## Dileptonic-helium ground-state energy

P. du T. van der Merwe

Atomic Energy Corporation, P.O. Box 582, Pretoria 0001, Republic of South Africa

(Received 9 December 1987)

The large-dimensional approach to atomic physics is extended to accommodate mass-polarization and recoil contributions. This approach, which does not rely on partitioning of the potential into subterms, but instead treats the Hamiltonian for large dimension exactly and incorporates corrections order by order in the dimension, is of interest for exotic atoms and molecules. Application of the results to the helium atom and the dimuonic-helium ground-state energy is considered.

# I. INTRODUCTION

Recent developments<sup>1-3</sup> based on the large-dimensional approach<sup>4</sup> suggest that light atomic systems may possess novel collective features contained within electronic levels. lt has furthermore been found that this view provides a natural habitat for structural aspects' and electronic correlations<sup>5</sup> which generate vibrations and rotations and provide a new perspective of dynamic molecular modes complementary to the group-theoretical<sup>6</sup> and hyperspherical supermultiplet classification schemes.<sup>7</sup>

The purpose of this investigation is to bring recoil and inertial effects into the realm of the large-dimensional approach. The general foundation has already been established in a previous work<sup>2</sup> in which the three-particle Schrödinger equation for general masses was formulated in terms of appropriate collective Jacobi coordinates in an inflated number of spatial dimensions  $N$ . A summary of these aspects is given in Sec. II. The role of inertial effects is delineated in Secs. III and IV and is illustrated by considering the ground-state energies of two physical systems of interest. These effects should be of particular relevance for the vibrational modes promoted by the relative collective motion of the constituents with respect to their common center of momentum. The largedimensional approach has been shown to provide a powerful nonperturbative approach where the leading approximation addresses structural aspects, while higher approximations describe fluctuations relative to the integrable "semiclassical" situation. Section III treats the vibrational eigenrnodes in detail. Although recoil effects provide only small contributions to the helium atomic ground-state energy as discussed in Sec. IV, they are nevertheless of potential importance in high-precision calculations<sup>8</sup> with a view to, for example, chemical-reaction theory. More substantial effects are encountered in the new dimuonic helium atom, also treated in Sec. IV, where inertial effects come into their own. In view of the circumstance that the large-dimensional approach does not rely on the usual ad hoc partitioning of the potential into parts, but instead treats the full Hamiltonian for large N exactly and then incorporates corrections order by order in  $1/N$ , it is of particular interest for dimuonic atoms and muonic molecules where standard adiabatic perturbation schemes along the lines of Born-Oppenheimer adiabatic separation of leptonic and nuclear motions become somewhat tenuous, particularly in view of their artifactual symmetry-breaking aspects.<sup>9</sup>

## II. DIMENSIONAL INFLATION

In order to establish the notation, we review as introduction to this section the general framework for the three-particle Schrodinger equation for general masses in N spatial dimensions given in a previous work.<sup>2</sup> The essence of the large-dimensional method entails a change of variables to collective coordinates represented by rescaled Jacobi variables in the potential model under discussion.

Consider the motion of three particles in an Ndimensional space with respect to their center of mass. It is expedient to introduce collective coordinates in terms of which the kinetic part of the Hamiltonian is diagonal, given by the Jacobi coordinates denoted by  $X$  and  $Y$ ,

$$
MR = m_3R_3 + m_1R_1 + m_2R_2, \qquad (2.1)
$$

$$
\mathbf{X} = a\left(\mathbf{R}_1 - \mathbf{R}_2\right) \,,\tag{2.2}
$$

$$
Y = b (R_3 - Z) , \qquad (2.3)
$$

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

$$
Z = (m_1 R_1 + m_2 R_2)(m_1 + m_2)^{-1}
$$
 (2.4)

and the symbol a denotes a normalization factor of the relative displacement vectors of particles  $(1,2)$ , while b is a normalization factor of the vector from the c.m. of the pair (1,2) to the third particle given by

$$
a^2 \mu_{12}^{-1} = \frac{2}{m} = b^2 \mu_{(1+2),3}^{-1} \tag{2.5}
$$

Let  $\mu_{12}$  denote the reduced mass of particles 1 and 2, while the reduced mass of the pair (1,2) relative to 3 is given by  $\mu_{12}$  denote the reduce<br>le the reduced mass of<br>n by<br> $\mu_{(1+2),3} = m_3(m_1 + m_2)$ 

