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An exactly solvable model where properties of a fermion assembly are dominated by the highest occupied level: case of harmonic confinement in *d* dimensions

I A Howard[1], I V Komarov[2], N H March[1,3] and L M Nieto[4]

[1] Department of Physics, University of Antwerp (RUCA), Antwerpen, Belgium
[2] Institute of Physics, St Petersburg State University, St Petersburg, Russia
[3] Oxford University, Oxford, UK
[4] Departamento de Física Teórica, Universidad de Valladolid, 47005 Valladolid, Spain

E-mail: luismi@metodos.fam.cie.uva.es

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Abstract
It is shown explicitly that the fermion particle density $\varrho(r)$ in d dimensions for isotropic harmonic confinement and odd d is determined by the one-dimensional wavefunctions of the highest occupied state. Knowledge of the Dirac density matrices for $d = 1$ and 2 suffices to completely determine the general d-dimensional matrices.

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Our groups have been working independently on the properties of a fermion assembly of particles subject to isotropic harmonic confinement [1–3] in d dimensions. Folklore has it that the properties of large fermion assemblies are dominated by eigenfunctions of the highest occupied level.

The purpose of this paper is to use the results of [1–3] to give an explicit proof, for harmonic confinement of independent fermions in d dimensions, of the above assertion. In fact, it turns out that given solutions of the $d = 1$ and 2 models of harmonic forces, one can generate solutions for arbitrary d.

As Lawes and March in [4] summarize, the corresponding Dirac density matrix of $N + 1$ occupied lowest states in one dimension reads

$$\varrho_N^{(1)}(x, x') = \frac{1}{2}\psi_N(x)\psi_N(x') + \frac{1}{2(x - x')}[\psi_N(x)\psi'_N(x') - \psi_N(x')\psi'_N(x)] \tag{1}$$

then for the density $\varrho_N^{(1)}(x)$ one has

$$\varrho_N^{(1)}(x) = \varrho_N^{(1)}(x, x')|_{x'=x} = \frac{1}{2}[\psi_N'(x)]^2 + \left(N - \frac{x^2}{2}\right)\psi_N^2(x). \tag{2}$$

Here $\psi_N(x)$ stands for the normalized harmonic oscillator function with N nodes, $N = 0, 1, \ldots$. Below we clearly distinguish the Dirac density matrix for $N+1$ occupied lowest levels with $n = 0, 1, \ldots, N$ and that of the shell with a given energy. Thus we have denoted the complete Dirac density matrix in one dimension for maximal N filled shells as $\varrho_N^{(1)}(x, x')$. The superscript and subscript indicate the dimension d of the configuration space and the value of the Fermi energy $E_F = N + d/2$ respectively.

These results (1) and (2) go back to Husimi [5]. Relation (1) was already known in the nineteenth century as the Christoffel–Darboux formula for the classical orthogonal polynomials (e.g., [6]).

Introducing the differential operator [1]

$$\mathcal{L}(x, x') = \frac{1}{x - x'}\left(\frac{\partial}{\partial x'} - \frac{\partial}{\partial x}\right) \tag{3}$$

one can rewrite equation (1) as the action of the operator $\mathcal{L}$ on products of the oscillator functions at the Fermi level:

$$\varrho_N^{(1)}(x, x') = \tfrac{1}{2}(\mathcal{L}(x, x') + 1)\psi_N(x)\psi_N(x'). \tag{4}$$

In fact, it turns out that given solutions of the $d = 1$ and 2 models of harmonic forces, one can generate solutions for arbitrary dimensionality d. The d-dimensional Dirac density matrix for the (N)th closed shell will be written below as $\gamma_N^{(d)}(\mathbf{r}, \mathbf{r}')$ and the coordinates to be used (see also [7]) are defined by

$$x = \frac{|\mathbf{r} + \mathbf{r}'| + |\mathbf{r} - \mathbf{r}'|}{2} \geqslant 0 \qquad y = \frac{|\mathbf{r} + \mathbf{r}'| - |\mathbf{r} - \mathbf{r}'|}{2} \geqslant 0. \tag{5}$$

These variables allow one to discard symbols of the absolute value and dot product in the following equalities:

$$\begin{array}{ll} |\mathbf{r} + \mathbf{r}'| = x + y & |\mathbf{r} - \mathbf{r}'| = x - y \\ |\mathbf{r}|^2 + |\mathbf{r}'|^2 = x^2 + y^2 & (\mathbf{r} \cdot \mathbf{r}') = xy. \end{array} \tag{6}$$

