \) in explicit expressions for analogous integrals involving the more convenient Yukawa potential.

Often, this indirect approach is very effective. However, it is no panacea. Moreover, it can easily lead to problems: The limiting process \( 1/r = \lim_{\beta \to 0} \exp(-\beta r)/r \) is not necessarily continuous in integrals, and it is not guaranteed that it produces a finite result.

These possible problems can be illuminated easily by considering integrals of the following kind:

\[
\mathcal{J}(f; \beta) = \int [f(r)]^* \frac{\exp(-\beta r)}{r} d^3r
\]

(2.1)

As usual, integration extends over the whole \( \mathbb{R}^3 \).
For $\beta > 0$, the Yukawa potential belongs to the Hilbert space $L^2(\mathbb{R}^3)$ of square integrable functions defined by (B.3). If we also have $f \in L^2(\mathbb{R}^3)$, the integral (2.1) is a special case of the inner products (B.3), and it is finite. This follows at once from the Cauchy-Schwarz Inequality (see for example [47, Theorem 7.7 on p. 177]) which can be expressed as follows:

$$
|\langle f | g \rangle|^2 \leq \langle f | f \rangle \langle g | g \rangle = \| f \|^2 \| g \|^2 .
$$

(2.2)

If we perform the limit $\beta \to 0$ in (2.1), we formally obtain integrals of the following kind:

$$
K(f) = \int [f(r)]^* \frac{1}{r} g(r') \, dr \, dr' \quad (2.3)
$$

Since the Coulomb potential does not belong to $L^2(\mathbb{R}^3)$ or to any of those Hilbert spaces, which are considered in this Reply and which all involve an integration over the whole $\mathbb{R}^3$, the Cauchy-Schwarz Inequality cannot be used to guarantee the existence of $K(f)$ for arbitrary $f \in L^2(\mathbb{R}^3)$. Instead, the integral $K(f)$ makes sense only if $f$ belongs to a suitably restricted (proper) subset of $L^2(\mathbb{R}^3)$ prior to other function spaces.

The possible discontinuity of the limit $\beta \to 0$ also becomes evident in the six-dimensional integrals

$$
C(f, g) = \int \int [f(r)]^* \frac{1}{|r - r'|} g(r') \, dr \, dr' \quad (2.4)
$$

and

$$
\mathcal{Y}(f, g; \beta) = \int \int [f(r)]^* \frac{\exp(-\beta|r - r'|)}{|r - r'|} g(r') \, dr \, dr' , \quad (2.5)
$$

which describe the interaction of two charge densities $f, g : \mathbb{R}^3 \to \mathbb{C}$ via the Coulomb and the Yukawa potential, respectively, and which involve an integration over the whole six-dimensional space $\mathbb{R}^3 \times \mathbb{R}^3$.

Obviously, we have $C(f, g) = \lim_{\beta \to 0} \mathcal{Y}(f, g; \beta)$, but it would be grossly negligent to perform this limit without explicitly knowing criteria, which the charge densities $f$ and $g$ have to satisfy in order to guarantee that the limit $\beta \to 0$ is continuous and produces a finite result.

This question can be analyzed with the help of Fourier transformation. If we use the symmetrical version of Fourier transformation according to (A.1) and (A.2), the six-dimensional integrals (2.4) and (2.5) can be expressed as three-dimensional Fourier integrals via the following general expression introduced into electronic structure calculations by Geller [58, Eqs. (1) and (2)]:

$$
\int \int f^*(r) \, g(r') \, h(r - r') \, dr \, dr' = (2\pi)^3/2 \int \int [\tilde{f}(p)]^* \tilde{g}(p) \tilde{h}(p) \, d^3p .
$$

(2.6)

If we choose $h(r - r') = \exp(-\beta|r - r'|)/|r - r'|$, we only need the Fourier transform of the Yukawa potential (see for example [59, Eqs. (6.8) and (6.9)]),

$$
(2\pi)^{-3/2} \int \exp(-ip \cdot r) \exp(-\beta r) \, d^3r = \frac{(2/\pi)^{1/2}}{\beta^2 + p^2} , \quad \beta > 0 ,
$$

(2.7)
to obtain:

$$\mathcal{Y}(f, g; \beta) = 4\pi \int \left[ \tilde{f}(p) \right]^* \frac{1}{\beta^2 + p^2} \tilde{g}(p) \, d^3 p.$$  \hfill (2.8)

Fourier transformation maps $L^2(\mathbb{R}^3)$ onto $L^2(\mathbb{R}^3)$ in a one-to-one manner such that inner products are conserved [60, Theorem IX.6 on p. 10]. Thus, $u, v \in L^2(\mathbb{R}^3)$ implies $\bar{u}, \bar{v} \in L^2(\mathbb{R}^3)$, and the coordinate and momentum space inner products (B.3) and (B.9), respectively, are identical:

$$\int [u(r)]^* v(r) \, d^3 r = \int [\bar{u}(p)]^* \bar{v}(p) \, d^3 p$$  \hfill (2.9)

It follows at once from the Cauchy-Schwarz Inequality [2.2] that $\mathcal{Y}(f, g; \beta)$ is finite if $\tilde{f}(p)/[\beta^2 + p^2]^{1/2}, \tilde{g}(p)/[\beta^2 + p^2]^{1/2} \in L^2(\mathbb{R}^3)$. Unfortunately, this condition is not particularly helpful in practice since it is not so easy to find convenient coordinate representations for the functions $\tilde{f}(p)/[\beta^2 + p^2]^{1/2}$ and $\tilde{g}(p)/[\beta^2 + p^2]^{1/2}$ (they have to be expressed as convolution integrals containing $f(r)$ and $g(r)$, respectively, multiplied by a modified Bessel function).

Fortunately, a slightly more restrictive, but much more convenient condition on the charge densities $f$ and $g$ can be constructed easily. For all $p \in \mathbb{R}^3$ and for all $\beta > 0$, we have $1/(\beta^2 + p^2) \leq 1/\beta^2$. Thus,

$$\left| \int \left[ \tilde{f}(p) \right]^* \frac{1}{\beta^2 + p^2} \tilde{g}(p) \, d^3 p \right| \leq \frac{1}{\beta^2} \left| \int \left[ \tilde{f}(p) \right]^* \tilde{g}(p) \, d^3 p \right|, \quad \beta > 0.$$  \hfill (2.10)

By applying the Cauchy-Schwarz Inequality [2.2] to the integral on the right-hand side we find that $\mathcal{Y}(f, g; \beta)$ with $\beta > 0$ is finite if $\tilde{f}, \tilde{g} \in L^2(\mathbb{R}^3)$ or – since Fourier transformation is an isometric isomorphism of $L^2(\mathbb{R}^3)$ – if $f, g \in L^2(\mathbb{R}^3)$.

If we perform the limit $\beta \to 0$ in the Fourier integral (2.8), we formally obtain:

$$C(f, g) = 4\pi \int \left[ \tilde{f}(p) \right]^* \frac{1}{p^2} \tilde{g}(p) \, d^3 p.$$  \hfill (2.11)

The momentum space integral on the right-hand side can be interpreted to be an inner product of the type of (B.11) that gives rise to a suitable Hilbert space.

The Cauchy-Schwarz Inequality [2.2] now requires $\tilde{f}(p)/p, \tilde{g}(p)/p \in L^2(\mathbb{R}^3)$ to guarantee that $C(f, g)$ is finite. Obviously, this is much more restrictive than the requirement $\tilde{f}, \tilde{g} \in L^2(\mathbb{R}^3)$ or even $\tilde{f}(p)/[\beta^2 + p^2]^{1/2}, \tilde{g}(p)/[\beta^2 + p^2]^{1/2} \in L^2(\mathbb{R}^3)$, which both guarantee that $\mathcal{Y}(f, g; \beta)$ is finite (alternative criteria, which also guarantee the existence of the Coulomb integrals $C(f, g)$, are for instance formulated in [60, Example 3 (Sobolev’s inequality) on p. 31] or [61, Section 4.3 (Hardy-Littlewood-Sobolev inequality)])

This example clearly shows that the limit $\beta \to 0$ in integrals involving the Yukawa potential $\exp(-\beta r)/r$ is not necessarily continuous and does not always produce a finite result for arbitrary square integrable charge densities $f$ and $g$.

If we set $\beta = 0$ in the Fourier transform (2.7) of the Yukawa potential, we formally obtain the Fourier transform of the Coulomb potential (see for example [62, Eq. (2) on p. 194]):

$$(2\pi)^{-3/2} \int \frac{\exp(-ip \cdot r)}{r} \, d^3 r = \frac{(2/\pi)^{1/2}}{p^2}.$$  \hfill (2.12)
There is a fundamental difference between the Fourier transforms (2.7) and (2.12). The Fourier integral in (2.7) is well defined and exists in the sense of classical analysis, whereas the Fourier integral in (2.12) diverges in the sense of classical analysis and becomes mathematically meaningful only if certain limiting or summation procedures are applied. Thus, the Fourier transform (2.7) of the Yukawa potential is a function in the ordinary sense. In contrast, the Fourier transform (2.12) of the Coulomb potential is a generalized function or distribution which is meaningful in suitably restricted functionals only.

So, whenever we perform the limit $\beta \to 0$ in integrals involving the Yukawa potential $\exp(-\beta r)/r$, we have to be cautious and take into account that this limit may be discontinuous and that it does not necessarily produce a finite result in the case of an essentially arbitrary integrand. It will become clear in later Sections that these problems are not restricted to integrals and that they can also occur in orthogonal expansions of the Yukawa potential.

3 Divergent Orthogonal Expansions

Hilbert spaces, whose basic features are reviewed in Appendix B, play a major role in various branches of mathematics and mathematical physics and in particular also in approximation theory. They also provide a rigorous mathematical framework for quantum mechanics.

As discussed in Section 4 or in more details in [41, Section 3], one-range addition theorems can also be viewed to be special approximation procedures: A function $f(r \pm r')$ belonging to suitable Hilbert space is expanded in terms of a complete and orthonormal function set in such a way that the two argument vectors $r, r' \in \mathbb{R}^3$ are separated. By construction, such an orthogonal expansion converges in the mean with respect to the norm of the corresponding Hilbert space.

Therefore, it certainly makes sense to discuss the basic properties of orthogonal expansions in Hilbert spaces – including their power as well as their limitations – in a relatively detailed way. Hilbert spaces are linear vector spaces over the complex numbers equipped with an inner product $(\cdot|\cdot)$ satisfying (B.1) and a norm $\| \cdot \|$ satisfying (B.2), which has to be finite. A vector space with these properties is called a Hilbert space if it is complete with respect to its norm $\| \cdot \|$.

