Momentum density and spatial form of correlated density matrix in model two-electron atoms with harmonic confinement

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The detailed nature of the correlated first-order density matrix for the model atoms in the title for arbitrary interparticle interaction $u(r_{12})$ is studied. One representation with contracted information is first explored by constructing the momentum density $\rho(\mathbf{p})$ in terms of the wave function of the relative motion, say $\Psi_R(r_{12})$, which naturally depends on the choice of $u(r_{12})$. For $u(r_{12})=e^2/r_{12}$, the so-called Hookean atom, and for the inverse square law $u(r_{12})=\lambda/r_{12}^2$, plots are presented of the above density $\rho(\mathbf{p})$ in momentum space. The correlated kinetic energy is recovered from averaging $p^2/2m$, m denoting the electron mass, with respect to $\rho(\mathbf{p})$. The second method developed is in coordinate space and expands the density matrix $\gamma(\mathbf{r}_1,\mathbf{r}_2)$ in Legendre polynomials, using relative coordinate $\mathbf{r}_1-\mathbf{r}_2$, center-of-mass coordinate $(\mathbf{r}_1+\mathbf{r}_2)/2$ and the angle, θ say, between these two vectors. For the Moshinsky atom in which $u(r_{12})=\frac{1}{2}kr_{12}^2$ only the s term ($l=0$) contributes to the Legendre polynomial expansion. The specific example we present of the inverse square law model is shown to be characterized by the low-order terms ($s+d$) of the Legendre expansion. The Wigner function is finally calculated analytically for both Moshinsky and inverse square law models.

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I. INTRODUCTION

It remains of outstanding interest for atomic physics to make analytical progress on the theory of the ground-state of the helium atom. The difficulty, of course, resides in the interelectronic repulsion of the two electrons with opposite spins, at separation r_{12} and given by e^2/r_{12}. To attempt to gain insight into the effect of such Coulombic repulsion between spin-half fermions, Kestner and Sinanoglu [1] proposed the study of a model in which the electron-nuclear attraction was replaced by harmonic confinement with potential energy $\frac{1}{2}kr^2$, but e^2/r_{12} was retained as the interparticle interaction. For the special case $k=1/4$, Kais, Herschbach, and Levine [2] obtained the exact spatial ground-state wave function $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ in closed form and the above model is now termed the Hookean atom. Holas, Howard, and March [3], referred to as HHM below, subsequently constructed a theory for such two-electron "artificial atoms," characterized by an arbitrary interparticle interaction $u(r_{12})$, but always with harmonic confinement. The ground-state wave function $\Psi(\mathbf{r}_1,\mathbf{r}_2)$ then separates as a product of center-of-mass (c) wave function $\Psi_c(\mathbf{c})$ and relative motion (R) contribution $\Psi_R(\mathbf{b})$ where

$$\mathbf{b}=\mathbf{r}_1-\mathbf{r}_2, \quad \mathbf{c}=(\mathbf{r}_1+\mathbf{r}_2)/2 \tag{1}$$

The center-of-mass part $\Psi_c(\mathbf{c})=\Psi_c(c)$ can be obtained as a Gaussian function. Naturally $\Psi_R(\mathbf{b})=\Psi_R(b)$ depends on $u(r_{12})$, but requires only the solution of a one-particle Schrödinger equation with potential $V_{\text{eff}}(r)$ given by [3]

$$V_{\text{eff}}(r)=\frac{1}{4}kr^2+u(r). \tag{2}$$

We study in full detail below the correlated first-order density matrix denoted by $\gamma(\mathbf{r}_1,\mathbf{r}_2)$. In terms of $\Psi_c(c)$ and $\Psi_R(b)$ introduced above, Eq. (17) in Ref. [3] reads

$$\gamma(\mathbf{r}_1,\mathbf{r}_2)=\tilde{\gamma}(\mathbf{b},\mathbf{c})=2\int d\mathbf{x}\Psi_c\left(\frac{1}{2}\left|\mathbf{x}+2\mathbf{c}+\frac{1}{2}\mathbf{b}\right|\right)\times\Psi_c\left(\frac{1}{2}\left|\mathbf{x}+2\mathbf{c}-\frac{1}{2}\mathbf{b}\right|\right)\times\Psi_R\left(\left|\mathbf{x}+\frac{1}{2}\mathbf{b}\right|\right)\Psi_R\left(\left|\mathbf{x}-\frac{1}{2}\mathbf{b}\right|\right), \tag{3}$$

where $\tilde{\gamma}(\mathbf{b},\mathbf{c})$ is the same density matrix but with different variables. As already noted, Ψ_c is found to have the normalized form

$$\Psi_c(c)=\frac{1}{a^{3/2}\pi^{3/4}}\exp\left(-\frac{1}{2}\frac{c^2}{a^2}\right), \quad a=\left(\frac{\hbar}{2m\omega}\right)^{1/2}, \quad \omega^2=k/m \tag{4}$$

We retain $\Psi_R(b)$ in its general form, until it becomes necessary to make specific evaluations as in, say, the Hookean atom.

We shall first consider "contracting" the information content in Eq. (3) by focusing in Sec. II below on the momentum density $\rho(\mathbf{p})$. This is defined such that the total correlated kinetic energy T can be calculated by averaging the kinetic energy $p^2/2m$ with respect to $\rho(\mathbf{p})$. Section III considers the three model atoms referred to in the abstract, plots of $\rho(\mathbf{p})$ being presented for each case. Section IV then treats the so-called Wigner function $\gamma_w(\mathbf{r},p)$ which generalizes the corresponding classical phase space probability distribution.

