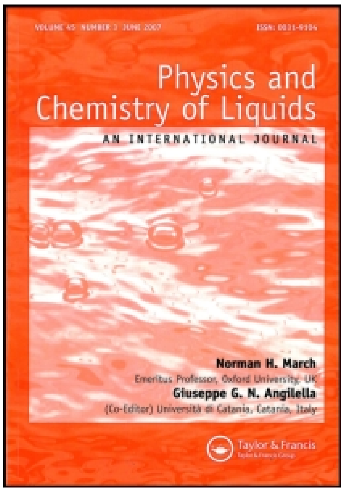

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

Interacting inhomogeneous electron liquids with harmonic confinement: *s*-wave model

I. A. Howard[a]; N. H. March[b]
[a] Department of Physics, University of Antwerp, B-2020 Antwerp, Belgium [b] Donostia International Physics Center (DIPC), E-20080 San Sebastian, Spain

To cite this Article Howard, I. A. and March, N. H.(2005) 'Interacting inhomogeneous electron liquids with harmonic confinement: *s*-wave model', Physics and Chemistry of Liquids, 43: 6, 559 — 565
To link to this Article: DOI: 10.1080/00319100500231703
URL: http://dx.doi.org/10.1080/00319100500231703

Physics and Chemistry of Liquids
Vol. 43, No. 6, December 2005, 559–565

Taylor & Francis
Taylor & Francis Group

Interacting inhomogeneous electron liquids with harmonic confinement: *s*-wave model

I. A. HOWARD*† and N. H. MARCH‡

†Department of Physics, University of Antwerp, Groenenborgerlaan 171,
B-2020 Antwerp, Belgium
‡Donostia International Physics Center (DIPC), E-20080 San Sebastian, Spain and
Oxford University, Oxford, England

(*Received 25 May 2005*)

In an earlier work by Holas *et al.* [A. Holas, I.A. Howard, N.H. March. *Phys. Lett. A*, **310**, 451 (2003)], the ground-state electron density $\rho(r)$ for model two-electron spin-compensated atoms was obtained in terms of the relative motion wave function for the case of harmonic confinement and arbitrary interparticle interaction $u(r_{12})$. Following recent interest in the *s*-wave approximation to $\rho(r)$ for Coulombic potential energy e^2/r_{12} at separation r_{12} between the electrons, we here consider both harmonic interaction $u(r_{12})$ proportional to r_{12}^2 and also the inverse square law $1/r_{12}^2$. The interplay between correlation and confinement clearly emerges in such spin-compensated models of interacting inhomogeneous electron liquids.

Keywords: Inhomogeneous electron liquids; *s*-Wave model; Electron correlation

1. Introduction

There is currently some interest, motivated by the search for analytic forms of the electron density $\rho(r)$ in the ground state of the He atom, in the so-called *s*-wave model. This was set down as early as 1962 by Temkin [1] and has independently been studied by the present authors [2]. Somewhat different forms of this *s*-wave approximation were considered in [1] and [2], and a synthesis was made in a very recent study by Howard and March [3], aided by the use of the analytically solvable Hookean atom [4,5] for a specific force constant. It seems of interest for the *s*-wave model to explore in more detail the interplay between external potential $V_{\text{ext}}(r)$ and the model electron–electron repulsion adopted. To do so, we have taken as starting point the treatment of Holas *et al.* [5] for harmonic confinement, namely

$$V_{\text{ext}}(r) = \frac{kr^2}{2} \tag{1}$$

but general interparticle repulsion $u(r_{12})$.

---

*Corresponding author. Email: iris.howard@ua.ac.be

Physics and Chemistry of Liquids
ISSN 0031-9104 print: ISSN 1029-0451 online © 2005 Taylor & Francis
DOI: 10.1080/00319100500231703

2. Moshinsky atom with $V_{\mathrm{ext}}(r)$ and interparticle repulsion both harmonic

To make analytical progress, we take first the case when $u(r_{12})$ is also harmonic, namely

$$u(r_{12}) = K\frac{r_{12}^2}{2}, \tag{2}$$

which is the so-called Moshinsky atom (see, e.g., [6] and earlier references therein). The ground-state wavefunction for the two-electron atom within this model is

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{(1+2K)^{3/8}}{\pi^{3/2}} \exp(-(r_1^2 + r_2^2)/2) \exp\Big[-(\sqrt{1+2K}-1)(r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta)/4\Big]. \tag{3}$$