Let us assume that $f$ is an element of some Hilbert space $\mathcal{H}$, and that the functions $\{\varphi_n\}_{n=0}^{\infty}$ are linearly independent and complete in $\mathcal{H}$. Then, $f$ can be approximated by finite linear combinations

$$f_N = \sum_{n=0}^{N} C_n^{(N)} \varphi_n, \quad N \in \mathbb{N}_0.$$  \hspace{1cm} (3.1)

The coefficients $C_n^{(N)}$ are chosen in such a way that the mean square deviation

$$\|f - f_N\|^2 = (f - f_N|f - f_N)$$  \hspace{1cm} (3.2)

becomes minimal.
The determination of the coefficients $C_n^{(N)}$ in (3.1) by minimizing the mean square deviation (3.2) only makes sense if both $f$ and the functions $\{\varphi_n\}_{n=0}^\infty$ are normalizable according to $\|f\| < \infty$ and $\|\varphi_n\| < \infty$, respectively. Thus, $f$ as well as the functions $\{\varphi_n\}_{n=0}^\infty$ have to belong to the Hilbert space $\mathcal{H}$.

The finite approximation (3.1) converges to $f$ as $N \to \infty$ if the mean square deviation (3.2) can be made as small as we like by increasing the summation limit $N$. In the case of convergence, it looks natural to assume that $f$ possesses an infinite expansion

$$f = \sum_{n=0}^\infty C_n \varphi_n$$

in terms of the linearly independent and complete functions $\{\varphi_n\}_{n=0}^\infty$ with coefficients $C_n = \lim_{N \to \infty} C_n^{(N)}$.

Unfortunately, this is not true. In general, the coefficients $C_n^{(N)}$ in (3.1) do not only depend on $n$, $f$, and $\{\varphi_n\}_{n=0}^\infty$, but also on the summation limit $N$. It is not a priori clear whether the coefficients $C_n^{(N)}$ in (3.1) possess well defined limits $C_n = \lim_{N \to \infty} C_n^{(N)}$, or to put it differently, whether an infinite expansion of the type of (3.3) exists. Expansions of the type of (3.3) may or may not exist.

It is one of the central results of approximation theory that for functions $f \in \mathcal{H}$ the mean square deviation (3.2) becomes minimal if the functions $\{\varphi_n\}_{n=0}^\infty$ are not only linearly independent and complete, but also orthonormal satisfying $(\varphi_n | \varphi_{n'}) = \delta_{nn'}$ for all indices $n, n' \in \mathbb{N}_0$, and if the coefficients are chosen according to $C_n^{(N)} = (\varphi_n | f)$ (see for example [49, Theorem 9 on p. 51]).

If the functions $\{\varphi_n\}_{n=0}^\infty$ are complete and orthonormal in $\mathcal{H}$ and if the expansion coefficients are chosen according to $C_n^{(N)} = (\varphi_n | f)$, then the coefficients $(\varphi_n | f)$ in $f_N$ do not depend on the truncation order $N$. Thus, $f \in \mathcal{H}$ possesses an infinite series expansion

$$f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n$$

in terms of the complete and orthonormal function set $\{\varphi_n\}_{n=0}^\infty$, and this expansion converges in the mean with respect to the norm $\| \cdot \|$ of the Hilbert space $\mathcal{H}$.

This is all well known and described in countless books on functional analysis or approximation theory. In these books, it is always emphasized that orthogonal expansions of the type of (3.4) are mathematically meaningful and converge in the mean if and only if $f \in \mathcal{H}$.

However, in practical applications we are often confronted with functions that are not normalizable and thus do not belong to the corresponding Hilbert space $\mathcal{H}$. In some cases it may be desirable to expand such a function $f \notin \mathcal{H}$ in terms of functions $\{\varphi_n\}_{n=0}^\infty$, that are complete and orthonormal in $\mathcal{H}$. It is thus a practically relevant question whether and under which conditions the concept of orthogonal expansions in a Hilbert space $\mathcal{H}$ can be extended to functions $f \notin \mathcal{H}$.

If this is indeed possible, we also have to analyze in which respect orthogonal expansions of a function $f \in \mathcal{H}$ differ from those of a function $f \notin \mathcal{H}$. In particular,
we have to analyze whether and under which conditions orthogonal expansions \( f = \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \) can be used in inner products \((f|g)\) with \( f \notin \mathcal{H} \) and \( g \in \mathcal{H} \).

There is one obvious complication: If \( f \in \mathcal{H} \), then it follows from the Cauchy-Schwarz Inequality (2.2) that the map \( g \mapsto (f|g) \) is bounded and thus continuous for all \( g \in \mathcal{H} \). If, however, \( f \notin \mathcal{H} \), we have to take into account the Riesz Representation Theorem (see for example [47, Theorem 7.60 on p. 199]):

For every continuous and thus bounded linear functional \( U : \mathcal{H} \to \mathbb{C} \) there exists a unique \( u \in \mathcal{H} \) such that \( U(v) = (u|v) \) for all \( v \in \mathcal{H} \).

Thus, the map \( g \mapsto (f|g) \) with \( f \notin \mathcal{H} \) cannot be continuous and bounded for all \( g \in \mathcal{H} \). Consequently, for a given \( f \notin \mathcal{H} \), there must be at least one \( g \in \mathcal{H} \) that yields an unbounded inner product \((f|g)\).

Accordingly, the following discussion has to be limited to those \( g \in \mathcal{H} \) that yield for a given \( f \notin \mathcal{H} \) bounded inner products \((f|g)\). Therefore, we have to assume that \( g \) belongs to the subset \( \mathcal{F} \subset \mathcal{H} \) defined by

\[
\mathcal{F} = \{ g | g \in \mathcal{H}, f \notin \mathcal{H}, |(f|g)| < \infty \}. \tag{3.5}
\]

For arbitrary \( f \notin \mathcal{H} \), it can happen that there is no \( g \in \mathcal{H} \) satisfying \(|(f|g)| < \infty\), i.e., that \( \mathcal{F} \) is empty. In the following text, it will be assumed that this is not the case. However, it follows from the Riesz Representation Theorem that we cannot have \( \mathcal{F} = \mathcal{H} \), i.e., \( \mathcal{F} \) is either empty or a proper subset of \( \mathcal{H} \).

A divergent orthogonal expansion \( f = \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \) makes sense only if the inner products \((\varphi_n|f)\) are finite for all finite indices \( n \). If \( f \in \mathcal{H} \), this is guaranteed by the Cauchy-Schwarz Inequality (2.2), but for \( f \notin \mathcal{H} \) we have to assume explicitly that \( \varphi_n \in \mathcal{F} \) holds for all finite values of the index \( n \).

On the basis of these assumptions, it is at least formally possible to construct an orthogonal expansion \( f = \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \) even if \( f \notin \mathcal{H} \). It is, however, not at all clear whether and in which sense the formal series expansion \( \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \) represents \( f \notin \mathcal{H} \). In particular, we have no a priori reason to assume that this expansion might converge in the mean according to the norm \( \| \cdot \| \) of \( \mathcal{H} \), which would imply that \( \sum_{n=0}^{\infty} |(\varphi_n|f)|^2 < \infty \) holds.

The divergence of the series \( \sum_{n=0}^{\infty} |(\varphi_n|f)|^2 \) can be made plausible by analyzing the mean square deviation of the difference between a function \( f \) and its (possibly divergent) orthogonal expansion \( \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \):

\[
\begin{align*}
\| f - \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \|^2 &= \left( f - \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n \right) \left( f - \sum_{m=0}^{\infty} (\varphi_m|f) \varphi_n \right) \\
&= (f|f) - \sum_{n=0}^{\infty} (\varphi_n|f)^* (\varphi_n|f) \\
&\quad - \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} (\varphi_n|f)^* (\varphi_m|f) (\varphi_m|\varphi_n) + \sum_{m=0}^{\infty} (\varphi_m|f) (f|\varphi_m) \\
&\quad = (f|f) - \sum_{m=0}^{\infty} |(\varphi_m|f)|^2. \tag{3.6}
\end{align*}
\]
If \( f \in \mathcal{H} \), we have \( \|f\|_2^2 = (f|f) < \infty \), and it follows from Parseval’s Equality (see for example [63, Eq. (II.2) on p. 45])

\[
\|f\|_2^2 = \sum_{n=0}^{\infty} |(\varphi_n|f)|^2
\]

that (3.6) vanishes.

If, however, \( f \notin \mathcal{H} \), then \( \|f\|_2^2 = (f|f) \) diverges. In this case, the mean square deviation (3.6) can only vanish if \( \sum_{n=0}^{\infty} |(\varphi_n|f)|^2 \) also diverges. Of course, this is hand-waving and not a rigorous mathematical proof. In particular, it is not at all clear whether the mean square deviation (3.6) makes sense at all if \( f \notin \mathcal{H} \). Nevertheless, this non-rigorous argument should suffice to convince even a skeptical reader that it would be overly optimistic to expect that the formal expansion \( \sum_{n=0}^{\infty} (\varphi_n|f)\varphi_n \) converges in the mean to something finite if \( f \notin \mathcal{H} \).

We should also take into account that series expansions – or actually all approximation schemes – are practically useful only if they reproduce the essential features of the function they represent. At least in quantum mechanical bound state calculations, the norm of a function is of considerable importance and should be preserved by an orthogonal expansion. Otherwise, a function \( f \notin \mathcal{H} \) could be transformed to a function belonging to \( \mathcal{H} \) simply by expanding \( f \) in terms of a complete and orthonormal function set. This would truly be a miraculous achievement with revolutionary and most likely highly undesirable consequences.

Plausibility arguments are no substitute for a rigorous proof. Such a proof can be formulated with the help of the Riesz-Fischer Theorem (see for example [47, Theorem 7.43 on p. 191]):

Let \( \{\varphi_n\}_{n=0}^{\infty} \) be a complete and orthonormal function set in a Hilbert space \( \mathcal{H} \), and let \( c_0, c_1, c_2, \ldots \) be a sequence of numbers such that \( \sum_{n=0}^{\infty} |c_n|^2 \) converges. Then, the expansion \( \sum_{n=0}^{\infty} c_n \varphi_n \) converges in the mean to some \( w \in \mathcal{H} \) such that \( c_n = (\varphi_n|w) \).

This theorem shows that there is no sequence \( (\varphi_0|f), (\varphi_1|f), (\varphi_2|f), \ldots \) of inner products such that \( \| \sum_{n=0}^{\infty} (\varphi_n|f)\varphi_n \|^2 = \sum_{n=0}^{\infty} |(\varphi_n|f)|^2 < \infty \) and \( f \notin \mathcal{H} \) simultaneously hold. Accordingly, \( f \notin \mathcal{H} \) implies that \( \sum_{n=0}^{\infty} (\varphi_n|f)\varphi_n \) diverges in the mean with respect to the norm of \( \mathcal{H} \). Thus, normalization is preserved by orthogonal expansions even if \( f \notin \mathcal{H} \).

