The central role of the von Weizsäcker kinetic energy density in determining the energy functional of a model two-electron atom with harmonic confinement and inverse square interparticle repulsion

D. Geldof · C. Van Alsenoy · N. H. March

Abstract This study uses an analytically known expression for the relative motion wave function $\Psi_{RM}(r)$ for the Crandall et al. two-electron model atom with harmonic confinement plus inverse square law interparticle repulsion. This wavefunction is then employed to calculate the kinetic energy density for chosen values of both the harmonic force constant and the strength of the interaction coupling. Further consideration is then given to the Gál–March energy density functional which is shown to depend on the von Weizsäcker kinetic energy density in a fundamental manner.

Keywords Exactly soluble two-electron atomic model · Energy functional · von Weizsäcker kinetic energy

Crandall, Whitnell and Bettega [1] (CWB) solved analytically the two-electron harmonically confined model atom with inverse square interparticle repulsion $u(r_{12}) = \lambda/r_{12}^2$ for the ground state wave function $\Psi(\vec{r}_1, \vec{r}_2)$. Their result was recently utilized by Capuzzi, March and Tosi [2] (CMT) to extract the relative motion (RM) wave function from the product form $\Psi_{CM}(\frac{\vec{r}_1+\vec{r}_2}{2})\Psi_{RM}(r_{12})$ of the CWB $\Psi(\vec{r}_1, \vec{r}_2)$ as

$$\Psi_{RM}(r) = \left(\frac{m\omega}{2\hbar}\right)^{\alpha/2+3/4} \left(\frac{2}{\Gamma(\alpha + 3/2)}\right)^{1/2} r^{(\alpha+1)} exp\left(-m\omega r^2/4\hbar\right) \quad (1)$$

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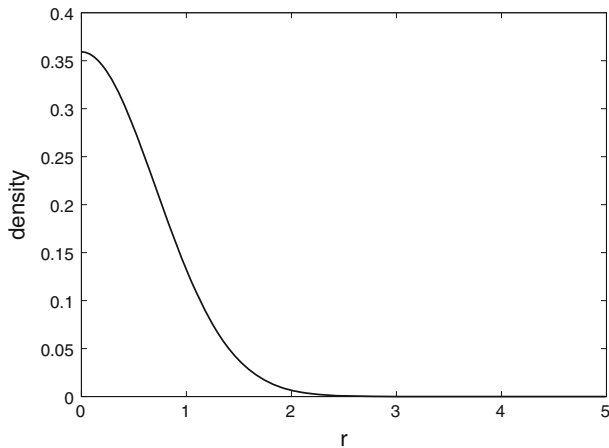Oxford University, Oxford, England

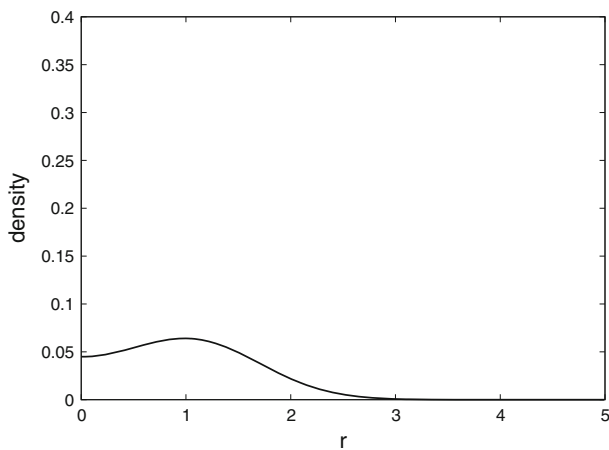**Fig. 1** Density as a function of r (in a.u.) for $\alpha = 0$ and $\omega = 1$

Fig. 2 Density as a function of r (in a.u.) for $\alpha = 3$ and $\omega = 1$

as well as the resulting density

$$\rho(r) = \frac{exp\left(-2m\omega r^2/\hbar\right)}{\pi^{3/2}4^\alpha \Gamma(\alpha + 3/2)} \frac{m\omega}{\hbar r} \int\limits_0^\infty exp(-y^2/2)y^{2\alpha+1}sinh(ry/a)dy \qquad (2)$$

In Eq. (1) the harmonic confinement potential is $\frac{1}{2}m\omega^2 r^2$ while the quantity α subsumes the strength λ of the interparticle repulsion $u(r_{12}) = \lambda/r_{12}^2$ through the definition [1]

