Differential equation for the ground-state density of artificial two-electron atoms with harmonic confinement

2005 J. Phys. A: Math. Gen. 38 L439

(http://iopscience.iop.org/0305-4470/38/24/L01)

J. Phys. A: Math. Gen. **38** (2005) L439–L442 doi:10.1088/0305-4470/38/24/L01

LETTER TO THE EDITOR

Differential equation for the ground-state density of artificial two-electron atoms with harmonic confinement

P Capuzzi[1], **N H March**[2,3] **and M P Tosi**[1]

[1] NEST-INFM and Classe di Scienze, Scuola Normale Superiore, Piazza dei Cavalieri 7, I-56126 Pisa, Italy
[2] Department of Physics, University of Antwerp, 171 Groenenborgerlaan, B-2020 Antwerp, Belgium
[3] Oxford University, Oxford, UK

E-mail: capuzzi@sns.it

Received 3 March 2005, in final form 15 April 2005
Published 1 June 2005
Online at stacks.iop.org/JPhysA/38/L439

Abstract

A long-term aim of density functional theory is to obtain a differential equation for the ground-state electron density $\rho(r)$ in a closed-shell atom, the simplest example being He. Since He remains intractable analytically, artificial atoms with harmonic repulsive potential energy $u(r_{12})$ have therefore been studied. Here we exploit recent work on $\rho(r)$ for such a two-electron system, with $u(r_{12}) = \lambda/r_{12}^2$, to construct a second-order linear differential equation for $\rho(r)$. This is compared and contrasted with available results for different choices of $u(r_{12})$.

PACS numbers: 01.55.+b, 02.30.Hq, 02.30.Qp, 71.10.−w

Harmonic confinement of quantum particles using magnetic trapping at low densities is now commonplace for both bosons [1, 2] and fermions [3] at ultralow temperatures. Neglecting interparticle interactions, we considered earlier such confinement for fermions occupying an arbitrary number of closed shells in two [4] and three [5] dimensions, and in both cases differential equations have been given for the ground-state density $\rho(r)$.

Of course, it is of considerable interest to effect the generalization of such differential equations to include interparticle interactions. Here, therefore, we utilize recent results obtained on Wigner bosonic molecules with repulsive interactions and harmonic confinement [6] to construct a differential equation for a He-like artificial atom with (a) harmonic confinement $V(r) = m\omega^2 r^2/2$ and (b) an interparticle repulsive potential energy $u(r_{12})$ given by

$$u(r_{12}) = \lambda/r_{12}^2. \tag{1}$$

We follow Crandall *et al* [7] in writing the unnormalized spatial symmetric wavefunction for the ground state as

$$\Psi(\mathbf{r}_1,\mathbf{r}_2) = \mathrm{e}^{-m\omega r_1^2/2\hbar}\,\mathrm{e}^{-m\omega r_2^2/2\hbar}\,r_{12}^{\alpha} \tag{2}$$

where $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is the particle separation while α measures the strength of the repulsive coupling through

$$\alpha = [(1 + 4\lambda m/\hbar^2)^{1/2} - 1]/2. \tag{3}$$

In the work on Wigner bosonic molecules we were able to analytically calculate $\int \Psi^2(\mathbf{r}_1,\mathbf{r}_2)\,\mathrm{d}\mathbf{r}_2$ and this is what we require, when normalized such that

$$\int \rho(r)\,\mathrm{d}\mathbf{r} = 2, \tag{4}$$

to obtain the ground-state density of the present artificial two-electron atom. The result [6] is given by

$$\rho(r) = \frac{1}{2^{\alpha-1}\pi^{3/2}}\left(\frac{m\omega}{\hbar}\right)^{3/2}\mathrm{e}^{-2m\omega r^2/\hbar}\,{}_1F_1\left(\frac{3}{2}+\alpha;\frac{3}{2};\frac{m\omega r^2}{\hbar}\right) \tag{5}$$

where ${}_1F_1$ is the confluent hypergeometric function [8].

The aim of the present study is then to obtain the differential equation satisfied by $\rho(r)$ in equation (5). To this end, we multiply both sides of equation (5) by $\exp(2m\omega r^2/\hbar)$ and then note that the product of this Gaussian times $\rho(r)$ satisfies the same linear homogeneous differential equation as the confluent hypergeometric function ${}_1F_1$.

From Morse and Feshbach [9], the function ${}_1F_1(\gamma;\varrho;z)$ satisfies the differential equation

$$z\frac{\mathrm{d}^2y}{\mathrm{d}z^2} + (z-\varrho)\frac{\mathrm{d}y}{\mathrm{d}z} - \gamma y = 0. \tag{6}$$

Replacing y in equation (6) by $\rho(r)\exp(2m\omega r^2/\hbar)$ we find the corresponding differential equation for the ground-state density $\rho(r)$. This second-order, linear, homogeneous differential equation takes the explicit form

$$\frac{\hbar}{4m\omega}r\,\rho''(r) + \left[\frac{\hbar}{2m\omega}+\frac{3}{2}r^2\right]\rho'(r) + r\left[\frac{3}{2}-\alpha+2\frac{m\omega}{\hbar}r^2\right]\rho(r) = 0. \tag{7}$$

It is of interest to compare equation (7) with those appropriate to other forms of interparticle interaction $u(r_{12})$ again combined with harmonic confinement. Thus March, Gál and Nagy [10] took $u(r_{12}) = e^2/r_{12}$, the so-called Hookean atom, and derived the third-order differential equation

$$\sum_{i=0}^{3} P_i(r)\rho^{(i)}(r) = 0 \tag{8}$$

where $P_i(r)$ are polynomials tabulated in [10]. For the more elementary choice $u(r_{12}) = \frac{1}{2}kr_{12}^2$, March and Ludeña [11] obtained a second-order differential equation paralleling the result (7): namely

$$\nabla^2\rho = (-6\beta + 4\beta^2r^2)\rho(r), \tag{9}$$

where $\beta = (2\gamma-1)/\gamma$ while $\gamma = \frac{1}{2}\{(1+2k)^{1/2}+1\}$, the confinement potential energy being $\frac{1}{2}r^2$.

