Exotic atoms as a prototype of the general three-particle Coulomb problem

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The three-particle quantum-mechanical Coulomb problem for general masses is treated based on the large-dimensional method. This extends the theory to anisotropic systems. A perspective of the bonded configurations of diverse three-particle systems is provided specified by radial and angular correlations. It is shown that proper dissociation behavior is embedded, being a culmination of appropriate treatment of mass polarization and recoil effects. Vibrational effects rooted in interparticle correlations and which materialize beyond the leading approximation are delineated. The accompanying force constants, knowledge of which is a prerequisite for determining the wave functions and spectral features, are investigated. A special premium is placed on exotic atoms which display enhanced anisotropic features and serve to illuminate the underlying physical aspects.

I. INTRODUCTION

This paper is a sequel to previous works[1,2] in which a nonrelativistic framework was developed for treating general three-particle quantum systems based on the method of dimensional inflation.[3-6] By embedding the physical system in a space of arbitrary dimension N, which may be exploited as an expansion parameter, the theory has been structured in such a way that the physical attributes of the system remain intact. It is shown in this paper that this culminates in a precise formulation of recoil and mass polarization contributions (referred to collectively as inertial effects in the following discussion) which are of particular relevance for exotic atoms and molecules involving heavy constituents such as muons. The approach provides insight into the physical features of anisotropic systems and is of importance for deriving scaling features. A perspective of exotic atoms along these lines as a prototype of the general three-particle Coulomb problem is presented.

Section II addresses the structural aspects in terms of an effective potential which incorporates quantum fluctuations and is central to the method. General solutions for radial and angular correlations are reported corresponding to bonded structures determined by the stationary points of the effective potential. In Sec. III the vibrational aspects engendered by the bonded structures are investigated. Force constants and wave functions are derived and implemented to yield general results for three-particle ground-state energy eigenvalues. Section IV is devoted to the neutral muonic helium atom and concluding remarks.

II. BONDED THREE-PARTICLE COULOMB CONFIGURATIONS

A convenient starting point is the three-particle (s-state) Schrödinger equation for particles of general masses, in N spatial dimensions, given by[2]

$$\eta E\phi=-\varepsilon\left[\frac{\partial^2}{\partial P^2}+\frac{\partial^2}{\partial Q^2}+\left[\frac{1}{P^2}+\frac{1}{Q^2}\right]\frac{\partial^2}{\partial\gamma^2}\right]\phi+V_e\phi\ , \tag{2.1}$$

where E denotes the three-particle energy and the effective potential reads

$$V_e=\sum_{i=1}^{3}g_iP_i^{-1}+\frac{\Delta}{\eta}\left[\frac{1}{P^2}+\frac{1}{Q^2}\right]\left[\frac{(N-2)(N-4)}{\sin^2\gamma}-1\right] \tag{2.2}$$

and

$$\varepsilon=\frac{\hbar^2}{m\eta}\ , \tag{2.3}$$

while

$$\Delta=\frac{\hbar^2}{4m}\ . \tag{2.4}$$

The derivation of Eq. (2.1) is detailed in Sec. III of the first paper listed under Ref. 2 whereas the relationship of the wave function ϕ to the standard Schrödinger wave function is given by Eqs. (3.3) and (3.4) of the same paper.

The reduced mass of the three-particle system is denoted by

$$m=(m_1m_2+m_2m_3+m_3m_1)M^{-1} \tag{2.5}$$

with

$$M=m_1+m_2+m_3\ . \tag{2.6}$$

Apart from the basic requirement that η behaves as N^2 for large N it may be left arbitrary until Sec. III where the constraint imposed by the dissociation limit can be addressed. Meanwhile the scaling factor may be represented in the convenient form

$$\eta=[(N-1)-\delta_1][(N-1)-\delta_2]\ . \tag{2.7}$$

The effective potential to the required order is expressed as

$$V_e=V_e^L+R\frac{(\delta_1+\delta_2-4)}{(N-1)}+O\left[\frac{1}{(N-1)^2}\right]\ , \tag{2.8}$$

where the leading contribution to the effective potential reads

$$V_e^L=\sum_{i=1}^{3} g_i P_i^{-1}+\frac{\Delta}{\sin^2\gamma}\left[\frac{1}{P^2}+\frac{1}{Q^2}\right], \tag{2.9}$$

while the residual term is given by

$$R=\frac{\Delta}{\sin^2\gamma}\left[\frac{1}{P^2}+\frac{1}{Q^2}\right]. \tag{2.10}$$

Furthermore, the rescaled Jacobi vectors denoted by P and Q are defined by

$$x=\eta P,\quad y=\eta Q\ , \tag{2.11}$$

where the lengths of the Jacobi vectors are given by

$$x^2=\sum_{i=1}^{N} X_i^2,\quad y^2=\sum_{i=1}^{N} Y_i^2\ . \tag{2.12}$$

The center-of-mass (c.m.) coordinates and the Jacobi vectors, in turn, are given by

$$M\mathbf{R}=m_1\mathbf{R}_1+m_2\mathbf{R}_2+m_3\mathbf{R}_3\ , \tag{2.13}$$

$$\mathbf{X}=a(\mathbf{R}_1-\mathbf{R}_2)\ , \tag{2.14}$$

$$\mathbf{Y}=b(\mathbf{R}_3-\mathbf{Z})\ , \tag{2.15}$$

where the (1,2)-particle c.m. vector reads

$$\mathbf{Z}=(m_1\mathbf{R}_1+m_2\mathbf{R}_2)(m_1+m_2)^{-1} \tag{2.16}$$

and the normalization of the relative displacement vectors is determined by

$$a^2\mu_{12}^{-1}=\frac{2}{m}=b^2\mu_{(1+2),3}^{-1} \tag{2.17}$$

in terms of the reduced mass μ_{12} of particles 1 and 2; while the reduced mass of the pair (1,2) relative to 3 reads

