On the four-body problem in the Born-Oppenheimer approximation

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Abstract

The quantum problem of four particles in $\mathbb{R}^d$ ($d \geq 3$), with arbitrary masses $m_1, m_2, m_3$ and $m_4$, interacting through an harmonic oscillator potential is considered. This model allows exact solvability and a critical analysis of the Born-Oppenheimer approximation. The study is restricted to the ground state level. We pay special attention to the case of two equally heavy masses $m_1 = m_2 = M$ and two light particles $m_3 = m_4 = m$. It is shown that the sum of the first two terms of the Puiseux series, in powers of the dimensionless parameter $\sigma = \frac{m}{M}$, of the exact phase $\Phi$ of the wave function $\psi_0 = e^{-\Phi}$ and the corresponding ground state energy $E_0$, coincide exactly with the values obtained in the Born-Oppenheimer approximation. A physically relevant rough model of the $H_2$ molecule and of the chemical compound $H_2O_2$ (Hydrogen peroxide) is described in detail. The generalization to an arbitrary number of particles $n$, with $d$ degrees of freedom ($d \geq n - 1$), interacting through an harmonic oscillator potential is briefly discussed as well.
I. INTRODUCTION

Recently, a many-body quantum reduced Hamiltonian was presented in Ref. [1]. It describes the ground state level of a $d$-dimensional $n$-body quantum system, $d \geq n - 1$, with an arbitrary potential that solely depends on relative distances between the particles. The dynamical variables of the reduced Hamiltonian are the $\frac{n(n-1)}{2}$ relatives distances between the bodies. In particular, in Refs. [2]-[3] the three-body system was considered in detail while in the work [4] the four-body case was analyzed. Also, for the four-body quantum system Jacobi-like-variables were introduced in Ref. [5, 6] to reduce the Schrödinger equation to generalized radial equations where only six internal variables are involved. It is worth mentioning that even in the planar case $d = 2$, the dynamics of the classical 4-body problem is very rich [7]-[9]. Unfortunately, in all these important conceptual works few applications are mentioned and not explicit examples were worked out in detail.

The Born-Oppenheimer approximation (BOA) [10, 11] is a landmark in atomic and molecular physics. Even the well-established notion of molecular electronic states is deeply connected to this approximation.

The general assumption of this approximation is physically transparent: when the masses of the nuclei are much heavier than the electronic ones then an approximate separation of the electronic and nuclear motions (pseudo-separation of variables) is possible and, consequently, the task of solving the Schrödinger equation or the classical Hamilton’s equations become considerably simpler.

The nature of the BOA is essentially perturbative. In the case of a quantum Coulomb system of electrons and nuclei, the small expansion parameter $\lambda = \sigma^{\frac{1}{4}}$ involves the ratio of the electron mass $m$ to the nuclear mass $M$, namely $\sigma = m/M$ [10, 11]. Accordingly, the Hamiltonian is expressed as the sum of two terms, the so-called clamped-nuclei electronic Hamiltonian (which is $\sigma$-independent) and the nuclear kinetic energy operator ($\propto \sigma$). As a result, in the BOA the total approximate molecular wavefunction is factorized as a product of an electronic and a nuclear wavefunction. In fact, Hunter [12] suggested that the exact wavefunction also admits such a factorization. Remarkably, using a variational principle Cederbaum showed that this factorization occurs indeed [13].

In order to examine the accuracy of the Born-Oppenheimer approximation, Moshinsky and Kittel [14] discussed the 3-dimensional ($d = 3$) elementary problem of a light particle (the
electron) and two heavy particles (the nuclei) which are coupled to each other by harmonic forces. This model, originally used in nuclear physics [15], can be solved both exactly and within BOA, thus allowing a critical discussion of such an approximation. The analysis in Ref. [14] concluded that the Born-Oppenheimer approximation provides accurate results for both the energy and the ground-state wave function, even for the extreme case in which the light particle is a proton in a hydrogen bond.

In a recent paper, Sutcliffe and Woolley made a careful reformulation of the conventional Born-Oppenheimer argument drawing on results from the modern mathematical literature and proved that the correct $\sigma$-independent part of Hamiltonian is not the clamped-nuclei electronic Hamiltonian but a different operator which was given there explicitly. Until now, due to its enormous importance in contemporary experimental atomic and molecular physics, the BOA continues to be a fruitful object of study and it is used in a plethora of applications. The purpose of the present work is two fold. On the one hand, for a 3-body ($n = 3$) exactly solvable model in $\mathbb{R}^3$ ($d = 3$), based on the formalism described in Ref. [2], we will re-derive the known results [14] in a cleaner and more elegant manner. Afterwards, we extend these 3D results to the case of an arbitrary dimension $d > 3$. Secondly, along the same lines we aim to determine quantitatively the accuracy of the Born-Oppenheimer approximation for a 4-body closed chain of interacting harmonic oscillators with $d$-degrees of freedom ($d > 2$). At $d = 3$, such a system is a rough model of the $H_2$ molecule and of the chemical compound $H_2O_2$ (Hydrogen peroxide). Valuable results for the $n$-body case in $d$-dimensions are derived as well.

II. THREE BODY PROBLEM

In this Section we first consider a three-body quantum system in $d$-dimensions ($d > 1$). The Hamiltonian is of the form

\[ H = - \sum_{i=1}^{3} \frac{1}{2m_i} \Delta_i^{(d)} + V(r_{12}, r_{13}, r_{23}), \quad (1) \]

where $V$ is a scalar potential that solely depends on the relative distances

\[ r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|, \quad r_{13} = |\mathbf{r}_1 - \mathbf{r}_3|, \quad r_{23} = |\mathbf{r}_2 - \mathbf{r}_3|, \]
and \( \Delta_i \) is the individual \( d \)-dimensional Laplacian

\[
\Delta_i = \frac{\partial^2}{\partial r_i \partial r_i},
\]

associated to the \( i \)th body with mass \( m_i \) and coordinate vector \( r_i = (x_{i,1}, x_{i,3}, \ldots, x_{i,d}) \in \mathbb{R}^d \).

Thus, in total the Hamiltonian (1) possesses \( 3d \) degrees of freedom. After separating the center of mass motion, the number of degrees of freedom of the system reduces to \( 2d \) in the space of relative motion.

For this reduced system there exists a quadratic potential \( V \) in terms of relative distances \( r_{12}, r_{23}, r_{13} \), for which uncountable number of quantum \( S \)-states (zero total angular momentum) of the eigenvalue problem \( \mathcal{H} \Psi = E \Psi \) can be found by algebraic means. Their eigenfunctions are the elements of the finite-dimensional representation space(s) of \( \mathfrak{sl}(4, \mathbb{R}) \) algebra of differential operators [2]. In general, assuming that the potential

\[
V = V(r_{12}, r_{13}, r_{23}),
\]

solely depends on the \( \rho \)-variables

\[
\rho_{12} = r_{12}^2, \quad \rho_{13} = r_{13}^2, \quad \rho_{23} = r_{23}^2,
\]