Then, again projecting out the $l = 0$ component analytically from the Moshinsky ground-state wavefunction, we find

$$\begin{aligned}\Psi_0(r_1, r_2) = \Big\{ & -\exp(r_1 r_2/2)(1+2K)^{3/8} \Big/ \Big[\exp\Big(\sqrt{1+2K}r_1 r_2/2\Big)\pi^{3/2} r_1 r_2 \Big(\sqrt{1+2K}-1\Big)\Big] \\ & + \exp\Big(\sqrt{1+2K}r_1 r_2/2\Big)(1+2K)^{3/8} \Big/ \Big[\exp(r_1 r_2/2)\pi^{3/2} r_1 r_2 \Big(\sqrt{1+2K}-1\Big)\Big]\Big\} \\ & \times \exp\Big(-(r_1^2 + r_2^2)\Big(1+\sqrt{1+2K}\Big)\Big/4\Big).\end{aligned} \tag{4}$$

The exact density $\rho(r)$ resulting from equation (3) is compared with its *s*-wave counterpart from equation (4) in figure 1(a) for the choice $K = 5$, and in figure 1(b) $K = 1$. In the latter case, there is good agreement, the *s*-wave projection already containing 0.946 of the integrated electron density (normalized to unity rather than two in both figures 1a and b). As one changes the confinement relative to the interparticle interaction, figure 1(a) shows a substantial difference, the terms in the density for $l > 0$ now contributing 0.228 of the total integrated electron density.

3. Harmonic confinement with inverse square law repulsion $u(r_{12}) = \lambda/r_{12}^2$

As a second example in which we can vary the interplay between harmonic confinement and 'interelectronic' repulsion, we choose

$$u(r_{12}) = \frac{\lambda}{r_{12}^2}, \tag{5}$$

which was already considered in the earlier work by Crandall *et al.* [7]. This model has also been studied very recently by Capuzzi *et al.* [8,9]. The symmetric spatial wave function $\Psi(\mathbf{r}_1, \mathbf{r}_2)$ then takes the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2) = C\exp(-\omega r_1^2)\exp(-\omega r_2^2)\big[r_1^2 + r_2^2 - 2r_1 r_2 \cos\theta\big]^{\alpha/2}, \tag{6}$$