In Sec. IV we also introduce a Legendre polynomial expansion of the first-order density matrix, motivated by the facts emphasized already that the "natural" coordinates are b and c given in Eq. (1), plus the angle between them. We then exemplify the complete theory by specific introduction of the relative motion wave functions $\Psi_R(b)$ for the three model atoms in the abstract. Section V constitutes a summary, plus some proposals for future work that have been prompted by the findings presented here. In Appendix A we get a general expression for atomic scattering for these two-electron systems that relates it to the relative motion wave function. It then reflects the effect of different inter-particle interaction and we calculate it for the three models in Abstract. As for another aspect of the density matrix, Appendix B tries to show how the density matrix for these systems departures from idempotency by turning on the interaction between particles and how big it can be.

II. MOMENTUM DENSITY $\rho(\mathbf{p})$ FOR MODEL TWO-ELECTRON ATOMS

From the spatial density matrix $\gamma(\mathbf{r}_1,\mathbf{r}_2)$ we define the momentum density $\rho(\mathbf{p})$ in the usual way via Fourier transforms between $\mathbf{r}$ and $\mathbf{p}$ space as

$$\rho(\mathbf{p}) = \int \gamma(\mathbf{r}_1,\mathbf{r}_2)\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot(\mathbf{r}_1-\mathbf{r}_2)\right)d\mathbf{r}_1 d\mathbf{r}_2. \tag{5}$$

Introducing the coordinates $\mathbf{b}$ and $\mathbf{c}$ in Eq. (1), and noting that in the transformation $(\mathbf{r}_1,\mathbf{r}_2)\rightarrow(\mathbf{b},\mathbf{c})$ the Jacobian is unity, we readily obtain

$$\rho(\mathbf{p}) = \int \tilde{\gamma}(\mathbf{b},\mathbf{c})\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{c}d\mathbf{b}. \tag{6}$$

Thus, Eq. (6) immediately focuses on $\int\tilde{\gamma}(\mathbf{b},\mathbf{c})d\mathbf{c}$. Introducing the explicit form (4) for the center-of-mass wave function into Eq. (3) we then find

$$\begin{aligned}\int \tilde{\gamma}(\mathbf{b},\mathbf{c})d\mathbf{c} = \frac{2}{a^3\pi^{3/2}}\int d\mathbf{x}\Psi_R\left(\left|\mathbf{x}-\frac{1}{2}\mathbf{b}\right|\right)\\ \times\Psi_R\left(\left|\mathbf{x}+\frac{1}{2}\mathbf{b}\right|\right)\exp\left(-\frac{b^2}{16a^2}\right)\\ \times\int d\mathbf{c}\exp\left(-\frac{4c^2+4\mathbf{c}\cdot\mathbf{x}+x^2}{4a^2}\right).\end{aligned} \tag{7}$$

For the second integral on the right hand side, we have

$$\int d\mathbf{c}\exp\left(-\frac{4c^2+4\mathbf{c}\cdot\mathbf{x}+x^2}{4a^2}\right) = a^3\pi^{3/2}. \tag{8}$$

Hence we find by inserting Eq. (8) into Eq. (7) and then utilizing Eq. (6):

$$\begin{aligned}\rho(\mathbf{p}) = 2\int\int\Psi_R\left(\left|\mathbf{x}-\frac{1}{2}\mathbf{b}\right|\right)\Psi_R\left(\left|\mathbf{x}+\frac{1}{2}\mathbf{b}\right|\right)\\ \times\exp\left(-\frac{b^2}{16a^2}\right)\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{x}d\mathbf{b}.\end{aligned} \tag{9}$$

This equation is the basic result from which we exemplify the theory by inserting for the three models referred to in the abstract the appropriate forms of the relative motion wave function $\Psi_R(r)$.

III. EXPLICIT RESULTS FOR MOMENTUM DENSITY FOR THREE CHOICES OF THE INTERPARTICLE INTERACTION $u(r_{12})$

Let us take in turn, Moshinsky, Hookean, and inverse square law models of the interaction $u(r_{12})$.

A. Moshinsky atom with $u(r_{12})=\frac{1}{2}Kr_{12}^2$

The relative motion wave function is evidently of Gaussian form, which we write as

$$\Psi_R(r) = \frac{1}{a'^{3/2}\pi^{3/4}}\exp\left(-\frac{1}{2}\frac{r^2}{a'^2}\right),\quad a' = \left(\frac{2\hbar}{m\omega'}\right)^{1/2}, \tag{10}$$

where

$$K+\frac{k}{2} = \frac{m}{2}\omega'^2 \tag{11}$$

and therefore

$$a' = \frac{2}{\beta}a,\quad \beta = \left(\frac{2K+k}{k}\right)^{1/4}. \tag{12}$$

Then the momentum density follows by inserting Eq. (10) into Eq. (9) when we obtain

$$\rho(\mathbf{p}) = \frac{128\pi^{3/2}a^3}{(1+\beta^2)^{3/2}}\exp\left(-\frac{4a^2p^2}{(1+\beta^2)\hbar^2}\right). \tag{13}$$

Thus the total kinetic energy of the Moshinsky atom is simply

$$T = \frac{1}{(2\pi\hbar)^3}\int_0^\infty (p^2/2m)\rho(\mathbf{p})4\pi p^2dp = \frac{3(1+\beta^2)\hbar^2}{8ma^2}. \tag{14}$$

As a test we can calculate T using Eq. (23) of Ref. [3]

$$T = \frac{\hbar^2}{4m}\int d^3C\left(\frac{d}{dC}\Psi_c(C)\right)^2 + \frac{\hbar^2}{m}\int d^3r\left(\frac{d}{dr}\Psi_R(r)\right)^2, \tag{15}$$

resulting in $\frac{3\hbar^2}{8ma^2}$ and $\frac{3\beta^2\hbar^2}{8ma^2}$ for the center-of-mass-motion contribution and the relative-motion contribution respectively, in agreement with Eq. (14), as expected. Of course, the Gaussian form (10) crucially simplifies equation (9) as will become quite apparent when we turn to treat the Hookean atom with the confinement force constant k taken to be (1/4), in atomic units.