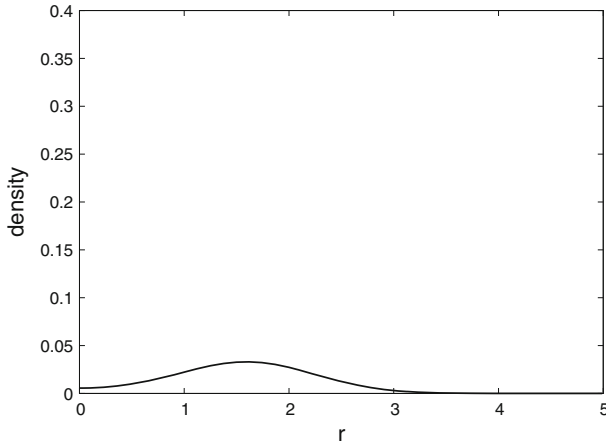$$\alpha = \left[\left(1 + \frac{4\lambda m}{\hbar^2}\right)^{1/2} - 1\right]/2 \qquad (3)$$

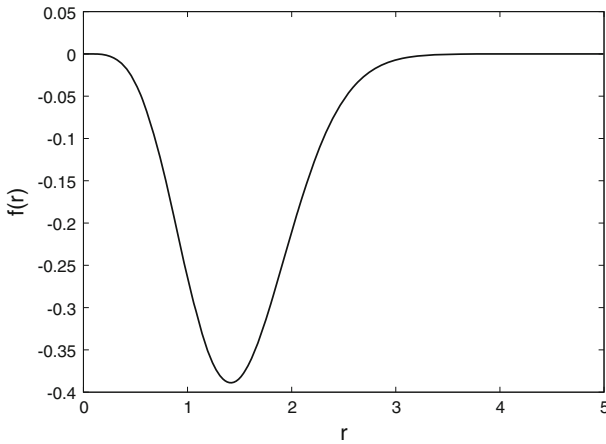**Fig. 3** Density as a function of r (in a.u.) for $\alpha = 6$ and $\omega = 1$

Fig. 4 f(r), defined in Eq. 11, as a function of r (in a.u.) for $\alpha = 0$ and $\omega = 1$

We next recall the result of Holas, Howard and March [3] (HHM) that one form of the correlated kinetic energy density $t(r)$ for the CWB model and indeed for general $u(r_{12})$ is given by

$$T = \int t(r)d\vec{r} \tag{4}$$

where $t(r) = t_{CM}(r) + t_{RM}(r)$: the separate terms having forms $t_{CM}(r) = (\hbar^2/4m)[\frac{d}{dr}\Psi_{CM}(r)]^2$ and $t_{RM}(r) = (\hbar^2/m)[\frac{d}{dr}\Psi_{RM}(r)]^2$. Ψ_{CM} is Gaussian and known for all $u(r_{12})$, the total kinetic energy contribution being explicitly $T_{CM} = \int t_{CM}(r)d\vec{r} = 3\hbar\omega/4$, independent of the interaction between the particles.

Using Eq. (2) above for $\rho(r)$, we display in Figs. 1, 2 and 3 the density for α equal to 0, 3 and 6 and ω equal to 1.
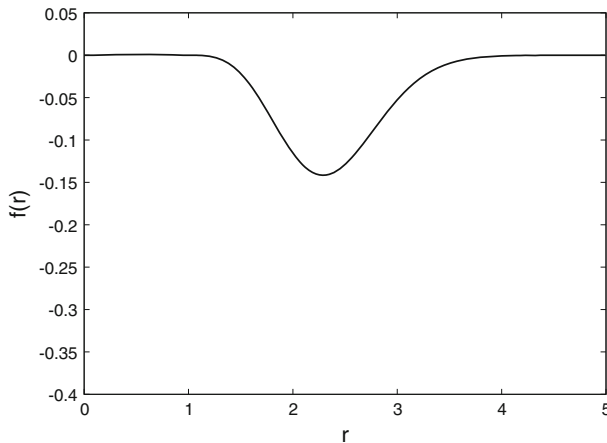
Fig. 5 f(r), defined in Eq. 11, as a function of r (in a.u.) for $\alpha = 3$ and $\omega = 1$
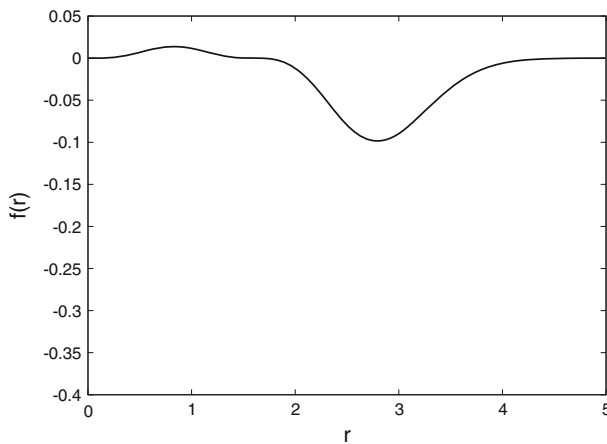