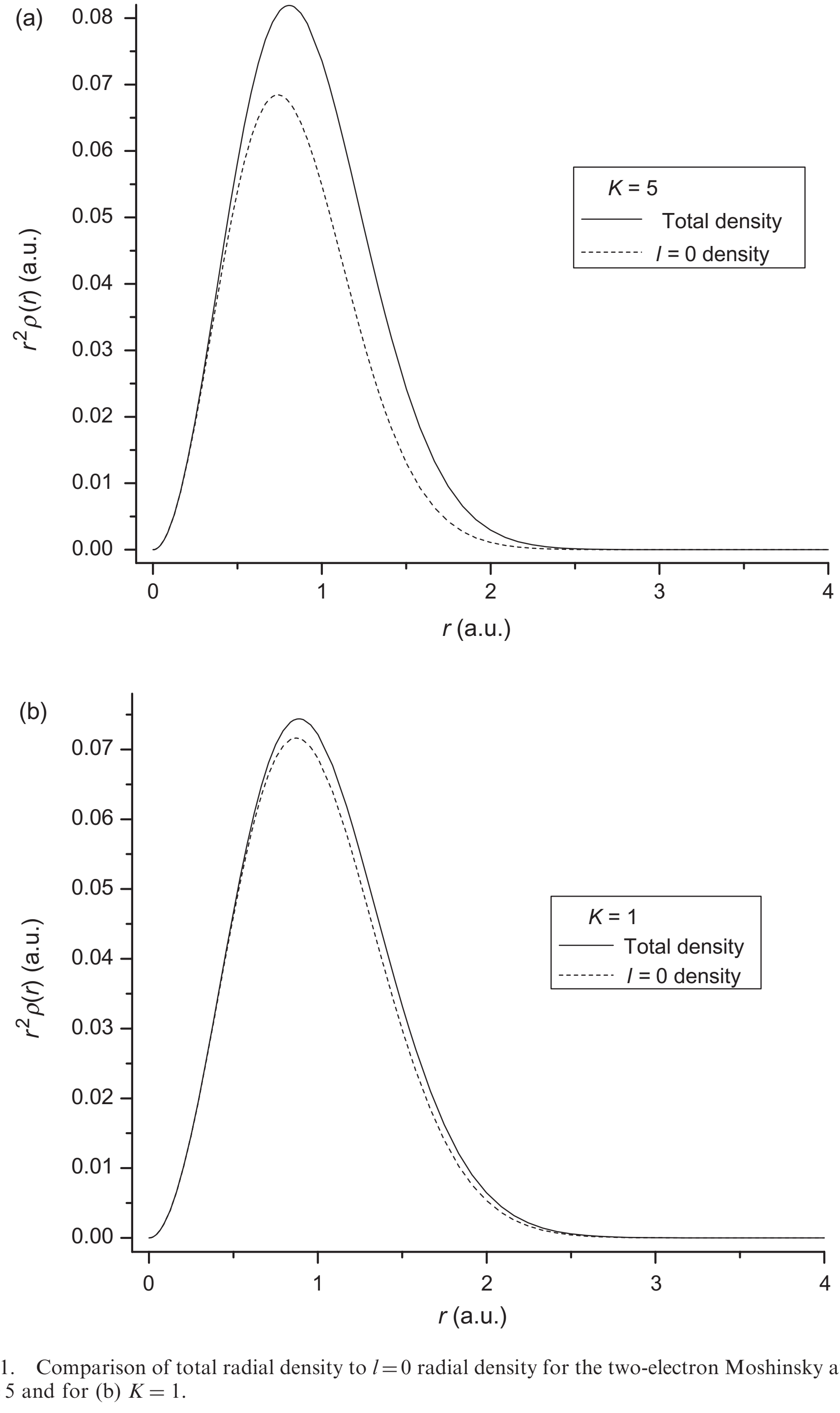

Figure 1. Comparison of total radial density to $l = 0$ radial density for the two-electron Moshinsky atom for (a) $K = 5$ and for (b) $K = 1$.

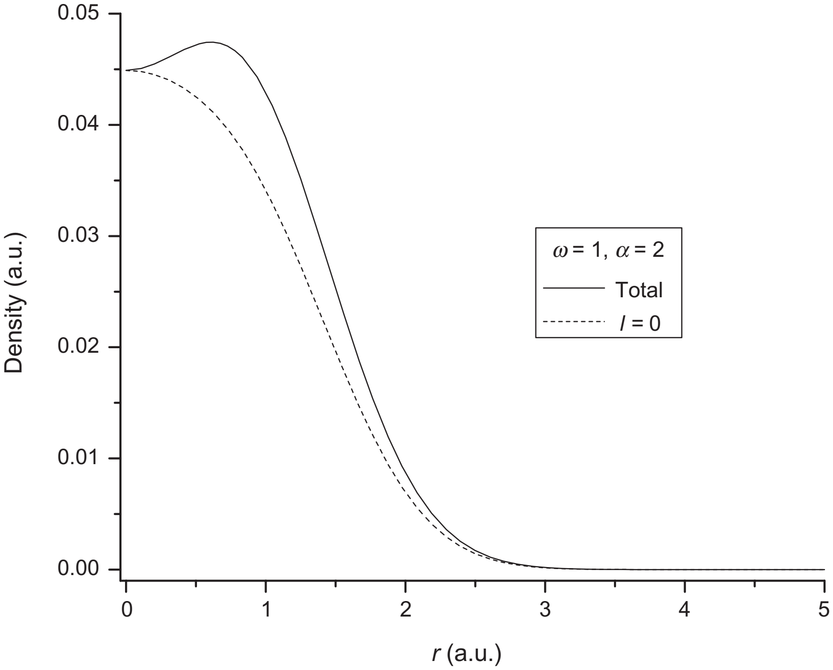

Figure 2. Comparison of total density to $l=0$ density for the case of harmonic confinement with inverse square law repulsion, here with $\omega=1$ and $\alpha=2$. Note that electron repulsion is underestimated by the *s*-wave model, a Wigner 'molecule' being apparent in the total density plot.

where θ is the angle between the vectors $\mathbf{r}_1$ and $\mathbf{r}_2$, while α is defined by

$$\alpha = \frac{\sqrt{1+4\lambda m/\hbar^2}-1}{2}. \tag{7}$$

One now extracts the *s*-($l=0$) term, $\Psi_0(r_1, r_2)$ from equation (4) by multiplying both sides by $\sin\theta\,\mathrm{d}\theta$ and integrating over θ to find

$$\Psi_0(r_1,r_2) = C\exp\left[-\frac{\omega(r_1^2+r_2^2)}{2}\right]\left[(r_1^2+r_2^2+2r_1r_2)^{\alpha/2}-(r_1^2+r_2^2-2r_1r_2)^{\alpha/2}\right] \times \frac{(r_1^2+r_2^2-2r_1r_2)}{2r_1r_2(\alpha+2)}. \tag{8}$$