$$
\mu_{(1+2),3} = m_3(m_1 + m_2)M^{-1}, \qquad (2.6)
$$

and furthermore, denote the reduced mass of the threeparticle system by

$$
m = (m_1 m_2 + m_2 m_3 + m_3 m_1) M^{-1}, \qquad (2.7)
$$

38 1187 1988 The American Physical Society

where

$$
M = m_1 + m_2 + m_3 \tag{2.8}
$$

$$
x^{2} = \sum_{i=1}^{N} X_{i}^{2}, \quad y^{2} = \sum_{i=1}^{N} Y_{i}^{2}, \quad (2.9)
$$

$$
\cos \gamma = \hat{\mathbf{X}} \cdot \hat{\mathbf{Y}} \tag{2.10}
$$

The wave function of an S state is a function of the rotationally invariant quantities, i.e., the lengths of the Jacobi vectors and the angle between these vectors, defined as follows:

Expressed in terms of these collective variables the kinetic energy assumes the form<sup>2</sup>

$$
T_{S}\psi = -\frac{\hbar^{2}}{m} \left[ \frac{\partial^{2}}{\partial x^{2}} + \frac{(N-1)}{x} \frac{\partial}{\partial x} + \frac{\partial^{2}}{\partial y^{2}} + \frac{(N-1)}{y} \frac{\partial}{\partial y} + \left[ \frac{1}{x^{2}} + \frac{1}{y^{2}} \right] \left[ \frac{\partial^{2}}{\partial \gamma^{2}} + (N-2) \cot \gamma \frac{\partial}{\partial \gamma} \right] \right] \psi .
$$
 (2.11)

The Hamiltonian may be cast into a Hermitian form by the transformation

$$
\psi(x, y, \gamma) = J\Phi(x, y, \gamma) \tag{2.12}
$$

where

$$
J = (xy)^{-(1/2)(N-1)} (\sin \gamma)^{-(1/2)(N-2)}
$$
\n(2.13)

denotes the square root of the Jacobian of the transformation, so that

$$
T_S \Phi = -\frac{\hbar^2}{m} \left[ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \left[ \frac{1}{x^2} + \frac{1}{y^2} \right] \frac{\partial^2}{\partial \gamma^2} - \frac{1}{4} \left[ \frac{1}{x^2} + \frac{1}{y^2} \right] \left[ \frac{(N-2)(N-4)}{\sin^2 \gamma} - 1 \right] \right] \Phi .
$$
 (2.14)

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

$$
x = \eta P, \quad y = \eta Q \tag{2.15}
$$

The scaling factor  $\eta$  is arbitrary apart from the requirement that it behaves as  $N^2$  for large N. Equation (2.14) suggests that it be chosen as

$$
\eta = (N-2)(N-4) \tag{2.16}
$$

a choice which facilitates the treatment of higher-1/N terms.<sup>3</sup> The equation of motion is given by

$$
\eta E \Phi = \eta H \Phi = -\frac{\hbar^2}{m\eta} \left[ \frac{\partial^2}{\partial P^2} + \frac{\partial^2}{\partial Q^2} + \left[ \frac{1}{P^2} + \frac{1}{Q^2} \right] \left[ \frac{\partial^2}{\partial \gamma^2} + \frac{1}{4} - \frac{(N-2)(N-4)}{4\sin^2\gamma} \right] \right] \Phi + V(G, P, Q, \gamma) \Phi , \qquad (2.17)
$$

where the rescaled potential reads

$$
V(G, P, Q, \gamma) = \eta V(x, y, \gamma) = G_1 P_1^{\alpha} + G_2 P_2^{\alpha} + G_3 P_3^{\alpha}.
$$
\n(2.18)

The rescaled coupling constants are defined by  $G_i = \eta^{\alpha+1}g_i$ , while the rescaled interparticle separations  $P_i$ , in turn, are given by

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

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

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

where  $\sigma = m_1 + m_2$ . For convenience, the center of the coordinates may be chosen to coincide with the c.m.  $(R=0)$ .