This applies also to expansions in terms of Guseinov’s functions \( k \Psi_{n,\ell}^{m}(\beta, r) \) defined by (D.1). As discussed in [41, p. 20], the Yukawa potential belongs for \( k = 0, 1, 2, \ldots \) to the weighted Hilbert space \( L^2_{r_k}(\mathbb{R}^3) \) defined by (D.3), but not for \( k = -1 \) (see also [64, p. 410]). Consequently, the expansion of the Yukawa potential in terms of Guseinov’s functions converges in the mean for \( k = 0, 1, 2, \ldots \) and diverges for \( k = -1 \). In Appendix [E] it is explicitly shown that this is indeed the case.

We thus arrive at the conclusion that conventional Hilbert space theory and the related concept of convergent orthogonal expansions of the type of (3.4) in terms of complete and orthonormal functions \( \{\varphi_n\}_{n=0}^{\infty} \) only make sense if \( f \in \mathcal{H} \). Divergent
expansions \( f = \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n \) with \( f \notin \mathcal{H} \) are *generalized functions* in the sense of Schwartz [18] that can converge *weakly* when used in suitably restricted functionals.

In the context of one-range addition theorems, which are to be used in multicenter integrals, it is essential that orthogonal expansions \( f = \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n \) can safely be used in inner products \( (f | g) \). If \( f, g \in \mathcal{H} \), this can be shown by applying the Cauchy-Schwarz Inequality (2.2) to the inner product \( (f - \sum_{n=0}^{N} (\varphi_n | f) \varphi_n | g) \). We obtain:

\[
| (f - \sum_{n=0}^{N} (\varphi_n | f) \varphi_n | g) |^2 \leq \| f - \sum_{n=0}^{N} (\varphi_n | f) \varphi_n \|^2 \| g \|^2. \tag{3.8}
\]

The assumption \( g \in \mathcal{H} \) implies \( \| g \|^2 < \infty \), and the assumption \( f \in \mathcal{H} \) implies that \( \| f - \sum_{n=0}^{N} (\varphi_n | f) \varphi_n \|^2 \) vanishes as \( N \to \infty \). Accordingly, the right-hand side of (3.8) vanishes as \( N \to \infty \).

If \( g \in \mathcal{H} \) but \( f \notin \mathcal{H} \), we cannot use the Cauchy-Schwarz Inequality (2.2). Moreover, the inner products \( (f | g) \) is not necessarily finite. As discussed above, the map \( g \mapsto (f | g) \) with \( f \notin \mathcal{H} \) cannot be continuous and bounded for all \( g \in \mathcal{H} \). Thus, it is essential to assume that \( g \) belongs to the subset \( \mathcal{F} \subset \mathcal{H} \) defined by (3.5).

Next, we have to formulate criteria, which guarantee that the divergent orthogonal expansion \( f = \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n \) can safely be used in inner products \( (f | g) \) with \( g \in \mathcal{F} \). Thus, we have to analyze under which conditions

\[
(f - \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n | g) = 0 \tag{3.9}
\]

with \( f \notin \mathcal{H} \) holds for suitable \( g \in \mathcal{F} \).

There is a very simple situation in which (3.9) is obviously valid. Let us assume that there is some \( \tilde{g} \in \mathcal{F} \) that possesses a *finite* expansion in terms of the complete and orthonormal functions \( \{ \varphi_n \}_{n=0}^{\infty} \):

\[
\tilde{g} = \sum_{m=0}^{M} \tilde{\gamma}_m \varphi_m = \sum_{m=0}^{M} (\tilde{g} | \varphi_m) \varphi_m, \quad M \in \mathbb{N}_0. \tag{3.10}
\]

Since we always assume that the inner products \( (\varphi_n | f) \) are finite for all finite values of \( n \), we obtain:

\[
(f - \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n | \tilde{g}) = (f | \tilde{g}) - \left( \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n | \tilde{g} \right)
\]

\[
= \sum_{m=0}^{M} \tilde{\gamma}_m (f | \varphi_m) - \sum_{n=0}^{\infty} \sum_{m=0}^{M} (\varphi_n | f) \tilde{\gamma}_m (\varphi_n | \varphi_m)
\]

\[
= \sum_{m=0}^{M} \tilde{\gamma}_m (f | \varphi_m) - \sum_{m=0}^{M} (\varphi_m | f) \tilde{\gamma}_m = 0. \tag{3.11}
\]

Thus, for functions \( \tilde{g} \in \mathcal{F} \) satisfying (3.10), the divergent orthogonal expansion \( f = \sum_{n=0}^{\infty} (\varphi_n | f) \varphi_n \) produces the correct result in the inner product \( (f | \tilde{g}) \).
As a mild generalization of (3.10), let us now consider some \( g \in \mathcal{F} \) that possesses an infinite expansion in terms of the complete and orthonormal function \( \{ \varphi_n \}_{n=0}^\infty \):

\[
g = \sum_{m=0}^\infty \gamma_m \varphi_m = \sum_{m=0}^\infty (\varphi_m | g) \varphi_m. \tag{3.12}
\]

Since \( g \in \mathcal{F} \subset \mathcal{H} \), this expansion converges in the mean. However, the convergence of this expansion alone does not suffice to guarantee that (3.9) is satisfied. The problem is that we are now confronted with infinite series that do not necessarily converge:

\[
(f - \sum_{n=0}^\infty (\varphi_n | f) \varphi_n | g) = (f | g) - \left( \sum_{n=0}^\infty (\varphi_n | f) \varphi_n | g \right)
\]

\[
= \sum_{m=0}^\infty \gamma_m (f | \varphi_m) - \sum_{n=0}^\infty (\varphi_n | f^* (\varphi_n | g)
\]

\[
= \sum_{m=0}^\infty \gamma_m (f | \varphi_m) - \sum_{n=0}^\infty \sum_{m=0}^\infty (\varphi_n | f^* \gamma_m (\varphi_n | \varphi_m)
\]

\[
= \sum_{m=0}^\infty \gamma_m (f | \varphi_m) - \sum_{n=0}^\infty (\varphi_n | f^* \gamma_n. \tag{3.13}
\]

If \( \sum_{m=0}^\infty \gamma_m (f | \varphi_m) \) and \( \sum_{n=0}^\infty (\varphi_n | f^* \gamma_n \) both converge to \( (f | g) \), (3.9) is satisfied, and the use of the divergent orthogonal expansion \( f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) in the inner product \( (f | g) \) produces the correct result.

The requirement, that the infinite series in (3.13) have to converge, makes it possible to characterize the subset \( \mathcal{F} \subset \mathcal{H} \) defined by (3.5) more precisely. The expansion \( g = \sum_{n=0}^\infty (\varphi_n | g) \varphi_n \) converges in the mean if the coefficients \( (\varphi_n | g) \) decay more rapidly than \( n^{-1/2} \) as \( n \to \infty \). Since \( f \notin \mathcal{H} \), the coefficients \( (\varphi_n | f) \) of the expansion \( f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) either decay less rapidly than \( n^{-1/2} \) as \( n \to \infty \) or they may even diverge as \( n \to \infty \). Thus, the coefficients \( (\varphi_n | g) \) in (3.12) have to decay so fast as \( n \to \infty \) that the infinite series \( (f | g) = \sum_{n=0}^\infty (f | \varphi_n)(\varphi_n | g) \) converges. This is certainly the case if the coefficients \( (f | \varphi_n)(\varphi_n | g) \) decay more rapidly than \( 1/n \) as \( n \to \infty \).

Divergent orthogonal expansions \( f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) with \( f \notin \mathcal{H} \) possess the characteristic features of generalized functions in the sense of Schwartz [3]: Although divergent in the mean, such an expansion is meaningful in inner products \( (f | g) \) as long as \( g \) is restricted to the proper subset \( \mathcal{F} \subset \mathcal{H} \) defined by (3.3). If \( g \notin \mathcal{F} \), the divergent orthogonal expansion \( f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) cannot be used in the inner product \( (f | g) \) since the infinite series \( (f | g) = \sum_{m=0}^\infty (f | \varphi_m)(\varphi_m | g) \) diverges.

Conceptually, this situation very much resembles the theory of rigged Hilbert spaces or Gelfand triplets \( \Phi \subset \mathcal{H} \subset \Phi^\times \). Here, \( \mathcal{H} \) is a Hilbert space, \( \Phi \) is a suitably restricted subset of \( \mathcal{H} \), and \( \Phi^\times \) is its dual space defined by the condition that inner product \( (u | v) \) with \( u \in \Phi^\times \) and \( v \in \Phi \) remains finite. Loosely speaking, we may say that the more we restrict the subset \( \Phi \subset \mathcal{H} \), the larger its dual space \( \Phi^\times \) becomes. A very readable account of rigged Hilbert spaces from the perspective of quantum
mechanics and their relationship with Dirac’s bra and ket formalism can be found in the book by Ballentine [65, Chapter 1.4].

The insight, that divergent orthogonal expansions \( f = \sum_{n=0}^{\infty}(\varphi_n|f)\varphi_n \) with \( f \notin \mathcal{H} \) are essentially generalized functions and can be used in a mathematical rigorous way in inner products \((f|g)\) with \( g \in \mathcal{F} \), does not imply that all problems with the use of these divergent series are solved. The characterization of the subset \( \mathcal{F} \subset \mathcal{H} \) is the crucial step that makes these divergent expansions mathematically meaningful in inner products \((f|g)\). But in real life applications, the characterization of \( \mathcal{F} \) may turn out be the most difficult problem that can occur in this context.

4 One-Range Addition Theorems for the Coulomb Potential

Let us assume that \( f \) belongs to the Hilbert space \( L^2(\mathbb{R}^3) \) of square integrable functions defined by (B.5) and that the functions \( \{\varphi_{n,\ell}^m(r)\}_{n,\ell,m} \) are complete and orthonormal in \( L^2(\mathbb{R}^3) \). As discussed in more details in [41, Section 3], a one-range addition theorem for \( f(r \pm r') \), which converges in the mean with respect to the norm of \( L^2(\mathbb{R}^3) \), can be constructed by expanding \( f \) in terms of the orthonormal functions \( \{\varphi_{n,\ell}^m(r)\}_{n,\ell,m}^m \):

\[
\begin{align*}
    f(r \pm r') &= \sum_{n,\ell,m} C_{n,\ell}^m(f; \pm r') \varphi_{n,\ell}^m(r), \quad (4.1a) \\
    C_{n,\ell}^m(f; \pm r') &= \int \left[\varphi_{n,\ell}^m(r)\right]^* f(r \pm r') d^3r. \quad (4.1b)
\end{align*}
\]

The expansion (4.1) is indeed a one-range addition theorem, since the variables \( r \) and \( r' \) are completely separated: The dependence on \( r \) is entirely contained in the functions \( \varphi_{n,\ell}^m(r) \), whereas \( r' \) occurs only in the expansion coefficients \( C_{n,\ell}^m(f; \pm r') \) which are overlap integrals.

