

Models including electron correlation in relation to Fock's proposed expansion of the ground-state wave function of He-like atomic ions

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Here attention is first drawn to the importance of gaining insight into Fock's early proposal for expanding the ground-state wave function for He-like atomic ions in hyperspherical coordinates. We approach the problem via two solvable models, namely, (i) the s -term model put forth by Temkin [Phys. Rev. **126**, 130 (1962)] and (ii) the Hookean atom model proposed by Kestner and Sinanoglu [Phys. Rev. **128**, 2687 (1962)]. In both cases the local kinetic energy can be obtained explicitly in hyperspherical coordinates. Separation of variables occurs in both model wave functions, though in a different context in the two cases. Finally, a \mathbf{k} -space formulation is proposed that should eventually result in distinctive identifying characteristics of Fock's nonanalyticities for He-like atomic ions when both electrons are close to the nucleus.

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I. INTRODUCTION

Because of the present intractability of the exact analytic solution of the Schrödinger solution for the ground-state of He-like atomic ions, we approach the problem here via two solvable models. The first model we discuss was put forth by Kestner and Sinanoglu [1], who proposed the replacement of the Coulomb confinement form of the external potential $V_{\text{ext}}(\vec{r})$ by a harmonic restoring potential given by $\frac{1}{2}kr^2$ but retaining the full Coulombic interaction e^2/r_{12} . It was natural to refer to this model as the two-electron Hookean atom. The model's great merit is that the center-of mass motion can be separated from the relative motion (see, for instance, Ref. [2]). Kais *et al.* quote the exact ground-state wave function $\Psi(\vec{r}_1, \vec{r}_2)$ for the solvable case of the Hamiltonian $H_{\text{Hooke}} = -\nabla_1^2 - \nabla_2^2 + e^2/r_{12} + (k/2)(r_1^2 + r_2^2)$ for $k = \frac{1}{4}$ a.u. as

$$\Psi(\vec{r}_1, \vec{r}_2) = N_0 \left(1 + \frac{1}{2}|\vec{r}_1 - \vec{r}_2|\right) \exp\left[-\frac{1}{4}(r_1^2 + r_2^2)\right], \quad (1)$$

which corresponds to ground-state energy $E_0 = 2$ a.u. ($E_{\text{HF}} = 2.039325$ a.u., where E_{HF} represents the Hartree-Fock energy). Following Fock's proposal [3], we immediately rewrite Eq. (1) in hyperspherical coordinates R , Θ , and α defined by

$$\begin{aligned} R &= \sqrt{r_1^2 + r_2^2}, & r_1 &= R \cos \alpha, \\ r_2 &= R \sin \alpha, & \cos \Theta &= \frac{\vec{r}_1 \cdot \vec{r}_2}{r_1 r_2} \end{aligned} \quad (2)$$

to obtain

$$\Psi(R, \alpha, \Theta) = \Psi_g(R) - \sqrt{1 - \sin 2\alpha \cos \Theta} \frac{\partial \Psi_g(R)}{\partial R}, \quad (3)$$

where $N_0 \exp[-\frac{1}{4}R^2] = \Psi_g(R)$.

For He-like atomic ions Fock proposed expanding the ground-state wave function for small R in a form involving not only non-negative-integer powers of R , but also positive-integer powers of $\ln R$. We refer to the important subsequent work of Refs. [4–9], which have demonstrated the convergence and usefulness of Fock's expansion. It is also relevant here to note two recent papers on the Hookean model [10,11].

Here we note that while Eq. (3) is not directly separable in hyperspherical coordinates, it is the sum of a part $\Psi_g(R)$, independent of the angles α and Θ , plus a piece with an R dependence determined by $\partial \Psi_g(R)/\partial R$, times the known function $\sqrt{1 - \sin 2\alpha \cos \Theta}$ of angles α and Θ . Clearly, both R -dependent parts can be expanded to all orders in R^2 and there are no logarithmic terms at small R . Since for small R both electrons are near the origin of harmonic confinement, it is clear that e^2/r_{12} alone for small r_{12} does not lead to Fock-like nonanalytic terms for small r . Thus, Coulomb confinement with $V_{\text{ext}}(r) = -Z/r$ replacing the harmonic form needs to be invoked in He if Fock's nonanalytic behavior is to be recovered.