(relative distances squared) we arrive at the reduced three-dimensional radial equation in the \( \rho \)-space [2]

\[
\mathcal{H}_{\text{rad}} \psi(\rho) = [-\Delta_{\text{rad}}(\rho) + V(\rho)] \psi(\rho) = E \psi(\rho),
\]

where the radial operator defined by

\[
\Delta_{\text{rad}}(\rho) = 2 \left[ \frac{1}{\mu_{13}} \rho_{13}^2 \partial_{\rho_{13}}^2 + \frac{1}{\mu_{23}} \rho_{23}^2 \partial_{\rho_{23}}^2 + \frac{1}{\mu_{12}} \rho_{12}^2 \partial_{\rho_{12}}^2 + \right.
\]

\[
\frac{(\rho_{13} + \rho_{12} - \rho_{23})}{m_1} \partial_{\rho_{13},\rho_{12}} + \frac{(\rho_{13} + \rho_{23} - \rho_{12})}{m_3} \partial_{\rho_{13},\rho_{23}} + \frac{(\rho_{23} + \rho_{12} - \rho_{13})}{m_2} \partial_{\rho_{23},\rho_{12}} +
\]

\[
\left. \frac{d}{\mu_{13}} \partial_{\rho_{13}} + \frac{d}{\mu_{23}} \partial_{\rho_{23}} + \frac{d}{\mu_{12}} \partial_{\rho_{12}} \right],
\]

governs the kinetic (radial) dynamics of the relative motion, and

\[
\mu_{ij} = \frac{m_i m_j}{m_i + m_j},
\]

is the reduced mass for particles \( i \) and \( j \). The radial Hamiltonian (4) is equivalent, up to a gauge transformation, to a three-dimensional Schrödinger operator, see Ref. [2].
The operator (4) describes all the eigenfunctions with zero angular momentum of the original Hamiltonian (1). In particular, it describes the ground state level we usually are interested in.

For the operator $\mathcal{H}_{\text{rad}}$ (4), the configuration space is given by $S_{\Delta} \geq 0$ where

$$S_{\Delta} = \frac{1}{4} \sqrt{2 (\rho_{12} \rho_{13} + \rho_{12} \rho_{23} + \rho_{13} \rho_{23}) - (\rho_{12}^2 + \rho_{13}^2 + \rho_{23}^2)},$$

(7)

is the area of the triangle of interaction whose vertices are the individual positions $r_i$ of the three particles.

The reduced Hamiltonian $\mathcal{H}_{\text{rad}}$ (4) is essentially self-adjoint with respect to the radial measure

$$d\varrho = (S_{\Delta})^{d-3} d\rho_{12} d\rho_{13} d\rho_{23}.$$

(8)

Although the radial Hamiltonian $\mathcal{H}_{\text{rad}}$ is self-adjoint it is not in the form of a Laplace-Beltrami operator plus a potential. For this to be true a further $d-$dependent gauge transformation is needed, as shown in Ref. [2]. For $d = 3$, a case partially studied in Ref. [14], the radial measure (8) is greatly simplified.

### III. THREE-BODY HARMONIC OSCILLATOR

Now, let us consider the Hamiltonian (4) with potential

$$V^{(es)} = 2 \omega^2 \left[ \nu_{12} \rho_{12} + \nu_{13} \rho_{13} + \nu_{23} \rho_{23} \right],$$

(9)

where $\omega$ and $\nu_{12}, \nu_{13}, \nu_{23}$ are positive constants. Equivalently, in terms of the relative distances $r_{ij}$ (3) between particles, (9) is an harmonic pairwise potential. It is easy to verify that the eigenfunctions $\Psi$ of the radial Hamiltonian (4) with potential (9),

$$\mathcal{H}^{(es)}_{\text{rad}} = -\Delta_{\text{rad}}(\rho) + 2 \omega^2 \left[ \nu_{12} \rho_{12} + \nu_{13} \rho_{13} + \nu_{23} \rho_{23} \right],$$

(10)

occur in the form

$$\Psi(\rho_{12}, \rho_{13}, \rho_{23}) = \Psi^{(es)}_0(\rho_{12}, \rho_{13}, \rho_{23}) \times P_N(\rho_{12}, \rho_{13}, \rho_{23}),$$

where $\Psi^{(es)}_0$ (the ground state) is a global common factor and $P_N$ is a multivariable polynomial function in the $\rho$-variables [2]. Its spectra is linear in quantum numbers. Moreover,
the operator (10) is exactly solvable which implies that one can compute the spectrum and the eigenfunctions by pure algebraic methods. In particular, the ground state can be taken in the following form

$$
\Psi_{0}^{(es)} = \mathcal{N} e^{-\omega (a \mu_{12} \rho_{12} + b \mu_{13} \rho_{13} + c \mu_{23} \rho_{23})},
$$

(11)

where $\mathcal{N}$ is a normalization factor. The parameters $a$, $b$, $c$ in the exponent can be related to those of the potential (9) through the algebraic equations

$$
\begin{align*}
\nu_{12} &= a^{2} \mu_{12} + a b \frac{\mu_{12} \mu_{13}}{m_{1}} + a c \frac{\mu_{12} \mu_{23}}{m_{2}} - b c \frac{\mu_{13} \mu_{23}}{m_{3}}, \\
\nu_{13} &= b^{2} \mu_{13} + a b \frac{\mu_{12} \mu_{13}}{m_{1}} + b c \frac{\mu_{13} \mu_{23}}{m_{3}} - a c \frac{\mu_{12} \mu_{23}}{m_{2}}, \\
\nu_{23} &= c^{2} \mu_{23} + a c \frac{\mu_{12} \mu_{23}}{m_{2}} + b c \frac{\mu_{13} \mu_{23}}{m_{3}} - a b \frac{\mu_{12} \mu_{13}}{m_{1}},
\end{align*}
$$

(12)

such that the ground state energy is given by

$$
E_{0}^{(es)} = \omega d (a + b + c).
$$

(13)

In the three $\rho$-variables, the exactly-solvable Hamiltonian (10) does not admit separation of variables. However, the ground state eigenfunction (11) can be trivially factored as the product of three functions, each of them depending on a single $\rho$ variable.

*By construction, the eigenfunctions of the three-dimensional Hamiltonian (10) are also eigenfunctions (with the same energy) of the original 3d-dimensional Hamiltonian (1).*

**A. Case of equal masses**

In this Section we consider the case of three particles of equal masses $m_{1} = m_{2} = m_{3} = m$, but arbitrary constants $a, b, c > 0$. The harmonic oscillator potential (9) becomes

$$
V^{(3m)} = \frac{1}{2} m \omega^2 \left[ (2 a^2 + a(b+c) - b c) \rho_{12} + (2 b^2 + b(a+c) - c a) \rho_{13} + (2 c^2 + c(a+b) - a b) \rho_{23} \right].
$$

(14)

It is a type of non-isotropic 3-body harmonic oscillator with different spring constants. In this case the exact ground state function (11) and the associated energy (13) are given by

$$
\Psi_{0}^{(3m)} = e^{-\frac{m}{2} (a \rho_{12} + b \rho_{13} + c \rho_{23})},
$$

(15)

$$
E_{0}^{(3m)} = \omega d (a + b + c).
$$

(16)

The case of 3 identical spring constants in (14) corresponds to $a = b = c$. 

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B. Case of two equal massive particles

Now, we move to the case where two of the three particles are identical, i.e. we put

\[ m_1 = m_2 = 1 ; \quad m_3 = m , \]

and interact through an harmonic oscillator potential, namely

\[ V = \frac{1}{4} \rho_{12} + \frac{1}{2} K \rho_{13} + \frac{1}{2} K \rho_{23} , \quad K > 0 . \]  \hspace{1cm} (17)

By putting

\[ a = \frac{1}{2} \left( \sqrt{K} + 1 - \sqrt{K m \over m+2} \right) , \quad b = c = \frac{\sqrt{K(m+1)}}{2 \sqrt{m(m+2)}} , \quad \omega = 1 , \]

in Eqs. (9) and (12) we arrive to the expression (17). For the three-dimensional case \( d = 3 \), this physically important problem was studied in Ref. [14]. In order to make a comparison, we adopted the same units of mass and spring constants used in Ref. [14].