$$\mu_{(1+2),3}=\sigma m_3 M^{-1},\quad \sigma=m_1+m_2\ . \tag{2.18}$$

The rescaled interparticle separations, denoted by P_i, which specify the geometry of the three-particle system assume the form

$$r_1^2=r_{23}^2=\eta^2\left[\frac{m_1^2P^2}{\sigma^2a^2}+\frac{2m_1PQ\cos\gamma}{\sigma ab}+\frac{Q^2}{b^2}\right]=\eta^2P_1^2\ , \tag{2.19}$$

$$r_2^2=r_{31}^2=\eta^2\left[\frac{m_2^2P^2}{\sigma^2a^2}-\frac{2m_2PQ\cos\gamma}{\sigma ab}+\frac{Q^2}{b^2}\right]=\eta^2P_2^2\ , \tag{2.20}$$

$$r_3^2=r_{12}^2=\eta^2\frac{P^2}{a^2}=\eta^2P_3^2\ , \tag{2.21}$$

where the directions of the Jacobi vectors have been chosen such that

$$\cos\gamma=\hat{\mathbf{X}}\cdot\hat{\mathbf{Y}}\ . \tag{2.22}$$

The merits of analytic continuation in the number of spatial dimensions have been discussed at some length in the literature.[1-6] At the heart of the method lies the fact that it represents a rigorous interpretation in the large-dimensional limit of highly correlated motions and concomitant geometrical aspects also in nonintegrable three-particle problems.[1] In this ideal limit the frozen bonded structures of the three-particle systems are then specified by the stationary points of the effective potential Eq. (2.9). The Jacobi coordinates play an essential role in that mass polarization contributions, which would be present in the kinetic term in a formalism based on relative interparticle coordinates, are automatically incorporated into the effective potential as are quantum-mechanical pressure effects responsible for the modified nature of the potential.[2] These modifications are most striking in the proximity of strong gradients generated by the Coulomb contribution to the potential represented by the first term of Eq. (2.2). Quantum fluctuations around the bonded structures are incorporated in Sec. III by including correction terms in the form of a $1/N$ expansion which engender rovibrational modes. By structuring the formalism in this particular way, physical aspects related, among others, to inertial effects are left intact. The main concern of this work is to clarify these features as manifested in three-particle exotic systems where they become pronounced through the presence of muons.

According to Eq. (2.1), the three-particle energy to leading order in η is given by the stationary points of the effective potential

$$E(3,s)=\frac{1}{\eta}V_e^L(P_s,Q_s,\gamma_s)\ , \tag{2.23}$$

where the index s designates the corresponding values at the stationary points determined by the solution of the set of equations:

$$0=\frac{2\Delta}{\sin^2\gamma P^2}+\frac{ag_3}{P}+\frac{g_1}{P_1^3}\left[\frac{A^2P^2}{a^2}+\frac{APQ\cos\gamma}{ab}\right]+\frac{g_2}{P_2^3}\left[\frac{B^2P^2}{a^2}-\frac{BPQ\cos\gamma}{ab}\right], \tag{2.24}$$

$$0=\frac{2\Delta}{\sin^2\gamma Q^2}+\frac{g_1}{P_1^3}\left[\frac{Q^2}{b^2}+\frac{APQ\cos\gamma}{ab}\right]+\frac{g_2}{P_2^3}\left[\frac{Q^2}{b^2}-\frac{BPQ\cos\gamma}{ab}\right], \tag{2.25}$$

$$\frac{2\Delta\cos^2\gamma}{\sin^4\gamma}\left[\frac{1}{P^2}+\frac{1}{Q^2}\right]=\frac{g_1}{P_1^3}\left[\frac{APQ\cos\gamma}{ab}\right]-\frac{g_2}{P_2^3}\left[\frac{BPQ\cos\gamma}{ab}\right], \tag{2.26}$$

where

$$A=m_1/\sigma,\quad B=m_2/\sigma\ . \tag{2.27}$$

The "exclusion" notation is furthermore employed for the coupling constant, viz., $g_1=g_{23}$ denotes the mutual coupling of the particles 2 and 3. Combining the first two

equations, it follows that

$$\frac{2\Delta}{\sin^2\gamma}\left[\frac{1}{P^2}+\frac{1}{Q^2}\right]=-\frac{ag_3}{P}-\frac{g_1}{P_1}-\frac{g_2}{P_2}\ . \tag{2.28}$$

This result may be recognized as an expression of the virial theorem. Although the way it has emerged in this approach may seem somewhat foreign compared to standard treatments, the fact that the individual components of the effective potential are related in this particular manner at the stationary points serves to emphasize the kinetic origin of the extra term accompanying the usual Coulomb contribution. Combining Eqs. (2.9), (2.23), and (2.28) yields the leading-order contribution of the stationary point energy:

$$E(3,s)=\frac{1}{2\eta}\left[\frac{ag_3}{P}+\frac{g_1}{P_1}+\frac{g_2}{P_2}\right]\ . \tag{2.29}$$

This particular form of the energy displays the partition of energy among the individual constituents once the geometry of the bonded structure is known. The treatment of the variational problem is facilitated by solving for a particular bond length in terms of the other internal variables. With a view to solving for P_1, we define the auxiliary quantity

$$v=P_2/P_1 \tag{2.30}$$

and furthermore record the following relationships which form a bridge between the Jacobi and the relative (internal) coordinates:

$$\cos\gamma=\frac{\Omega}{rt},\quad \sin\gamma=\frac{v(1-c^2)^{1/2}}{rt}\ , \tag{2.31}$$