If the overlap integrals \( C_{n,\ell}^m(f; \pm r') \) can be expanded in terms of the functions \( \varphi_{n,\ell}^m(r') \) according to

\[
\begin{align*}
    C_{n,\ell}^m(f; \pm r') &= \sum_{n',\ell',m'} T_{n',\ell',m'}^{n\ell m}(f; \pm r') \varphi_{n',\ell'}^m(r'), \quad (4.2a) \\
    T_{n',\ell',m'}^{n\ell m}(f; \pm) &= \int \left[\varphi_{n',\ell'}^m(r')\right]^* C_{n,\ell}^m(f; \pm r') d^3r', \quad (4.2b)
\end{align*}
\]

then the addition theorem (4.1) assumes a completely symmetrical form:

\[
\begin{align*}
    f(r \pm r') &= \sum_{n,\ell,m} \sum_{n',\ell',m'} T_{n,\ell,n',\ell',m'}^{n\ell m}(f; \pm) \varphi_{n,\ell}^m(r) \varphi_{n',\ell'}^m(r'). \quad (4.3)
\end{align*}
\]

As is well known in approximation theory, a nontrivial weight function \( w(r) \neq 1 \) can give more weight to those regions of space in which \( f \) is large, while deemphasizing the contribution from those regions in which \( f \) is small. Accordingly, the inclusion
of a suitable weight function \( w : \mathbb{R}^3 \to \mathbb{R}_+ \) can improve convergence. It is thus an obvious idea to construct one-range addition theorems that converge with respect to the norm of a weighted Hilbert space \( L^2_w(\mathbb{R}^3) \) defined in (B.8). If \( f \in L^2_w(\mathbb{R}^3) \), we can construct a one-range addition theorem by expanding \( f(r \pm r') \) with respect to a function set \( \{ w_{n,\ell}^{m}(r) \} \) that is complete in \( L^2_w(\mathbb{R}^3) \) and orthonormal with respect to the modified inner product (B.6) \( \langle \psi, \phi \rangle = \int \psi^* \phi \, w \, d^3r \).

In the articles [3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37], Guseinov and coworkers derived and applied one-range addition theorems in connection with the special weight function \( w(r) = r^k \) with \( k = -1, 0, 1, 2, \ldots \) and used Guseinov’s functions \( k \Psi_{n,\ell}^{m}(\beta, r) \) defined by (D.1) as expansion functions. This yields one-range addition theorems of the following general kind:

\[
f(r \pm r') = \sum_{n, \ell, m} k \Gamma_{n,\ell,m}^{n',\ell',m'}(f; \beta, \pm) \, k \Psi_{n,\ell}^{m}(\beta, r) \, k \Psi_{n',\ell'}^{m'}(\beta, r'), \tag{4.4a}
\]

\[
k \Gamma_{n,\ell,m}^{n',\ell',m'}(f; \beta, \pm) = \int \left[ k \Psi_{n',\ell'}^{m'}(\beta, r') \right]^* \left( r'^k \right) k \Psi_{n,\ell}^{m}(f; \beta, \pm r') \, d^3r', \tag{4.4b}
\]

\[
k C_{n,\ell}(f; \beta, \pm r') = \int \left[ k \Psi_{n,\ell}^{m}(\beta, r) \right]^* r^k f(r \pm r') \, d^3r. \tag{4.4c}
\]

If \( f \in L^2_{r,k}(\mathbb{R}^3) \), this addition theorem converges in the mean according to the norm (D.3) of the weighted Hilbert space \( L^2_{r,k}(\mathbb{R}^3) \).

As discussed in more details in [41 Section 4], Guseinov derived in this way one-range addition theorems, for example for Slater-type functions with integral and nonintegral principal quantum numbers defined by (1.1). For fixed \( k = -1, 0, 1, 2, \ldots \), Guseinov’s functions satisfy the orthogonality condition (D.2) and they are complete and orthonormal in the weighted Hilbert space \( L^2_{r,k}(\mathbb{R}^3) \) defined by (D.5). As long as the Slater-type functions, which are to be expanded, belong to the weighted Hilbert space \( L^2_{r,k}(\mathbb{R}^3) \), this is a completely legitimate approach that leads to one-range addition theorems for Slater-type functions which converge in the mean with respect to the norm (D.4) of \( L^2_{r,k}(\mathbb{R}^3) \).

The Coulomb potential plays a central role in electronic structure calculations, and the evaluation of inter-electronic repulsion integrals of the type of (2.4) leads to formidable computational problems, in particular if the densities \( f \) and \( g \) in (2.4) are two-center charge densities of the type of \( u(r - A)v(r - B) \) with \( A, B \in \mathbb{R}^3 \). Therefore, it would be desirable to have a one-range addition theorem for the Coulomb potential. In [17], Guseinov tried to accomplish this by expanding \( 1/|r - r'| \) in terms of functions \( k \Psi_{n,\ell}^{m}(\beta, r) \). Formally, Guseinov’s approach leads to the following symmetrical one-range addition theorems:

\[
\frac{1}{|r - r'|} = \sum_{n, \ell, m} k \Gamma_{n,\ell,m}^{n',\ell',m'}(\beta) \, k \Psi_{n,\ell}^{m}(\beta, r) \, k \Psi_{n',\ell'}^{m'}(\beta, r'), \tag{4.5a}
\]

\[
k \Gamma_{n,\ell,m}^{n',\ell',m'}(\beta) = \int \left[ k \Psi_{n',\ell'}^{m'}(\beta, r') \right]^* r^k \, k C_{n,\ell}^{m}(\beta, r') \, d^3r', \tag{4.5b}
\]
\[ \kappa C_{n,\ell}^m(\beta, \mathbf{r}') = \int [k \Psi_{n,\ell}^m(\beta, \mathbf{r})]^* \frac{r^k}{|\mathbf{r} - \mathbf{r}'|} \, d^3\mathbf{r}. \]  

(4.5c)

There are, however, some principal problem with these orthogonal expansions which Guseinov had either overlooked or ignored in his earlier work and which he still ignored in his most recent preprints [44, 45, 46], although I had emphasized their importance in [41]. In order to convince both Guseinov as well as other skeptical readers, I presented in Section 3 a detailed discussion of the properties of orthogonal expansions. The central features of these expansions can be summarized as follows:

1. If \( f \) belongs to some Hilbert space \( \mathcal{H} \), then \( f \) can be expanded in terms of a function set \( \{\varphi_n\}_{n=0}^\infty \) that is complete and orthonormal in \( \mathcal{H} \), and the expansion \( \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) converges to \( f \) in the mean with respect to the norm of \( \mathcal{H} \).

2. If \( f \notin \mathcal{H} \), the formal orthogonal expansion \( f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) diverges in the mean with respect to the norm of \( \mathcal{H} \).

3. Nevertheless, such a divergent orthogonal expansion \( f = \sum_{n=0}^\infty (\varphi_n | f) \varphi_n \) can produce meaningful results in inner products \( (f | g) \) as long as \( g \) is restricted to the proper subset \( \mathcal{F} \subset \mathcal{H} \) defined by (3.5).

The weighted Hilbert spaces \( L^2_{r^k}(\mathbb{R}^3) \) with \( k = -1, 0, 1, 2, \ldots \) are based on the inner product (D.3) which involves an integration over the whole three-dimensional space \( \mathbb{R}^3 \) with weight function \( w(r) = r^k \). The Coulomb potential \( 1/|\mathbf{r} - \mathbf{r}'| \) does not belong to any of the weighted Hilbert spaces \( L^2_{r^k}(\mathbb{R}^3) \) which Guseinov implicitly used in his work. This implies that the one-range addition theorems (4.5) of the Coulomb potential diverge for \( k = -1, 0, 1, 2, \ldots \) in the mean with respect to the norms (D.4) of the weighted Hilbert spaces \( L^2_{r^k}(\mathbb{R}^3) \).

Guseinov was not the first one who had derived a divergent expansion for the Coulomb potential in terms of a complete and orthonormal function set. Salmon, Birss, and Ruedenberg [66] derived a bipolar expansion of the Coulomb potential in terms of the Gaussian-type eigenfunctions of a three-dimensional isotropic harmonic oscillator which are complete and orthonormal in the Hilbert space \( L^2(\mathbb{R}^3) \) of square integrable functions. However, Silverstone and Kay [67] demonstrated that this expansion diverges, which was confirmed by Ruedenberg and Salmon [68]. Apparently, this observation was some kind of death sentence for the bipolar expansion of Salmon, Birss, and Ruedenberg [66]. As far as I know, nobody has ever used this expansion.

The divergence of the one-range addition theorems (4.5) for the Coulomb potential cannot be ignored. So, we are confronted with the question what we should do with these addition theorems. We could dismiss them as practically useless and ignore them, as it was done with the divergent bipolar expansion of Salmon, Birss, and Ruedenberg [66]. However, I think that this would be premature. Salmon, Birss, and Ruedenberg published their divergent bipolar expansion in 1968, and we now have a much better understanding of generalized functions and we also know much more about numerically efficient summation techniques which often can associate a finite value to a divergent series (see also the discussion in [41, pp. 24 - 25]).
As discussed in Section 3, divergent expansions of the type of (4.5) can nevertheless be practically useful as long as they are exclusively used in suitably restricted functionals. Thus, these functions are essentially generalized functions in the sense of Schwartz [48]. Obviously, this offers new perspectives, but one must not forget that in relationships involving generalized functions one always has to be extremely careful about their domains of validity.

Consequently, it is not acceptable to proceed like Guseinov and to ignore the distributional nature of divergent one-range addition theorems of the type of (4.5) and to treat them like ordinary orthogonal expansions that converge in the mean. It is absolutely essential to formulate regularity conditions for functionals – in our case multicenter integrals – and to take them into account. Otherwise, the use of distributional one-range addition theorems in multicenter integrals would be purely experimental. Virtually every outcome would be possible, depending on the other functions occurring in the integral. The fact that Guseinov apparently encountered no problems in his numerical examples does not prove anything.