1. Exact result

The exact ground state energy (13) and the eigenfunction (11) reduce to

\[ E_0 = \frac{1}{2} d \left( \sqrt{K (m+2) \over m} + \sqrt{K+1} \right) , \]  \hspace{1cm} (18)

\[ \psi_0 = \left( \sqrt{\pi} \Gamma(d/2) \Gamma(d-1/2) \right)^{-1/2} \left( K m \over m+2 \right)^{d/4} e^{1/4 \left( \sqrt{K m \over m+2} (\rho_{12} - 2(\rho_{13} + \rho_{23})) - \sqrt{K+1} \rho_{12} \right)} , \]  \hspace{1cm} (19)

respectively. The function (19) is normalized with respect to the radial measure \( d \rho \) (8).

The following remark is in order. For the three-dimensional case \( d = 3 \), Moshinsky and Kittel [14] studied the original Hamiltonian (1) with potential (17). After separation of the center of mass, the 9-dimensional problem reduces to a 6-dimensional one in the space of relative motion. In this space, they introduce two 3-dimensional vectorial Jacobi coordinates \( \mathbf{r}_{1}^{(J)} \) and \( \mathbf{r}_{2}^{(J)} \). Hence, for the normalization of the eigenfunctions they do not use (8) but the factorizable integration measure

\[ d^3 \mathbf{r}_{1}^{(J)} d^3 \mathbf{r}_{2}^{(J)} = d \Omega d \rho , \]  \hspace{1cm} (20)
where \(d\Omega\) involves 3 angular variables alone.

Now, the ground state function of (1) must depend on the relative distances only \([16]\). This fundamental fact is not evident in \([14]\), whereas in the present formalism it does, see eq. \([19]\). Using the measure \((20)\), immediately we see that the ground state eigenfunction \((19)\) reproduces up to the corresponding constant factor coming from the trivial integration over \(d\Omega\), the result reported in \([14]\). The energy \((18)\) is exactly the same value obtained in \([14]\), as it should be. That way, we nicely reproduce the results presented in \([14]\) and extend them to arbitrary dimension \(d\).

2. Approximate solution

As for the Born-Oppenheimer approximation one starts with the assumption that the two identical particles \(m_1 = m_2 = 1\) are much heavier than the third one \(m\), thus \(m \ll 1\). The masses \(m_1\) and \(m_2\) are fixed at positions \(r_1\), \(r_2\), respectively. In this case \(\rho_{12}\) is also fixed, and one solves first the electronic radial Hamiltonian

\[
H_{\text{rad}}^{(\text{electronic})} \psi^{(e)} = \left[ -\Delta_{\text{rad}}^{(\text{electronic})} + \frac{1}{2} K \rho_{13} + \frac{1}{2} K \rho_{23} \right] \psi^{(e)} = E^{(e)} \psi^{(e)}, \tag{21}
\]

where the operator

\[
\Delta_{\text{rad}}^{(\text{electronic})} = \frac{2}{m} \left[ \rho_{13} \partial_{\rho_{13}}^2 + \rho_{23} \partial_{\rho_{23}}^2 + (\rho_{13} + \rho_{23} - \rho_{12}) \partial_{\rho_{13},\rho_{23}} + \frac{d}{2} \partial_{\rho_{13}} + \frac{d}{2} \partial_{\rho_{23}} \right]. \tag{22}
\]

depends on \(\rho_{12}\) parametrically, in other words \(\rho_{12}\) plays the role of a classical variable. Formally, the operator \((22)\) can be obtained from \((5)\) in the limit \(m_1 = m_2 \to \infty\) together with \(m_3 \to m\).

For the electronic eigenvalue problem \((21)\) we obtain the ground state function

\[
\psi_0^{(e)} = \pi^{-\frac{d}{4}} \sqrt{2Km} \frac{d}{4} e^{\frac{i}{4} \sqrt{\frac{K}{2m}} (\rho_{12} - 2(\rho_{13} + \rho_{23}))}, \tag{23}
\]

with energy

\[
E_0^{(e)} = d \sqrt{\frac{K}{2m}} + \frac{K \rho_{12}}{4}. \tag{24}
\]

The ground state \((23)\) obeys the \(L^2\)-condition
\[ \int (\psi_0^{(e)})^2 dr_3 = 1, \]  

where the integration is over the electronic variable \( r_3 \in \mathbb{R}^d \) only.

For \( d = 3 \), using standard spherical coordinates \( r_3 = (r_3, \theta, \phi) \) we easily find the relation
\[ d^3r_3 = r_3^2 \sin \theta \, dr_3 \, d\theta \, d\phi = \frac{1}{4\sqrt{r_{12}}} \, d\rho_{13} \, d\rho_{23} \, d\phi. \]

Then, at \( d = 3 \) the solution (23) coincides with that presented in Ref. [14].

Expression (24), under the name of a potential curve, is the one we must add to the Hamiltonian of the two heavy particles \( m_1 = m_2 = 1 \), namely \((-4 \rho_{12} \partial_{\rho_{12}}^2 - 2 d \partial_{\rho_{12}} + \frac{1}{4} \rho_{12})\), to get the nuclear Hamiltonian, i.e.
\[
\mathcal{H}^{\text{(nuclear)}} = \left[ -4 \rho_{12} \partial_{\rho_{12}}^2 - 2 d \partial_{\rho_{12}} + \frac{1}{4} \rho_{12} \right] + d \sqrt{\frac{K}{2m}} + \frac{K \rho_{12}}{4}. \]

Clearly, the ground state of (26)
\[ \psi^{(n)}_0 \propto e^{-\frac{\sqrt{2(K+1)}}{4} \rho_{12}}, \]

is the one of zero quanta with frequency \( \sqrt{K+1} \). Therefore, the normalized total wave function in the Born-Oppenheimer approximation (BOA) takes the form
\[
\psi_0^{(BO)} = \left( \frac{\sqrt{\pi} \Gamma\left(\frac{d}{2}\right) \Gamma\left(\frac{d-1}{2}\right)}{2^{d-1}} \right)^{-\frac{1}{2}} \left( \frac{K(1+K)}{2} \right)^{\frac{d}{2}} e^{-\frac{\sqrt{2(K+1)}}{4} \rho_{12}} \times e^{\frac{i}{4} \sqrt{\frac{Km}{2}} (\rho_{12} - 2(\rho_{13} + \rho_{23}))}
\]

\[ \propto \psi_0^{(e)} \times \psi_0^{(n)}, \]

with respect to the measure (8). The corresponding ground state energy is given by
\[
E_0^{(BO)} = \frac{1}{2} d \left( \sqrt{\frac{2K}{m}} + \sqrt{K+1} \right). \]

This expression corresponds to the generalization to \( d \)-dimensions of the result obtained in Ref. [14].

3. Accuracy of the Born-Oppenheimer approximation

Assuming \( m \ll 1 \), we first compare the energies \( E_0 \) (18) and \( E_0^{(BO)} \) (28).
\[ \Delta E \equiv \frac{E_0 - E_0^{(BO)}}{E_0} = 1 - \frac{E_0^{(BO)}}{E_0} = 1 - \frac{\sqrt{\frac{2K}{m}} + \sqrt{K + 1}}{\sqrt{\frac{K(m+2)}{m}} + \sqrt{K + 1}} \]

\[ \approx \frac{1}{4} m - \frac{1}{4} \sqrt{\frac{K + 1}{2K}} m^{3/2} + \frac{(K + 4)}{32K} m^2 + \ldots . \]  

(29)

FIG. 1. The ratio \( \Delta E \) (29) as a function of the spring constant \( K \) for (left) the hydrogen molecular ion \( H_2^+ \) (\( m = \frac{1}{2000} \)) and (right) the proton in a hydrogen bond between two nitrogen or oxygen atoms (\( m = \frac{1}{15} \)). The ratio \( \Delta E \) is a monotonic increasing (bounded) function of \( K \).