$$P=aP_1r,\quad Q=bP_1t\ , \tag{2.32}$$

$$PQ\cos\gamma=abP_1^2\Omega\ , \tag{2.33}$$

where

$$\Omega=B-Av^2+vc(A-B)\ , \tag{2.34}$$

$$r^2=1+v^2-2vc\ , \tag{2.35}$$

$$t^2=B^2+A^2v^2+2ABvc\ , \tag{2.36}$$

and $c=\cos\theta_3=\cos\theta_{12}=\hat{P}_1\cdot\hat{P}_2$, where θ_3 denotes the angle subtended by the particles 1 and 2 at the third. The expectation values of the inner products of the relative vectors (in conjunction with the interparticle separations) serve as a natural measure for interparticle correlations. In view of the circumstance that the large-dimensional limit represents a novel "semiclassical" limit providing direct access to expectation values, the cosine of the angle referred to above may for brevity in the following discussion be termed the correlation angle. Equations (2.25) and (2.30)–(2.36) yield the following expression for the interparticle separation:

$$P_1=-\frac{2\Delta r^2}{b^2(1-c^2)W}\ , \tag{2.37}$$

where

$$W=g_1v^2(B+Avc)+g_2(vA+Bc) \tag{2.38a}$$

and

$$\frac{b^2}{\Delta}=\frac{8}{\hbar^2}\left[\frac{m_3\sigma}{M}\right]\ . \tag{2.38b}$$

Employing Eq. (2.37) to eliminate P_1 from Eqs. (2.24)–(2.26) the following system of coupled equations for v and c results:

$$v^2rg_3+r^2[g_1v^2A(1-vc)+g_2B(v-c)]$$
$$=b^2t^2a^{-2}[g_1v^2(B+Avc)+g_2(vA+Bc)] \tag{2.39}$$

and

$$r(g_2B-Av^3g_1)(1-c^2)=[vg_3+r(vg_1+g_2)]$$
$$\times[B-Av^2+(A-B)vc]\ . \tag{2.40}$$

Furthermore, equivalent forms of the equations needed in later development are recorded

$$rv^2g_3+vr^2(vg_1+g_2)=TW\ , \tag{2.41}$$

$$vr^2(g_2B-Av^3g_1)(1-c^2)=TW\Omega\ , \tag{2.42}$$

where

$$T=r^2+b^2t^2a^{-2}\ . \tag{2.43}$$

Before investigating the general solutions, a special case is considered to make contact with previous work. When two of the constituents possess equal mass and charge ($m_1=m_2$, $A=B$, $g_1=g_2$) a symmetrical configuration results. Equation (2.40) is satisfied by $v=1$ expressing, via Eq. (2.30), the fact that the equal-mass particles are located on the base points of an isosceles triangle. Equation (2.39) in turn fixes the correlation angle.

Returning to the general situation, the following convention is adopted: Regard the particle of mass m_3 as the attracting center, and in order to display clustering features of the solutions, the particle masses are ordered according to $m_3\geq m_2\geq m_1$. The multiplicity of solutions generated by the system of Eqs. (2.39) and (2.40) corresponds to different stationary points which the three-particle system and its subsystems may assume. Attention is, first of all, restricted to the particular solution $v=c=0$, which describes the dissociation limits. In order to avoid subtle issues that arise in the indefinite form of Eq. (2.37) in this limit, the equivalent form for the interparticle separation is noted

$$P_1=\frac{2\Delta T\Omega}{vb^2(g_1Av^3-g_2B)(1-c^2)^2} \tag{2.44}$$

which follows from Eqs. (2.24), (2.31)–(2.36), and (2.41). When v approaches zero, one of the constituent particles (m_2) tends to dissociate. The accompanying behavior of the correlation angle, specified by c approaching zero, is a general feature of this highly fragmented regime.[1] The scaling of the interparticle separation with the masses of the particles that remain bound is of significance. Utilizing Eqs. (2.30) and (2.44) and employing the result that

$$\left[\frac{\Delta T}{b^2}\right]_{v=c=0}=\frac{\Delta}{a^2b^2}(a^2+b^2B^2)$$
$$=\left[\frac{\Delta}{b^2}\right]\frac{\sigma(m_1+m_3)}{m_1M}\ , \qquad (2.45)$$

it follows that

$$r_2=\eta P_2=\left[\frac{\eta}{4}\right]\left[\frac{\hbar^2}{-g_2}\right]\left[\frac{m_1+m_3}{m_1m_3}\right],\quad g_2<0\ . \qquad (2.46)$$

This result guarantees that the stationary point energy

$$E(3,s)=\frac{1}{\eta}V_e^L(s)$$
$$=\frac{TW}{2\eta P_1v^2r^2}=\frac{1}{2\eta P_2}\left[\frac{vg_3}{r}+vg_1+g_2\right] \qquad (2.47)$$

exhibits the proper threshold behavior,

$$E(3,s,v=c=0)=-\left[\frac{4}{\eta}\right]\left[\frac{g_2^2}{2\hbar^2}\right]\left[\frac{m_1m_3}{m_1+m_3}\right]\ . \qquad (2.48)$$

The multiplicative scaling factor $4/\eta$ is specific to the large-dimensional approach. It is apparent that the proper ionization energy to the leading order is guaranteed by $\eta=(N-1)^2$. The three-particle binding energy differs from that of the related two-particle system by genuine three-particle features subsumed under the heading correlation effects conveniently incorporated by the dependence on the variable c. As has been discussed above, it transpires that in the fragmentation regime angular correlation effects tend to wash out as c tends to zero. In this asymptotic regime where the extra particle acts as a mere spectator, the integrability of the residual three-particle situation inevitably leads to the suggested singularity structure in $(N-1)^2$, characteristic of the two-particle Coulomb problem. The asymptotic limit when v become large elicits the analogous behavior where particle m_1 plays the role of spectator. Cognizance of the role of inertial effects culminates in proper threshold characteristics, which is not a matter of course even in more standard approaches as attested by recent investigations.[7] These results augur well for the treatment of the truly three-particle bound states, which is next on the agenda.