In order to facilitate implementation of the large- $N$ technique it is appropriate to express the equation of motion for Coulomb interactions ( $\alpha = -1$ ) in the form

$$
\eta E \Phi = -\frac{\hbar^2}{m\eta} \left[ \frac{\partial^2}{\partial P^2} + \frac{\partial^2}{\partial Q^2} + \left[ \frac{1}{P^2} + \frac{1}{Q^2} \right] \frac{\partial^2}{\partial \gamma^2} \right] \Phi + V_e \Phi , \quad (2.22)
$$

where the effective potential reads

(2.19) 
$$
V_e = \sum_{i=1}^{3} g_i P_i^{-1} + \Delta \left[ \frac{1}{P^2} + \frac{1}{Q^2} \right] \left[ \frac{1}{\sin^2 \gamma} - \frac{1}{\eta} \right]
$$
 (2.23)

and

$$
\Delta = \frac{\hbar^2}{4m} \tag{2.24}
$$

The advantage of the effective potential is that contributions due to quantum fluctuations, mass polarization, and recoil are incorporated directly into the effective potential, while the remaining part of the kinetic term is quenched in the large-dimensional limit. Corrections to

38

this exactly solvable semiclassical limit, in general, are accommodated in the form of corrections of order  $1/\eta$ relative to the coherent limit discussed in detail in Sec. III.

#### III. GROUND-STATE ENERGY AND VIBRATIONAL EIGENMODES

According to Eq. (2.22), the three-particle ground-state energy to leading order in  $\eta$  is given by the minimum of the effective potential

$$
E(3)_m = \frac{1}{\eta} V_e(P_m, Q_m, \gamma_m)
$$
 (3.1)

$$
= -\left[\frac{4}{\eta}\right] \frac{fg^{2}(1+c)^{3}}{\hbar^{2}(1-c)} \frac{[1+\xi(1-c)]}{(1+2\xi)^{2}} , \qquad (3.2)
$$

where the subscript  $m$  designates evaluation at its minimum and  $f = m_1 = m_2$  denotes the mass of the leptons, whereas  $\xi = f/m_3$ , where  $m_3$  denotes the mass of the third particle of charge Ze, i.e.,  $g = -Ze^2$ . Furthermore,  $c = \cos\theta_{12}$  is a measure of the correlation angle [see Eqs. (3.5) and (3.6)], which in the ground state is determined by the formula $2$ 

$$
\Sigma(1+2\xi)[2(1-c)]^{1/2} = 8c - 4\xi(1-c)^2 , \qquad (3.3)
$$

with  $\Sigma = g_3/g = -1/Z$ . For leptons of equal mass and if  $Z \ge 2$ , <sup>10</sup> the geometrical arrangement of the three particles is that of an isosceles triangle (cos $\gamma=0$ ), where the Jacobi coordinates are related to the relative coordinates by

$$
P_1^2 = P_2^2 = P_0^2 = \frac{P^2}{4a^2} + \frac{Q^2}{b^2} \tag{3.4}
$$

$$
P^2 = 2a^2 P_0^2 (1 - c) , \qquad (3.5)
$$

and

$$
Q^2 = \frac{1}{2}b^2 P_0^2 (1+c) , \qquad (3.6)
$$

where  $c = cos\theta_{12} = \hat{\mathbf{P}}_1 \cdot \hat{\mathbf{P}}_2$  at the stationary point and  $P_0$  in the ground state is determined by

$$
P_0 = -\frac{\hbar^2 (1+2\xi)}{4fg (1+c)^2}, \quad g < 0 \tag{3.7}
$$

For sufficiently large  $N$  the system would be frozen in this geometrical configuration. The next-to-leading term in Eq. (2.22) in  $\eta$  describes harmonic vibrations about the minimum of the effective potential. Denoting the vibrational energy by  $E_y$  we expand the potential about the minimum as follows:

$$
V_e(P,Q,\gamma) = V_e(P_m, Q_m, \gamma_m) + p^2 V_1 + q^2 V_2 + 2pqV_3
$$
  
+  $(\gamma - \gamma_m)^2 V_{\gamma\gamma} + 2p(\gamma - \gamma_m) V_{P\gamma}$   
+  $2q(\gamma - \gamma_m) V_{Q\gamma}$ , (3.8)

where  $p = P - P_m$ ,  $q = Q - Q_m$ , while

and

$$
V_{\gamma\gamma} = \frac{1}{2} \left[ \frac{\partial^2 V_e}{\partial \gamma^2} \right]_m ,
$$
  