B. Hookean atom with $u(r_{12})=e^2/r_{12}$

Here, from Ref. [2], the normalized relative motion wave function is found for force constant $k=\frac{1}{4}$ to be

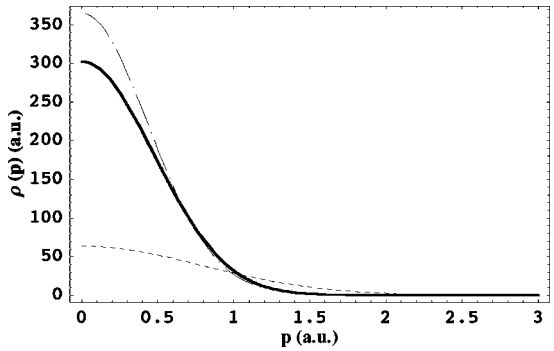

FIG. 1. Ground-state density $\rho(p)$ for the three models of harmonically confined two-electron atoms $(k=\frac{1}{4})$. (Dashed line) Moshinsky model with $\beta=2$. (Solid curve) Hookean atom. (Dashed-point line) Inverse square law repulsion with $\alpha=2$.

$$\Psi_R(r) = [4\pi(8+5\sqrt{\pi})]^{-1/2}\left(1+\frac{r}{2}\right)\exp\left(-\frac{r^2}{8}\right), \quad (16)$$

where atomic units are now being employed in the relative motion wave function $(a=1)$.

Inserting this result (16) into Eq. (9) we find (p is in atomic units)

$$\rho(\mathbf{p}) = \frac{1}{2\pi(8+\sqrt{5\pi})}\int\int\left(1+\frac{1}{2}\left|\mathbf{x}-\frac{1}{2}\mathbf{b}\right|\right)\times\left(1+\frac{1}{2}\left|\mathbf{x}+\frac{1}{2}\mathbf{b}\right|\right)\times\exp\left(-\frac{b^2}{8}\right)\exp\left(-\frac{x^2}{4}\right)\exp(i\mathbf{p}\cdot\mathbf{b})d\mathbf{x}d\mathbf{b} \quad (17)$$

If we focus first on the $\mathbf{x}$ integration the result (17) can be simplified by taking $\mathbf{b}$ as the z axis, followed by using elliptic coordinates [4]. The final result turns out to be

$$\rho(\mathbf{p}) = \frac{\pi}{8+\sqrt{5\pi}}\int_0^\infty db\frac{\sin(pb)}{p}e^{-3b^2/16}\left\{8b(4+b) - 64\pi\left[\mathrm{erf}\left(\frac{b}{4}\right)-1\right]\mathrm{erf}\left(\frac{b}{4}\right)e^{b^2/8} + \sqrt{\pi}[(8-b^2)b + 2(4+b)(8+b^2)]e^{b^2/16}\right\}, \quad (18)$$

where $\mathrm{erf}(x)$ is the error function. But since the remaining integration in Eq. (18) has not been achieved analytically, we show the shape of the spherical momentum density $\rho(p)$ for comparison with that for the Moshinsky atom in Fig. 1, after numerical integration.

As in the previous case we calculate the total kinetic energy, using

$$T = \frac{1}{(2\pi\hbar)^3}\int_0^\infty (p^2/2m)\rho(\mathbf{p})4\pi p^2 dp = 0.664418 \text{ a.u.}, \quad (19)$$

where the center-of-mass-motion contribution and the relative-motion contribution are 3/8 and 0.289418 a.u, respectively, via Eq. (15).

C. Inverse square law repulsion with $u(r_{12})=\lambda/r_{12}^2$

For this model the work of Crandall [5] leads to the relative motion wave function $\Psi_R(r)$ as

$$\Psi_R(r) = n_R r^\alpha \exp\left(-\frac{r^2}{8a^2}\right),$$

$$n_R = 2^{-(\alpha+1)}a^{-(3+2\alpha)/2}\left(4\pi\Gamma\left(\frac{3}{2}+\alpha\right)\right)^{-1/2}, \quad (20)$$

where

$$\alpha = \left(\sqrt{1+\frac{4m\lambda}{\hbar^2}}-1\right)/2. \quad (21)$$

Inserting Eq. (20) into Eq. (9) we find

$$\rho(\mathbf{p}) = 2n_R^2\int\int\left(\left(x^2+\frac{1}{4}b^2\right)^2-(\mathbf{x}\cdot\mathbf{b})^2\right)^{\alpha/2}\times\exp\left(-\frac{x^2}{4a^2}\right)\exp\left(-\frac{b^2}{8a^2}\right)\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{x}d\mathbf{b}. \quad (22)$$

For the special case when $\alpha=2$, this becomes

$$\rho(\mathbf{p}) = \frac{8\sqrt{2}}{15}\pi^{3/2}a^3\left(87-\frac{56p^2a^2}{\hbar^2}+\frac{16p^4a^4}{\hbar^4}\right)\exp\left(-\frac{2p^2a^2}{\hbar^2}\right) \quad (23)$$

which is also plotted in Fig. 1. Finally the total kinetic energy, putting $a=1$ in atomic units, is $T=0.65$ a.u. where the center-of-mass-motion contribution and the relative-motion contribution are 3/8 a.u. and 11/40 a.u., respectively.