Table I collates the results of the numerical solution of Eqs. (2.39) and (2.40) for the ratio of the interparticle separation v and the correlation angle for a number of representative systems. The first entry of the table ($^{\infty}$He) assumes the center of attraction to be infinitely massive and serves as a point of reference where inertial effects are negligible. The values of the parameters[8] employed in the calculation are given by

$$m_e/m_\mu=4.836\,332\,18\times10^{-3}\ ,$$
$$m_e/m_p=5.446\,170\,13\times10^{-4}\ ,$$
$$m_e/m_d=2.724\,437\,07\times10^{-4}\ ,$$
$$m_e/m_{^4\mathrm{He}}=1.370\,933\,54\times10^{-4}\ ,$$
$$m_e/m_{^3\mathrm{He}}=1.819\,529\times10^{-4}\ ,$$
$$m_\mu/m_{\pi^-}=0.757\,042\,4\ ,$$
$$m_d/m_{^3\mathrm{He}}=0.667\,851,\quad m_d/m_t=0.667\,737\,0\ .$$

A cursory glance at the table reveals the pivotal role played by the coupling constants (expressed in units of e^2) as is to be expected, i.e., for fixed coupling-constant ratios the values of the geometrical attributes tend to cluster around common values. The spread within each subclass

TABLE I. Values of v and c determined by numerical solution of Eqs. (2.39) and (2.40) for a number of prototype systems. The first entry of the table ($^{\infty}$He) assumes the center of attraction to be sufficiently massive to suppress inertial effects.

Physical system	Assembly of coupling constants g_1	g_2	g_3	Solutions v	c
$^{\infty}He^{2+}e^-e^-$	−2	−2	1	1	−0.092 380 87
$^4He^{2+}e^-e^-$	−2	−2	1	1	−0.092 321 92
$^4He^{2+}\mu^-\mu^-$	−2	−2	1	1	−0.080 539 47
$^4He^{2+}\mu^-e^-$	−2	−2	1	402.187 399	$6.536\,579\times10^{-5}$
$^3He^{2+}\mu^-e^-$	−2	−2	1	1	−0.092 302 63
$^3He^{2+}\mu^-\mu^-$	−2	−2	1	1	−0.076 809 73
$^3He^{2+}\mu^-e^-$	−2	−2	1	398.608 915	$8.770\,447\times10^{-5}$
$^3He^{2+}\mu^-e^+$	−2	+2	−1	1.000 001 38	0.999 998 61
$^3He^{2+}\mu^+e^-$	2	−2	−1	0.962 694 74	0.927 023 04
$^4He^{2+}\pi^-\mu^-$	−2	−2	1	1.833 997 08	−0.057 166 2
$^4He^{2+}\pi^+\mu^-$	2	−2	−1	0.984 363 66	0.977 482 68
$^3He^{2+}d^+\mu^-$	2	−2	−1	0.960 274 36	0.930 327 61
$^4He^{2+}d^+\mu^-$	2	−2	−1	0.961 611 36	0.931 382 97
$p^+e^-e^-$	−1	−1	1	1	−0.192 898 09
$d^+d^+\mu^-$	1	−1	−1	0.778 691 88	0.642 102 49
$t^+d^+\mu^-$	1	−1	−1	0.791 497 02	0.652 827 88
$e^+e^-e^-$	−1	−1	1	1	−0.017 384 4
$\mu^-e^+e^+$	−1	−1	1	1	−0.191 386 97

originates from inertial effects. The solutions with constant value $v=1$ obtain for systems built up of two equal-mass particles sharing equal interactions and reflects the underlying isosceles symmetry. A dramatic illustration of the import of inertial effects is for the neutral helium muonic system ($He^{2+}\mu^-e^-$), where v is catapulted to 402.2 and 398.6 for the ^{4}He and ^{3}He isotopes, respectively. Further discussion of this important physical system is relegated to Sec. IV. Suffice it to remark here that although the picture of close proximity of the muon to the central nucleus to form an attractive core orbited by the widely separated electron may be gleaned from physical reasoning and confirmed by a variational treatment, for example, the general framework provided here for the first time furnishes a unified description subsuming the diverse Coulomb systems under a single heading.

In conclusion to this section, attention is drawn to a special class of systems which exhibit spontaneous symmetry breakdown. As has been shown by a stability analysis,[9] symmetry breakdown is a generic feature of systems where the central nuclear charge falls below a critical value ($Z<2$). The treatment of the ground state of this special class of delicately bound anisotropic systems which, in spite of the symmetry in masses and coupling constants spontaneously assume a scalene configuration, constitutes an important open problem for future work in the large-dimensional method. The isosceles arrangements which materialize in these cases are actually autoionization states. This impediment should not detract from the validity of the general theory of anisotropic systems above this divide, which is the concern of the present paper.

Before going afield with higher-order results in the next section, it is recalled that apart from the useful role of the leading approximation to articulate essential physical features, the rigorous large-N results can be surprisingly accurate when implemented for $N=3$. This is particularly the case when dealing with ratios of interparticle separations, for example,[10] or alternatively conformally invariant objects such as the cosines of bond angles which are immune to rescalings.

III. VIBRATIONAL STATES FOR ANISOTROPIC SYSTEMS

In the preceding section attention was focussed on structural configurations and the ordered values of bond lengths and angles sustained by the effective potential were emphasized. Vibrations provide probes of the structural order and entail distortions of the stationary geometrical degrees of freedom by bond bending and stretching. The next to leading term in the large-dimensional expansion describes the harmonic deviations relative to the stationary configurations by the equation of motion

$$\eta E\phi=-\varepsilon\left[\frac{\partial^2}{\partial P^2}+\frac{\partial^2}{\partial Q^2}+\frac{\partial^2}{\partial\Gamma^2}\right]\phi+V_e^L(s)\phi+R_s\frac{(\delta_1+\delta_2-4)}{(N-1)}\phi$$
$$+[p^2V_1+q^2V_2+2pqV_3+(\Gamma-\bar{\Gamma}_s)^2\Gamma_sV_{\gamma\gamma}+2p(\Gamma-\bar{\Gamma}_s)\Gamma_s^{1/2}V_{P\gamma}+2q(\Gamma-\bar{\Gamma}_s)\Gamma_s^{1/2}V_{Q\gamma}]\phi\ . \tag{3.1}$$