\n
$$
V_{P\gamma} = \frac{1}{2} \left[ \frac{\partial^2 V_e}{\partial P \partial \gamma} \right]_m ,
$$
  
\n
$$
V_{Q\gamma} = \frac{1}{2} \left[ \frac{\partial^2 V_e}{\partial Q \partial \gamma} \right]_m .
$$
  
\n(3.10)

The eigenvalue problem for the vibrational modes is defined by

$$
\eta E_v \phi_v = [-\varepsilon T(h) + V_e(h)] \phi_v , \qquad (3.11)
$$

where  $T(h)$  and  $V<sub>e</sub>(h)$  denote the harmonic contributions for the kinetic and effective potential of Eq. (2.17) and

$$
\Sigma(1+2\xi)[2(1-c)]^{1/2} = 8c - 4\xi(1-c)^2, \qquad (3.3) \qquad \qquad \varepsilon = -\frac{\hbar^2}{m\eta} \ . \tag{3.12}
$$

In view of the circumstance that the asymmetrical and symmetrical vibrations are uncoupled,

$$
V_{P\gamma} = V_{Q\gamma} = 0 \tag{3.13}
$$

the modes may be separated by the Ansätze  $\phi_v = \phi_s \phi_A$ and

$$
E_v = E_S + E_\gamma \tag{3.14}
$$

where the vibrational energy  $E_{\gamma}$  corresponding to the asymmetric stretching mode is determined by

$$
\eta E_{\gamma} \phi_A = \left( -\epsilon \Gamma_0 \frac{\partial^2}{\partial \gamma^2} + (\gamma - \gamma_m)^2 V_{\gamma \gamma} \right) \phi_A , \quad (3.15)
$$

with

$$
\Gamma_0 = \left[\frac{1}{P^2} + \frac{1}{Q^2}\right]_m = \frac{(2+\xi)[1+\xi(1-c)]}{P_0^2(1-c^2)(1+2\xi)}\tag{3.16}
$$

and

escribes harmonic vibrations about the effective potential. Denoting the vibra-  
\n
$$
E_y
$$
 we expand the potential about the  
\nws:  
\n
$$
V_e(P_m, Q_m, \gamma_m) + p^2 V_1 + q^2 V_2 + 2pqV_3
$$
\n
$$
+ (\gamma - \gamma_m)^2 V_{\gamma\gamma} + 2p(\gamma - \gamma_m) V_{P\gamma}
$$
\n
$$
= \sum_{i=1}^{\infty} \frac{1}{2} \int_{-\infty}^{\infty} \int
$$

The treatment of the symmetrical vibrations is facilitated by performing an orthogonal transformation to normal coordinates

 $V_1 = \frac{1}{2} \left| \frac{\partial^2 V_e}{\partial P^2} \right|$  $V_2 = \frac{1}{2} \left| \frac{\partial^2 V_e}{\partial Q^2} \right|$  $V_3 = \frac{1}{2} \left( \frac{\partial^2 V_e}{\partial P \partial Q} \right)_{m}$  $\partial P$ ao <sup>.</sup> (3.9)

$$
\begin{bmatrix} p \\ q \end{bmatrix} = \begin{bmatrix} \cos \rho & -\sin \rho \\ \sin \rho & \cos \rho \end{bmatrix} \begin{bmatrix} p_1 \\ p_2 \end{bmatrix}
$$
 (3.18)

such that  $E_S = E_1 + E_2$ , where the eigenmodes are determined by

$$
\eta E_i \phi_i = \left[ -\varepsilon \frac{d^2}{dp_i^2} + p_i^2 \lambda_i \right] \phi_i, \quad i = 1, 2 \tag{3.19}
$$

where

$$
\tan(2\rho) = \frac{2V_3}{V_1 - V_2}
$$

and  $\lambda_1$  and  $\lambda_2$  denote the eigenvalues of the symmetric part of the harmonic potential,

$$
\lambda_i^2 = \frac{1}{2}(V_1 + V_2) \pm \frac{1}{2} [(V_1 - V_2)^2 + 4V_3^2]^{1/2} . \tag{3.20}
$$