Remarkably, the ratio \( \Delta E \) (29) does not depend on the dimension \( d \). In Figure 1 we plot \( \Delta E \) (29) as a function of the spring constant \( K \) in the case of two relevant systems, namely the hydrogen molecular ion \( H_2^+ \) (\( m = \frac{1}{2000} \)) and the proton in a hydrogen bond between two nitrogen or oxygen atoms (\( m = \frac{1}{15} \)).

In powers of the small parameter \( m \ll 1 \) we have

\[ E_0 = E_0^{(BO)} + \frac{d \sqrt{K}}{4 \sqrt{2}} \left( m^{\frac{1}{2}} - \frac{1}{8} m^{\frac{3}{2}} + \frac{1}{32} m^{\frac{5}{2}} + \ldots \right) , \]  

(30)

hence, \( E_0^{(BO)} \) is nothing but the sum of the first two terms of the Puiseux series of the exact result \( E_0 \) (18). Similarly, we obtain that the exponent in (27), i.e. the phase

\[ \Phi_{BO} \equiv \frac{1}{4} \sqrt{\frac{K m}{2}} (\rho_{12} - 2(\rho_{13} + \rho_{23})) - \frac{\sqrt{(K + 1)}}{4} \rho_{12} \]

of the ground state function in the Born-Oppenheimer approximation, coincides exactly with the sum of the first two terms of the Puiseux series of the exact result (19)

\[ \Phi = \frac{1}{4} \left( \sqrt{\frac{K m}{m + 2}} (\rho_{12} - 2(\rho_{13} + \rho_{23})) - \sqrt{K + 1} \rho_{12} \right) . \]
Explicitly,

$$\Phi = \Phi_{\text{BO}} - \frac{1}{16} \sqrt{\frac{K}{2}} (\rho_{12} - 2 (\rho_{13} + \rho_{23})) \left( m^{\frac{3}{2}} - \frac{3}{8} m^{\frac{5}{2}} + O(m^{7}) \right). \quad (31)$$

To compare the wave functions, we consider the overlap $T \equiv \langle \psi_{0}^{(\text{BO})} | \psi_{0} \rangle^2$, which from (27) and (19) is given by

$$T = 2^{\frac{d}{2}} (m + 2)^{d/4} \left( \sqrt{2 (m + 2)} + 2 \right)^{-d} \simeq 1 - \frac{d m^2}{128} + \frac{d m^3}{256} + O(m^4). \quad (32)$$

The overlap $T$ does not depend on the spring constant $K$. However, it depends on the dimension $d$.

FIG. 2. The overlap $T$ as a function of the mass $m$ of the light particle at $d = 2, 3, 4$. The two marked circles stand for the hydrogen molecular ion $H_2^+ (m = \frac{1}{2000})$ and for the proton in a hydrogen bond between two nitrogen or oxygen atoms ($m = \frac{1}{15}$), respectively.

For the physically important cases of $H_2^+ (m = \frac{1}{2000})$ and hydrogen bond ($m = \frac{1}{15}$) in three-dimensions $d = 3$, the overlap (32) differs from 1 by terms of the order less than one part in $10^8$ and four parts in $10^4$, respectively [14]. The new results (30)-(32) show that also for the physically relevant two-dimensional case $d = 2$, the Born-Oppenheimer approximation provides accurate values for the energy as well as for the ground state wave function.
IV. FOUR BODY CASE

Similarly to the three-body case, assuming \( d \geq 3 \) and that the potential \( V = V(\rho) \) solely depends on the six independent relative variables

\[
\rho_{12} = r_{12}^2, \quad \rho_{13} = r_{13}^2, \quad \rho_{23} = r_{23}^2, \quad \rho_{14} = r_{14}^2, \quad \rho_{24} = r_{24}^2, \quad \rho_{34} = r_{34}^2,
\]

one arrives at the six-dimensional radial equation in the \( \rho \)-space of the relative motion

\[
\left[ -\Delta^{(4)}_{\text{rad}}(\rho) + V(\rho) \right] \psi(\rho) = E \psi(\rho),
\]

(33)

where

\[
\Delta^{(4)}_{\text{rad}}(\rho) = 2 \left[ \frac{1}{\mu_{12}} \rho_{12} \frac{\partial^2}{\partial \rho_{12}^2} + \frac{1}{\mu_{13}} \rho_{13} \frac{\partial^2}{\partial \rho_{13}^2} + \frac{1}{\mu_{14}} \rho_{14} \frac{\partial^2}{\partial \rho_{14}^2} + \frac{1}{\mu_{23}} \rho_{23} \frac{\partial^2}{\partial \rho_{23}^2} \\
+ \frac{1}{\mu_{24}} \rho_{24} \frac{\partial^2}{\partial \rho_{24}^2} + \frac{1}{\mu_{34}} \rho_{34} \frac{\partial^2}{\partial \rho_{34}^2} \right]
\]

\[
+ \frac{2}{m_1} \left( (\rho_{12} + \rho_{13} - \rho_{23}) \frac{\partial}{\partial \rho_{12}} \frac{\partial}{\partial \rho_{13}} + (\rho_{12} + \rho_{14} - \rho_{24}) \frac{\partial}{\partial \rho_{12}} \frac{\partial}{\partial \rho_{14}} + (\rho_{13} + \rho_{14} - \rho_{34}) \frac{\partial}{\partial \rho_{13}} \frac{\partial}{\partial \rho_{14}} \right)
\]

\[
+ \frac{2}{m_2} \left( (\rho_{12} + \rho_{23} - \rho_{13}) \frac{\partial}{\partial \rho_{12}} \frac{\partial}{\partial \rho_{23}} + (\rho_{12} + \rho_{24} - \rho_{14}) \frac{\partial}{\partial \rho_{12}} \frac{\partial}{\partial \rho_{24}} + (\rho_{23} + \rho_{24} - \rho_{34}) \frac{\partial}{\partial \rho_{23}} \frac{\partial}{\partial \rho_{24}} \right)
\]

\[
+ \frac{2}{m_3} \left( (\rho_{13} + \rho_{23} - \rho_{12}) \frac{\partial}{\partial \rho_{13}} \frac{\partial}{\partial \rho_{23}} + (\rho_{13} + \rho_{34} - \rho_{14}) \frac{\partial}{\partial \rho_{13}} \frac{\partial}{\partial \rho_{34}} + (\rho_{23} + \rho_{34} - \rho_{24}) \frac{\partial}{\partial \rho_{23}} \frac{\partial}{\partial \rho_{34}} \right)
\]

\[
+ \frac{2}{m_4} \left( (\rho_{14} + \rho_{24} - \rho_{12}) \frac{\partial}{\partial \rho_{14}} \frac{\partial}{\partial \rho_{24}} + (\rho_{14} + \rho_{34} - \rho_{13}) \frac{\partial}{\partial \rho_{14}} \frac{\partial}{\partial \rho_{34}} + (\rho_{24} + \rho_{34} - \rho_{23}) \frac{\partial}{\partial \rho_{24}} \frac{\partial}{\partial \rho_{34}} \right)
\]

\[
+ d \left[ \frac{1}{\mu_{12}} \frac{\partial}{\partial \rho_{12}} + \frac{1}{\mu_{13}} \frac{\partial}{\partial \rho_{13}} + \frac{1}{\mu_{14}} \frac{\partial}{\partial \rho_{14}} + \frac{1}{\mu_{23}} \frac{\partial}{\partial \rho_{23}} + \frac{1}{\mu_{24}} \frac{\partial}{\partial \rho_{24}} + \frac{1}{\mu_{34}} \frac{\partial}{\partial \rho_{34}} \right],
\]