Fig. 6 f(r), defined in Eq. 11, as a function of r (in a.u.) for $\alpha = 6$ and $\omega = 1$

Turning to the correlated potential energy contribution we can appeal to the result of Gál and March [4] for the functional $F[\rho]$ defined from the energy functional $E_V[\rho]$, with V denoting the external potential, by

$$E_V[\rho] = F[\rho] + \int \rho(r)V(r)d\vec{r} \qquad (5)$$

The desired interparticle correlated potential energy is then simply $F - T$ where T has already been treated in Eq. (4) and immediately below that equation. For the CWB model which is the focus of the present article, Gál et al. [4] write F explicitly as [Eq. (20) of [4]]
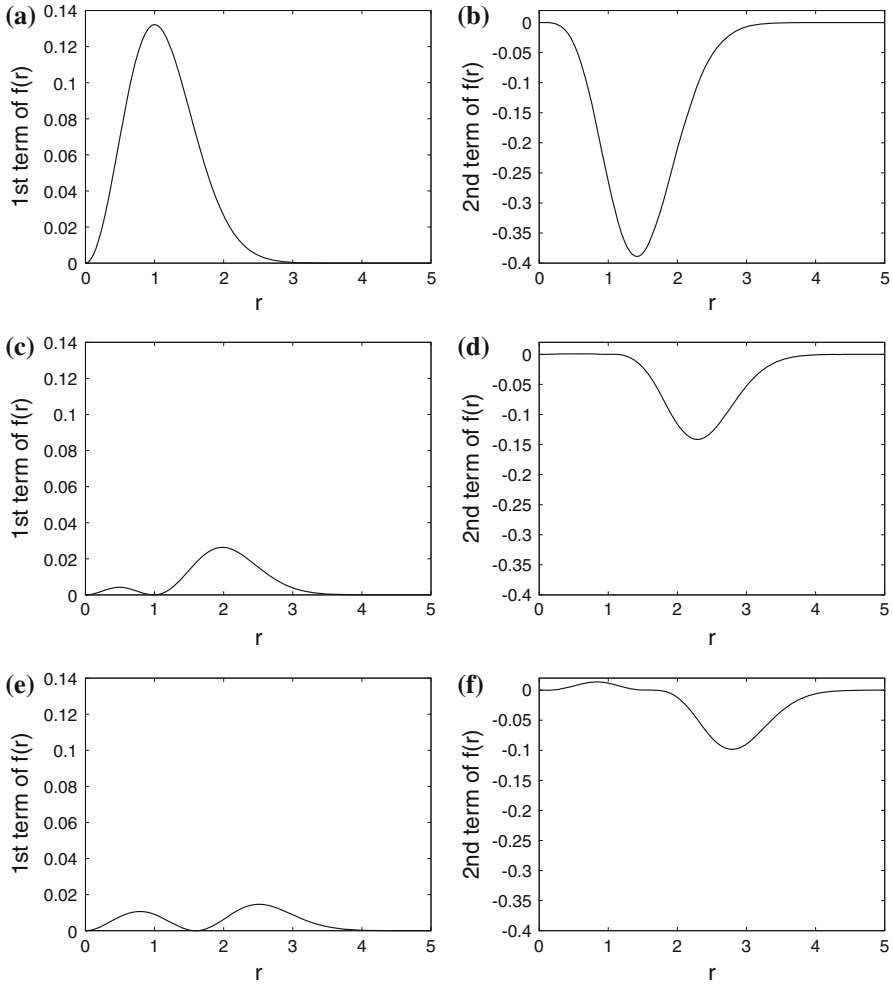
Fig. 7 *Plot* of the two terms separately of f(r) as a function of r (in a.u.) and $\omega = 1$. **a** 1st term of f(r) ($\alpha = 0$). **b** 2nd term of f(r) ($\alpha = 0$). **c** 1st term of f(r) ($\alpha = 3$). **d** 2nd term of f(r) ($\alpha = 3$). **e** 1st term of f(r) ($\alpha = 6$). **f** 2nd term of f(r) ($\alpha = 6$)