IV. WIGNER FUNCTION FOR TWO-ELECTRON FAMILY WITH GENERAL INTERPARTICLE INTERACTION $u(r_{12})$

We have seen in the study of momentum density that the correlated density matrix $\tilde{\gamma}(\mathbf{b},\mathbf{c})$ is somewhat simplified by Fourier transform. This has motivated us to consider therefore the "mixed" $\mathbf{r}$ and $\mathbf{p}$ representation introduced by Wigner [6,7]. We choose to define this function as

$$\gamma_w\left(\frac{\mathbf{r}_1+\mathbf{r}_2}{2},\mathbf{p}\right) = \int\gamma(\mathbf{r}_1,\mathbf{r}_2)\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{b}. \quad (24)$$

Inverting the Fourier transform, we can therefore write, using again coordinates $\mathbf{b}$ and $\mathbf{c}$

$$\tilde{\gamma}(\mathbf{b},\mathbf{c}) = \frac{1}{(2\pi\hbar)^3}\int \gamma_w(\mathbf{c},\mathbf{p})\exp\left(-i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{p}. \quad (25)$$

From this equation, by putting $\mathbf{r}_1=\mathbf{r}_2=\mathbf{r}$, we find

$$n(\mathbf{r}) = \frac{1}{(2\pi\hbar)^3}\int \gamma_w(\mathbf{r},\mathbf{p})d\mathbf{p}. \quad (26)$$

Similarly, the momentum density $\rho(\mathbf{p})$ considered in Secs. II and III is given by

$$\rho(\mathbf{p}) = \int \gamma_w(\mathbf{r},\mathbf{p})d\mathbf{r}. \quad (27)$$

A. Form of $\gamma_w(\mathbf{r},\mathbf{p})$ for two-electron model atoms

Returning to Eq. (3) and using Eqs. (4) and (24), we obtain the form for $\gamma_w(\mathbf{c},\mathbf{p})$

$$\gamma_w(\mathbf{c},\mathbf{p}) = \frac{2}{a^3\pi^{3/2}}\int\int \Psi_R\left(\left|\mathbf{x}-\frac{1}{2}\mathbf{b}\right|\right)\Psi_R\left(\left|\mathbf{x}+\frac{1}{2}\mathbf{b}\right|\right) \times\exp\left(-\frac{b^2}{16a^2}\right)\exp\left(-\frac{4c^2+4\mathbf{c}\cdot\mathbf{x}+x^2}{4a^2}\right) \times\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{x}d\mathbf{b}, \quad (28)$$

where we recall that $\Psi_R(r)$ is the wave function for relative motion governed by the effective potential $V_{\text{eff}}(r)$ in Eq. (2).

One can usefully write the kinetic energy density $t(\mathbf{r})$ in terms of the mixed function $\gamma_w(\mathbf{r},\mathbf{p})$ as

$$t(\mathbf{r}) = \frac{1}{(2\pi\hbar)^3}\int \frac{p^2}{2m}\gamma_w(\mathbf{r},\mathbf{p})d\mathbf{p} + \frac{1}{64m\hbar\pi^3}\int \nabla_r^2\gamma_w(\mathbf{r},\mathbf{p})d\mathbf{p}. \quad (29)$$

Since the momentum density studied in Secs. II and III is given by relation (27), we have for the total correlated kinetic energy T the result

$$\mathbf{T} = \int t(\mathbf{r})d\mathbf{r} = \frac{1}{(2\pi\hbar)^3}\int d\mathbf{r}\int \frac{p^2}{2m}\gamma_w(\mathbf{r},\mathbf{p})d\mathbf{p} + \frac{1}{64m\hbar\pi^3}\int d\mathbf{r}\int \nabla_r^2\gamma_w(\mathbf{r},\mathbf{p})d\mathbf{p}. \quad (30)$$

Provided, for the particular choice of interaction $u(r_{12})$ one verifies that the order of the $\mathbf{r}$ and $\mathbf{p}$ integrations can be interchanged (as well as the order of ∇_r^2 and the $\mathbf{p}$ integration) in Eq. (30) one finds, as expected, that the kinetic energy per electron is given by

$$\mathbf{T} = \frac{1}{(2\pi\hbar)^3}\int \frac{p^2}{2m}\rho(\mathbf{p})d\mathbf{p}. \quad (31)$$

Inserting the Legendre polynomial expansion for $\tilde{\gamma}(\mathbf{b},\mathbf{c})$, for $\gamma_w(\mathbf{c},\mathbf{p})$ we find, with $\cos\theta=\mathbf{b}\cdot\mathbf{c}/bc$