The harmonic coefficients in the expansion of the potential around the stationary points are defined by

$$V_1=\frac{1}{2}\left[\frac{\partial^2V_e^L}{\partial P^2}\right]_s,\quad V_2=\frac{1}{2}\left[\frac{\partial^2V_e^L}{\partial Q^2}\right]_s,$$
$$V_3=\frac{1}{2}\left[\frac{\partial^2V_e^L}{\partial P\partial Q}\right]_s \tag{3.2}$$

and

$$V_{\gamma\gamma}=\frac{1}{2}\left[\frac{\partial^2V_e^L}{\partial\gamma^2}\right]_s,\quad V_{P\gamma}=\frac{1}{2}\left[\frac{\partial^2V_e^L}{\partial P\partial\gamma}\right]_s,$$
$$V_{Q\gamma}=\frac{1}{2}\left[\frac{\partial^2V_e^L}{\partial Q\partial\gamma}\right]_s, \tag{3.3}$$

where

$$\Gamma=\Gamma_s^{-1/2}\gamma,\quad \bar{\Gamma}_s=\Gamma_s^{-1/2}\gamma_s\ , \tag{3.4}$$

$$\Gamma_s=\left[\frac{1}{P^2}+\frac{1}{Q^2}\right]_s=T(bP_1tr)^{-2}\ , \tag{3.5}$$

and

$$p=P-P_s,\quad q=Q-Q_s\ .$$

The wave function which describes the internal dynamics of this localized structure is given by the Gaussian form

$$\phi=N_0\exp(-\tfrac{1}{2})[w_1(P-P_s)^2+2W_1(P-P_s)(Q-Q_s)$$
$$+w_2(Q-Q_s)^2+w_3(\Gamma-\bar{\Gamma}_s)^2$$
$$+2W_2(P-P_s)(\Gamma-\bar{\Gamma}_s)$$
$$+2W_3(Q-Q_s)(\Gamma-\bar{\Gamma}_s)]\ , \tag{3.6}$$

where N_0 denotes a normalization factor.

Combining Eqs. (3.1) and (3.6) and comparing coefficients, the energy eigenvalue is given by

$$E_s=E(3,s)+\left[\frac{\varepsilon}{\eta}\right](w_1+w_2+w_3)$$
$$+\frac{R_s}{\eta}\left[\frac{\delta_1+\delta_2-4}{N-1}\right], \tag{3.7}$$

where the vibrational energies are determined by the coupled set of equations

$$\varepsilon(w_1^2+W_1^2+W_2^2)=V_1\ , \tag{3.8a}$$

$$\varepsilon(w_2^2+W_1^2+W_3^2)=V_2\ , \tag{3.8b}$$

$$\varepsilon(w_3^2+W_2^2+W_3^2)=\Gamma_s V_{\gamma\gamma} , \tag{3.8c}$$

$$\varepsilon(w_1W_1+w_2W_1+W_2W_3)=V_3 , \tag{3.8d}$$

$$\varepsilon(w_1W_2+w_3W_2+W_1W_3)=\Gamma_s^{1/2}V_{P\gamma} , \tag{3.8e}$$

$$\varepsilon(w_2W_3+w_3W_3+W_1W_2)=\Gamma_s^{1/2}V_{Q\gamma} . \tag{3.8f}$$

Employing the relationships

$$\frac{\varepsilon}{P_1^2}=-\left[\frac{4}{\eta}\right]\frac{2V_e^L(s)v^2(1-c^2)(\xi_1+\xi_2)}{T(\xi_1+\xi_2+\xi_1\xi_2)} , \tag{3.9}$$

$$a^2=\frac{2\xi_1(1+\xi_1+\xi_2)}{(1+\alpha)(\xi_1+\xi_2+\xi_1\xi_2)} , \tag{3.10}$$

$$b^2=\frac{2\xi_2(1+\alpha)}{(\xi_1+\xi_2+\xi_1\xi_2)} \tag{3.11}$$

(where $\alpha=m_1/m_2$, $\xi_1=m_1/m_3$, and $\xi_2=m_2/m_3$) the required force constants, constrained by the stationary-state conditions, may in terms of the appropriate three-particle energy units be cast into the forms

$$V_1=-V_e^L(s)\frac{H_{11}}{a^2P_1^2r^2}=\rho V_{11} , \tag{3.12}$$

$$V_2=-V_e^L(s)\frac{r^2H_{22}}{b^2P_1^2t^2T}=\rho V_{22} , \tag{3.13}$$

$$V_3=-V_e^L(s)\frac{H_{12}}{abP_1^2}=\rho V_{12} , \tag{3.14}$$

$$\Gamma_s V_{\gamma\gamma}=\rho V_{33} , \tag{3.15}$$

$$\Gamma_s^{1/2}V_{P\gamma}=-V_e^L(s)\frac{T^{1/2}H_{13}}{abtr^2P_1^2(1-c^2)^{1/2}}=\rho V_{13} , \tag{3.16}$$

and

$$\Gamma_s^{1/2}V_{Q\gamma}=-V_e^L(s)\frac{T^{1/2}H_{23}}{b^2P_1^2t^2r(1-c^2)^{1/2}}=\rho V_{23} , \tag{3.17}$$

where

$$\rho^{1/2}=-\left[\frac{4\eta}{\varepsilon}\right]^{1/2}E(3,s) . \tag{3.18}$$

The fact that $E(3,s)$ is negative is to be kept in mind generally. The auxiliary quantities are defined as follows:

$$V_{11}=\frac{v^2(1-c^2)H_{11}(1+\alpha)(\xi_1+\xi_2)}{r^2T\xi_1(1+\xi_1+\xi_2)} , \tag{3.19}$$

$$\begin{aligned}H_{11}=1&-\frac{3r^2}{T}+\frac{2r^2v(vg_1+g_2)}{TW}\\&+\frac{r^4}{vTW}(g_1A^2v^3+g_2B^2)\\&-\frac{3g_1r^2v^2}{TW}(A^2r^2+A\Omega)^2\\&-\frac{3g_2r^2}{v^3TW}(B^2r^2-B\Omega)^2 ,\end{aligned} \tag{3.20}$$