It will be valuable below to supplement the operator $\mathcal{L}$ in equation (3) with a further operator $\mathcal{M}$. This we define as the even part of $\mathcal{L}(x, y)$ with respect to its second argument by

$$\mathcal{M}(x, y) = \frac{1}{2}(\mathcal{L}(x, y) + \mathcal{L}(x, -y)) = \frac{1}{x^2 - y^2}\left(y\frac{\partial}{\partial y} - x\frac{\partial}{\partial x}\right). \tag{7}$$

By direct operation of $\mathcal{M}(x, y)$ on $\varrho_N^{(1)}(x, y)$, and using the explicit forms of $\varrho_N^{(3)}(x, y)$ for small values of the number of shells N, we find after some calculation

$$\varrho_N^{(3)}(x, y) = \frac{1}{\pi}\varrho_N^{(1)}(x, y) \tag{8}$$

for $N = 0$ and 1,

$$\varrho_3^{(3)}(x, y) = \frac{1}{\pi}\left(\varrho_3^{(1)}(x, y) + \varrho_1^{(1)}(x, y)\right) \tag{9}$$

and

$$\varrho_4^{(3)}(x, y) = \frac{1}{\pi}\left(\varrho_4^{(1)}(x, y) + \varrho_2^{(1)}(x, y)\right). \tag{10}$$

We infer from the above a much more general result,

$$\varrho_N^{(d)}(x, y) = \frac{1}{2\pi}(\mathcal{M}(x, y) + 1)\varrho_N^{(d-2)}(x, y). \tag{11}$$

Equations (8)–(10), culminating in equation (11), to which we shall return below, represent the central findings of the present letter, showing that for odd d the three-dimensional Dirac matrix, for instance, is determined for an arbitrary number of closed shells by the one-dimensional form $\varrho_N^{(1)}(x, y)$. In fact, since equation (11) applies to general d, all the Dirac matrices $\varrho_N^{(d)}(x, y)$ for odd d are determined through equation (1) by the wavefunction $\psi_N(x)$. This establishes the folklore referred to in the first paragraph of this letter for odd values of the dimensionality d.

Let us next comment on the dependence of $\gamma_N^{(3)}(\mathbf{r}, \mathbf{r}')$,

$$\gamma_N^{(3)}(\mathbf{r}, \mathbf{r}') = \sum_{n_1+n_2+n_3=N} \psi_{n_1n_2n_3}(\mathbf{r})\psi_{n_1n_2n_3}(\mathbf{r}') = \frac{1}{2\pi}(M(x, y) + 1)\psi_N(x)\psi_N(y) \tag{12}$$

on its spatial variables. For a general one-particle $d = 3$ Hamiltonian the Dirac density matrix depends on two vectors $\mathbf{r}$ and $\mathbf{r}'$. For a central field Hamiltonian due to rotational symmetry one can introduce the Dirac density matrix for a subshell of fixed angular momentum, which depends not on six values of components of vectors $\mathbf{r}$ and $\mathbf{r}'$ but on three scalar variables $r = |\mathbf{r}|, r' = |\mathbf{r}'|$ and $|\mathbf{r} - \mathbf{r}'|$ only. For the isotropic harmonic oscillator with $d = 3$, due to additional $SU(3)$ symmetry, the Dirac density matrix of closed shells with the same energy and number of variables can be reduced to the two scalar combinations x, y defined in equation (5). This property holds true for any $d \geqslant 2$. It is worth noting that the free particle density matrix of the shell depends on one variable $|\mathbf{r} - \mathbf{r}'|$ only. Equation (11) implies that one need only calculate two basic density matrices for $d = 1$ and 2, and subsequently to differentiate them. Thus for $d = 3$, one has

$$\varrho_N^{(3)}(\mathbf{r}, \mathbf{r}') = \sum_{n=0}^{N} \gamma_N^{(3)}(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi}\left(\mathcal{M}(x, y) + 1\right)\frac{1}{2}(\mathcal{L}(x, y) + 1)\psi_N^{(1)}(x)\psi_N^{(1)}(y). \tag{13}$$