This leads us directly to a second model, proposed by Temkin [12], which is now referred to as the Temkin-Poet [13] model for He-like atomic ions. Particularly relevant to this study is Ref. [14], where it is pointed out that the wave function considered by Howard and March [15], namely,

$$\Psi_{\text{HM}}(\vec{r}_1, \vec{r}_2) = C \exp\left[-(Z - 1/2)(r_1 + r_2) + \frac{|r_1 - r_2|}{2}\right], \quad (4)$$

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is the exact ground-state wave function for the Hamiltonian

$$\hat{H}'_s = -\frac{1}{2}\nabla_1^2 - \frac{Z}{r_1} - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_2} + \frac{1}{r_>} + \delta(r_1 - r_2). \quad (5)$$

This differs from the Temkin-Poet model $H_{TP} = \hat{H}'_s - \delta(r_1 - r_2)$ by the presence of the δ function, with the quantity $r_>$ given by

$$r_> = \frac{1}{2}(r_1 + r_2 + |r_1 - r_2|) = \max(r_1, r_2). \quad (6)$$

As put forth in Ref. [12], only the s term in the expansion of $1/r_{12}$ is retained to obtain the Hamiltonian in Eq. (5). Inserting hyperspherical coordinates from Eq. (2) into the Howard-March (HM) wave function in Eq. (4) then yields

$$\Psi_{\text{HM}} = C \exp \left[- (Z - 1/2)R(\sin \alpha + \cos \alpha) + \frac{R}{2} |\sin \alpha - \cos \alpha| \right], \quad (7)$$

with no explicit dependence on Θ .

II. LOCAL-ENERGY AND KINETIC-ENERGY OPERATORS IN HYPERSPHERICAL COORDINATES

When the ground-state wave function Ψ is written in terms of the hyperspherical coordinates R , α , and Θ described above,

$$E_{\text{LK}} = \frac{12 \sin^2 \Theta + 16 \cos \Theta \cos^2(2\alpha) \csc(2\alpha) - 8\phi + 2[r(12 - R^2) - 12]\phi^2 - (R^4 - 16R^2 + 12)\phi^3 + 12\phi^4}{16R\phi^3(\alpha, \Theta) \left[1 + \frac{R}{2}\phi(\alpha, \Theta) \right]}. \quad (10)$$

Here $\phi(\alpha, \Theta) = \sqrt{1 - \sin(2\alpha) \cos \Theta}$, while the potential-energy term $U(R, \alpha, \Theta)$ is

$$U(R, \alpha, \Theta) = \frac{1}{8}R^2 + \frac{e^2}{R\phi(\alpha, \Theta)}. \quad (11)$$

Given the explicit kinetic-energy operator

$$\hat{T}(R, \alpha) = -\frac{1}{2} \left[\partial_R^2 + \frac{5}{R} \partial_R + \frac{1}{R^2} [\partial_\alpha^2 + 4 \cot(2\alpha) \partial_\alpha] \right], \quad (12)$$

we write the potential-energy entering \hat{H}'_s in Eq. (5) as

$$U(R, \alpha) = -\frac{1}{R} [\mu(\alpha) - \delta(\sin \alpha - \cos \alpha)]. \quad (13)$$

It should be noted that here we have used the relation

$$\delta(Rx) = \frac{1}{R} \delta(x) \quad (14)$$

and have defined $\mu(\alpha)$ in Eq. (13) as

$$\mu(\alpha) = (Z - 1/2)(\sec \alpha + \csc \alpha) + \frac{1}{2} \frac{|\sin \alpha - \cos \alpha|}{\sin \alpha \cos \alpha}. \quad (15)$$

we find it convenient to work with the local L ground-state energy E_L defined by

$$E_L = \frac{\hat{H}\Psi(R, \alpha, \Theta)}{\Psi(R, \alpha, \Theta)} = -\frac{1}{2} \frac{[\nabla_1^2 + \nabla_2^2]\Psi}{\Psi} + U(R, \alpha, \Theta). \quad (8)$$

Here $U(R, \alpha, \Theta)$ is the total potential energy entering the Hamiltonian \hat{H} . At this point we return to the Hookean atom with $k = 1/4$ and note immediately that $U_{\text{external}} = U_{\text{ext}}$ is given by

$$U_{\text{ext}}(r_1, r_2) = \frac{1}{8}(r_1^2 + r_2^2) = \frac{1}{8}R^2 \quad (9)$$

in hyperspherical coordinates. This, of course, is a crucial simplification and means that the entire dependence of $U(R, \alpha, \Theta)$ on α and Θ for this Hookean atom model comes from the Coulomb repulsion potential energy $e^2/|r_1 - r_2|$.