The total vibrational energy is summarized by

$$
E_v = \frac{\varepsilon^{1/2}}{\eta} \left[ \lambda_1 (2n_1 + 1) + \lambda_2 (2n_2 + 1) + (\Gamma_0 V_{\gamma \gamma})^{1/2} (2n_\gamma + 1) \right],
$$
 (3.21)

where  $n_1$ ,  $n_2$ , and  $n<sub>y</sub>$  denote the vibrational quantum numbers.

We now attend to the task of finding the required force constants. Equations (2.23) and (3.9), subject to the constraints (3.3)—(3.7), lead to the following results valid in the ground state:

$$
V_1 = -\frac{g(2+\xi)}{8P_0^3(1-c)^2(1+2\xi)^2}
$$
  
×[5+c-c<sup>2</sup>+3c<sup>3</sup>-6\xi(1-c)<sup>3</sup>], (3.22)

$$
V_2 = -\frac{g}{8P_0^3}(2+\xi)(5-3c) ,
$$
 (3.23)

$$
V_3^2 = \frac{9g^2(\xi + 2)^2}{64(1 + 2\xi)P_0^6}(1 - c^2)
$$
 (3.24)

The auxiliary quantities required to find the eigenvalues may be cast into the form

$$
V_1 + V_2 = \left(\frac{-g}{4P_0^3}\right) \frac{(2+\xi)}{(1-c)^2(1+2\xi)^2}
$$
  
 
$$
\times [\Omega + \xi(1-c)^2(7-3c)
$$
  
 
$$
+ 2\xi^2(1-c)^2(5-3c)], \qquad (3.25)
$$

where

$$
\Omega = 5 - 6c + 5c^2 \tag{3.26}
$$

Furthermore, defining

$$
R^2 = (V_1 - V_2)^2 + 4V_3^2 \t\t(3.27)
$$

it follows that

$$
R^{2} = \frac{g^{2}(2+\xi)^{2}}{16P_{0}^{6}(1-c)^{4}(1+2\xi)^{4}}R_{1}^{2} ,
$$
 (3.28)

with

$$
R_1^2 = S_0 + S_1 \xi + S_2 \xi^2 + S_3 \xi^3 + S_4 \xi^4 , \qquad (3.29)
$$

where

$$
S_0 = 9 - 36c + 94c^2 - 84c^3 + 33c^4 , \qquad (3.30)
$$

$$
S_1 = 2(1-c)^2(27-145c+141c^2-39c^3), \qquad (3.31)
$$

$$
S_2 = (1 - c)^2 (277 - 928c + 922c^2 - 312c^3 + 9c^4), \qquad (3.32)
$$

$$
S_3 = 4(1-c)^4(83 - 84c + 9c^2), \qquad (3.33)
$$

and

$$
S_4 = 4(1-c)^4(5-3c)^2
$$
 (3.34)

It is of importance to observe that all of the above quantities, Eqs. (3.25)—(3.34), associated with the eigenvalues of the symmetric stretching mode and bending motion, are positive definite (since  $g$  and  $c$  are negative). This is a result of the physical circumstance that energy is expended in exciting the symmetrical vibrations. Consequently, these oscillations cannot induce instabilities into the system.

The asymmetric stretching mode decouples from the symmetric modes previously treated. Its harmonic coefficient is determined from the expression

$$
\Gamma_0 V_{\gamma\gamma} = \frac{16g^4 f^3 (2+\xi) K \Omega_{\gamma} (1+c)^6}{\hbar^6 (1+2\xi)^5 (1-c)^2} , \qquad (3.35)
$$

 $\lambda$  where

$$
K = 1 + \xi(1 - c) \tag{3.36}
$$

and

$$
\Omega_{\gamma} = 1 - 2\xi + 2(3 + 4\xi)c - 3(1 + 2\xi)c^{2}.
$$
 (3.37)

The conditions under which this mode may induce instabilities and trigger symmetry breakdown are analyzed in a separate paper.<sup>10</sup> Suffice it to remark that for  $Z \ge 2$ these issues do not play a role in the rest of the paper.