$$V_{22}=\frac{r^2v^2(1-c^2)H_{22}}{t^2T^2} , \tag{3.21}$$

$$\begin{aligned}H_{22}=3&+\frac{t^2}{Wv}(g_1v^3+g_2)\\&-\frac{3g_1v^2}{W}(t^2+A\Omega)^2-\frac{3g_2}{Wv^3}(t^2-B\Omega)^2 ,\end{aligned} \tag{3.22}$$

$$V_{12}=\frac{v^2(1-c^2)H_{12}}{T}\left[\frac{(\xi_1+\xi_2)^2}{\xi_1\xi_2(1+\xi_1+\xi_2)}\right]^{1/2} , \tag{3.23}$$

$$\begin{aligned}H_{12}=&-\frac{\Omega^2}{v^2rt(1-c^2)}\\&+\left[\frac{3r}{tTWv^3}\right][\Omega r^2(B^3g_2-A^3v^5g_1)\\&+\Omega t^2(g_2B-Av^5g_1)\\&-(g_1A^2v^5+g_2B^2)(r^2t^2+\Omega^2)] ,\end{aligned} \tag{3.24}$$

$$V_{33}=\frac{H_{33}}{r^2t^2} , \tag{3.25}$$

$$\begin{aligned}H_{33}=&v^2(1-c^2)+4\Omega^2\\&-\frac{3vr^2(1-c^2)^2}{TW}(g_1A^2v^5+g_2B^2) ,\end{aligned} \tag{3.26}$$

$$V_{13}=\frac{v^2(1-c^2)^{1/2}H_{13}}{tr^2T^{1/2}}\left[\frac{(\xi_1+\xi_2)^2}{\xi_1\xi_2(1+\xi_1+\xi_2)}\right]^{1/2} , \tag{3.27}$$

$$\begin{aligned}H_{13}=&\frac{3\Omega}{v}-\frac{2\Omega r^2}{Tv}\\&+\frac{3(1-c^2)r^2}{TWv^2}[r^2(g_1A^3v^5-g_2B^3)\\&+\Omega(g_1A^2v^5+g_2B^2)] ,\end{aligned} \tag{3.28}$$

$$V_{23}=\frac{v^2(1-c^2)^{1/2}H_{23}}{t^2rT^{1/2}} , \tag{3.29}$$

and

$$\begin{aligned}H_{23}=&\frac{\Omega}{v}+\frac{2\Omega r^2}{Tv}-\frac{3r^2t^2(1-c^2)}{TWv^2}(g_2B-g_1Av^5)\\&-\frac{3\Omega r^2(1-c^2)}{TWv^2}(g_2B^2-g_1A^2v^5) .\end{aligned} \tag{3.30}$$

Knowledge of the force constants embodied by Eqs. (3.19)–(3.30) is a prerequisite for determining the wave functions and spectral features via Eqs. (3.6) and (3.7). The relative values of the force constants listed in Tables I and II serve as a measure for the mixing of states and indicate that the luxury of the most general treatment of the eigenvalue problem is unnecessary in the majority of cases. To avoid extensive calculations it is fruitful to opt for a simplified procedure of diagonalization by neglecting the weak dependence on the off-diagonal matrix elements V_{13} and V_{23}. The vanishing of these coefficients is a consequence of isosceles configurations and effectively

TABLE II. Values of the (dimensionless) vibrational constants defined by Eqs. (3.19)–(3.30).

System	V_{11}	V_{22}	V_{12}	V_{33}	V_{13}	V_{23}
$^4He\mu^-e^-$	$4.687\,76\times10^{-3}$	0.995 789 5	−0.060 699 6	0.997 042 5	−0.031 301 9	$-9.069\,7\times10^{-4}$
$^3He\mu^-e^-$	$4.645\,96\times10^{-3}$	0.995 824 6	−0.060 314 9	0.997 027	−0.031 383 5	$-8.854\,7\times10^{-4}$
$^4He\mu^-\mu^-$	0.599 463 95	0.804 172 5	−0.446 290 4	0.102 181	0	0
$^4He\pi^-\mu^-$	0.534 417 5	0.778 744 7	−0.443 513 6	0.286 477 6	−0.131 534 3	−0.070 275 9
$^4Hee^-e^-$	0.612 027 3	0.787 233 6	−0.445 576 6	0.105 013 28	0	0

persists in a number of relevant cases. We concentrate on these special systems in the sequel which suffices to illustrate the general procedure. It then follows that $W_2=W_3=0$, which culminates in the solution

$$w_3=\left[\frac{\rho}{\varepsilon}\right]^{1/2}\lambda_\gamma,\quad \lambda_\gamma=V_{33}^{1/2}\ , \tag{3.31}$$

$$W_1=\left[\frac{\rho}{\varepsilon}\right]\frac{V_{12}}{d\sqrt{2}}(\lambda_+-\lambda_-)\ , \tag{3.32}$$

$$(2)^{3/2}dw_1=(d+V_{11}-V_{22})\left[\frac{\rho\lambda_+}{\varepsilon}\right]^{1/2}+(d-V_{11}+V_{22})\left[\frac{\rho\lambda_-}{\varepsilon}\right]^{1/2}\ , \tag{3.33}$$

$$(2)^{3/2}dw_2=(d-V_{11}+V_{22})\left[\frac{\rho\lambda_+}{\varepsilon}\right]^{1/2}+(d+V_{11}-V_{22})\left[\frac{\rho\lambda_-}{\varepsilon}\right]^{1/2}\ , \tag{3.34}$$

$$w_1+w_2=\frac{1}{\sqrt{2}}\left[\frac{\rho}{\varepsilon}\right]^{1/2}(\lambda_++\lambda_-)\ , \tag{3.35}$$