It should be added here, at this point, that proof of the above formulae [2] can be given by using recurrence relations between the one-dimensional harmonic oscillator wavefunctions and the time-dependent Green function for the one-dimensional oscillator, known to mathematicians as the bilinear generating function for Hermite polynomials [6]. We may write the diagonal ($x = x'$) form of this relation as

$$F^{(1)}(x, x, t) = \sum_{n=0}^{N} t^n \gamma_n^{(1)}(x, x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/2} \frac{1}{\sqrt{1 - t^2}} \exp\left(-\frac{m\omega}{\hbar}x^2\frac{1 - t}{1 + t}\right) \tag{14}$$

where we have, for illustrative purposes, retained units such that

$$V = \tfrac{1}{2}m\omega^2x^2. \tag{15}$$

Generalizing to d dimensions, and for $\mathbf{r}' \neq \mathbf{r}$, one finds for the d-dimensional analogue of equation (14)

$$\sum_{m=0}^{\infty} t^m \gamma_m^{(d)}(\mathbf{r}, \mathbf{r}') = \left(\frac{m\omega}{\pi\hbar}\right)^{d/2} \frac{1}{(1 - t^2)^{d/2}} \exp\left(\frac{m\omega}{2\hbar}\frac{4(\mathbf{r}\cdot\mathbf{r}')t - (r^2 + r'^2)(1 + t^2)}{1 - t^2}\right). \tag{16}$$

On the diagonal, and for the illustrative case $d = 3$, this then gives

$$\sum_{m=0}^{\infty} t^m \gamma_m^{(3)}(\mathbf{r}, \mathbf{r}) = \left(\frac{m\omega}{\pi\hbar}\right)^{3/2} \frac{1}{(1 - t^2)^{3/2}} \exp\left(-\frac{m\omega}{\hbar}r^2\frac{1 - t}{1 + t}\right). \tag{17}$$

To make direct contact with the result of Sondheimer and Wilson [8] for the canonical density matrix $C(\mathbf{r}, \mathbf{r}', \beta)$, one simply replaces t by $\exp(-\beta\hbar\omega)$, which leads to

$$C(\mathbf{r}, \mathbf{r}', \beta) = \left(\frac{m\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}\right)^{d/2} \exp\left\{-\frac{m\omega}{\hbar}\left[(r^2 + r'^2)\tanh\left(\frac{\beta\hbar\omega}{2}\right) + \frac{(\mathbf{r}-\mathbf{r}')^2}{4}\coth\left(\frac{\beta\hbar\omega}{2}\right)\right]\right\}. \tag{18}$$

Due to the properties of the x, y variables in equation (6), the right-hand side of equation (16) takes the form of the one-dimensional generating function in the scalar variables x, y in equation (5) and the coordinate-independent factor $(1-t^2)^{-(d-1)/2}$. For $d = 3$ this factor is a geometric series

$$\frac{1}{1-t^2} = \sum_{k=0}^{\infty} t^{2k} \tag{19}$$

that gives the sum over states with the fixed parity

$$\gamma_N^{(3)}(x, y) = \sum_{k=0}^{[N/2]} \psi_{N-2k}(x)\psi_{N-2k}(y) \tag{20}$$

which leads to relation (13). Here $[N/2]$ denotes the integer part. Similar considerations prove the recurrence relation (11).

For $d = 2$ we need to expand $1/\sqrt{1-t^2}$ instead of $1/(1-t^2)$ in equation (16). So for $\gamma_N^{(2)}(x, y)$ we have the following sum:

$$\gamma_N^{(2)}(x, y) = \sum_{k=0}^{[(N+1)/2]} \frac{(k-1)!!}{k!!}\psi_{N-2k}(x)\psi_{N-2k}(y). \tag{21}$$

Here the double factorial symbol $k!! = k(k-2)(k-4)\cdots$ denotes the product of all positive integers of the same parity as k up to k. For two dimensions, in fact, we can write the shell density matrix $\gamma_N^{(2)}$ in a compact differential form. Using polar coordinates, the shell density matrix has the form

$$\gamma_N^{(2)}(\mathbf{r}, \mathbf{r}') = \frac{1}{2\pi\sqrt{rr'}} \sum_{m+2n=N,\, m\geqslant 0,\, n\geqslant 0} \varepsilon_m \chi_{nm}(r)\chi_{nm}(r')\cos(m(\vartheta)) \tag{22}$$

where

$$\chi_{nm}(r) = \left(\frac{2n!}{(m+n)!}\right)^{1/2} r^{m+\frac{1}{2}}\,\mathrm{e}^{-r^2/2} L_n^m(r^2) \tag{23}$$

and $\varepsilon_m = 1$ for $m = 0$, $\varepsilon_m = 2$ for $m \neq 0$. Transforming to coordinates (x, y) then yields

$$\gamma_N^{(2)}(\mathbf{r}, \mathbf{r}') = \gamma_N^{(2)}(x, y) = \frac{1}{2\pi\sqrt{xy}} \sum_{m+2n=N+1} \varepsilon_m \chi_{nm}(x)\chi_{nm}(y). \tag{24}$$