#### IV. DILEPTONIC-HELIUM GROUND-STATE ENERGY

The total ground-state energy, which is the sum of Eq. (3.1) and the zero-point vibrational energy, is given by

$$
E_G = E(3)_m + E_1 + E_2 + E_\gamma \tag{4.1}
$$

By virtue of the results derived in Sec. III, the three-body ground-state energy may be expressed in the following form:

where

$$
S = \Omega + \xi (7 - 3c)(1 - c)^2 + 2\xi^2 (5 - 3c)(1 - c)^2.
$$
 (4.3)

The last result provides an expression for the groundstate energy which incorporates recoil and masspolarization contributions. In view of the harmonic expansion invoked in Sec. III, the result is valid to order  $1/N<sup>3</sup>$  in the large-N expansion. Before displaying the result in the appropriate form, stock has to be taken of certain features pertaining to the analytic properties of the energy as a function of  $N$ . Analogous with the analytic behavior of the integrable hydrogen case where the ground-state energy displays a second-order pole in  $N-1$ , it has been conjectured that  $N-1$  may be an appropriate expansion parameter $11$  in the helium problem. On physical grounds it has been shown<sup>1</sup> that the correct ionization threshold behavior is obtained by factorizing the three-particle energies in a multiplicative form, the first factor [see also Eq. (4.3) below] of which displays the two-particle substructure and the desired dipole structure appropriate for widely separated electrons, while the second factor reflects the dynamic polarizability and screening aspects. The notion of factorization formed a key idea in identifying the asymptotic nature<sup>12</sup> of the large-N expansion in the three-body system, which would otherwise be masked by the presence of convergent hydrogenic subterms in the expansion. Dimensional interpolation<sup>12</sup> has furthermore shown that, aside from the hydrogenic factor, treating the remainder terms as an expansion in  $1/N$  and truncating the asymptotic series optimally at the term of order  $1/N$  just before the semiconvergent aspect becomes operative in the asymptotic expansion, affords an accuracy better than  $1\%$  (for  $N=3$ and nuclear charge of two units). This procedure, which facilitates comparison of the general results with the norecoil situation, is adopted in the sequel. '

Implementing the foregoing procedure, it follows that the ground-state energy may be expressed in the following form:

$$
E_G = E(3) \left[ 1 + \frac{1}{N} (4 - \beta) + O\left[\frac{1}{N^2}\right] \right],
$$
 (4.4)

where

$$
\beta = \frac{1}{\sqrt{2}(K)} [(S + R_1)^{1/2} + (S - R_1)^{1/2}] + \left[ \frac{\Omega_{\gamma}}{K} \right]^{1/2}
$$
 (4.5)

and

$$
E(3) = -\frac{fZ^{2}e^{4}}{\hbar^{2}(1+2\xi)^{2}} \left[\frac{2}{N-1}\right]^{2} \frac{(1+c)^{3}}{(1-c)} [1+\xi(1-c)] .
$$
\n(4.6)

The application of the results to the dileptonic-helium systems, i.e., the helium atom and the helium dimuoni atom (indicated by He- $\mu\mu$ ) is now considered. The results of the calculation for the helium atomic groundstate energy, Eq. (4.4), correlation angle, Eq. (3.3), and harmonic coefficients, Eqs.  $(3.22)$ – $(3.37)$ , are listed in Table I. Two cases are distinguished for comparison: The results listed under (b) where recoil and masspolarization contributions have been neglected, and the general results which appear under the heading (a). Because recoil contributions are rather small in normal atoms, these effects are investigated in Table II for the dimuonic helium atom where recoil and masspolarization contributions become significant. The data employed in the calculations are  $R_\infty = 13.605804$  eV, employed in the calculations are  $K_{\infty} = 15.003$  604 ev<br>  $\xi(e) = m_e / m_{\text{4He}} = 1.3709337 \times 10^{-4}$ , and  $\xi(\mu) = m_{\mu}$  $e) = m_e / m_{^4\text{He}} = 1.3 / 0.9$ <br> $m_{^4\text{He}} = 2.834.652 \times 10^{-2}$ .