where

$$d=[(V_{11}-V_{22})^2+4V_{12}^2]^{1/2} \tag{3.36}$$

and

$$\lambda_\pm=(V_{11}+V_{22}\pm d)^{1/2}\ . \tag{3.37}$$

Furthermore, Eqs. (2.10), (2.28), and (2.29) yield

$$R_s=-\eta E(3,s)\ , \tag{3.38}$$

so that the ground-state energy according to Eq. (3.7) is given by

$$E_G=E(3,s)\left[1-\frac{(\delta_1+\delta_2-4)}{(N-1)}-\left[\frac{4}{\eta}\right]^{1/2}\lambda+O\left[\frac{1}{N^2}\right]\right]\ , \tag{3.39}$$

where

$$\lambda=\lambda_\gamma+\frac{1}{\sqrt{2}}(\lambda_++\lambda_-) \tag{3.40a}$$

and

$$E(3,s)=-\left[\frac{4}{\eta}\right]\frac{\sigma m_3(1-c^2)W^2T}{2\hbar^2Mv^2r^4} \tag{3.40b}$$

by virtue of Eqs. (2.37) and (2.47). In order to display the ground-state energy in a form in keeping with the discussion in Sec. II of the dissociation behavior, it is appropriate to factor the leading contribution to exhibit the analytic properties as a function of $(N-1)$ as

$$E_L=-\left[\frac{2}{N-1}\right]^2\left[\frac{\sigma m_3}{2\hbar^2M}\right]\frac{(1-c^2)W^2T}{v^2r^4}\ . \tag{3.41}$$

The three-particle energy thus consists of a hydrogenic-type contribution modulated by a multiplicative term which is rooted in collective effects. The latter is accompanied in its wake by zero-point vibrational contributions as displayed in Eq. (3.39). Dimensional interpolation[5] furthermore suggests[6] that, apart from the leading term, the remaining terms in the expansion be treated as an expansion in $1/N$ and that the resulting series, which is an asymptotic one, be truncated optimally at the term of order $1/N$ just before the semiconvergent aspects become operative. The accuracy achieved in this way of better than 1% (for $N=3$ and nuclear change of two units) is more than adequate for our purpose.

Implementing the foregoing procedure, the energy may be expressed in the following form:

$$E_G=E_L\left[1+\frac{1}{N}(4-2\lambda)+O\left[\frac{1}{N^2}\right]\right]\ , \tag{3.42}$$

where λ is given by Eq. (3.40a) provided that the matrix elements V_{13} and V_{23} are negligible compared to the other elements of V_{ij}. When these conditions are not satisfied, the above approximation may be transcended for the ground-state energy itself by computing λ by means of

$$\lambda=\lambda_1^{1/2}+\lambda_2^{1/2}+\lambda_3^{1/2}\ , \tag{3.43}$$

where λ_1, λ_2, and λ_3 denote the eigenvalues of the matrix defined by V_{ij}. The ground-state energy which incorporates inertial effects are given in Table III for a number of representative systems. For computational purposes the reference energy is expressed as

$$E_L=-\left[\frac{2}{N-1}\right]^2R_\infty\left[\frac{m_2}{m_e}\right]\frac{(1+\alpha)(1-c^2)W^2T}{(1+\xi_1+\xi_2)v^2r^4} \tag{3.44}$$

TABLE III. Values of the ground-state energy (in eV) determined from Eq. (3.42). The quantity v serves to label the anisotropy of the system, e.g., Eq. (2.30). The variational ground-state energy is denoted by E_G^V (in keV) as given by Ref. 11.

System	$-E_G$ (eV)	$-E_L$ (eV)	v	2λ	$-E_G^V$ (keV)[a]
$^4He\mu^-e^-$	10 956.3	10 956.3	402.2	4	10.96
$^3He\mu^-e^-$	10 858.5	10 858.5	398.6	4	10.86
$^4He\pi^-\mu^-$	17 873.6	17 651.0	1.8	3.962 170 8	
$^4He\mu^-\mu^-$	16 035.1	14 943.7	1	3.780 906 1	
$^4Hee^-e^-$	79.767	74.487	1	3.787 365 4	

[a]Reference 11.

and the Rydberg is taken as 13.605 698 1 eV.[8] Table III also lists auxiliary quantities in order to assess the relative importance of the different contributions to the energy covered in this section. It is to be expected that the contribution due to the zero-point energy of the vibrational effects represented by the second term in Eq. (3.42) will be suppressed in highly fragmented systems. This is quantified in Table III by the close proximity of λ to 2 in this regime. This is, in turn, a consequence of the circumstance that the zero-point vibrational contributions to the ground-state energy enters only via the (invariant) trace of the vibrational energy eigenvalues, which conforms to the sum rule. Individual vibrational effects manifest themselves through the dependence of the wave functions on these attributes. In the fragmentation regime even the "leading N approximation," subject to the proper treatment of threshold effects, yields excellent values for the ground-state energies as can be seen by comparing the results of Table III to the variational results[11] of 10.96 keV and 10.86 keV for the ($^4He\mu^-e^-$) and ($^3He\mu^-e^-$) systems, respectively. The reliability of the results for the ground-state energy may be inferred from the properties of asymptotic expansions as is the case in point. The error estimate for an asymptotic expansion (barring some rather exceptional cases) is based on the circumstance that the error is less than or equal to the first neglected term. In the case of systems possessing isosceles arrangement where higher-order terms are known, the error in the ground-state energy is less than 1%. In the case of fragmented systems the uncertainty may be gauged by the next to leading term which yields an error estimate of less than 1.3% for the system $He\pi\mu$ and about 0.01% for the highly fragmented system $He\mu e$. Finally, the difference in ionization potentials between ($He^{2+}\mu^-e^-$) and ($H^{2+}e^-e^-$) implies that it is not energetically possible for $(He\mu^-)^+$ to capture an electron from a helium atom. This affords a particular stability to the $(He\mu^-)^+$ system, so that an electron donor is required for the formation of neutral muonic helium.