Writing the kinetic-energy operator (following, e.g., Macek [16]) in hyperspherical coordinates, the He-atom ground-state Schrödinger equation reads

$$-\frac{1}{2} \left[\frac{\partial^2}{\partial R^2} + \frac{5}{R} \frac{\partial}{\partial R} - \frac{\Lambda^2}{R^2} \right] \Psi - \left(\frac{Ze^2}{r_1} + \frac{Ze^2}{r_2} - \frac{e^2}{r_{12}} \right) \Psi = E\Psi,$$

where Λ^2 is Casimir's operator [cf. Eq. (12)]. We can immediately use the Hookean atom wave function Ψ in Eq. (1) to calculate the kinetic-energy term on the right-hand side of Eq. (8) as

The total energy is $E_{\text{HM}} = -(Z^2 - Z + 1/2)$, while the local kinetic energy is $E_{\text{HM}}^K = \frac{1}{R}\mu(\alpha) - (Z^2 - Z + 1/2)$. The wave function in Eq. (4) has been written in the form

$$\Psi_{\text{HM}}(R, \alpha) = C e^{-R\lambda(\alpha)}, \quad (16)$$

where

$$\lambda(\alpha) = (Z - 1/2)(\sin \alpha + \cos \alpha) - \frac{1}{2} |\sin \alpha - \cos \alpha|. \quad (17)$$

For the HM model it is in $\ln \Psi_{\text{HM}}$ that the variables R and α separate, in contrast to the Hookean atom Ψ in Eq. (3). The quantity $y(\alpha) = \lambda(\alpha)$ must satisfy the two differential equations

$$y'' + 4 \cot(2\alpha)y' + 5y = (2Z - 1)(\sec \alpha + \csc \alpha) + \frac{|\sin \alpha - \cos \alpha|}{\sin \alpha \cos \alpha}$$

and

$$(y')^2 + y^2 = 2(Z^2 - Z + 1/2).$$

III. DETAILED TREATMENT OF BOTH MODELS IN \mathbf{k} SPACE

We turn now to the representations of our models in \mathbf{k} space. It is convenient to introduce a dummy integration vector \vec{R} whose magnitude is the coordinate R .

The Hookean atom is the simplest to start with. The angle-independent term $\Psi_g(R)$ clearly has a Gaussian Fourier transform and the Fourier transform of Eq. (3) is

$$\begin{aligned} \Phi(k, \alpha, \Theta) &= 4\pi N_0 \left\{ 2\sqrt{\pi} e^{-k^2} - \left[2 + \sqrt{\pi} \left(\frac{1}{k} - 2k \right) e^{-k^2} \text{Erfi}(k) \right] \right. \\ &\quad \left. \times \sqrt{1 - \sin(2\alpha) \cos \Theta} \right\}. \end{aligned} \quad (18)$$

[Here $\text{Erfi}(z)$ denotes the error function of an imaginary argument.] Similarly, the Fourier transform of the Howard-March wave function in Eq. (4) is

$$\Phi_{\text{HM}}(k, \alpha) = \frac{8\pi C\lambda}{(k^2 + \lambda^2)^2}, \quad (19)$$

where $\lambda = (Z - 1/2)(\cos \alpha + \sin \alpha) - \frac{1}{2}|\cos \alpha - \sin \alpha|$.

For the Howard-March and Temkin-Poet models we have

$$E\Psi(R, \alpha) - U(R, \alpha)\Psi(R, \alpha) = \hat{T}(R, \alpha)\Psi(R, \alpha), \quad (20)$$

where we write

$$\hat{T}(R, \alpha) = \frac{1}{2} \left[\Delta_R + \frac{1}{R^2} \Delta_\alpha \right], \quad \Delta_R = \partial_R^2 + \frac{5}{R} \partial_R, \quad (21)$$

$$\Delta_\alpha = \partial_\alpha^2 + 4 \cot(2\alpha) \partial_\alpha, \quad U(R, \alpha) = -\frac{1}{R} f(\alpha), \quad (22)$$

where $f = \mu$ for the Temkin-Poet case and $\mu - 2^{-1/2} \delta(\alpha - \pi/4)$ for the Howard-March case. The Fourier transform on the left-hand side of Eq. (20) with respect to the vector \vec{R} gives

$$E\Phi(k, \alpha) + \frac{f(\alpha)}{2\pi^2} \int \frac{d\vec{k}'}{|\vec{k} - \vec{k}'|^2} \Phi(\vec{k}', \alpha), \quad (23)$$