Although the primary objective of this work centered around the question of the generalization of the largedimensional approach to include inertial effects, it is perhaps appropriate at this point to address the question of the promise of the method itself and its accuracy. The first issue has already been discussed at some length in the literature,  $1-4, 12-14$  where it has been shown that the approach is particularly suited in physical problems not amenable to perturbation theory. Furthermore, dimensional inflation provides a new perspective also in nonintegrable three-particle problems,  $1-\overline{3}$  where it provides a rigorous interpretation of, among other things, highly correlated motions which are not indicated by the Hamiltonian itself. That the method is also promising for achieving high accuracy in calculating binding energies in atomic physics derived from the investigation of Goodson and Herschbach, $8$  where the large-dimensional approach was used as a starting point for a recursive method in conjunction with a Pade summation to achieve an accuracy of ten significant figures for the helium ground-state energy (neglecting recoil and masspolarization contributions, though). The accuracy which could eventually be achieved along these lines is more

TABLE I. Helium atom ground-state energy (in eV), Eq. (4.4), labeled (a), while results neglecting recoil and mass-polarization effects ( $\xi = 0$ ) appear under (b). The correlation angle is determined from Eq.  $(3.3)$  and the harmonic coefficients from Eqs.  $(3.22)$ – $(3.37)$ .

	$c = cos\theta_1$	$E_G$ (eV)	$(S+R_1)^{1/2}$	$(S - R_1)^{1/2}$	$\Omega_{\nu}^{1/2}$				
(a)	$-0.092322$	$-79.777117$	3.038.399	1.401 288	0.648 163	3.786978			
(b)	$-0.092381$	$-79.77864$	3.038 036	1.401 517	0.648 161	3.787399			

TABLE II. Helium dimuonic atom (He- $\mu\mu$ ) ground-state energy (in eV), Eq. (4.4), labeled (a), while results neglecting recoil and mass-polarization effects ( $\xi=0$ ) appear under (b). The correlation angle is determined from Eq. (3.3) and the harmonic coefficients from Eqs. (3.22)—(3.37).

	$c = cos \theta_1$	$E_G$ (eV)	$(S+R_1)^{1/2}$	$(S - R_1)^{1/2}$	$\Omega^{1/2}$	
(a)	$-0.080539$	$-16420.19$	3.115312	1.350 993	0.649032	3.703 612
(b)	$-0.092381$	$-16495.67$	3.038 036	1.401 517	0.648 161	3.787399

difficult to anticipate as the large- $N$  approach is a relative new entry compared to time-honored methods such as the variational approach. The physical insight provided by the large- $N$  approach may also assist in tailoring variational wave functions where an optimal choice of basis functions (to describe correlations and desirable analytic structure) is essential for rapidly converging variational energies.<sup>15</sup> Apart from such possible spin-offs of the  $1/N$ expansion, the fact that it yields rigorous solutions in the large-dimensional limit while incorporating further corrections nonperturbatively (avoiding the partitioning of the potential into subterms) without special assumptions about the structure of the wave function as well as the nonperturbative treatment of recoil and masspolarization effects, makes the method attractive for also treating excited states. The global picture the method has provided of electronic excitations, as well as collective features exhibited by three-particle systems,<sup>1</sup> further more illustrate the potential of the approach for uncovering novel physical behavior.

Since the dimuonic-helium atom appears not to have been detected experimentally or discussed theoretically previously, it is of interest in conclusion to take note of the recent observation of related muonic-helium systems, namely <sup>4</sup>He- $\mu$ e, <sup>3</sup>He- $\mu$ e (Ref. 16) and the negative muonic ion  $(\mu^+e^-e^-)$ .<sup>17</sup> It is of importance to point out that the symmetry properties of the muonic systems just mentioned are on general grounds quite distinct from those of the dimuonic-helium atom which possesses isosceles symmetry.<sup>10</sup> It may, furthermore, be inferred from the ground-state features treated in this paper that collective features discussed in connection with the helium atomic spectrum are expected to be enhanced by masspolarization effects in exotic atoms. Of particular interest would be the affiliated dimuon excitations which represent novel doubly excited states' where identical leptons exhibit concerted motions. We hope to return to these aspects in subsequent work.