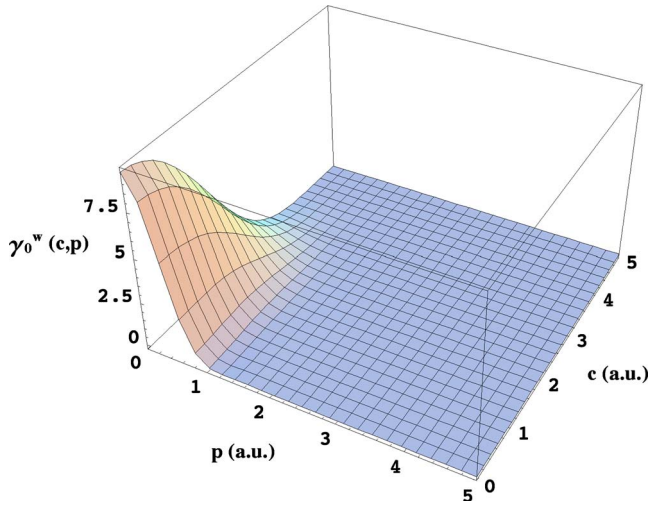

FIG. 2. (Color online) Wigner function $\gamma_w(c,p)$ for the Moshinsky model with $k=\frac{1}{4}$ in a.u. and $\beta=2$.

$$\gamma_w(\mathbf{c},\mathbf{p}) = \int \sum_{l=0}^{\infty}(2l+1)\tilde{\gamma}_l(b,c)P_l(\cos\theta)\exp\left(i\frac{\mathbf{p}}{\hbar}\cdot\mathbf{b}\right)d\mathbf{b} = \sum_{l=0}^{\infty}(2l+1)\gamma_l^w(c,p)P_l(\cos\delta), \quad (32)$$

where δ is the angle between $\mathbf{c}$ and $\mathbf{p}$. $\gamma_l^w(c,p)$ can be extracted from the appropriate forms of $\gamma^w(\mathbf{c},\mathbf{p})$ by employing the addition theorem for spherical harmonics.

B. Moshinsky atom

For the Moshinsky model it is straightforward from relations (3), (10), and (24) to obtain

$$\gamma_w(\mathbf{c},\mathbf{p}) = \frac{128\beta^3}{(1+\beta^2)^3}\exp\left(-\frac{4a^2p^2}{(1+\beta^2)\hbar^2}\right)\exp\left(-\frac{\beta^2c^2}{(1+\beta^2)a^2}\right). \quad (33)$$

This form (33) shows that in this example there are no negative regions of the Wigner function, which is encouraging for semiclassical phase space comparisons. The plot of Eq. (33) is presented in Fig. 2.

We turn below to compare and contrast this result (33), which shows for the Moshinsky atom that only the $s(l=0)$ term in Eq. (32) is nonzero, with that for the inverse square law repulsion.

C. Inverse square law repulsion $u(r_{12})=\lambda/r_{12}^2$

While for this case it appears difficult generally to derive a closed formula, for the special case $\alpha=2$ it follows by inserting Eqs. (4) and (20) into Eq. (3) and then using Eq. (24) that

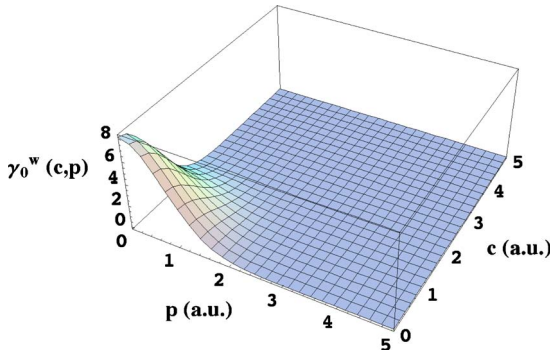

FIG. 3. (Color online) s-state ($l=0$) component $\gamma_0^w(c,p)$ of Wigner function $\gamma_w(c,p)$ in Eq. (34), for inverse square law $u(r_{12})=\lambda/r_{12}^2$, with $k=\frac{1}{4}$ in a.u., λ related to α in relation (21) and $\alpha=2$.

$$\gamma_w(\mathbf{c},\mathbf{p}) = \frac{4}{15}\left[\frac{c^4}{a^4} + 12\frac{c^2}{a^2} + 36 - 48p^2a^2 + 16p^4a^4 - 8c^2p^2 + 16p^2c^2\cos^2(\delta)\right]\exp(-2a^2p^2)\exp\left(-\frac{c^2}{2a^2}\right), \tag{34}$$

where p is written in atomic units. If we integrate the result (34) over $\mathbf{c}$ we correctly recover Eq. (23). Now, by rewriting Eq. (34) in the form of Eq. (32) it turns out that

$$\gamma_0^w(c,p) = \frac{4}{15}\left(\frac{c^4}{a^4} + 12\frac{c^2}{a^2} + 36 - 48p^2a^2 + 16p^4a^4 - \frac{8p^2c^2}{3}\right)\times\exp(-2a^2p^2)\exp\left(-\frac{c^2}{2a^2}\right) \tag{35}$$

and

$$\gamma_2^w(c,p) = \frac{128}{225}p^2c^2\exp(-2a^2p^2)\exp\left(-\frac{c^2}{2a^2}\right), \tag{36}$$

all the rest of the terms in the series (32) being identically zero. Plots of Eq. (35) for the s-wave contribution and Eq. (36) for the d-wave part of the Wigner function are shown in Figs. 3 and 4, respectively. Again, we have shown from Eq. (34) that the total Wigner function is never negative for the interaction strength measured by $\alpha=2$ in this model with inverse square law repulsion.

V. SUMMARY AND FUTURE DIRECTIONS

As to the general family of harmonically confined two-electron model atoms with arbitrary interaction $u(r_{12})$, the major equations obtained here are Eq. (9) for the momentum density $\rho(\mathbf{p})$ and Eq. (28) for the Wigner function. Both Eqs. (9) and (28) are characterized by the relative motion wave function $\Psi_R(r)$. In turn, this is to be determined, for specified interparticle repulsion interaction $u(r_{12})$, from the one-electron Schrödinger equation with potential $V_{\text{eff}}(r)$ given in Eq. (2).