$$F^{CWB} = \frac{\hbar^2}{16m} \frac{\int \left(\frac{\rho'^2(r)}{\rho(r)} + \frac{r}{2} \frac{\rho'(r)\rho''(r)}{\rho(r)} \right) d\vec{r}}{\left(1 + \frac{27}{4(\alpha+3)} - \frac{3}{4(\alpha+3)} \frac{\int r^2 \frac{\rho'^2(r)}{\rho(r)} d\vec{r}}{\int \rho(r) d\vec{r}} \right)} \tag{6}$$

Rewriting this equation as

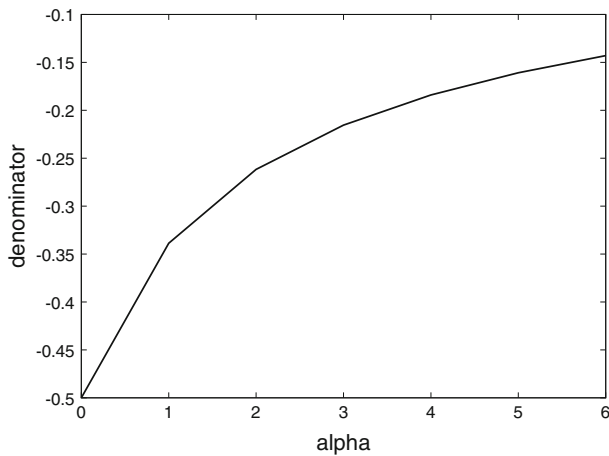$$\frac{16m}{\hbar^2} F^{CWB} = \frac{\mathcal{N}}{\mathcal{D}} \tag{7}$$

Fig. 8 Denominator $\mathcal{D}$, defined in Eq. 12, as a function of α for $\omega = 1$

and defining $\tau(r) = \rho'^2(r)/\rho(r)$ we can now remove the term involving $\rho'\rho''/\rho$ in Eq. (5) by differentiating $\tau(r)$ in the form $\rho(r)\tau(r) = \rho'^2(r)$, to get

$$\frac{2\rho'(r)\rho''(r)}{\rho(r)} = \tau'(r) + \frac{\rho'(r)}{\rho(r)}\tau(r) \tag{8}$$

Then we find for the numerator $\mathcal{N}$ in Eq. (7) above:

$$\mathcal{N} = \int \tau(r)d\vec{r} + \frac{1}{4}\int r\tau'(r)d\vec{r} + \frac{1}{4}\int r\frac{\tau(r)\rho'(r)}{\rho(r)}d\vec{r} \tag{9}$$

Integrating the second term on the RHS of Eq. (9) 'by parts' using spherical symmetry as an intermediate step we find

$$\mathcal{N} = \int f(r)\,d\vec{r} \tag{10}$$

with $f(r)$ defined as

$$f(r) = \frac{1}{4}\tau(r) + \frac{1}{4}r\frac{\tau(r)\rho'(r)}{\rho(r)} \tag{11}$$