The density $\rho(r)$ derived from equation (3.2) was given by Capuzzi *et al.* [8,9] as

$$\rho(r) = \frac{2^{1-\alpha}}{\pi^{3/2}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\exp\left(-\frac{2m\omega r^2}{\hbar}\right){}_1F_1\left(3/2+\alpha, 3/2, \frac{m\omega r^2}{\hbar}\right) \tag{9}$$

where ${}_1F_1$ is the confluent hypergeometric function [10]. For $\omega=1$ and $\alpha=2$, this is plotted in the continuous curve of figure 2. The *s*-density $\rho_0(r)$ derived from

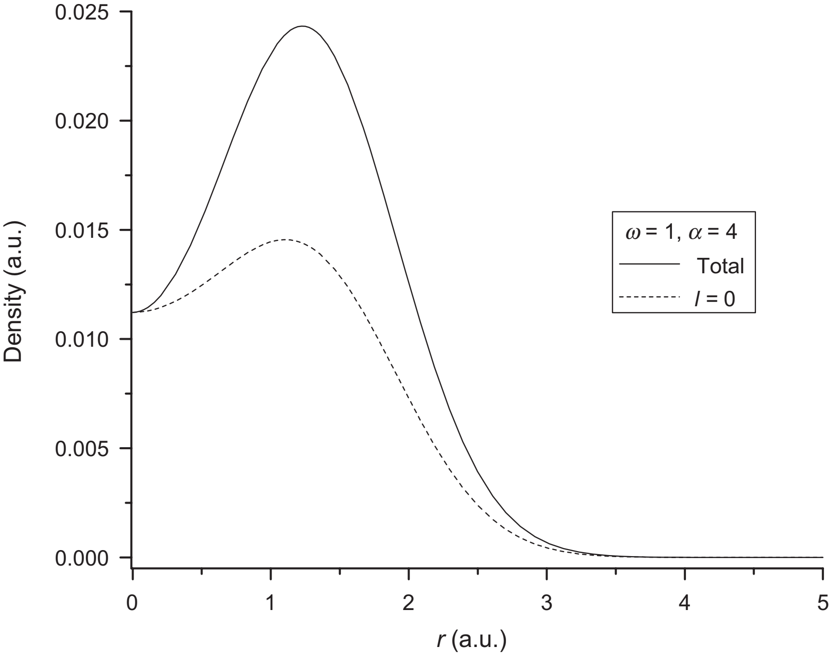

Figure 3. Comparison of total density to $l=0$ density as in figure 2, but with $\omega=1$ and $\alpha=4$. Now, in contrast to figure 2, both curves show fingerprints of a Wigner 'molecule'.

equation (6) is

$$\rho_0(r) = \int \Psi_0^2(\mathbf{r}_1, \mathbf{r}_2)\mathrm{d}\mathbf{r}_2 \tag{10}$$

is plotted for comparison in the same figure. The total charge contained in the *s*-wave component is 0.800 of the volume integral of equation (4).

One comment that is called for on figure 2 is that the fact that the maximum of the total density is moved away from the origin is due to the strong 'electron–electron' repulsion for $\alpha=2$, a Wigner-like 'molecule' being formed as emphasized by Capuzzi *et al.* [8]. As seen clearly from figure 2, the *s*-wave model does not capture this feature at $\alpha=2$. However, when the interaction strength is increased, such that $\alpha=4$, and retaining the same harmonic confinement characterized by $\omega=1$, the *s*-wave density does reveal now a Wigner-like 'molecule' with about the same bond length (see figure 3). However, the *s*-wave contribution of density $\rho_0(r)$ only contains now 0.598 of the total charge corresponding to the exact density $\rho(r)$ for this model. As a final example, figure 4 shows the choice of parameters $\omega=1$ and $\alpha=10$. Now the *s*-wave density only contains 0.319 of the total charge, though again the 'Wigner molecule' is in evidence with about the correct bond length.