For the three models for which one-body solutions for $\Psi_R(r)$ are known for this specified potential, we have obtained explicit results for $\rho(\mathbf{p})$, one notable example being Eq. (23) for a special case of the inverse square law repulsion $u(r_{12})=\lambda/r_{12}^2$. This form of $\rho(\mathbf{p})$ is then rederived by first calculating the Wigner function $\gamma_w(\mathbf{r},\mathbf{p})$, which has the analytical form (34). For this example, the spatial density matrix $\tilde{\gamma}(\mathbf{b},\mathbf{c})$, where these vectors $\mathbf{b}$ and $\mathbf{c}$ are defined in Eq. (1), is shown to truncate at $l=2$ in the Legendre polynomial expansion in Eq. (32) in terms of $\cos\theta=\mathbf{b}\cdot\mathbf{c}/bc$.

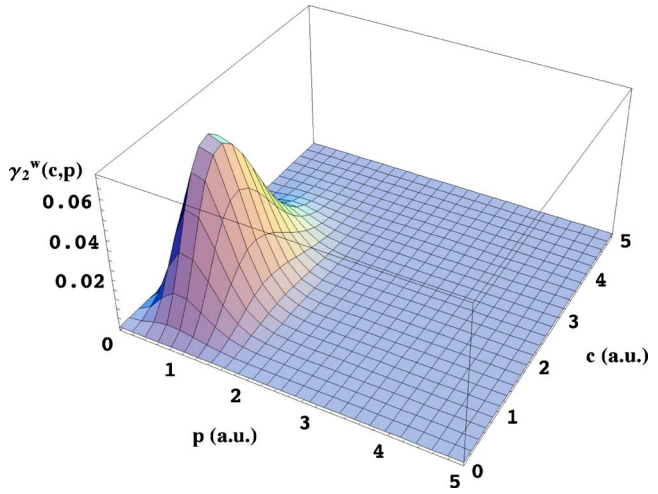

FIG. 4. (Color online) d-state ($l=2$) component $\gamma_2^w(c,p)$ of Wigner function $\gamma_w(c,p)$ in Eq. (34), for Inverse square law $u(r_{12})=\lambda/r_{12}^2$, with $k=\frac{1}{4}$ in a.u., λ being related to α as in relation (21) and $\alpha=2$.

Future directions prompted by the above findings take us back to the first sentence of the Introduction, referring to the helium atom. This, of course, calls for study of electron confinement by an external potential energy $-\frac{Ze^2}{r}$, where atomic number Z equals 2 for helium. Two areas then call for fuller study: (i) the large Z limit (nonrelativistic) limit of the two-electron heliumlike atomic ions sequence and (ii) use of existing variational (and therefore approximate) wave functions for the above series.

In area (i) cited above, pioneering work of Schwartz [8] on the diagonal ground-state electron density $n(r)$ was generalized by Hall, Jones, and Rees [9,10], to yield $\gamma(\mathbf{r}_1,\mathbf{r}_2)$ for large Z; i.e., for Coulomb confinement rather than the harmonically confined family treated in the present study. We propose that the time is right to reopen this area, but perhaps to attempt to construct a family of simplified interactions in which only radial correlation appears as a first step. As for area (ii) we note some recent analytical progress associated with the ground-state variational wave function proposed by Chandrasekhar [11]. In particular, Howard and March [12] have exploited the analytical form of $n(r)$ as a function of atomic number Z to impose, by choice of Chandrasekhar's parameters, the Kato electron-nuclear cusp condition plus the correct asymptotic behavior of $n(r)$ at large r. In view of our present results on the truncation of the Legendre polynomial expansion of $\tilde{\gamma}(\mathbf{b},\mathbf{c})$ entering Eq. (32) above, the convergence of such a form of expansion of $\gamma(\mathbf{r}_1,\mathbf{r}_2)$ for Chandrasekhar's wave function would seem worthy of careful investigation, even though numerical study may be called for

except for $\mathbf{r}=\mathbf{r}_1=\mathbf{r}_2$, when the density matrix $\gamma(\mathbf{r}_1,\mathbf{r}_2)$ reduces to the analytically known electron density $n(r)$.

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APPENDIX A. ATOMIC SCATTERING FACTOR

The atomic scattering factor $f(\mathbf{G})$ is defined as the Fourier transform of the electron density $n(\mathbf{r})$

$$f(\mathbf{G}) = \int n(\mathbf{r})\exp(i\mathbf{G}\cdot\mathbf{r})d\mathbf{r}. \tag{A1}$$

Using Eq. (14) of Ref. [3] and assuming the order of integration over r and y can be interchanged, we require the integral $I(\mathbf{G},y)$ defined by

$$I(\mathbf{G},y) = \int \exp\left(-\frac{r^2}{a^2}\right)\exp(i\mathbf{G}\cdot\mathbf{r})\frac{\sinh\left(\frac{ry}{a}\right)}{\frac{ry}{a}}d\mathbf{r}. \tag{A2}$$

The result for this integral becomes

$$I(\mathbf{G},y) = \int_0^\infty 4\pi r^2 \exp\left(-\frac{r^2}{a^2}\right)\frac{\sinh\left(\frac{ry}{a}\right)}{\frac{ry}{a}}\frac{\sin(Gr)}{Gr}dr$$

$$= \frac{2\pi^{3/2}a^2}{Gy}\sin\left(\frac{Gay}{2}\right)\exp\left(\frac{y^2-(Ga)^2}{4}\right). \tag{A3}$$