(34)

where \( \mu_{ij} \) is defined in Eq. (6) and \( \Delta^{(4)}_{\text{rad}} \) plays the role of kinetic radial operator cf.(5). The operator

\[
\mathcal{H}^{(4)}_{\text{rad}} = -\Delta^{(4)}_{\text{rad}} + V,
\]

(35)

is equivalent to a six-dimensional radial Schrödinger operator, for further details see [4]. It can be called six-dimensional radial Hamiltonian. As a function of the six \( \rho \)-variables, the operator (34) is not \( S_6 \) permutationally-invariant. Nevertheless, it remains \( S_4 \) invariant under the permutations of the particles. For the three-body case, where the number of \( \rho \) variables (relative distances squared) equals the number of particles, the corresponding operator \( \Delta_{\text{rad}} \) is indeed \( S_3 \) permutationally-invariant.

For the Hamiltonian \( \mathcal{H}^{(4)}_{\text{rad}} \) (35), the configuration space is given by \( V \geq 0 \) where
\[ V \equiv \frac{1}{12} \left[ \left( (\rho_{13} + \rho_{14} + \rho_{23} + \rho_{24}) \rho_{34} - (\rho_{13} - \rho_{14}) (\rho_{23} - \rho_{24}) - \rho_{34}^2 \right) \rho_{12} 
- \rho_{13}^2 \rho_{24} - \rho_{34} \rho_{12}^2 + \rho_{23} \left[ (\rho_{14} - \rho_{24}) \rho_{34} - \rho_{14} (\rho_{14} + \rho_{23} - \rho_{24}) \right] 
+ \rho_{13} \left[ (\rho_{14} (\rho_{23} + \rho_{24} - \rho_{34}) + \rho_{24} (\rho_{23} - \rho_{24} + \rho_{34}) \right] \right]^{\frac{1}{2}}, \]

is the volume of the tetrahedron of interaction whose vertices correspond to the positions of the particles.

The reduced Hamiltonian \( H_{\text{rad}}^{(4)} \) is essentially self-adjoint with respect to the radial measure

\[ d\rho = V^{d-4} d\rho_{12} d\rho_{13} d\rho_{14} d\rho_{23} d\rho_{24} d\rho_{34}. \]

Although the radial Hamiltonian is essentially self-adjoint it is not in the form of a Laplace-Beltrami operator plus potential. For this to be true a further gauge transformation is needed, see [4].

V. FOUR-BODY HARMONIC OSCILLATOR

For the four-body system, let us introduce the harmonic potential

\[ \tilde{V}^{(es)} = 2 \omega^2 \nu_{12} \rho_{12} + \nu_{13} \rho_{13} + \nu_{14} \rho_{14} + \nu_{23} \rho_{23} + \nu_{24} \rho_{24} + \nu_{34} \rho_{34}, \]

where \( \omega \) and the \( \nu \)'s are positive constants. It is easy to verify that the eigenfunctions of the Hamiltonian \( \tilde{H}_{\text{rad}}^{(es)} \) with potential \( \tilde{V}^{(es)} \)

\[ \tilde{H}_{\text{rad}}^{(es)} = -\Delta_{\text{rad}}^{(4)}(\rho) + \tilde{V}^{(es)}, \]

occur in the form

\[ \tilde{\Psi}(\rho) = \tilde{\Psi}_0^{(es)}(\rho) \times \tilde{P}_N(\rho), \]

where \( \tilde{\Psi}_0^{(es)} \) (the ground state) is a global common factor and \( \tilde{P}_N \) is a multivariable polynomial function in the six \( \rho \)-variables. Its spectra is linear in quantum numbers. Again, the operator \( \tilde{H}_{\text{rad}}^{(es)} \) is exactly solvable. The ground state function takes the following form

\[ \tilde{\Psi}_0^{(es)} = N e^{-\omega (a \mu_{12} \rho_{12} + b \mu_{13} \rho_{13} + c \mu_{14} \rho_{14} + e \mu_{23} \rho_{23} + f \mu_{24} \rho_{24} + g \mu_{34} \rho_{34})}, \]

\[ (40) \]
where $N$ is a normalization factor and the parameters $a, b, c, e, f, g$ in the exponent are related to those of the potential (38) through the six algebraic equations

$$
\nu_{12} = a^2 \mu_{12} + a b \frac{\mu_{12} \mu_{13}}{m_1} + a c \frac{\mu_{12} \mu_{14}}{m_1} + a e \frac{\mu_{12} \mu_{23}}{m_1} + a f \frac{\mu_{12} \mu_{24}}{m_2} + b e \frac{\mu_{13} \mu_{23}}{m_3} - e f \frac{\mu_{14} \mu_{24}}{m_4},
$$

$$
\nu_{13} = b^2 \mu_{13} + b a \frac{\mu_{13} \mu_{12}}{m_1} + b c \frac{\mu_{13} \mu_{14}}{m_1} + b e \frac{\mu_{13} \mu_{23}}{m_3} + b g \frac{\mu_{13} \mu_{34}}{m_3} - a e \frac{\mu_{12} \mu_{23}}{m_2} - e f \frac{\mu_{14} \mu_{34}}{m_4},
$$

$$
\vdots
$$

$$
\nu_{34} = g^2 \mu_{34} + g b \frac{\mu_{34} \mu_{13}}{m_3} + g c \frac{\mu_{34} \mu_{14}}{m_4} + g e \frac{\mu_{34} \mu_{24}}{m_3} + g f \frac{\mu_{34} \mu_{24}}{m_4} - b c \frac{\mu_{13} \mu_{14}}{m_1} - e f \frac{\mu_{23} \mu_{24}}{m_4}.
$$

and the ground state energy takes the simple form

$$
\tilde{E}^{(es)}_0 = \omega d (a + b + c + e + f + g).
$$

**A. Case of equal masses**

Let us consider the case of four particles of equal masses $m_1 = m_2 = m_3 = m_4 = m$, but arbitrary constants $a, b, c, e, f, g > 0$. From (41), it follows that the harmonic oscillator potential (38) reduces to

$$
V^{(4m)} = \frac{1}{2} m \omega^2 \left[ (2a^2 + a(b + c + e + f) - be - cf) \rho_{12} + (2b^2 + b(a + c + e + g) - ae - cg) \rho_{13} + (2c^2 + c(a + b + f + g) - af - bg) \rho_{14} + (2e^2 + e(a + b + f + g) - ab - fg) \rho_{23} + (2f^2 + f(a + c + e + g) - ac - eg) \rho_{24} + (2g^2 + g(b + c + e + f) - bc - ef) \rho_{34} \right].
$$

It is a type of non-isotropic 4-body harmonic oscillator with different spring constants. In this case the exact ground state function (40) is given by

$$
\Psi^{(4m)}_0 = e^{-\frac{\omega m}{2} (a \rho_{12} + b \rho_{13} + c \rho_{14} + e \rho_{23} + f \rho_{24} + g \rho_{34})},
$$

with energy

$$
E^{(4m)}_0 = \omega d (a + b + c + e + f + g).
$$
B. Case of two equal massive particles