4. Summary and future directions

Three examples now exist in which the common ingredient is the external potential, reflecting harmonic confinement, but with different choices of the 'electron–electron'

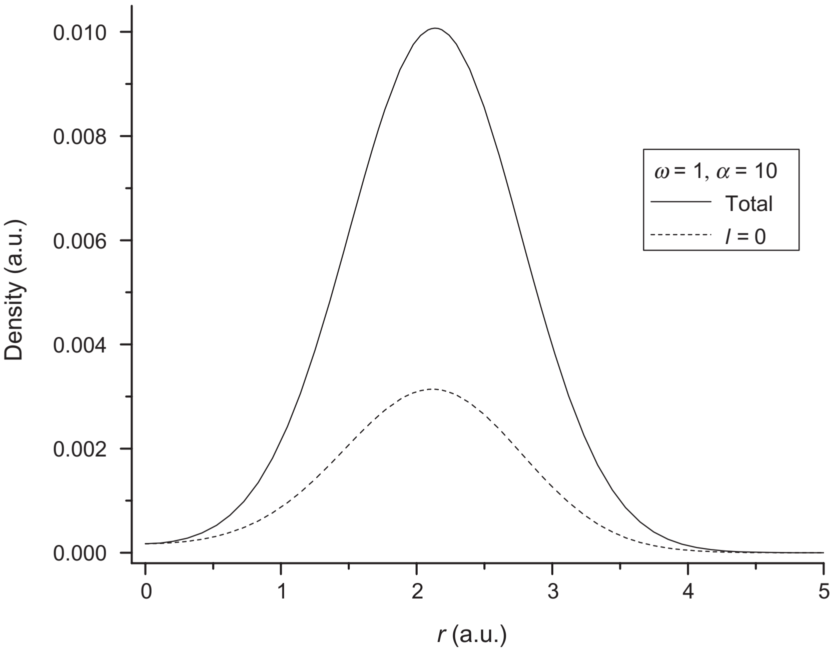

Figure 4. Comparison of total density to $l = 0$ density with $\omega = 1$ and $\alpha = 10$. A similar conclusion concerning a Wigner 'molecule' can be drawn as in figure 2, but now the s-wave contribution contains only a modest fraction of the total charge.

repulsion potential energy $u(r_{12})$. The major merit of the two choices treated in the present study is that the interplay between confinement and interparticle repulsion can be varied by changing the strength of $u(r_{12})$ measured by α, relative to the confinement potential energy, characterized by ω. For the inverse square repulsion λ/r_{12}^2, figures 2–4 show that the influence of the s-term in the total wave function decreases with increasing α. In particular from $\alpha = 2$ to 10, the integrated charge density in the s-wave reduces from 0.800 of the total to 0.319 at $\alpha = 10$. However, provided α is substantial, say ≈ 4, the 'Wigner molecule' heralded by the presence of a maximum in the particle density away from the origin has approximately the same bond length from the total density profile and from the its s-wave counterpart.

It will be interesting to study the Hookean atom further in future, for different force constants, for comparison with He-like two-electron atomic ions.

Acknowledgements

IAH acknowledges support from the IWT-Flanders under grant no. IWT-161. NHM acknowledges that his contribution to this study was brought to fruition during a visit to the Donostia International Physics Center, San Sebastian, Spain. NHM wishes to thank Professors P.M. Echenique and A. Rubio for their very generous hospitality.

References

[1] A. Temkin. *Phys. Rev.*, **126**, 130 (1962).
[2] I.A. Howard, N.H. March. *Phys. Rev. A*, **71**, 042501 (2005).
[3] I.A. Howard, N.H. March. *Chem. Phys. Lett.*, (accepted).
[4] N.R. Kestner, O. Sinanoglu. *Phys. Rev.*, **128**, 2687 (1962).
[5] A. Holas, I.A. Howard, N.H. March. *Phys. Lett. A*, **310**, 451 (2003).
[6] N.H. March, I.A. Howard, I. Nagy, A. Rubio. *Phys. Lett. A*, **288**, 101 (2001).
[7] R. Crandall, R. Whitnell, R. Bettega. *Am. J. Phys.*, **52**, 438 (1984).
[8] P. Capuzzi, N.H. March, M. Tosi. *Phys. Lett. A*, **339**, 207 (2005).
[9] P. Capuzzi, N.H. March, M. Tosi. *J. Phys. A: Math. Gen.*, **38**, L439 (2005).
[10] M. Abramowitz, I.A. Stegun (Eds), *Handbook of Mathematical Functions*, Dover, New York (1972).
[11] S. Kais, D.R. Herschbach, R.D. Levine. *J. Chem. Phys.*, **91**, 7791 (1989).