where Φ denotes the Fourier transform of Ψ . We next evaluate the right-hand side of Eq. (20), which can be written, by expressing Ψ as an inverse Fourier transform and expanding the kernel $e^{-i\vec{k} \cdot \vec{R}}$ in spherical Bessel functions,

$$\begin{aligned} &4\pi \int_0^\infty \hat{T}(R, \alpha) [j_0(k'R)\Phi(k', \alpha)] k'^2 dk' \\ &= 2\pi \int_0^\infty \left\{ \left[j_0(k'R) + \frac{3}{k'R} j_1(k'R) \right] \Phi(k', \alpha) \right. \\ &\quad \left. - \frac{j_0(k'R)}{(k'R)^2} \Delta_\alpha \Phi(k', \alpha) \right\} k'^4 dk'. \end{aligned} \quad (24)$$

The Fourier transform of Eq. (24) is

$$\begin{aligned} &\frac{4\pi^3}{k^2} \Phi(k, \alpha) \\ &+ \frac{12\pi^2}{k} \int_0^\infty \left\{ \left[\ln \left| \frac{k+k'}{k-k'} \right| - \frac{2kk'}{|k^2 - k'^2|} \right] \Phi(k', \alpha) \right. \\ &\quad \left. - \pi k k' k_{<} \Delta_\alpha \Phi(k', \alpha) \right\} k' dk'. \end{aligned} \quad (25)$$

Consequently, both the Howard-March and Temkin-Poet model equations have the form

$$\begin{aligned} &(E - 4\pi^3 k^2) \Phi(k, \alpha) \\ &+ \frac{f(\alpha) - 12\pi^3}{\pi k} \int_0^\infty \ln \left| \frac{k+k'}{k-k'} \right| \Phi(k', \alpha) k' dk' \\ &+ 12\pi^3 \int_0^\infty k'^2 k_{<} \Delta_\alpha \Phi(k', \alpha) dk' = 0. \end{aligned} \quad (26)$$

Remarkably, Eq. (26) with the Howard-March value of E is a solution of Eq. (20), whereas it is not, for any values of E and $\lambda(\alpha)$, for the Temkin-Poet model. The reason, of course, is that the second derivative in Δ_α operating on Eq. (16) produces the δ function necessary to cancel that in $f(\alpha)$, but the latter is absent in the Temkin-Poet case.

We have focused on the two model wave functions in Eqs. (3) and (7) in hyperspherical coordinates so far because Eq. (3) for the Hookean atom involves e^2/r_{12} exactly, while Eq. (4) has Coulomb confinement through the Hamiltonian \hat{H}'_s in Eq. (5), but a modified electron-electron interaction in which the s -wave term only, namely, $e^2/r_{>}$, is retained, plus an additional radial correlation through the δ -function contribution to \hat{H}'_s . The Hookean atom results presented here then make it clear that for small R , Fock-like terms in the He atom wave function must arise from an interplay between Coulomb confinement and the full electron-electron interaction e^2/r_{12} ; while Coulomb confinement is exactly incorporated in the model Hamiltonian \hat{H}'_s in Eq. (5), the electron-electron interaction terms are too primitive to yield terms like $R^2 \ln R$, for instance, at small R .

IV. A THIRD MODEL WITH HARMONIC CONFINEMENT BUT INVERSE SQUARE INTERPARTICLE INTERACTION

We think it will be of interest to mention here yet a third exactly solvable model in which the wave function itself has clear nonanalytic behavior at small R . This is the case for the wave function derived by Crandall *et al.* [17] for the two-electron model, $H_c = -(\nabla_1^2 + \nabla_2^2)/2 + (\omega/2)(r_1^2 + r_2^2) + \lambda/r_{12}^2$, which parallels the Hookean atom by having harmonic confinement, but with an inverse quadratic interaction instead of e^2/r_{12} as in the Hookean model. The Crandall ground-state wave function $\Psi(\vec{r}_1, \vec{r}_2)$ has the explicit form

$$\Psi_C(\vec{r}_1, \vec{r}_2) = \exp[-m\omega r_1^2/2\hbar] \exp[-m\omega r_2^2/2\hbar] r_{12}^\gamma, \quad (27)$$

