Quantum-mechanical calculations on gravitational systems

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The correlation among particles in a quantum-mechanical gravitational system is discussed. It is found with the help of correlated exponential wave functions that the correlation energies in the ground state of three- and four-body gravitational systems are 35% and 30% of the total binding energy of the system. The correlation energy decreases with the number of particles N. In the limit $N\to\infty$ it is less than 2% of the binding energy of the system. Several general properties of correlated exponential wave functions are demonstrated. These properties are useful for calculations on Coulomb and gravitational many-body systems.

INTRODUCTION

Studies of quantum-mechanical systems of particles which interact with each other by gravitational forces are pertinent to astrophysics[1] and elementary particle physics.[2] Calculations on such systems were carried out in Refs. 1 and 2 in the one-particle, self-consistent-field (SCF) approximation. Limits on their energies as a function of the number of particles making up the system were studied in Refs. 3 and 4.

The absence of repulsive forces makes the correlation in the motion of particles in a gravitational system quite different from that of the electrons in atoms, molecules, or solids. Specifically, the particles in a gravitational system try to come as close to each other as possible, while the correlation of electrons is basically an attempt to avoid each other. For this reason one might expect the particle correlation in a gravitational system to cause a substantial increase in the particle packing density and an increase in the binding energy of the system in comparison with the uncorrelated one-particle SCF approximation. In an effort to identify the role played by a correlation in the motion of particles in gravitational systems, we carry out some variational calculations below, using trial wave functions which are exponential functions of the instantaneous distances between all particles. As a result we find energies for three- and four-body gravitational systems which are substantial refinements of the results calculated by the SCF method. The results show that the correlation energy in these systems reaches a level equal to a third of the total binding energy of the system. We also examine the behavior of the correlation energy in the limit as the number of particles in the gravitational system goes to infinity, $N\to\infty$. The calculations below are based on general properties of correlated exponential wave functions, which are almost ideally suited for a description of gravitational systems.

CORRELATED EXPONENTIAL WAVE FUNCTIONS FOR GRAVITATIONAL SYSTEMS OF PARTICLES

We consider a system of N identical particles (bosons) with masses m interacting through gravitational forces. The energy operator of the system is

$$H=T+U=-\frac{\hbar^2}{2m}\sum_{j=1}^{N}\Delta_j-Gm^2\sum_{j<k}^{N}\frac{1}{r_{jk}}, \tag{1}$$

where G is the gravitational constant, and the operators T and U represent the kinetic energy of the particles and the potential energy of their mutual attraction.

An exact solution of the Schrödinger equation

$$(T+U)\Psi=E\Psi \tag{2}$$

is known only for a two-particle gravitational system. The ground state of that system corresponds to the wave function of a hydrogen-like atom,

$$\Psi=\exp\left(-\frac{Gm^3r_{12}}{2\hbar^2}\right)$$

and its energy is

$$E=-G^2m^5/4\hbar^2.$$

For an approximate description of the ground state of a gravitational system of an arbitrary number of particles N, we introduce a trial wave function which is an exponential function of all the interparticle distances:

$$\Phi_\alpha=\exp\left(-\frac{Gm^3\alpha}{\hbar^2}\sum_{j<k}^{N}r_{jk}\right). \tag{3}$$

This wave function contains the variable parameter α, whose optimum value is to be found by minimizing the mathematical expectation of the energy,

$$\bar{E}=\frac{\langle\Phi_\alpha|T+U|\Phi_\alpha\rangle}{\langle\Phi_\alpha|\Phi_\alpha\rangle}. \tag{4}$$

Making use of the uniformity properties of the operators T and U, we reduce the condition for the minimum of the energy to the equation

$$2\langle\Phi_\alpha|T|\Phi_\alpha\rangle+\langle\Phi_\alpha|U|\Phi_\alpha\rangle=0, \tag{5}$$

which must be satisfied by the optimum value of the parameter α.