I do not expect that it will be easy to formulate the necessary regularity conditions. Firstly, the Coulomb potential is in spite of its apparent simplicity a relatively complicated mathematical object (see for example [61, Chapter 9]). Secondly, I fear that for every type of multicenter integral containing the Coulomb potential a new set of regularity conditions has to be formulated.

In [41, p. 23], a possible strategy based on orthogonal expansions of the charge densities \( f \) and \( g \) in Coulomb integrals \( C(f, g) \) defined by (2.4) was sketched. It cannot be denied that this approach would be highly pedestrian, and more elegant and more powerful alternatives would be highly desirable. It seems that a lot of work remains to be done before distributional one-range addition theorems of the type of (4.5) can safely and effectively be applied in multicenter integrals.

The idea of using distributional orthogonal expansions, which diverge in the mean and converge only weakly in suitably restricted functionals, is not new. In [69], I derived expansions of the plane wave \( \exp(i \cdot r) \) in terms of complete orthonormal and biorthogonal function sets that converge only weakly. In some cases, these expansions simplify the evaluation of Fourier transforms, and they can also be used for the construction of one-range addition theorems (see [64] or [69, Section VII]).

Expansions for the plane wave, that closely resemble those derived in [69], were also constructed by Guseinov [6, Eqs. (45) - (46)]. Guseinov, who did not mention [69] in [6], either overlooked or deliberately ignored the obvious fact that the plane wave does not belong to any of the Hilbert spaces which he implicitly used. Accordingly, Guseinov’s expansion diverge in the mean and can only converge weakly. Guseinov’s oversight is hard to understand because he had cited [69] in several other articles [3, 11, 12, 18, 19, 27, 28, 32].

5 Guseinov’s Rearranged Addition Theorems

As discussed in Section 3, orthogonal expansions play a central role in Hilbert spaces and also in approximation theory. In contrast, nonorthogonal expansions are largely
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ignored. Of course, there are many good reasons for this neglect. In the context of one-range addition theorems, the most important evidence speaking against the use of nonorthogonal functions is the following well established fact: If a function set \( \{ \varphi_n \}_{n=0}^{\infty} \) is only complete in a given Hilbert space \( \mathcal{H} \), but not orthogonal, then it is general only possible to construct finite approximations to \( f \in \mathcal{H} \) of the type of (3.1) by minimizing the mean square deviation (3.2), but the existence of formal expansions of the type of (3.3) in terms of nonorthogonal functions is not guaranteed: Thus, nonorthogonal expansions may or may not exist. This fact is documented quite extensively in the mathematical literature (see for example [49, Theorem 10 on p. 54] or [50, Section 1.4]) or also in the literature on electronic structure calculations [51, 52, 53, 54, 55, 56]). Horrifying examples of pathologies of nonorthogonal expansions can be found in [55, Section III.I].

Of course, there are situations in which nonorthogonal expansions offer computational advantages (see for example the discussion in [70]). However, in the vast majority of all cases, orthogonal expansions have clearly superior properties. Consequently, one should not voluntarily abandon the highly useful feature of orthogonality unless there are truly compelling reasons.

In [41, 42], Guseinov derived one-range addition theorems for Slater-type functions with integral and nonintegral principal quantum numbers of the type of (4.1) by expanding them in terms of his complete and orthonormal functions \( k \Psi_{n,\ell}^m(\beta, \mathbf{r}) \). As long as the Slater-type functions belong to the weighted Hilbert spaces \( L^2_{\alpha}(\mathbb{R}^3) \) defined by (D.5) with \( k = -1, 0, 1, 2, \ldots \), these addition theorem converge in the mean with respect to the norms (D.4) of these Hilbert spaces.

For reasons, which I do not really understand, Guseinov considered it to be advantageous to replace in his one-range addition theorems for Slater-type functions his complete and orthonormal functions \( k \Psi_{n,\ell}^m(\beta, \mathbf{r}) \) by nonorthogonal Slater-type functions with integral principal quantum numbers via [41, Eq. (6.4)]

\[
k \Psi_{n,\ell}^m(\beta, \mathbf{r}) = 2^\ell \left[ \frac{(2\beta)^{k+3} (n + \ell + k + 1)!}{(n - \ell - 1)!} \right]^{1/2} \sum_{\nu=0}^{n-\ell-1} \frac{(-n + \ell + 1)^\nu 2^n}{(2\ell + k + \nu + 2)! (2\ell + k + \nu)!} \chi_{\nu+\ell+1,\ell}^m(\beta, \mathbf{r})
\]

and to rearrange the order of summations of the resulting expansions. Guseinov constructed in this way expansions of Slater-type functions \( \chi_{N,L}^M(\beta, \mathbf{r} \pm \mathbf{r}') \) with in general nonintegral principal quantum numbers \( N \in \mathbb{R} \setminus \mathbb{N} \) in terms of Slater-type functions \( \chi_{n,\ell}^m(\beta, \mathbf{r}) \) with integral principal \( n \in \mathbb{N} \) quantum numbers located at a different center (see also [41, Section 6]).

As is well known, Slater-type functions are complete in all Hilbert space implicitly used by Guseinov (for a proof, see [53, Section 4]), but not orthogonal. In view of the principal problems mentioned above, it is therefore not at all clear whether Guseinov’s rearranged addition theorems are mathematically meaningful. Accordingly, I claimed in [41, Section 6]) that Guseinov’s rearrangements of his one-range addition theorems, which are expansions in terms of his functions \( k \Psi_{n,\ell}^m(\beta, \mathbf{r}) \) and thus
ultimately expansions in terms of generalized Laguerre polynomials $L_{n-\ell-1}^{(2\ell+k+2)}(2\beta r)$, are dangerous and potentially disastrous and that their validity has to be checked.

In [44, p. 7], Guseinov disagreed and claimed this his Eq. (3.11) – a finite nested sum containing his functions $\Psi_{n,\ell}^m(\beta, r)$ on the left-hand side and Slater-type functions $\chi_{n,\ell}^m(\beta, r)$ with integral principal quantum numbers on the right-hand side – proves the validity and mathematical soundness of his approach.

I do not question the validity of Guseinov’s Eq. (3.11), but I very much disagree with Guseinov’s conclusion that his Eq. (3.11) proves the validity of his rearrangements. The problem with Guseinov’s reasoning is that he does not distinguish carefully between rearrangements of finite and infinite sums. Obviously, a finite sum

$$F_N(x) = \sum_{n=0}^{N} \lambda_n^{(\alpha)} L_n^{(\alpha)}(x), \quad N \in \mathbb{N}_0, \quad (5.2)$$

of generalized Laguerre polynomials $L_n^{(\alpha)}(x)$ multiplied by purely numerical coefficients $\lambda_n^{(\alpha)}$ can always be rearranged. If we insert the explicit expression (C.1) of the generalized Laguerre polynomials into (5.2) and rearrange the order of summations, we obtain

$$F_N(x) = \sum_{\nu=0}^{N} \frac{(-x)^\nu}{\nu!} \sum_{\mu=0}^{N-\nu} \frac{(\alpha + \nu + 1)^\mu}{\mu!} \lambda_{\mu+\nu}^{(\alpha)}. \quad (5.3)$$

But if we now perform in the finite sum (5.2) the limit $N \to \infty$ and consider instead the rearrangement of the infinite series

$$F(x) = \lim_{N \to \infty} F_N(x) = \sum_{n=0}^{\infty} \lambda_n^{(\alpha)} L_n^{(\alpha)}(x), \quad (5.4)$$

the situation is much more complicated and many things can go wrong. Formally, a rearrangement of $F(x)$ yields the following power series in $x$:

$$F(x) = \sum_{\nu=0}^{\infty} \frac{(-x)^\nu}{\nu!} \sum_{\mu=0}^{\infty} \frac{(\alpha + \nu + 1)^\mu}{\mu!} \lambda_{\mu+\nu}^{(\alpha)}. \quad (5.5)$$

This power series for $F(x)$ makes sense if and only if the inner series on the right-hand side of (5.5) converges for every $\nu \in \mathbb{N}_0$. In addition, the inner series in $\mu$ has to produce values that do not increase too strongly with increasing $\nu$, because otherwise the right-hand side of (5.5) diverges for every $|x| > 0$. In the case of an essentially arbitrary function $F(x)$, these two conditions are not necessarily satisfied. It is also easy to show that the convergence of the Laguerre expansion for $F(x)$ with respect to the norm of the Laguerre-type Hilbert space $L^2_{e^{-\alpha x}}(\mathbb{R}_+)$ defined by (C.3) does not imply the convergence of the inner series over $\mu$ on the right-hand side of (5.5) for every $\nu \in \mathbb{N}_0$.

Special attention deserves the case that $F(x)$ is not an analytic function in the sense of complex analysis at the expansion point $x = 0$. In this case, the rearranged power series on right-hand side of (5.5) cannot exist because all but a finite number
of series coefficients are infinite, even if the Laguerre expansion for $F(x)$ exists and converges in the mean with respect to the norm of $L^2_{e^{-x^2}}(\mathbb{R}^+)$. Accordingly, I see no reason to alter my assessment [41, p. 18] that Guseinov’s rearrangements are dangerous and potentially disastrous, and that their validity must be checked explicitly.

The rearrangements of the finite sum $F_N(z)$ or of the infinite series $F(z)$ yielding (5.3) and (5.5), respectively, are special cases of the rearrangements of double series $\sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{m,n}$. This is an old and extensively studied topic in the theory of infinite series. The most detailed treatment, which I am aware of, can be found in the book by Bromwich [71, Chapter V]. Loosely speaking, the rearrangement of such a double series is safe if the double series converges absolutely. In the case of expansions in terms of orthogonal polynomials, we cannot tacitly assume absolute converge.

So, we have good reason to assume that Guseinov’s rearrangements of one-range addition theorems are dangerous and potentially disastrous. Of course, it is not satisfactory if we only know that a given mathematical manipulation is dangerous. Instead, we would like to know with certainty whether this operation is legitimate or not.

Unfortunately, one-range additions theorems for exponentially decaying functions are fairly complicated mathematical objects, and explicit proofs of their convergence and/or divergence are very difficult. Most likely, such an investigation would be a nontrivial research problem in its own right. Since I am convinced that Guseinov’s rearrangements are basically a bad idea, I saw no point in spending too much time and effort. Therefore, I looked for simpler alternatives to a detailed convergence analysis, even if these alternatives would not answer all questions of interest.