We display $f(r)$ derived in Eq. (11), using the densities plotted in Figs. 1, 2 and 3, in Figs. 4, 5 and 6. It may be of interest in the future to know how $f(r)$ is built up from the two terms on the RHS of Eq. (11), and these are therefore plotted separately in Fig. 7.
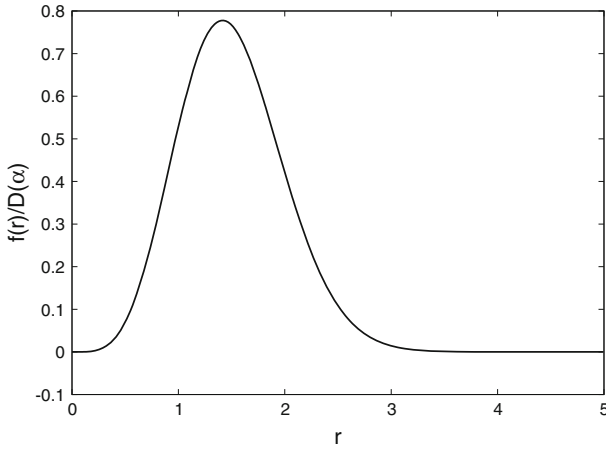
Fig. 9 f(r)/D(α) as a function of r (in a.u.) for $\alpha = 0$ and $\omega = 1$
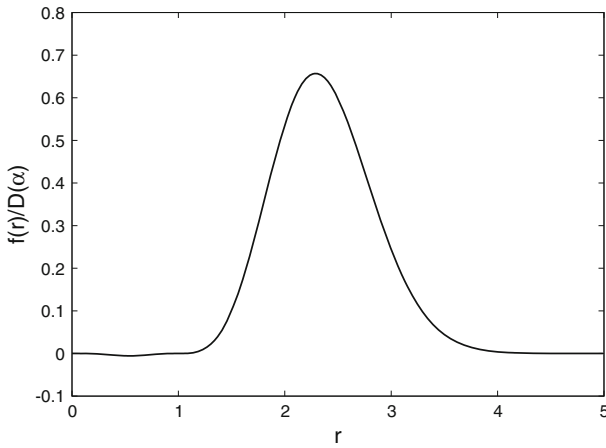

Fig. 10 f(r)/D(α) as a function of r (in a.u.) for $\alpha = 3$ and $\omega = 1$

For the denominator $\mathcal{D}$, using the definition for $\tau(r)$ as well as using the fact that $\int \rho(r)d\vec{r} = 2$ we arrive at the result from Eqs. (6) and (7) that

$$\mathcal{D} = 1 + \frac{27}{4(\alpha + 3)} - \frac{3}{8(\alpha + 3)} \int r^2 \tau(r) d\vec{r} \qquad (12)$$

This is plotted as a function of α in Fig. 8, for ω equal to 1.

In terms of these expressions, F^{CWB} can be written as:

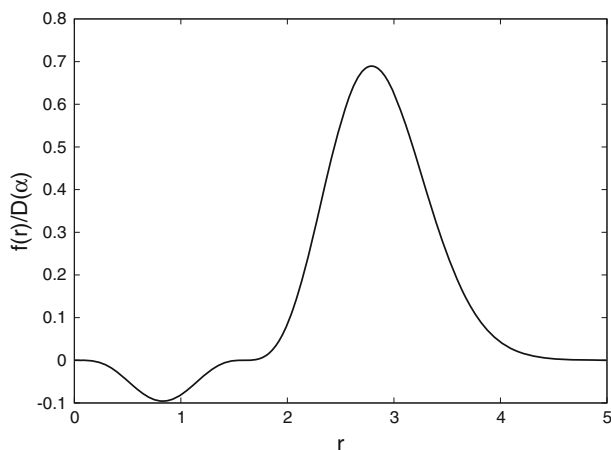$$\frac{16m}{\hbar^2} F^{CWB} = \int \frac{f(r)}{\mathcal{D}} d\vec{r} \qquad (13)$$

Fig. 11 f(r)/D(α) as a function of r (in a.u.) for $\alpha = 6$ and $\omega = 1$

and the integrand $\frac{f(r)}{D}$ is displayed in Figs. 9, 10 and 11, again for the three values of α.

To conclude, we have here calculated the DFT quantity $F[\rho]$ for the model atom of Crandall et al. [1] This functional was given first by Gál and March [4]. Here, we have defined a differential form of F, and have displayed numerically the results of inserting the exact ground-state density $\rho(r)$ in the integral form given by Capuzzi et al. [2], for a particular choice of the external potential but for different strengths of the interparticle interaction. We have shown explicitly the central role played by the von Weizsäcker kinetic energy in determining $F[\rho]$. It would, of course, be of considerable interest for the future if some aspects of the differential form of the functional $F[\rho]$, discussed in detail here for the Crandall atom, could be extended to apply, at least approximately, to the non-relativistic ground-state of the He-like ions with nuclear charge Ze.

References

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