1. Exact result

In this case we consider \( d \geq 3 \) and focus on the physically important case of two particles of equal mass \((m_1 = m_2 = 1)\) interacting between themselves and with another two particles \((m_3 = m_4 = m)\) through an harmonic oscillator potential, namely

\[
\tilde{V} = \frac{1}{4} \rho_{12} + \frac{K_1}{2} \rho_{34} + \frac{K_2}{2} (\rho_{13} + \rho_{14} + \rho_{23} + \rho_{24}) , \quad K_2 > 0 ; \ K_1 > 0 . \tag{46}
\]

For the Hamiltonian \((39)\), the exact ground state energy and the corresponding eigenfunction are given by

\[
\tilde{E}_0 = d (\alpha + 4 \beta + \gamma) = \frac{1}{2} d \left( \sqrt{1 + 2K_2} + \sqrt{\frac{2(K_1 + K_2)}{m}} + \sqrt{\frac{2K_2(1 + m)}{m}} \right) , \tag{47}
\]

\[
\tilde{\psi}_0 = \mathcal{N} e^{-\left(\frac{1}{2} \rho_{12} + \frac{\beta}{m(1+m)} \rho_{13} + \rho_{14} + \rho_{23} + \rho_{24}\right) + \frac{\gamma}{2} \rho_{34} ,} \tag{48}
\]

respectively, where

\[
\alpha = \frac{1}{2} \left( \sqrt{1 + 2K_2} - \sqrt{\frac{2K_2 m}{1 + m}} \right) ,
\]

\[
\beta = \frac{1}{2} \sqrt{\frac{K_2(1 + m)}{2m}} , \tag{49}
\]

\[
\gamma = \frac{1}{\sqrt{2m}} \left( \sqrt{K_1 + K_2} - \sqrt{\frac{K_2}{1 + m}} \right) ,
\]

and \( \mathcal{N} \) is a normalization constant.

2. Approximate solution

Now, for our problem at hand the Born-Oppenheimer approximation starts with the assumption that two masses \( m_1 = m_2 = 1 \) are much heavier than the other two \( m_3 = m_4 \ll 1 \), thus \( r_1 \) and \( r_2 \) are fixed \((\rho_{12} \) is constant) and then one solves first the electronic radial eigenvalue equation.
\[ \hat{H}^{\text{(electronic)}}_{\text{rad}} \tilde{\psi}^{(e)} = \left[ -\Delta^{\text{(electronic)}}_{\text{rad}} + \frac{K_1}{2} \rho_{34} + \frac{K_2}{2} (\rho_{13} + \rho_{14} + \rho_{23} + \rho_{24}) \right] \tilde{\psi}^{(e)} = \tilde{E}^{(e)} \tilde{\psi}^{(e)}, \]

where the operator

\[ \frac{m}{2} \Delta^{\text{(electronic)}}_{\text{rad}}(\rho) = \left[ \rho_{13} \partial^2_{\rho_{13}} + \rho_{14} \partial^2_{\rho_{14}} + \rho_{23} \partial^2_{\rho_{23}} + \rho_{24} \partial^2_{\rho_{24}} + 2 \rho_{34} \partial^2_{\rho_{34}} \right] + \left( (\rho_{13} + \rho_{23} - \rho_{12}) \partial_{\rho_{13}} \partial_{\rho_{23}} + (\rho_{13} + \rho_{34} - \rho_{14}) \partial_{\rho_{13}} \partial_{\rho_{34}} + (\rho_{23} + \rho_{34} - \rho_{24}) \partial_{\rho_{23}} \partial_{\rho_{34}} \right) + \left( (\rho_{14} + \rho_{24} - \rho_{12}) \partial_{\rho_{14}} \partial_{\rho_{24}} + (\rho_{14} + \rho_{34} - \rho_{13}) \partial_{\rho_{14}} \partial_{\rho_{34}} + (\rho_{24} + \rho_{34} - \rho_{23}) \partial_{\rho_{24}} \partial_{\rho_{34}} \right) + \frac{d}{2} \left[ \partial_{\rho_{13}} + \partial_{\rho_{14}} + \partial_{\rho_{23}} + \partial_{\rho_{24}} + 2 \partial_{\rho_{34}} \right], \]

depends on \( \rho_{12} \) parametrically. For the eigenvalue problem (50) we obtain the ground state function

\[ \tilde{\psi}^{(e)}_0 = \mathcal{N}^{(e)} e^{-\frac{1}{2} \sqrt{\frac{m}{2}} \left[ \sqrt{K_2} (\rho_{13} + \rho_{14} + \rho_{23} + \rho_{24} - \rho_{12} - \rho_{34}) + \sqrt{K_1 + K_2} \rho_{34} \right]}, \]

with energy

\[ \tilde{E}^{(e)}_0 = \frac{d}{\sqrt{2 m}} \left( \sqrt{K_2} + \sqrt{K_1 + K_2} \right) + \frac{K_2}{2} \rho_{12}, \]

where \( \mathcal{N}^{(e)} = \mathcal{N}^{(e)}(K_1, K_2, m, d) \) in (52) is a normalization factor. It is such that the \( L^2 \)-condition \( \int (\tilde{\psi}^{(e)}_0)^2 \, dr_3 \, dr_4 = 1 \) holds, where the integration is over the electronic variables \( r_3 \) and \( r_4 \) only.

Expression (53) is the one we must add to the Hamiltonian of the relative motion of the two heavy particles \( m_1 = m_2 = 1 \), namely \( (-4 \rho_{12} \partial^2_{\rho_{12}} - 2 d \partial_{\rho_{12}} + \frac{1}{4} \rho_{12}) \), to get the nuclear Hamiltonian, i.e.

\[ \hat{\mathcal{H}}^{\text{(nuclear)}} = \left[ -4 \rho_{12} \partial^2_{\rho_{12}} - 2 d \partial_{\rho_{12}} + \frac{1}{4} \rho_{12} \right] + \frac{d}{\sqrt{2 m}} \left( \sqrt{K_2} + \sqrt{K_1 + K_2} \right) + \frac{K_2}{2} \rho_{12}, \]

The ground state

\[ \tilde{\psi}^{(n)}_0 \propto e^{-\frac{1}{4} \sqrt{1 + 2 \frac{K_2}{m}} \rho_{12}}, \]
of (54) is the one of zero quanta with frequency $\sqrt{1 + 2K_2}$. Hence, the total wave function in the BOA takes the form

$$\tilde{\psi}_0^{(BO)} = N^{(BO)} e^{-\frac{1}{4}\sqrt{1 + 2K_2} \rho_{12} - \frac{1}{2}\sqrt{\frac{2}{9}\left[\sqrt{K_2 (\rho_{13} + \rho_{14} + \rho_{23} + \rho_{24} - \rho_{34})} + \sqrt{K_1 + K_2 \rho_{34}}\right]}},$$  (55)

where $N^{(BO)}$ is a normalization constant, and the corresponding energy is given by

$$\tilde{E}_0^{(BO)} = \frac{d}{2} \left( \sqrt{(1 + 2K_2)} + \sqrt{\frac{2K_2}{m}} + \sqrt{\frac{2(K_1 + K_2)}{m}} \right).$$  (56)