As shown in [41, Section 6], valuable insight can in some cases be gained by considering not the complicated one-range addition theorems themselves, but their much simpler one-center limits. Let us therefore assume that we succeeded in constructing a one-range addition theorem of the type of (4.4) for some function $f(\mathbf{r} \pm \mathbf{r}')$ by expanding it in terms of Guseinov’s functions. If we now consider its one-center limit by setting $\mathbf{r}' = 0$, our addition theorem must simplify to yield the expansion of $f(\mathbf{r})$ in terms of Guseinov’s functions:

$$f(\mathbf{r}) = \sum_{n, \ell} k F_{n, \ell}^m(\beta; f) k \Psi_{n, \ell}^m(\beta, \mathbf{r}), \quad (5.6a)$$

$$k F_{n, \ell}^m(\beta; f) = \int \left[ k \Psi_{n, \ell}^m(\beta, \mathbf{r}) \right]^* r^k f(\mathbf{r}) \, d\mathbf{r}. \quad (5.6b)$$

Under fortunate circumstances, the mathematical nature of such an identity allows conclusions about the legitimacy of Guseinov’s rearrangements.

Let us now assume that we succeeded in deriving a one-range addition theorem of the type of (4.4) by expanding Slater-type functions $\chi_{N,L}^N(\beta, \mathbf{r} \pm \mathbf{r}')$ with in general nonintegral principal quantum numbers $N \in \mathbb{R} \setminus \mathbb{N}$ in terms of Guseinov’s functions $k \Psi_{n, \ell}^m(\beta, \mathbf{r})$ with equal scaling parameters $\beta > 0$ (see for example [41, Eq. (6.1)] with $\beta = \gamma$). If we now set $\mathbf{r}' = 0$ in this addition theorem, it must simplify to yield the
following expansion of $\chi_{N,L}^M(\beta, r)$ in terms of Guseinov’s functions:

$$\chi_{N,L}^M(\beta, r) = \frac{(2\gamma)^{-(k+3)/2}}{2N-1} \Gamma(N + L + k + 2)$$

$$\times \sum_{\nu=0}^{\infty} \frac{(-N + L + 1)_\nu}{[(\nu + 2L + k + 2)]^\nu} \frac{1}{\nu!^2}$$

$$k \Psi_{\nu+1,L}^M(\beta, r), \quad N \in \mathbb{R} \setminus \mathbb{N}, \quad \beta > 0, \quad k = -1, 0, 1, 2, \ldots$$

(5.7)

If $N \in \mathbb{N}$ and $N \geq L + 1$, the infinite series on the right-hand side terminates because of the Pochhammer symbol $(-N + L + 1)_\nu$.

It is easy to show that the expansion (5.7) in terms of Guseinov’s function is a special case of the following expansion [41, Eq. (5.17)] which expresses a nonintegral power $x^\mu$ with $\mu \in \mathbb{R} \setminus \mathbb{N}_0$ as an infinite series of generalized Laguerre polynomials:

$$x^\mu = \frac{\Gamma(\mu + \alpha + 1)}{\Gamma(\alpha + 1)} \sum_{n=0}^{\infty} \frac{(-\mu)_n}{(\alpha + 1)_n} L_n^{(\alpha)}(x),$$

$$\mu \in \mathbb{R} \setminus \mathbb{N}_0, \quad \text{Re}(\mu + \alpha) > -1, \quad \text{Re}(\alpha) > -1.$$ (5.8)

If we set $\mu = m$ with $m \in \mathbb{N}_0$, the infinite series on the right-hand side terminates because of the Pochhammer symbol $(-m)_n$.

In [41 Eqs. (6.9) - (6.11)], it was shown that it is not possible to transform the Laguerre expansion (5.8) for $x^\mu$ with $\mu \in \mathbb{R} \setminus \mathbb{N}_0$ to a power series in $x$ by inserting the explicit expression (C.1) of the generalized Laguerre polynomials. Interchanging the order of the nested summations yields a formal power series in $x$ [41 Eq. (6.9)]. Superficially, this looks like success. However, the coefficients of this power series can be expressed as hypergeometric series $_1F_0$ which are for all but a finite number of indices infinite [41 Eq. (6.11)].

Of course, this failure is not really surprising: The general power function $z^\mu$ with $z \in \mathbb{C}$ and $\mu \in \mathbb{C} \setminus \mathbb{N}_0$ is not analytic at $z = 0$ in the sense of complex analysis. For $\mu = m$ with $m \in \mathbb{N}_0$, Taylor expansion of $z^m$ around $z = 0$ is, however, legitimate and yields the trivial identity $z^m = z^m$.

Thus, we can conclude that in the case of equal scaling parameters $\beta > 0$ the one-center limit $r' = 0$ of Guseinov’s rearranged addition theorem for Slater-type functions $\chi_{N,L}^M(\beta, r \pm r')$ does not exist if the principal quantum number $N$ is nonintegral, $N \in \mathbb{R} \setminus \mathbb{N}$.

Let us now assume that we succeeded in deriving a one-range addition theorem of the type of [41] by expanding Slater-type functions $\chi_{N,L}^M(\beta, r \pm r')$ with in general nonintegral principal quantum numbers $N \in \mathbb{R} \setminus \mathbb{N}$ in terms of Guseinov’s functions $k \Psi_{n,\ell}^m(\gamma, r)$ with different scaling parameters $\beta \neq \gamma > 0$ (see for example [41 Eq. (6.1)]) If we now set $r' = 0$ in this addition theorem, it must simplify to yield the following expansion of $\chi_{N,L}^M(\beta, r)$ in terms of Guseinov’s functions with different
scaling parameter $\gamma \neq \beta > 0$:

$$
\chi_{N,L}^{M}(\beta, r) = \frac{(2\gamma)^{L+(k+3)/2} \beta^{N-1}}{[\beta + \gamma]^{N+L+k+2}} \frac{\Gamma(N + L + k + 2)}{(2L + k + 2)!} \times \sum_{\nu=0}^{\infty} \left[ \frac{(\nu + 2L + k + 2)!}{\nu!} \right]^{1/2} k^{M}_{\nu+L+1,L}(\gamma, r) \times 2F_1 \left( -\nu, N + L + k + 2; 2L + k + 3; \frac{2\gamma}{\beta + \gamma} \right),$$

$$N \in \mathbb{R} \setminus \mathbb{N}, \quad \beta, \gamma > 0. \quad (5.9)$$

If we set $\gamma = \beta$, we of course obtain (5.7).

It is easy to show that (5.9) is a special case of the following expansion [41, Eq. (6.12)]:

$$
 x^{\mu} e^{ux} = (1-u)^{-\alpha-\mu-1} \frac{\Gamma(\alpha + \mu + 1)}{\Gamma(\alpha + 1)} \times \sum_{n=0}^{\infty} 2F_1 \left( -n, \alpha + \mu + 1; \alpha + 1; \frac{1}{1-u} \right) L_n^{(\alpha)}(x),

\mu \in \mathbb{R} \setminus \mathbb{N}_0, \quad \text{Re}(\mu + \alpha) > -1, \quad u \in (-\infty, 1/2). \quad (5.10)

The condition $-\infty < u < 1/2$ is necessary to guarantee that this expansion converges in the mean with respect to the norm of the weighted Hilbert space $L^2_{e^{-x}\alpha}(\mathbb{R}^+)$.

If we insert the explicit expression (C.1) of the generalized Laguerre polynomials into (5.10) and interchange the order of summations, we also obtain a formal power series in $x$. Unfortunately, an analysis of the resulting power series becomes very difficult because of the terminating Gaussian hypergeometric series $2F_1$ in (5.10) (probably, an analysis of the behavior of this $2F_1$ as $n \to \infty$ would be a nontrivial research project in its own right). However, we can argue that the function $z^{\mu} \exp(uz)$ with $\mu, u, z \in \mathbb{C}$ is only analytic at $z = 0$ in the sense of complex analysis if $\mu$ is a nonnegative integer, $\mu = m$ with $m \in \mathbb{N}_0$, yielding $z^{\mu} \exp(uz) = \sum_{n=0}^{\infty} u^n z^{m+n}/n!$. If $\mu$ is nonintegral, $\mu \in \mathbb{C} \setminus \mathbb{N}_0$, a power series expansion of $z^{\mu} \exp(uz)$ around $z = 0$ does not exist.

Thus, also for different scaling parameters $\beta \neq \gamma$, the one-center limit $r' = 0$ of the rearranged addition theorems for $\chi_{N,L}^{M}(\beta, r \pm r')$ does not exist if the principal quantum number $N$ is nonintegral, $N \in \mathbb{R} \setminus \mathbb{N}$.

Apparently, Guseinov deliberately ignores even now the fact that the Laguerre expansions (5.8) for $x^{\mu}$ and (5.10) for $x^{\mu} e^{ux}$ cannot be transformed to power series expansions in $x$ if $\mu \in \mathbb{R} \setminus \mathbb{N}_0$, although this had been emphasized in [41, pp. 18 - 19]. In [45, Eqs. (5) - (6)], Guseinov expanded Slater-type functions $\chi_{N,L}^{M}(\beta, r)$ with nonintegral principal quantum numbers as an infinite series of Slater-type functions $\chi_{n,L}^{m}(\beta, r)$ with integral principal quantum numbers, although these expansions do not exist since their terms are for all but a finite number of indices infinite. In [45, Eqs. (7) - (10)], Guseinov tried to resell essentially the same nonexisting expansion for
what he calls *Coulomb-Yukawa like correlated interaction potentials*, which are apart from a different normalization nothing but special Slater-type functions.

From a mathematical point of view, a one-range addition theorem for a function $f(r \pm r')$ is a mapping $\mathbb{R}^3 \times \mathbb{R}^3 \rightarrow \mathbb{C}$. In my opinion, one-range addition theorems have the highly advantageous feature that they provide a *unique* infinite series representation of $f(r \pm r')$ with *separated* variables $r$ and $r'$ that is valid for the *whole* argument set $\mathbb{R}^3 \times \mathbb{R}^3$. If we accept this premise, then we have to conclude that Guseinov’s manipulations, which produced his rearranged addition theorems for Slater-type functions $\chi^M_{N,L}(\beta, r \pm r')$, are at least in the case of nonintegral principal quantum numbers $N \in \mathbb{R} \setminus \mathbb{N}$ a complete failure.

The analysis of the one-center limits of rearranged one-range addition theorems provides valuable insight in the case of Slater-type functions with nonintegral principal quantum numbers, but it does not answer all questions. In particular, my nonanalyticity argument allows no conclusions about the validity of Guseinov’s rearrangements in the case of Slater-type functions with integral principal quantum numbers. Another interesting but open question is whether Guseinov’s rearrangements are in the case nonintegral principal quantum numbers invalid for the whole argument set $\mathbb{R}^3 \times \mathbb{R}^3$ or whether they are invalid only in the one-center limit. This is a practically very relevant question. If only the one-center limit is invalid, then it would be conceivable that Guseinov’s rearranged one-range addition theorems might be mathematically meaningful or possibly even numerically useful in a restricted sense as approximations, although they do not exist for the whole argument set $\mathbb{R}^3 \times \mathbb{R}^3$. This has to be investigated.