For system of $N\geqslant 3$ particles, the diagonal matrix elements of the operators T and U which appear in Eq. (5) are $3(N-2)$-dimensional integrals with nonseparable variables, because of "coupling" of the integration variables in the argument of the exponential function Φ_α. Exact analytical evaluations of these integrals are possible only for three-body systems (through the use of perimetric coordinates[5]). As soon as we get to $N=4$, an evaluation of these integrals requires a complicated Fourier-transform technique, followed by a one-dimensional numerical quadrature.[6] For $N\geqslant 5$, there are as yet no methods for evaluating these integrals. Accordingly, for the general case of a system with an arbitrary number of particles N, the matrix elements in Eq.

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(5) are unknown, and the problem of determining the optimum value of the parameter α looks at first glance to be beyond solution.

It turns out that the particular properties of the exponential trial wave function in Eq. (3) make it possible to solve Eq. (5) without evaluating any integrals at all. Let us demonstrate.

Direct differentiation of the wave function (3) with respect to the coordinates of the particles verifies that this function satisfies

$$(T+V_\alpha+W_\alpha)\Phi_\alpha=\varepsilon_\alpha\Phi_\alpha. \tag{6}$$

In Eq. (6)

$$\varepsilon_\alpha=-\frac{N(N-1)G^2m^5\alpha^2}{2\hbar^2}, \tag{7}$$

and V_α and W_α are the following functions of the coordinates of the particles:

$$V_\alpha=-2Gm^2\alpha\sum_{j<k}^{N}\frac{1}{r_{jk}}, \tag{8}$$

$$W_\alpha=-\frac{G^2m^5\alpha^2}{\hbar^2}\sum_{\substack{j,k<l\\k,l\neq j}}^{N}\cos\theta_{jkl}. \tag{9}$$

Here θ_{jkl} is the angle whose vertex is at particle j and whose sides link particle j to particles k and l. The cosine of this anlge can be expressed in terms of the interparticle distances:

$$\cos\theta_{jkl}=\frac{r_{jk}^2+r_{jl}^2-r_{kl}^2}{2r_{jk}r_{jl}}. \tag{10}$$

Equation (6) can be thought of as a Schrödinger equation for a system of N particles with identical masses m which are moving in a potential which is the sum of V_α and W_α, and Φ_α and ε_α are the eigenfunction and the eigenvalue of this equation.

Since V_α is a homogeneous function of the degree -1 of the particle coordinates, while W_α is a homogeneous function of degree 0, we draw the following conclusion regarding Eq. (6) from the virial theorem:

$$2\langle\Phi_\alpha|T|\Phi_\alpha\rangle+\langle\Phi_\alpha|V_\alpha|\Phi_\alpha\rangle=0. \tag{11}$$

This equation, which holds identically as the parameter α is varied, differs from (5) in that the actual potential energy U has been replaced by the function V_α. We now select a value of α such that the function V_α becomes equal to U. It can be seen from Eq. (8) that for this purpose we should set $\alpha=1/2$. In this particular case, Eq. (11) takes the form

$$2\langle\Phi_{1/2}|T|\Phi_{1/2}\rangle+\langle\Phi_{1/2}|U|\Phi_{1/2}\rangle=0. \tag{12}$$

The exponential trial function $\Phi_{1/2}$ found from Eq. (3) in the case $\alpha=1/2$ thus satisfies Eq. (5) and is therefore the optimum value in the variational calculation of the energy of the gravitational system. The surprising simiplicity of this result, which makes it possible to determine the optimum value of the scale factor ($\alpha=1/2$) and to satisfy the virial theorem (12) without going through calculations of any sort, is a characteristic feature of the correlated exponential trial wave function (3), whose structure reflects the nature of the gravitational interaction among particles.