Using standard boson ladder operators in rectangular coordinates (u_1, u_2) and (u_1', u_2')

$$\left[a_\alpha, a_\beta^\dagger\right] = \delta_{\alpha\beta} \qquad [a_\alpha, a_\beta] = 0 \qquad \alpha, \beta = 1, 2$$

we get

$$\gamma_N^{(2)}(u_1, u_2; u_1', u_2') = \frac{1}{N!}\left(a_1^\dagger a_1'^\dagger + a_2^\dagger a_2'^\dagger\right)^N |00\rangle|0'0'\rangle$$

and focus our attention on a further operator $A = a_1^\dagger a_1'^\dagger + a_2^\dagger a_2'^\dagger$ which, after some calculation, we can write in coordinates (x, y) as

$$A(x, y) = \frac{1}{2}\left(xy - y\left(1 + \frac{1}{x^2 - y^2}\right)\frac{\partial}{\partial x} - x\left(1 - \frac{1}{x^2 - y^2}\right)\frac{\partial}{\partial y} + \frac{\partial^2}{\partial x\,\partial y}\right). \tag{25}$$

This allows us to write

$$\gamma_N^{(2)}(u_1, u_2; u_1', u_2') = \gamma_N^{(2)}(x, y) = \frac{1}{N!}A(x, y)^N |0_x 0_y\rangle \tag{26}$$

where

$$|0_x 0_y\rangle = \frac{1}{\pi}\exp\left(-\frac{1}{2}(x^2 + y^2)\right). \tag{27}$$

It is straightforward to check, say for the first four shells, that equation (26) readily reproduces results directly calculable from known harmonic oscillator wavefunctions. Finally, we note that equation (26) may be formally summed over shells to give the density $\varrho_N^{(2)}$ as

$$\begin{aligned}\varrho_N^{(2)}(\mathbf{r}, \mathbf{r}') &= \sum_{n=0}^{N} \gamma_n^{(2)}(\mathbf{r}, \mathbf{r}') = \sum_{n=0}^{N} \frac{1}{n!}A(x, y)^n |0_x 0_y\rangle \\ &= \exp(A)\frac{\Gamma(N+1, A)}{\Gamma(N+1)}|0_x 0_y\rangle = \exp(A)\frac{\Gamma(N+1, A)}{\Gamma(N+1)}\varrho_0^{(2)}(x, y)\end{aligned} \tag{28}$$

where $\Gamma(a, x)$ denotes an incomplete gamma function [9].

We want to conclude by drawing attention to major simplifications which follow from the recent study of Howard *et al* [3]. We illustrate by taking the cases of two closed shells. These researchers use variables

$$\boldsymbol{\xi} = \frac{\mathbf{r} + \mathbf{r}'}{2} \qquad \boldsymbol{\eta} = \frac{\mathbf{r} - \mathbf{r}'}{2} \tag{29}$$

which embrace the (scalar) variables x and y in equation (5). In terms of the variables (29) $\varrho_2^{(1)}(\xi, \eta)$ is given in equation (3.9) of [3], and in their equation (5.5) for $\varrho_2^{(d)}(\xi, \eta)$ for $d = 4$. They are precisely the same functions of $|\boldsymbol{\xi}|$ and $|\boldsymbol{\eta}|$, the only difference being a d-dependent constant multiplying factor. This means that odd and even values of d are intimately related, in addition to equation (11) relating odd (even) d values. This suggests to us that, in equation (11) to be quite specific, $\varrho_N^{(d-2)}(x, y)$ is an eigenfunction of the operator $\mathcal{M}(x, y)$, with a d-dependent (also N-dependent) eigenvalue, but we have not established this.

In summary, the complete Dirac density matrices of the d-dimensional harmonic oscillator can be characterized solely by $d = 1$ and $d = 2$ matrices, through equation (11). But further, the matrices for odd values of d can be generated by the Fermi level wavefunctions for $d = 1$. In this model of isotropic harmonic confinement, the folklore mentioned in the first paragraph of the body of the letter has therefore been shown to be exact for such values of the dimensionality d.

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