These examples show that the situation is much more complicated than originally anticipated by Guseinov. Obviously, a lot of work remains to be done before we can claim with some confidence that we understand the subtleties of Guseinov’s rearrangements sufficiently well. It should also be clear that the burden of proof lies in all cases with Guseinov.

Nevertheless, I do not think that it would be a good idea to invest too much time and effort into an analysis of these most likely very difficult open questions. In my opinion, it is simply a bad idea to construct one-range addition theorems that use nonorthogonal functions as expansion functions. It would be much better to focus on those one-range addition theorems that are expansions in terms of complete and orthonormal function sets.

The principal superiority of orthogonal expansion functions becomes particularly evident in the case of one-range addition theorems of the type of (4.5) that do not converge in the mean with respect to the norm of an appropriate Hilbert space, but only weakly in the sense of generalized functions in suitably restricted functionals.

For example, in Section 3 I analyzed under which conditions inner products $(f|g)$ with $f \notin \mathcal{H}$ and $g \in \mathcal{H}$ are mathematically meaningful and whether the divergent orthogonal expansion $f = \sum_{n=0}^{\infty} (\varphi_n|f) \varphi_n$ can be used in these inner products. I showed that if $g$ belongs to the subset $\mathcal{F} \subset \mathcal{H}$ defined by (3.5), then the expansion $(f|g) = \sum_{n=0}^{\infty} (f|\varphi_n)(\varphi_n|g)$ converges if the expansion coefficients $(f|\varphi_n)(\varphi_n|g)$ decay more rapidly than $1/n$ as $n \rightarrow \infty$.

Ignoring all questions of convergence or existence, let us now assume that both $f$
and \( g \) can be expanded at least formally in terms of a complete, but nonorthogonal function set \( \{ \psi_n \}_{n=0}^{\infty} \):

\[
\begin{align*}
    f &= \sum_{m=0}^{\infty} F^{(\psi)}_m \psi_m, \\
    g &= \sum_{n=0}^{\infty} G^{(\psi)}_n \psi_n.
\end{align*}
\]

(5.11)

(5.12)

If we insert these expansions into the inner product \((f|g)\), we formally obtain the following double series:

\[
(f|g) = \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} [F^{(\psi)}_m]^* G^{(\psi)}_n (\psi_m|\psi_n).
\]

(5.13)

There can be no doubt that it would be much harder to formulate convergence criteria for this complicated double series than for the comparatively simple series \((f|g) = \sum_{m=0}^{\infty} (f|\varphi_m)(\varphi_m|g)\) which we obtain if we expand \( f \) and \( g \) in terms of a complete and orthonormal function set \( \{ \varphi_n \}_{n=0}^{\infty} \).

This simple example shows that it is a highly dubious idea to expand generalized functions in the sense of Schwartz [48] in terms of nonorthogonal function sets. At best, we would be confronted with nontrivial technical problems.

### 6 Summary and Conclusions

To some extent, divergent series are the dominant theme of this Reply. I am fully aware that divergent series have been and to some extent still are a highly controversial topic. There are still many who thoroughly dislike divergent series and think that they should be banned from the realm of rigorous mathematics. In their opinion, divergent series should at best be considered to be some kind of mathematical pornography. In addition, there are many others who – either because of ignorance or because of over-confidence – wrongly believe that divergent series cannot occur in their work and who thus tend to ignore questions of convergence.

It is now widely accepted that divergent series play a very useful role. They are indispensable tools in mathematics and in particular also in the mathematical treatment of scientific problems. Skeptical readers, who still prefer to ignore divergent series, should search Google Scholar (http://scholar.google.com/) for “divergent series” or for related topics. They will be surprised by the large number of applications of divergent series in different scientific disciplines.

There are principal differences between the divergent orthogonal expansions considered in this Reply and the more familiar divergent power series, which for instance occur abundantly in quantum mechanical perturbation expansions or as asymptotic expansions for special functions. Divergent power series can be used for the numerical evaluation of the function they represent: With the help of suitable summation techniques as for instance Borel summation, Padé approximants, or nonlinear sequence
transformations it is frequently possible to associate a finite value to a divergent power series.

In contrast, it is not intended to use the divergent orthogonal expansions of this Reply for the direct numerical evaluation of the function they represent. We only want to use these expansions in suitable functionals – typically multicenter integrals – because we hope for some formal simplifications. Actually, this applies to all one-range addition theorems: They are only intermediate results which ultimately produce series expansions for multicenter integrals.

The use of convergent expansions in integrals has the undeniable advantage that normally only comparatively mild assumptions are needed to guarantee that integration and summation can be interchanged and that the resulting expansions converge. Nevertheless, the use of convergent expansions in integrals is to some extent a luxury and not strictly necessary. We are free to use a divergent expansion in an integral and interchange integration and summation if we can guarantee that the resulting expansion converges to the correct result.

Obviously, such an approach gives us additional possibilities, but it would be naive to expect a free lunch: It is grossly negligent to use divergent series in integrals without explicitly knowing criteria of manageable complexity that guarantee the convergence of the resulting expansions. This is probably the most serious flaw of Guseinov’s work on one-range addition theorems. Since he is apparently completely unaware of the fact that divergent orthogonal expansions occur in his work, he has no reason to think about additional criteria which could justify the use of his divergent expansions in multicenter integrals.

In [44, Abstract], Guseinov claims that all his formulas were numerically tested, but this does not prove anything. A much more profound understanding of these divergent expansions and their domains of validity is needed, before they could be applied safely and in a mathematically rigorous way. Otherwise, the use of Guseinov’s divergent one-range addition theorems in multicenter integrals would be purely experimental.

Misconceptions about divergent series are also the core of Guseinov’s problems with his rearrangements of one-range addition theorems discussed in Section 5. It seems that Guseinov wrongly believes that it is always safe to rearrange the order of summations of double series \( \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} a_{m,n} \).

In recent years, Guseinov and coworkers were able to publish a remarkably large number of articles on one-range addition theorems [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34, 35, 36, 37, 38, 39, 40]. This fact and the dubious quality of these articles raise obvious doubts about the quality of our scientific publication system based on anonymous peer-refereeing, and also on the competence of Guseinov’s referees who also failed to understand the mathematical subtleties of one-range addition theorems.

Of course, Guseinov disagreed with this conclusion which was first expressed in [41, p. 5]. In [44, p. 3], he stated:

The respectable referees very well understand and examined the published by Guseinov and his coworkers in the years from 1978 to 2006 papers on
Unfortunately, I am not so optimistic. But it would be unfair to blame exclusively Guseinov’s referees. Refereeing Guseinov’s manuscripts is certainly not easy. It is Guseinov’s trademark to produce a large number of short and largely overlapping articles on essentially the same topic. This makes it very hard even for a very competent referee not to get lost in Guseinov’s flood of publications and to keep track of Guseinov’s truly new results. Moreover, as I know from my own experience as a referee, there is always the temptation to be less critical in the case of a short manuscript than in the case of a (very) long manuscript.

In my opinion, part of the problem are short articles. While there can be no doubt that short articles are well suited to present new experimental or computational results, they are basically unsuited for predominantly theoretical or mathematical topics.

For example, in a theoretical article on multicenter integrals, it is first necessary to provide a usually (very) long list of special functions and other abbreviations and conventions. Then, it is necessary to give a compact, but hopefully sufficiently comprehensive description of the mathematical techniques, which are to be employed. To do these things in a reasonable and for the reader beneficial way, we need at least a few pages before we can start with the derivation and description of new results.

If we nevertheless insist on writing (very) short articles, we can either shrink the in my opinion very important introductory part to an absolute minimum, or we can try to split the new results into numerous small pieces. Either alternative is undesirable: If we choose the first alternative, essential background information may be lacking and readability will most likely suffer quite a bit, and if we choose the latter alternative, we have to write numerous articles on essentially the same topic that contain virtually nothing new.

Of course, a compromise would also be possible: One could write a large number of articles with highly condensed and thus more or less incomprehensible introductory parts, that also present at best infinitesimal increments of insight.

The problems with short articles can be demonstrated convincingly by Guseinov’s recent reprint [46]. Guseinov’s only new result, which I could detect, are his Eqs. (6) - (7), which express a Slater-type function $\chi^{M}_{N,L} (\beta, r)$ with nonintegral principal quantum numbers as an infinite series of his functions $k \Psi^{m}_{n,\ell} (\gamma, r)$ and which corresponds to (5.9). In his Eqs. (8) - (9), Guseinov tried to resell his Eqs. (6) - (7) as an expansion for what he calls Coulomb-Yukawa like correlated interaction potentials, which are apart from a different normalization nothing but special Slater-type functions.

It is fairly easy to derive Guseinov’s new expansion. We only have to combine some well known properties of generalized Laguerre polynomials with a formula from the book by Gradshteyn and Ryzhik [72] Eq. (7.414.7) on p. 850]. Of course, Guseinov’s new expansion can be published, but one may wonder whether Guseinov’s new series expansion alone justifies a new article. A change of the editorial policy of scientific journals with respect to short articles on predominantly mathematical topics might be helpful.
A Terminology and Definitions

For the set of positive integers, I write \( \mathbb{N} = \{1, 2, 3, \ldots\} \), and for the set of non-negative integers, I write \( \mathbb{N}_0 = \{0, 1, 2, \ldots\} \). The real and complex numbers and the set of three-dimensional vectors with real components are denoted by \( \mathbb{R} \), \( \mathbb{C} \), and \( \mathbb{R}^3 \), respectively. \( \mathbb{R}_+ \) is the set of real numbers \( \geq 0 \).