The function $\Phi_{1/2}$ has another noteworthy property: From the Schrödinger equation (2) we find that the result of acting on the exact eigenfunction Ψ with the operator $T+U$ remains bounded regardless of the arrangement of the particles, even if the interparticle distances tend toward zero. The reason is that the right side of this equation contains the quantity $E\Psi$, which is bounded everywhere. We can show that the correlated exponential trial function $\Phi_{1/2}$ has an analogous property. Since the functions V_α and U are the same in the case $\alpha=1/2$, Eq. (6) for the function $\Phi_{1/2}$ can be written

$$(T+U)\Phi_{1/2}=(\varepsilon_{1/2}-W_{1/2})\Phi_{1/2}. \tag{13}$$

Since the function $W_{1/2}$ in Eq. (9) is bounded regardless of the arrangement of the particles, and since $\varepsilon_{1/2}$ in Eq. (7) is a constant number, the quantity $(T+U)\Phi_{1/2}$ is indeed bounded everywhere, even at points where particles collide, and where their interaction energy increases without bound.

The correlated exponential wave function $\Phi_{1/2}$ thus has the optimum scale, satisfies the virial theorem for the expectation values of the operators T and U, and furthermore suppresses the singularities in the potential energy at points where particles collide. This result, which holds for a gravitational system of N identical particles, can be generalized to gravitational and Coulomb systems of particles with arbitrary masses and charges. Using a method like that used here, one can show that the correlated exponential wave function

$$\Phi=\exp\left(\frac{1}{\hbar^2}\sum_{j<k}^{N}\frac{q_jq_km_jm_kr_{jk}}{m_j+m_k}\right) \tag{14}$$

satisfies the virial theorem, has the optimum scale, and suppresses the singularities in the potential energy at points where particles collide. The quantities q_j and m_j here are the charge and mass of particle j. In a gravitational system, the charges of the particles should be regarded as purely imaginary: $q_j=iG^{1/2}m_j$. For Coulomb systems, the products q_jq_k can have either sign, and Eq. (14) holds if the function Φ falls off exponentially, for any conceivable method of breaking up the system of N particles into two subsystems which are far apart. The properties of the function (14) which we have enumerated here were originally proved for a system of three charged particles by Demkov and Filinskiĭ.[7]

CORRELATION ENERGY FOR GRAVITATIONAL SYSTEMS

We now calculate the energy of a gravitational system of particles with the correlated exponential wave function $\Phi_{1/2}$ whose properties were discussed above. Using Eq. (12), we find that the mathematical expectation of the energy calculated using this function is

$$\bar{E}=\frac{\langle\Phi_{1/2}|U|\Phi_{1/2}\rangle}{2\langle\Phi_{1/2}|\Phi_{1/2}\rangle}. \tag{15}$$

Substituting in the explicit expressions for $\Phi_{1/2}$ and the gravitational potential energy U, making use of the interchange symmetry of the problem, and changing the scale of the integration variables, we find the formula

TABLE I. Ground-state energy of the gravitational system in the one-particle, self-consistent-field approximation found with the help of the correlated exponential wave function $\Phi_{1/2}$ (the energies are in units of $G^2m^5/\hbar^2$, where m is the mass of a particle).

Number of particles N	One-particle Hartree approximation	Correlation exponential wave function	Correlation energy
3	−0,6511	−1,0714	−0,4203
4	−1,9534	−2,7895	−0,8361

$$\bar{E} = -\frac{N(N-1)G^2m^5}{4\hbar^2}\frac{\int r_{12}^{-1}\exp\left(-\sum_{j<k}^{N} r_{jk}\right)d\tau}{\int \exp\left(-\sum_{j<k}^{N} r_{jk}\right)d\tau}. \quad (16)$$

Here $d\tau$ is the volume element of the $3(N-2)$-dimensional space of relative coordinates of the particles.