where γ measures the strength of the repulsive coupling through

$$\gamma = [(1 + 4\lambda m/\hbar^2)^{1/2} - 1]/2. \quad (28)$$

For γ nonintegral, as is usually the case for this model, we note below two features of the nonanalyticity, reflected in the term r_{12}^γ (which in hyperspherical coordinates is proportional to R^γ), times a known function of α and Θ . First, a physical property, the ground-state density $n(r) = \int \Psi_C^2(\vec{r}, \vec{r}') d\vec{r}'$, has

been obtained from Eq. (27) by Capuzzi *et al.* [18], which for the artificial two-electron atom reads

$$n(r) = \frac{(m\omega/\hbar)^{3/2}}{2^{a-1}\pi^{3/2}} \exp[-2m\omega r^2/\hbar] {}_1F_1\left(\frac{3}{2} + \gamma; \frac{3}{2}; \frac{m\omega r^2}{\hbar}\right). \quad (29)$$

The corresponding x-ray scattering factor $f(k)$, which is the Fourier transform of $n(r)$, can be calculated analytically from Eq. (29), with the result

$$f(k) = 2e^{-k^2 a^2/2} {}_1F_1\left(-\gamma; \frac{3}{2}; \frac{1}{4}k^2 a^2\right), \quad (30)$$

where $a = \sqrt{\hbar/2m\omega}$. Writing Eq. (27) in hyperspherical coordinates and then taking the Fourier transform with respect to R , we find that in \mathbf{k} space, the wave function of Crandall *et al.* is nonanalytic at small R and has the large- k behavior

$$\Phi_C(k, \alpha, \Theta) = f(\alpha, \Theta) \frac{1}{k^{\gamma+3}}, \quad (31)$$

where $f(\alpha, \Theta)$ is known.

V. DISCUSSION

Finally, returning to the specific Fock proposal of $\ln R$ behavior in the He atom, we note that White and Stillinger [19], using first-order perturbation theory on the angle-averaged wave function $\exp[-Z^*R]$ in Ref. [19] as the unperturbed result, found a term $R^2 \ln R$ times an angular function in He. In this regard, we consider the asymptotic behavior of the Fourier transforms below that are relevant to this work:

$$\begin{aligned} F(k) &= \int dR e^{i\mathbf{k}\cdot\mathbf{R}} R^\alpha e^{-aR^2} \\ &= \frac{2\pi}{a^{(\alpha+3)/2}} \Gamma(1 + \alpha/2) {}_1F_1\left(\frac{\alpha+3}{2}; \frac{3}{2}; -\frac{k^2}{4a}\right) \\ &\quad - \frac{\pi^{3/2} 2^{\alpha/2+2} \alpha}{k^{\alpha+3}} \frac{\Gamma(1 + \alpha/2)}{\Gamma(1 - \alpha/2)}, \end{aligned} \quad (32)$$

for large k and $\alpha \neq 0, 2, 4, \dots$, and

$$\begin{aligned} G(k) &= \int d\vec{R} e^{i\mathbf{k}\cdot\mathbf{R}} R^2 \ln R e^{-aR^2} \\ &= \frac{\pi \Gamma(5/2)}{a^{5/2}} \left\{ \frac{\partial}{\partial s} {}_1F_1\left(s; \frac{3}{2}; -\frac{k^2}{4a}\right) \right\}_{s=5/2} \\ &\quad + \left[\psi \frac{5}{2} - \ln a \right] \left(1 - \frac{k^2}{6a} \right) e^{-k^2/4a}. \end{aligned} \quad (33)$$

For large k ,

$$G(k) \sim \frac{2\pi^{3/2} [\ln a - \psi(5/2)] e^{-k^2/4a}}{a^2 k}. \quad (34)$$

The nonanalyticity in Eq. (31) is clearly reflected at large k in Eq. (32), while Eq. (33) is relevant to He itself in the context of the White-Stillinger first-order perturbation calculation [19].

VI. CONCLUSION

Following Fock's proposal [3], we have expressed the exact ground-state wave function for two solvable models in hyperspherical coordinates. While both wave functions are compact, we have been able to pull them together in \vec{k} space, leading to a common equation [Eq. (26)]. This is one of our principal results. Returning to Fock's ideas though, the Hookean atom model as presented above reveals that in hyperspherical coordinates, Fock-like terms in the He atom wave function for small R can arise only from the interplay between Coulomb confinement and the full electron-electron interaction e^2/r_{12} . We have also stressed that, while Coulomb confinement is exactly incorporated in the Hamiltonian \hat{H}'_s in Eq. (5), the electron-electron interaction terms included there are still too primitive to yield terms having, for example, the Fock term $R^2 \ln R$ at small R .

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