Fourier transformation is used in its symmetrical form, i.e., a function \( f: \mathbb{R}^3 \to \mathbb{C} \) and its Fourier transform \( \tilde{f} \) are connected by the integrals

\[
\tilde{f}(\mathbf{p}) = (2\pi)^{-3/2} \int e^{-i\mathbf{p} \cdot \mathbf{r}} f(\mathbf{r}) \, d^3 \mathbf{r},
\]

(A.1)

\[
f(\mathbf{r}) = (2\pi)^{-3/2} \int e^{i\mathbf{r} \cdot \mathbf{p}} \tilde{f}(\mathbf{p}) \, d^3 \mathbf{p},
\]

(A.2)

B Hilbert Spaces

Let \( \mathcal{V} \) be a vector space over the complex numbers \( \mathbb{C} \) that possesses an inner product \( (\cdot|\cdot): \mathcal{V} \times \mathcal{V} \to \mathbb{C} \), satisfying for all \( u, v, w \in \mathcal{V} \) and for all \( \alpha \in \mathbb{C} \) [63, p. 36]

\[
(u|u) \geq 0, \tag{B.1a}
\]

\[
(u|u) = 0 \iff u = 0, \tag{B.1b}
\]

\[
(u|v+w) = (u|v) + (u|w), \tag{B.1c}
\]

\[
(u|\alpha v) = \alpha (u|v), \tag{B.1d}
\]

\[
(u|v) = (v|u)^*. \tag{B.1e}
\]

Another essential concept is the norm \( \| \cdot \|: \mathcal{V} \to \mathbb{R} \) of the elements of a vector space \( \mathcal{V} \), satisfying for all \( u, v \in \mathcal{V} \) and for all \( \alpha \in \mathbb{C} \) [63, p. 8]

\[
\|u\| \geq 0, \tag{B.2a}
\]

\[
\|u\| = 0 \iff u = 0, \tag{B.2b}
\]

\[
\|\alpha u\| = |\alpha| \|u\|, \tag{B.2c}
\]

\[
\|u+v\| \leq \|u\| + \|v\|. \tag{B.2d}
\]

Obviously, \( \|u\| = \sqrt{(u|u)} \) with \( u \in \mathcal{V} \) is a norm satisfying these conditions.

A vector space \( \mathcal{V} \) over the complex numbers \( \mathbb{C} \) is called a Hilbert space, if it possesses an inner product \( (\cdot|\cdot) \) satisfying (B.1), and if \( \mathcal{V} \) is complete with respect to the norm defined by \( \|u\| = \sqrt{(u|u)} \). Completeness implies that every Cauchy sequence in \( \mathcal{V} \) converges with respect to this norm to an element of \( \mathcal{V} \).

In bound-state electronic structure calculations, we have to take into account Born’s statistical interpretation of the wave function. Thus, an obvious inner product for functions \( f, g: \mathbb{R}^3 \to \mathbb{C} \), that can be used as basis functions in atomic and molecular electronic structure calculations, can be defined according to

\[
(f|g)_2 = \int [f(\mathbf{r})]^* g(\mathbf{r}) \, d^3 \mathbf{r}. \tag{B.3}
\]
As usual, the integration extends over the whole $\mathbb{R}^3$.

On the basis of the inner product (B.3), the norm of a function $f: \mathbb{R}^3 \to \mathbb{C}$ is defined according to

$$\|f\|_2 = \sqrt{(f|f)_2}.$$  \hfill (B.4)

The Hilbert space $L^2(\mathbb{R}^3)$ of square integrable functions is defined via the norm (B.4) according to

$$L^2(\mathbb{R}^3) = \left\{ f: \mathbb{R}^3 \to \mathbb{C} \mid \int |f(r)|^2 \, d^3r < \infty \right\} = \left\{ f: \mathbb{R}^3 \to \mathbb{C} \mid \|f\|_2 < \infty \right\}.$$ \hfill (B.5)

The formalism of Hilbert spaces can be generalized to include weight functions. If $w: \mathbb{R}^3 \to \mathbb{R}_+$ is a suitable positive weight function, we define the inner product with respect to the weight function $w$ for functions $f, g: \mathbb{R}^3 \to \mathbb{C}$ according to

$$(f|g)_w,2 = \int [f(r)]^* w(r) g(r) \, d^3r.$$ \hfill (B.6)

As in (B.3), the integration extends over the whole $\mathbb{R}^3$. It is easy to show that $(f|g)_w,2$ with $w(r) \geq 0$ is indeed an inner product satisfying (B.1).

On the basis of the inner product (B.6), the norm of a function $f: \mathbb{R}^3 \to \mathbb{C}$ with respect to the weight function $w$ is defined according to

$$\|f\|_{w,2} = \sqrt{(f|f)_w,2}.$$ \hfill (B.7)

The Hilbert space $L^2_w(\mathbb{R}^3)$ of square integrable functions with respect to the weight function $w$ is defined via the norm (B.7) according to

$$L^2_w(\mathbb{R}^3) = \left\{ f: \mathbb{R}^3 \to \mathbb{C} \mid \int w(r) |f(r)|^2 \, d^3r < \infty \right\} = \left\{ f: \mathbb{R}^3 \to \mathbb{C} \mid \|f\|_{w,2} < \infty \right\}.$$ \hfill (B.8)

It is not necessary to use the coordinate representation for the definition of the Hilbert spaces $L^2(\mathbb{R}^3)$. Instead, the momentum representation can also be used. This is a consequence of the well-known fact that Fourier transformation defined via (A.1) and (A.2) maps $L^2(\mathbb{R}^3)$ onto $L^2(\mathbb{R}^3)$ in a one-to-one manner such that inner products are conserved [60, Theorem IX.6 on p. 10]. Thus, $f, g \in L^2(\mathbb{R}^3)$ implies that the Fourier transforms $\tilde{f}(p)$ and $\tilde{g}(p)$ are also elements of $L^2(\mathbb{R}^3)$. In addition, the inner product (B.3) satisfies

$$(f|g)_2 = \int [\tilde{f}(p)]^* \tilde{g}(p) \, d^3p.$$ \hfill (B.9)
C  Laguerre polynomials

The generalized Laguerre polynomials \( L_n^{(\alpha)}(x) \) possess the following explicit expressions [73, p. 240]:

\[
L_n^{(\alpha)}(x) = \sum_{\nu=0}^{n} (-1)^\nu \frac{(n+\alpha)}{n-\nu} \frac{x^\nu}{\nu!}
= \frac{(\alpha+1)_n}{n!} \; _1F_1(-n; \alpha+1; x).
\]

The generalized Laguerre polynomials satisfy for \( \text{Re}(\alpha) > -1 \) and \( m, n \in \mathbb{N}_0 \) the following orthogonality relationship [73, p. 241]:

\[
\int_0^\infty x^\alpha e^{-x} L_m^{(\alpha)}(x) L_n^{(\alpha)}(x) \, dx = \frac{\Gamma(\alpha+n+1)}{n!} \delta_{mn}.
\]

The completeness of the generalized Laguerre polynomials in the weighted Hilbert space \( L^2_{e^{-x^\alpha}}(\mathbb{R}_+) \) is a classic result of mathematical analysis (see for example [50, p. 33], [74, pp. 349 - 351], or [75, pp. 235 - 238]).

D  Guseinov’s Function Set

In [2, Eq. (1)], Guseinov introduced a fairly large class of complete and orthonormal functions which can be expressed as follows:

\[
k \Psi^m_{n,\ell}(\beta, r) = \left[ \frac{(2\beta)^{k+3} (n-\ell-1)!}{(n+\ell+k+1)!} \right]^{1/2} e^{-\beta r} L_{n-\ell-1}^{(2\ell+2k+2)}(2\beta r) \mathcal{Y}_{\ell}^m(2\beta r).
\]

The indices satisfy \( n \in \mathbb{N}, k = -1, 0, 1, 2, \ldots, \ell \in \mathbb{N}_0 \leq n - 1, -\ell \leq m \leq \ell \), and the scaling parameter \( \beta \) is positive.

Guseinov’s functions satisfy the orthonormality relationship (compare also [3, Eq. (4)])

\[
\int [k \Psi^m_{n,\ell}(\beta, r)]^* r^k k \Psi^{m'}_{n',\ell'}(\beta, r) \, d^3r = \delta_{nn'} \delta_{\ell\ell'} \delta_{mm'}.
\]

Accordingly, Guseinov’s functions are a complete and orthonormal set in the weighted Hilbert space \( L^2_{r^k}(\mathbb{R}^3) \) with \( k = -1, 0, 1, 2, \ldots \), which is defined via the inner product

\[
(f|g)_{r^k} = \int [f(r)]^* r^k g(r) \, d^3r
\]
and the norm
\[ \|f\|_{r^k,2} = \sqrt{(f|g)_{r^k,2}} \] (D.4)
according to
\[ L^2_{r^k}(\mathbb{R}^3) = \left\{ f: \mathbb{R}^3 \to \mathbb{C} \mid \int r^k |f(r)|^2 \, d^3r < \infty \right\} \]
\[ = \left\{ f: \mathbb{R}^3 \to \mathbb{C} \mid \|f\|_{r^k,2} < \infty \right\} . \] (D.5)

E Expansion of the Yukawa Potential

It is relatively easy to construct an expansion of the Yukawa potential in terms of Guseinov’s function \( k \psi^m_{\eta,\ell}(\beta, r) \). The Yukawa potential is a special Slater-type function satisfying
\[ e^{-\beta r} = (4\pi)^{1/2} \beta \chi^0_{0,0}(\beta, r) . \] (E.1)
Setting \( N = L = M = 0 \) in (5.7) yields:
\[ \frac{e^{-\beta r}}{r} = \left[ \frac{2\pi}{(2\beta)^k+1} \right]^{1/2} \frac{\Gamma(k+2)}{\nu} \sum_{\nu=0}^{\infty} \frac{\nu!}{[(\nu+k+2)! \nu!]^{1/2}} k^{\psi^0_{\nu+1,0}(\beta, r)} . \] (E.2)
This expansion converges in the mean with respect to the norm (D.4) of the weighted Hilbert space \( L^2_{r^k}(\mathbb{R}^3) \) with \( k = -1, 0, 1, 2, \ldots \) if the squares of the coefficients on the right-hand side decay more rapidly than \( 1/\nu \) as \( \nu \to \infty \).

The behavior of the coefficients in (E.2) can be analyzed with the help of the following asymptotic expression for the ratio of two gamma functions \([76, \text{Eq. (6.1.47)} \text{ on p. 257}]:\)
\[ \frac{\Gamma(z+a)}{\Gamma(z+b)} = z^{a-b} + O(z^{a-b-1}) , \quad z \to \infty . \] (E.3)
We then obtain the following asymptotic estimates for the \( \nu \)-dependent part of the square of the coefficients on the right-hand side of (E.2):
\[ \left[ \frac{\nu!}{[(\nu+k+2)! \nu!]^{1/2}} \right] = \frac{\nu!}{(\nu+k+2)!} = \nu^{-k-2} + O(\nu^{-k-3}) , \quad \nu \to \infty . \] (E.4)
Thus, the expansion (E.2) converges in the mean with respect to the norm (D.4) of the weighted Hilbert space \( L^2_{r^k}(\mathbb{R}^3) \) for \( k = 0, 1, 2 \ldots \) and diverges for \( k = -1 \). This is in agreement with the fact that the Yukawa potential belongs to the weighted Hilbert space \( L^2_{r^k}(\mathbb{R}^3) \) for \( k = 0, 1, 2 \ldots \), but not for \( k = -1 \).

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