3. Accuracy of the Born-Oppenheimer approximation

To estimate the accuracy of the BOA, we compute the ratio of the exact and approximate energies in powers of the small mass $m \ll 1$, namely

$$\Delta \tilde{E} \equiv \frac{\tilde{E}_0 - \tilde{E}_0^{(BO)}}{\tilde{E}_0} = 1 - \frac{\sqrt{(1 + 2K_2)} + \sqrt{\frac{2K_2}{m}} + \sqrt{\frac{2(K_1 + K_2)}{m}}}{\sqrt{1 + 2K_2} + \sqrt{\frac{2(K_1 + K_2)}{m}} + \sqrt{\frac{2K_2(1+m)}{m}}} \approx \frac{1}{2} \frac{\sqrt{K_2}}{\sqrt{K_2} + \sqrt{K_1 + K_2}} m - \frac{1}{2\sqrt{2}} \frac{\sqrt{(1 + 2K_2)K_2}}{\sqrt{K_2} + \sqrt{K_1 + K_2}} m^{3/2} \ldots .$$  (57)

If (i) $K_1$ and $K_2$ are of the order of 1, which implies that the strength of the interaction between light and heavy particles is of the same order as between the light particles and (ii) $m = 1/2000$, which is approximately the relation between the electron and proton masses, then the ratio (57) is $1.024 \times 10^{-4}$. It means that the BOA for the four-body system we study is slightly more accurate than for the three-body case. In the case of the chemical compound $H_2O_2$ (Hydrogen peroxide), $m \approx 1/15$, the fractional energy correction is approximately 0.012, see Fig 3.

The ratio $\Delta \tilde{E}$ does not depend on the dimension $d$. As a function of the light mass $m$, the expansion of the exact energy (47) is given by

$$\tilde{E}_0 = \tilde{E}_0^{(BO)} + \frac{d}{2\sqrt{2}} \left( m^{1/2} - \frac{1}{4} m^{3/2} + \frac{1}{8} m^{5/2} + \ldots \right),$$  (58)

hence, again the sum of the first two terms correspond to the energy (56) obtained in the BOA. Denoting the phases in (48) and (55) as $\tilde{\Phi}$ and $\tilde{\Phi}_{BO}$, respectively, we easily obtain the relation
FIG. 3. The ratio $\Delta \tilde{E}$ as a function of the spring constant $K \equiv K_1 = K_2$ for (left) the $H_2$ molecule ($m = \frac{1}{2000}$) and the chemical compound $H_2O_2$ ($m = \frac{1}{15}$). The ratio $\Delta \tilde{E}$ is a monotonic increasing (bounded) function of $K$.

\[ \tilde{\Phi} = \tilde{\Phi}_{BO} + \frac{1}{4} \sqrt{\frac{K_2}{2}} \left( m^2 - \frac{3}{4} m^2 + O(m^2) \right) (\rho_{13} + \rho_{14} + \rho_{23} + \rho_{24} - \rho_{12} - \rho_{34}) , \] 

that tell us that the BOA provides the lowest terms of the Puiseux series of the exact result.

VI. MANY-BODY SYSTEM

In this section, we generalize the three-body ($n = 3$) and four-body ($n = 4$) systems to the case of an arbitrary number of particles $n$. Assuming $d \geq (n - 1)$ and that the potential $V = V_n(\rho)$ solely depends on the $\frac{n(n-1)}{2}$ $\rho$-variables

\[ \rho_{ij} = \rho_{ij}^2 \quad i, j = 0, 1, 2, \ldots, n, \quad i < j , \]

we arrive, eventually, at the $\frac{n(n-1)}{2}$-dimensional eigenvalue problem

\[ [-\Delta^{(n)}_{\text{rad}}(\rho) + V_n(\rho)] \psi(\rho) = E \psi(\rho) , \] 

in the $\rho$-space of relative motion, where

\[ \Delta^{(n)}_{\text{rad}}(\rho) = 2 \sum_{i \neq j, i \neq k, j < k} \frac{1}{m_i} (\rho_{ij} + \rho_{ik} - \rho_{jk}) \frac{\partial}{\partial \rho_{ij}} \rho_{ik} \rho_{jk} + 2 \sum_{i < j} \left( \frac{m_i + m_j}{m_i m_j} \right) \rho_{ij} \frac{\partial^2}{\partial^2 \rho_{ij}} + \frac{d}{m_i m_j} \frac{\partial}{\partial \rho_{ij}} , \]
where $\mu_{ij}$ is as defined before and $\Delta^{(n)}_{\text{rad}}$ plays the role of kinetic radial operator cf. (5). It was conjectured that the operator

$$
\mathcal{H}^{(n)}_{\text{rad}} \equiv -\Delta^{(n)}_{\text{rad}} + V_n,
$$

is equivalent to a $\frac{n(n-1)}{2}$-dimensional radial Schrödinger operator, see [1]. As a function of the $\rho$-variables, the operator (61) is not $S_{n(n-1)}$ permutationally-invariant. Nevertheless, it remains $S_n$ invariant under the permutations of the $n$ particles.

For the Hamiltonian $\mathcal{H}^{(n)}_{\text{rad}}$ (62), the configuration space is given by $V_n \geq 0$ where $V_n$ is the simplex (volume) of the polytope of interaction whose vertices correspond to the positions of the particles. The quantity $V_n$ can be written as a Cayley-Menger determinant [17]. The reduced Hamiltonian $\mathcal{H}^{(n)}_{\text{rad}}$ (62) is essentially self-adjoint with respect to the radial measure

$$
d\rho_n = (V_n)^{d-n} \prod_{i,j=1; i<j}^n d\rho_{ij}.
$$

Although the radial Hamiltonian is essentially self-adjoint it is not in the form of a Laplace-Beltrami operator plus potential. For this to be true a further gauge transformation is needed, see [1].

VII. MANY-BODY HARMONIC OSCILLATOR

For the $n$-body problem in $d$ dimensions ($d \geq n - 1$), we consider the harmonic potential

$$
V_n^{(es)} = 2\omega^2 \sum_{i<j}^n \nu_{i,j} \rho_{ij},
$$

where $\omega$ and the $\nu$'s are positive constants. In this case, the reduced Hamiltonian (62)

$$
\mathcal{H}^{(es)}_{n,\text{rad}} = -\Delta^{(n)}_{\text{rad}} + V_n^{(es)},
$$

is an exactly solvable operator. The ground state function takes the following form

$$
\Psi_{n,0}^{(es)} = \mathcal{N} e^{-\omega(\sum_{i<j}^n a_{ij}\mu_{ij}\rho_{ij})},
$$

where $\mathcal{N}$ is a normalization factor and the parameters $a_{ij}$ in the exponent are related to those of the potential (64) through the $\frac{n(n-1)}{2}$ algebraic equations

$$
a_{ij} = a_{ij}^2 \mu_{ij} + a_{ij} \left( \sum_{i<k; k\neq j}^n \frac{1}{m_i} a_{ik} + \sum_{k<j; k\neq i}^n \frac{1}{m_j} a_{kj} \right)
\quad - \sum_{i<k<j}^n \frac{1}{m_k} a_{ik} a_{kj} - \sum_{i,j<k}^n \frac{1}{m_k} a_{ik} a_{jk} - \sum_{j<k<i}^n \frac{1}{m_k} a_{ki} a_{jk}.
$$
The ground state energy is given by

\[ E_{n,0}^{(es)} = \omega d \sum_{i<j}^{n} a_{i,j}. \]  

(68)