Putting this back in equation (A1), the result reads, when Eq. (14) of Ref. [3] is again invoked

$$f(\mathbf{G}) = \frac{16\pi}{G}\exp\left(-\frac{G^2a^2}{4}\right)\int_0^\infty y\sin\left(\frac{Gy}{2}\right)[\Psi_R(y)]^2dy. \tag{A4}$$

For the Moshinsky model, we readily obtain the scattering factor, using Eq. (10), as

$$f(\mathbf{G}) = 2\exp\left(-\frac{G^2a^2}{4}-\frac{G^2a^2}{4\beta^2}\right). \tag{A5}$$

For the inverse square law model $f(\mathbf{G})$ becomes

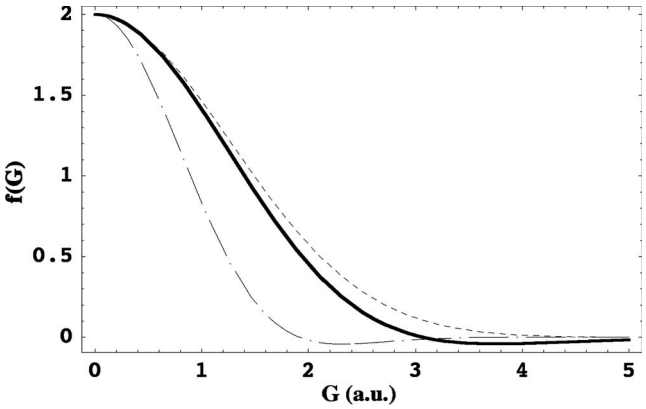

FIG. 5. Scattering factors $f(G)$, which are Fourier transforms of ground-state density $n(\mathbf{r})$ as in Eq. (A1). (Dashed line) Moshinsky model with $\beta=2$. (Solid curve) Hookean atom. (Dashed-point line) Inverse square law repulsion with $\alpha=2$. The harmonic confinement potential in the three curves is equal, chosen in such a way $a=1$ in a.u.

$$f(\mathbf{G}) = 2F_1\left(\frac{3}{2}+\alpha;\frac{3}{2};-\frac{1}{4}G^2a^2\right)\exp\left(-\frac{G^2a^2}{4}\right), \tag{A6}$$

where $F_1(a;b;z)$ is the confluent hypergeometric function of the first kind [13,14], for the special case when $\alpha=2$ is given explicitly by

$$F_1\left(\frac{7}{2};\frac{3}{2};-\frac{1}{4}G^2a^2\right) = \left(1-\frac{G^2a^2}{3}+\frac{G^4a^4}{60}\right)\exp\left(-\frac{G^2a^2}{4}\right). \tag{A7}$$

Inserting Eq. (A7) in relation (A6), the result for the scattering factor has the form

$$f(\mathbf{G}) = 2\left(1-\frac{G^2a^2}{3}+\frac{G^4a^4}{60}\right)\exp\left(-\frac{G^2a^2}{2}\right). \tag{A8}$$

Finally for the Hookean atom we have used Eq. (16) in Eq. (A4) to find, in atomic units,

$$f(G) = \frac{\exp\left(-\frac{G^2}{4}\right)}{G(8+5\sqrt{\pi})}\left\{G\left[8\exp\left(-\frac{G^2}{4}\right)+\sqrt{\pi}(10-G^2)\right]\right.$$

$$\left.+4\sqrt{\pi}(2-G^2)[\mathrm{erf}(iG)/i]\right\}, \tag{A9}$$

where $\mathrm{erf}(x)$ is the error function. The plot of $f(G)$ for the three models is presented in Fig. 5. Evidently for $G=0$, Eq. (A1) shows that $f(0)=\int n(\mathbf{r})d\mathbf{r}$, which is 2 for the family of models considered here.

APPENDIX B. DEPARTURES OF CORRELATED FIRST-ORDER DENSITY MATRICES FROM IDEMPOTENCY AS MEASURE OF WAVE FUNCTION ENTANGLEMENT

As was already known to Dirac [15] the first-order density matrix $\gamma(\mathbf{r},\mathbf{r}')$ for a single Slater determinant satisfies, for doubly filled levels

$$\frac{\gamma(\mathbf{r}_1,\mathbf{r}_2)}{2} = \int \frac{\gamma(\mathbf{r}_1,\mathbf{r}')}{2}\frac{\gamma(\mathbf{r}',\mathbf{r}_2)}{2}d\mathbf{r}'. \tag{B1}$$

Below we focus on the diagonal part

$$2n(\mathbf{r}) = \int [\gamma(\mathbf{r},\mathbf{r}')]^2 d\mathbf{r}'. \tag{B2}$$

It is well known that when one transcends independent-particle theory the condition (B1) in matrix language becomes $(\gamma/2)^2 < (\gamma/2)$.