IV. NEUTRAL MUONIC HELIUM AND CONCLUSIONS

In this section we zero in on the neutral muonic system ($He^{2+}\mu^-e^-$). Apart from the fact that it is an interesting system in its own right,[11,12] it serves as a prime example of a system exhibiting pronounced asymmetry. The treatment is not intended for computational purposes where the more precise numerical results of the previous sections are to be preferred, but rather to display the underlying physical features by dissecting further the formal expressions of the previous sections.

Because of the large disparity in the masses of the leptons, their separations from the center of attraction are also markedly different ($v \gg 1$). This implies that the interleptonic interaction plays a subsidiary role even in the ground state of the system. Correlation effects for this highly fragmented configuration hardly enter into the picture at all. This is formally expressed by the near vanishing of c. These special features lead to approximate analytic solutions of the set of Eqs. (2.39) and (2.40) for the attributes v and c to which we now turn. In keeping with the foregoing observations, retaining terms linear in c and exploiting the fact that v is large, lead to the following simplified form for Eq. (2.39):

$$cv(1+\alpha+\xi_1+\xi_2) = \xi_1+\xi_2-\frac{1}{(\alpha v)^2}\left[1-v\alpha(1+\xi_1+\xi_2)\times\left[\frac{g_3}{g_1}(1+\alpha)+\frac{g_2}{g_1}\right]\right] . \tag{4.1}$$

Treating Eq. (2.40) along the same lines it follows that

$$(1-\alpha)vc(g_3+g_2+vg_1)=g_3+vg_1-\alpha v^2(g_2+g_3) . \tag{4.2}$$

It turns out with the help of the numerical values of Table I that the second term of Eq. (4.1) is small due to a cancellation between the terms in the bracket. Neglecting this minor contribution greatly facilitates the solution for v and c and yields the transparent results

$$c=\alpha G\left[\frac{\xi_1+\xi_2}{1+\alpha(1+\xi_1+\xi_2)}\right]=\frac{Gm_1}{(m_1+m_3)} \tag{4.3}$$

and

$$v=\left[\frac{1}{\alpha G}\right]\left[\frac{1+\alpha(1+\xi_1+\xi_2)}{1+\alpha+\xi_1+\xi_2}\right] =\frac{m_2(m_1+m_3)}{m_1G(m_2+m_3)} , \tag{4.4}$$

where

$$G=\frac{g_3}{g_1}+\frac{g_2}{g_1} \tag{4.5}$$

has the significance of a screened Coulomb charge ratio. The multiplicative factors in large parentheses in the above equations derive from inertial effects. Equation (4.4) expresses the intuitive physical result that the ratio of the leptonic distances from the attractive center is determined (aside from the inertial contributions) by the product of the leptonic mass ratio and their screened charge ratio. Credence for the reliability of Eqs. (4.3) and (4.4) may be given by comparing the exact numerical results of $v=402.187$, $c=6.55\times10^{-5}$ and $v=398.609$, $c=8.77\times10^{-5}$ for ^{4}He and ^{3}He, respectively, to those obtained from the analytic expressions, namely $v=402.193$, $c=6.85\times10^{-5}$ and $v=398.615$, $c=9.1\times10^{-5}$. Thus the physical picture which emerges is that of a hydrogen atom embedded in a hydrogenic-type system. The prominent role of radial correlations is highlighted providing at the same time a concise form for inertial effects. The minor role played by angular-correlation effects owing to Coulomb interaction of the muon and electron provides independent justification for the neglect of this kind of correlation in Hylleraas-type correlated trial wave functions which serve as input in variational calculations.[13] Even for this ideal system a large number of hydrogenic-type basis functions need to be employed to effect the localization of the wave function the system.

Consider now the interparticle separation and ground-state energy applicable to this unique system. In the sequel the fragmentation regime $c=0$ and v large is labeled by the index f. It follows from Eqs. (2.44) and (2.30) in conjunction with the result

$$T(f)=\frac{v^2\sigma(m_2+m_3)}{Mm_2} \tag{4.6}$$

that the interparticle separations are given by

$$r_1=\eta P_1(f)=-\left[\frac{\eta}{4}\right]\frac{\hbar^2(m_2+m_3)}{g_1m_2m_3},\quad g_1<0 \tag{4.7}$$

and

$$r_2=\eta P_2(f)=-\left[\frac{\eta}{4}\right]\frac{\hbar^2(m_1+m_3)}{(g_2+g_3)m_1m_3},\quad (g_2+g_3)<0\ . \tag{4.8}$$

Employing the foregoing results, the second form of Eq. (2.47) implies that the ground-state energy may be exhibited as the sum of two hydrogenic-type contributions

$$E(3,s,f)=-\left[\frac{4}{\eta}\right]\frac{\hbar^{-2}}{2}\left[g_1^2\frac{m_2m_3}{(m_2+m_3)}+(g_2+g_3)^2\frac{m_1m_3}{(m_1+m_3)}\right], \tag{4.9}$$

this being a natural occurrence for a highly fragmented system. The bulk of the energy is carried by the muon which, in conjunction with the nucleus, constitutes a central core [of size determined by Eq. (4.7)] orbited by a loosely bound electron. While the central core may be optically active owing to muonic excitations, chemically the system acts like a heavy isotope of hydrogen. In general systems "independent" particle motion and cooperative features can coexist. The collective features are most striking in systems built up of equal-mass leptons, implying the existence of novel doubly excited states which entail the equal sharing of energy between affiliated leptons.[1] The pairing between leptons of the same charge is instituted by the intermediary action of an oppositely charged mobile nucleus. A large disparity in the masses of the constituent particles leads to pronounced anisotropy of the aggregate.

In summary, the framework treated in the paper provides a perspective of the three-particle problem which places a special premium on collective features quantified by a rigorous analytic procedure in an ideal limit and supplemented by a perturbation procedure freed from some of the constraints of more traditional approaches. This departure paved the way for a comprehensive formulation of the conformations of anisotropic systems and brings within reach further potential physical applications.

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