In conclusion, we note that a route exists, at least in principle, to unify the three equations (7)–(9) corresponding to the same harmonic confinement but different choices of the interparticle repulsion $u(r_{12})$. This route is via the general expression for $\rho(r)$ given by Holas *et al* (see their equation (14)) [12],

$$\rho(r) = \frac{8}{\pi^{1/2}} \exp\left(-\frac{r^2}{a^2}\right) \int_0^\infty y^2 \exp\left(-\frac{y^2}{4}\right) \{\Psi^{\mathrm{RM}}(ay)\}^2 \frac{\sinh(ry/a)}{(ry/a)}. \quad (10)$$

Here the length a is defined in terms of the harmonic confining potential energy as

$$a = \left(\frac{\hbar}{2m\omega}\right)^{\frac{1}{2}}. \quad (11)$$

It is worth recalling at this point that this approach may be considered as complementary to that of density-functional theory in which one obtains the differential equations for the ground-state density of systems subject to different external potentials but with fixed interparticle interaction.

The merit of equation (11) is that the interparticle repulsion $u(r_{12})$ is subsumed into the relative motion (RM) function $\Psi^{\mathrm{RM}}(r)$, which satisfies the radial Schrödinger equation

$$\left[-\frac{\hbar^2}{m}\frac{\partial^2}{\partial r^2} + V_{\mathrm{eff}}(r)\right]\psi^{\mathrm{RM}}(r) = E^{\mathrm{RM}}\psi^{\mathrm{RM}}(r) \quad (12)$$

where

$$V_{\mathrm{eff}}(r) = \tfrac{1}{4}m\omega^2 r^2 + u(r) \quad (13)$$

while

$$\psi^{\mathrm{RM}}(r) = (4\pi)^{1/2} r \Psi^{\mathrm{RM}}(r). \quad (14)$$

In equation (10), $\Psi^{\mathrm{RM}}(r)$ is normalized such that

$$\int_0^\infty \mathrm{d}r [\psi^{\mathrm{RM}}(r)]^2 = 1. \quad (15)$$

For the interaction (1), in fact $\psi^{\mathrm{RM}}(r)$ has the explicit form

$$\psi^{\mathrm{RM}}(r) = \left(\frac{m\omega}{2\hbar}\right)^{\alpha/2+3/4} \left[\frac{2}{\Gamma(\alpha+3/2)}\right]^{1/2} \mathrm{e}^{-m\omega r^2/(4\hbar)}\, r^{\alpha+1}. \quad (16)$$

Inserting this into equation (10) leads to the integral form

$$\rho(r) = \frac{\mathrm{e}^{-2m\omega r^2/\hbar}}{\pi^{3/2}4^\alpha\Gamma(\alpha+3/2)} \frac{m\omega}{\hbar r} \int_0^\infty \mathrm{e}^{-y^2/2} y^{2\alpha+1} \sinh(ry/a)\, \mathrm{d}y. \quad (17)$$

Comparing equations (17) and (5), one evidently has an integral representation for the hypergeometric function ${}_1F_1$ in the case when its second argument remains less than the first. The equivalence can be explicitly checked in general by comparing the series expansion of expressions (17) and (5).

To briefly summarize, the ground-state electron density of the model atom with harmonic confinement and interaction (1) satisfies the linear homogeneous second-order differential equation (7). For different interactions, with the same external potential, equation (10) provides a unification, but so far it has not proved possible to write a general single differential equation for arbitrary $u(r_{12})$.

Acknowledgments

This work has been partially supported by an Advanced Research Initiative of Scuola Normale Superiore di Pisa (SNS) and by the Istituto Nazionale di Fisica della Materia (INFM). N H March acknowledges that his contribution to this paper was largely made during a visit to SNS in 2005. He wishes to thank SNS for the very stimulating atmosphere where this study was carried out and for generous support.

References

[1] Cornell E A and Wieman C E 2002 *Rev. Mod. Phys.* **74** 875
[2] Ketterle W 2002 *Rev. Mod. Phys.* **74** 1131
[3] DeMarco B and Jin D S 1999 *Science* **285** 1703
[4] Minguzzi A, March N H and Tosi M P 2001 *Eur. Phys. J.* D **15** 315
[5] Minguzzi A, March N H and Tosi M P 2001 *Phys. Lett.* A **281** 192
[6] Capuzzi P, March N H and Tosi M P 2005 *Phys. Lett.* A **339** 207
[7] Crandall R, Whitnell R and Bettega R 1984 *Am. J. Phys.* **52** 438
[8] Abramowitz M and Stegun A (ed) 1972 *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables* (New York: Dover)
[9] Morse P M and Feshbach H 1953 *Methods of Theoretical Physics* vol 1 (New York: McGraw-Hill)
[10] March N H, Gál T and Nagy Á 1998 *Chem. Phys. Lett.* **292** 384
[11] March N M and Ludeña E V 2004 *Phys. Lett.* A **330** 16
[12] Holas A, Howard I A and March N H 2003 *Phys. Lett.* A **310** 451