Thus, for the two-electron family considered in the present article with general interaction $u(r_{12})$, we have in particular that since $n(\mathbf{r})$ has spherical symmetry

$$2n(r) > \int [\gamma(\mathbf{r},\mathbf{r}')]^2 d\mathbf{r}'. \tag{B3}$$

As an example, we have calculated both sides of the inequality (B3) for the Moshinsky atom with arbitrary interaction strength. It gives

$$n(r) = \frac{2\beta^3}{\pi^{3/2}a^3(1+\beta^2)^{3/2}} \times \exp\left(\left[\frac{(1-\beta^2)^2}{8a^2(1+\beta^2)} - \frac{1+6\beta^2+\beta^4}{8a^2(1+\beta^2)}\right]r^2\right) \tag{B4}$$

and

$$\int [\gamma(\mathbf{r},\mathbf{r}')]^2 d\mathbf{r}' = \frac{64\sqrt{2}\beta^6}{\pi^{3/2}a^3(1+\beta^2)^{3/2}(1+6\beta^2+\beta^4)^{3/2}} \times \exp\left(\left[\frac{(1-\beta^2)^2}{8a^2(1+\beta^2)(1+6\beta^2+\beta^4)} - \frac{1+6\beta^2+\beta^4}{8a^2(1+\beta^2)}\right]r^2\right). \tag{B5}$$

By integration of equations (B4) and (B5) over $\mathbf{r}$, one finds the difference between the two sides of the inequality (B3) as Δ_{diff} given by

$$\Delta_{\text{diff}} = 4 - \frac{2048\beta^3}{(14+37\beta^2+12\beta^4+\beta^6)^{3/2}}, \tag{B6}$$

where β is defined in Eq. (12). This result (B6) is illustrated in Fig. 6(a). In Fig. 6(b) we have plotted the right-hand side of the inequality (B3) for comparison with twice the Fermion density $n(r)$, for the specific interaction strength $\beta=2$. These Figs. 6(a) and 6(b) measure the degree of entanglement of the wave function. Therefore we shall conclude this appendix by giving the result for the inverse square law model for the specific interaction strength corresponding to the choice $\alpha=2$ in Eq. (21). We find it convenient to generate $\gamma(\mathbf{r},\mathbf{r}')$ from the Wigner function $\gamma_w(\mathbf{c},\mathbf{p})$ given in relation (34) for this value of α. Hence we find by using Eq. (34) Eq. (25)

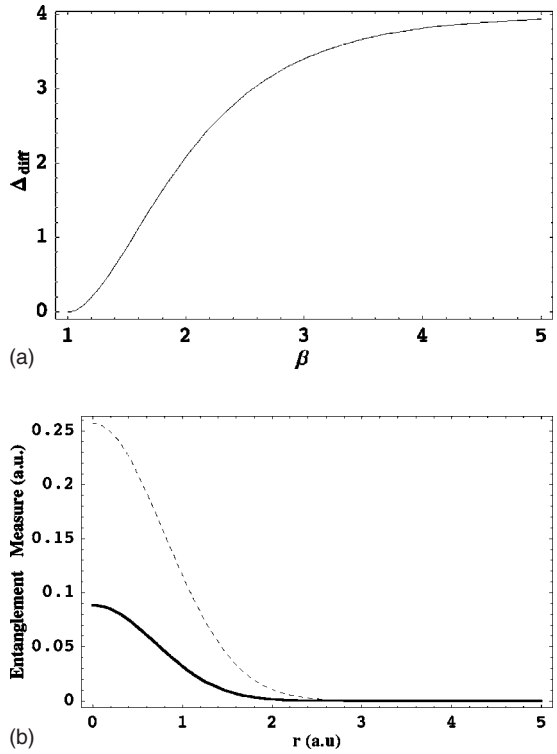

FIG. 6. Illustrates departures from idempotency for the Moshinsky model. (a) Integrated difference between sides of Eqs. (B3) and (B6), versus interaction strength represented by parameter β in Eq. (12). (b) Plot of Eqs. (B4) and (B5) for $2n(\mathbf{r})$ (dashed line) and $\int[\gamma(\mathbf{r},\mathbf{r}')]^2\, d\mathbf{r}'$ (solid curve), with $a=1$ in Eq. (4) and $\beta=2$ in relation (12).

$$\tilde{\gamma}(\mathbf{b},\mathbf{c}) = \frac{\pi^{3/2}}{15\sqrt{2}a^7}\left(30a^4 + \frac{(b^2+4c^2)^2}{8} + 20a^2c^2 + a^2b^2 - 2c^2b^2\cos^2(\theta)\right)\exp\left(-\frac{b^2}{8a^2}\right)\exp\left(-\frac{c^2}{2a^2}\right). \tag{B7}$$

Just as $\gamma_w(\mathbf{c},\mathbf{p})$, the Legendre polynomial expansion in $P_l(\cos\theta)$ entering Eq. (32), where θ is the angle between the vectors $\mathbf{b}$ and $\mathbf{c}$ in Eq. (1), contains only s ($l=0$) and d ($l=2$) components. By rewriting Eq. (B7) in the form of Eq. (32) it turns out that

$$\tilde{\gamma}_0(\mathbf{b},\mathbf{c}) = \frac{\pi^{3/2}}{15\sqrt{2}a^7}\left(30a^4 + \frac{(b^2+4c^2)^2}{8} + 20a^2c^2 + a^2b^2 - \frac{2}{3}c^2b^2\right) \times \exp\left(-\frac{b^2}{8a^2}\right)\exp\left(-\frac{c^2}{2a^2}\right) \tag{B8}$$

and

$$\tilde{\gamma}_2(\mathbf{b},\mathbf{c}) = -\frac{4\pi^{3/2}}{225\sqrt{2}a^7}c^2b^2\exp\left(-\frac{b^2}{8a^2}\right)\exp\left(-\frac{c^2}{2a^2}\right). \tag{B9}$$

We have verified that Eq. (B7) recovers the density $n(r)$ of Capuzzi *et al.* [13] for the case $\alpha=2$. This form (B7) can evidently be inserted in the inequality (B3) and Fig. 6(b) can be replicated for this case, but we shall not give further numerical details. For an arbitrary number of electrons in spin-compensated atoms (e.g. Ne, Ar, etc.), the inequality (B3) is a valuable measure of entanglement through the departure from idempotency.

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