A. Case of two equal massive particles

1. Exact result

Now, we focus on the special case where two particles of equal mass \((m_1 = m_2 = 1)\) interact between themselves and with \((n-2)\) identical particles \((m_3 = m_4 = \ldots = m_n = m)\) through an harmonic oscillator potential, namely

\[ V = \frac{1}{4} \rho_{12} + \frac{K_2}{2} \left( \sum_{j=2}^{n} \rho_{1j} + \sum_{j=3}^{n} \rho_{2j} \right) + \frac{K_1}{2} \sum_{i,j=3,i\neq j}^{n} \rho_{ij}. \]

(69)

For the Hamiltonian (65), the exact ground state energy and its eigenfunction are given by

\[ E_{n,0} = d \left[ \alpha + 2(n-2)\beta + \frac{1}{2}(n(n-5) + 6)\gamma \right] \]

\[ = \frac{1}{2}d \left[ \sqrt{1 + (n-2)K_2} + (n-3)\sqrt{\frac{2K_2 + (n-2)K_1}{m}} + \sqrt{\frac{K_2(2 + (n-2)m)}{m}} \right], \]

(70)

\[ \psi_{n,0} = \mathcal{N} e^{-\left(\alpha \frac{1}{2} \rho_{12} + \beta \frac{m}{2m+1} \left[ \sum_{j=2}^{n} \rho_{1j} + \sum_{j=3}^{n} \rho_{2j} \right] + \gamma \frac{m}{2} \sum_{i,j=3,i\neq j}^{n} \rho_{ij} \right)}, \]

(71)

respectively, where

\[ \alpha_n = \frac{1}{2} \left[ \sqrt{1 + (n-2)K_2} - (n-2)\sqrt{\frac{K_2 m}{2 + (n-2)m}} \right], \]

\[ \beta_n = \frac{1}{2} \frac{m+1}{m} \sqrt{\frac{K_2 m}{2 + (n-2)m}}, \]

(72)

\[ \gamma_n = \frac{1}{(n-2)\sqrt{m}} \left( \sqrt{(n-2)K_1 + 2K_2} - \sqrt{\frac{4K_2}{2 + (n-2)m}} \right), \]

and \( \mathcal{N} \) is a constant of normalization with respect to the radial measure \( d\rho_n \) (63).
2. **Accuracy of the Born-Oppenheimer approximation**

As for the Born-Oppenheimer approximation, we assume that the mass of two particles are equal \( m_1 = m_2 = 1 \) and much heavier than the remaining \((n - 2)\) particles which also have the same mass \( m \equiv m_3 = m_4 = \ldots = m_n \). As a function of the light mass \( m \), the sum of the first two terms of the expansion of the exact energy \((70)\)

\[
E_{n,0} = E_{n,0}^{(BO)} + \frac{d \sqrt{K_2 (n-2)}}{128 \sqrt{2}} \left( 32 m_1^2 - 4 m_3^2 (n-2) + m_5^2 (n-2)^2 + \ldots \right), \tag{73}
\]

coincide with the energy \( E_{n,0}^{(BO)} \) obtained in the BOA. For the phase

\[
\Phi_n \equiv -\left( \alpha_n \frac{1}{2} \rho_{12} + \beta_n \frac{m}{m+1} \left[ \sum_{j=2}^{n} \rho_{1j} + \sum_{j=3}^{n} \rho_{2j} \right] + \gamma_n \frac{m}{2} \sum_{i,j=3; i \neq j}^{n} \rho_{ij} \right),
\]

of the ground state in \((71)\), its Puiseux series expansion

\[
\Phi_n = \Phi_{n,BO} - \frac{(n-2)^2 \sqrt{K_2}}{16 \sqrt{2}} \left( m^{3/2} - \frac{3 m^{5/2} (n-2)}{8} + \ldots \right) \rho_{12}
+ \frac{(n-2)^2 \sqrt{K_2}}{8 \sqrt{2}} \left( m^{3/2} - \frac{3 m^{5/2} (n-2)}{8} + \ldots \right) \left[ \sum_{j=2}^{n} \rho_{1j} + \sum_{j=3}^{n} \rho_{2j} \right]
- \frac{\sqrt{K_2}}{4 \sqrt{2}} \left( m^{3/2} - \frac{3 m^{5/2} (n-2)}{8} + \ldots \right) \sum_{i,j=3; i \neq j}^{n} \rho_{ij}, \tag{74}
\]

also shows that its lowest terms reproduce the phase we calculated in the BOA. Finally, with \( m \ll 1 \), we compute the ratio

\[
\Delta E_n \equiv \frac{E_{n,0} - E_{n,0}^{(BO)}}{E_{n,0}} = \frac{\sqrt{K_2} (n-2)}{2 \sqrt{2} \left( (n-3) \sqrt{K_1 (n-2)} + 2 K_2 + \sqrt{2 K_2} \right) m}
- \frac{\sqrt{K_2} (n-2) \sqrt{K_2} (n-2) + 1}{2 \sqrt{2} \left( (n-3) \sqrt{K_1 (n-2)} + 2 K_2 + \sqrt{2 K_2} \right)^2} \frac{m^3}{m} + \ldots, \tag{75}
\]

to estimate the accuracy of the Born-Oppenheimer approximation. The ratio \((75)\), at \( n = 3 \) \((K_1 = 0)\) reduces to expression \((29)\) while at \( n = 4 \) coincides with \((57)\). Once again, the ratio \( \Delta E \) does not depend on the dimension \( d \). The first term, which is the dominant when \( m \ll 1 \), is always positive while the second term is negative. In the limit \( n \gg 1 \) the first and second term tend to \( \frac{1}{2} \sqrt{\frac{K_2}{2 K_1}} m \) and \( \frac{K_2}{2 \sqrt{2 K_1}} m^2 \), respectively.
CONCLUSIONS

In this paper we studied the quantum system of three particles coupled to each other by harmonic forces. We re-derived and extended to the $d$-dimensional case, using the formalism in Ref. [2], previous results (see [14]) such as the energies and eigenfunctions of the ground state. The exact results are compared with those obtained in the Born-Oppenheimer approximation (BOA), showing explicitly with examples the accuracy for the later.

We also studied the quantum 4-body problem in a $d$-dimensional space, $d > 2$, of two particles of equal heavy mass $m_1 = m_2 = 1$ interacting between themselves and with two light particles $m_3 = m_4 = m \ll 1$ through harmonic oscillator potentials. For the ground state level, this model is solved both exactly and within the framework of the Born-Oppenheimer approximation.

We have shown that the ratio between the energies of the approximate and exact solutions is $d$-independent and differs from unity by terms of the order of the dimensionless ratio $m$ of the masses. For the phase $\Phi$ of the ground state wave function and the corresponding ground state energy $E_0$, the approximate and exact solutions are related. The first terms of the Puiseux series expansion (in powers of $m$) of the exact results coincide exactly with the approximate solutions obtained in the BOA. Two physically relevant examples where considered where the light particles are either electrons ($H_2$ molecule) or protons ($H_2O_2$ compound).

The generalization to an arbitrary number $n$ of particles interacting through an harmonic oscillator potential in a $d$–dimensional space ($d \geq n - 1$) is discussed as well. In the case of two particles with equal heavy mass ($m_1 = m_2 = 1$) and $(n - 2)$ light particles ($m_3 = m_4 = \ldots = m_n = m \ll 1$), we found that the ratio between the energies of the approximate and exact solutions is again $d$-independent, and differs from unity by a term proportional to the ratio of the masses with an $n$-dependent coefficient that vanishes as $\sim \frac{1}{\sqrt{n}}$ at $n \to \infty$. We hope that the present consideration can be exploited and lead to approaches much better than the Born-Oppenheimer approximation.
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