Equation (16) holds for systems with an arbitrary number of particles. We have used it to calculate variational values of the energy of systems with $N=3$ (in which case all the necessary integrals can be evaluated in a simple manner by switching to perimetric coordinates) and also with $N=4$ (in this case, these integrals, calculated by the method of Ref. 6, were graciously furnished to us by K. Krauthuser of the University of Delaware). The results are shown in Table I, where they are compared with results calculated from the formula derived for the energy in the one-electron Hartree approximation[1,2] after the self-effects of the particles on themselves are eliminated.[3]

We see in Table I that the correlation treated using the wave function $\Phi_{1/2}$, which depends on all the interparticle distances, leads to a binding energy for the system which is substantially larger than that found in the SCF approximation. For the three-body system, this increase in binding energy (i.e., the correlation energy) is 65%, and for the four-body system it is 43%, of the binding energy calculated in the correlation-free one-particle SCF approximation. The role of interparticle correlations in gravitational systems is much greater than in the case of electrons in atoms. For the three-electron lithium atom and the four-electron beryllium atom, for example, the correlation energies are only 0.6% and 0.4% of the binding energies calculated in the SCF approximation.[8,9]

To find the accuracy of this calculation of the energy of a gravitational system with the help of the wave function $\Phi_{1/2}$, we carried out variational calculations of the energy of a three-body gravitational system with large bases consisting of from 10 to 60 functions. In these bases we included the function $\Phi_{1/2}$ and also functions of the type

$$f_k = P\exp(-\alpha_k r_{12} - \beta_k r_{23} - \gamma_k r_{31}), \quad (17)$$

where P represents symmetrization with respect to interchanges of all three particles. The exponential parameters α_k, β_k, and γ_k were found by the quasirandom method described in Refs. 10 and 11. As the basis is expanded, the energies found by the variational calculations rapidly converge on the value

$$E = -1{,}071779\ G^2m^5/\hbar^2, \quad (18)$$

which is essentially the exact value of the ground-state energy of a three-body gravitational system. This value is only 0.03% lower than the value $E = -15/14 = -1.071429$ which is found from Eq. (16) with the help of $\Phi_{1/2}$. This agreement is yet further demonstration of the excellence of the correlated exponential function $\Phi_{1/2}$ in calculations on gravitational systems.

Finally, we consider the role played by the correlation energy in gravitational systems with a large number of particles N. It was found in Ref. 3 that the energy of a gravitational system has the following lower bound in the limit $N\to\infty$:

$$E(N) \geqslant -0{,}05556\ N^3G^2m^5/\hbar^2. \quad (19)$$

The exact energy of a gravitational system as $N\to\infty$ obviously lies between its upper (Hartree) bound[1,2]

$$E(N) \leqslant -0{,}05426\ N^3G^2m^5/\hbar^2 \quad (20)$$

and the lower bound in Eq. (19). It follows that in the limit $N\to\infty$ the correlation energy of a gravitational system is less than 2% of the total binding energy of the system. This decrease in the relative size of the correlation energy with increasing number of particles arises because for large N the gravitational system forms a very compact cluster of matter, and each particle in this cluster "senses" primarily the average gravitational field of all the other particles, reacting only weakly to fluctuations in this field.

CONCLUSION

The results derived here show that the correlation energy in quantum-mechanical gravitational systems amounts to 35–30% of the total binding energy of the system when the number of particles is small ($N=3$ or 4), while as $N\to\infty$ it amounts to less than 2% of the total binding energy. Because of the differences in the signs of the interaction forces, the correlation among particles in gravitational systems is quite different from that among the electrons in Coulomb systems. The properties of the correlated exponential wave function $\Phi_{1/2}$ [and of the function Φ in Eq. (14)] which we have proved here—i.e., has the optimum scale, that it satisfies the virial theorem, and that it suppresses signularties in the potential energy—show that these functions hold promise for use in quantum-mechanical calculations on many-body Coulomb and gravitational systems in which the correlation in the motion of particles is taken into account.

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