- 'P. du T. van der Merwe, J. Chem. Phys. 81, 5976 (1984).
- P. du T. van der Merwe, Phys. Rev. D 33, 3383 (1986).
- 3D. R. Herschbach, J. Chem. Phys. 84, 838 (1986).
- 4E. Witten, Phys. Today 33, 38 (1980); L. D. Mlodinow and N. Papanicolaou, Ann. Phys. (N.Y.) 131, <sup>1</sup> (1981); 128, 314 (1980); R. A. Ferrel and D. J. Scalapino, Phys. Rev. A 9, 846 (1974).
- <sup>5</sup>P. du T. van der Merwe, J. Chem. Phys. 82, 5293 (1985); Phys. Rev. A 34, 3452 (1986).
- ${}^{6}D.$  R. Herrick, Adv. Chem. Phys. 52, 1 (1983); D. R. Herrick, M. E. Kellman, and R. D. Poliak, Phys. Rev. A 22, 1517 (1980); M. E. Kellman and D. R. Herrick, ibid. 22, 1535 (1980).
- <sup>7</sup>C. D. Lin, Phys. Rev. Lett. 51, 1348 (1983); G. S. Ezra and R. S. Berry, Phys. Rev. A 28, 1974 (1983); 28, 1989 (1983); S. Watanabe and C. D. Lin, ibid. 34, 823 (1986); 29, 1019 (1984); 36, 511 (1987}.
- <sup>8</sup>D. Z. Goodson and D. R. Herschbach, Phys. Rev. Lett. 58, 1628 (1987); J. Chem. Phys. 86, 4997 (1987).
- <sup>9</sup>O. Goscinski and V. Mujica, in *Density Matrices and Density* Functionals, edited by R. Erdahl and V. H. Smith, Jr. (Reidel, Dordrecht, 1987), p. 597; J. G. Loeser and D. R. Herschbach, J. Chem. Phys. 86, 3512 (1987); O. Goscinski and V. Mujica, Int. J. Quantum Chem. 29, 897 (1986); E. R. Davison and W. T. Borden, J. Phys. Chem. 87, 4783 (1983); R. G. Woolley,

Adv. Phys. 25, 27 (1976).

- <sup>10</sup>P. du T. van der Merwe, Phys. Rev. A 36, 3446 (1987).
- $^{11}$ L. C. Yaffe, Phys. Today 36, 50 (1983).
- <sup>12</sup>J. G. Loeser and D. R. Herschbach, J. Chem. Phys. 86, 2117 (1987). See also C. M. Bender and S. A. Orszag, Advanced Mathematical Methods for Scientists and Engineer (McGraw-Hill, New York, 1978); A. Erdelyi, Asymptotic Expansions (Dover, New York, 1956).
- <sup>13</sup>D. J. Doren and D. R. Herschbach, Chem. Phys. Lett. 118, 115 (1985); J. G. Loeser and D. R. Herschbach, J. Phys. Chem. 89, 3444 (1985);84, 3882 (1986);D.J. Doren and D. R. Herschbach, Phys. Rev. A 34, 2654; 34, 2665 (1986).
- <sup>14</sup>For further discussion of shifted  $1/N$  expansions see, e.g., E. Papp, Phys. Rev. A 36, 3550 (1987).
- <sup>15</sup>D. E. Freund, B. D. Huxtable, and J. D. Morgan, Phys. Rev. A 29, 980 (1984).
- <sup>16</sup>P. A. Souder, D. E. Casperson, T. W. Crane, V. W. Hughes, D. C. Lu, H. Orth, H. W. L. Reist, M. H. Yam, and G. zu Putlitz, Phys. Rev. Lett. 34, 1417 (1975); Phys. Rev. A 22, 33 (1980). H. Orth and V. W. Hughes, in Proceedings of the Workshop on Fundamental Muon Physics: Atoms, Nuclei and Particles, Los Alamos, 1986, edited by C. M. Hoffman, V. W. Hughes, and M. Leon (unpublished).
- $17K$ . P. Arnold et al., Bull. Am. Phys. Soc. 31, 35 (1986).