Available online at www.sciencedirect.com
ScienceDirect
Physics Letters A 361 (2007) 261–264
PHYSICS LETTERS A
www.elsevier.com/locate/pla

First-order density matrices in one dimension for independent fermions and impenetrable bosons in harmonic traps

P. Capuzzi [a,*], I.A. Howard [b], N.H. March [b,c], M.P. Tosi [a]

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

Received 28 August 2006; accepted 29 August 2006

Available online 27 September 2006

Communicated by V.M. Agranovich

Abstract

To complement existing knowledge of the density matrix $\gamma_F(x, y)$ of independent fermions for N particles in one dimension under harmonic confinement, the corresponding matrix $\gamma_{IB}(x, y)$ for impenetrable bosons is given for $N = 2$ and 3 (with the $N = 4$ form available also). For fermions the momentum density is then obtained and illustrated numerically for $N = 10$. The boson momentum density is studied analytically at high momentum p, the coefficients of the p^{-4} and p^{-6} terms being tabulated for $N = 2$–5 inclusive. Their dependence on powers of N is exhibited numerically. Finally, the functional relationship between $\gamma_{IB}(x, y)$ and $\gamma_F(x, y)$ is formally set out and illustrated.
© 2006 Elsevier B.V. All rights reserved.

PACS: 05.30.-d; 05.30.Fk; 05.30.Jp; 31.15.Ew

In a recent study, Howard et al. [1] have written the Dirac density matrix $\gamma_F(x, y)$ for N independent spinless fermions which are harmonically confined in one dimension in terms of the wave function $\psi_N(x)$ of the highest occupied level. Their result (see Eq. (4) of [1]) takes the form

$$\gamma_F(x, y) = \frac{1}{2}\big[\mathcal{L}(x, y) + 1\big]\psi_N(x)\psi_N(y), \tag{1}$$

where $\mathcal{L}$ is the differential operator [2] defined by

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

This expression (1) is quite explicit, since the wave function $\psi_N(x)$ of the highest occupied state, with confining potential $V(x) = x^2/2$, is given by

$$\psi_N(x) = \mathcal{C}_{N-1}\exp\big(-x^2/2\big)H_{N-1}(x), \tag{3}$$

where $H(x)$ denotes a Hermite polynomial, while the normalization factor is given by

$$\mathcal{C}_{N-1} = \frac{1}{\pi^{1/4}}\sqrt{\frac{1}{2^{N-1}(N-1)!}}. \tag{4}$$

It has been known for a long time that for one-dimensional impenetrable bosons (IB) the diagonal of the first-order density matrix, or the boson density, is identical with that of the above fermion problem, which we denote by $\rho(x)$, and is obtainable from Eq. (1) as

$$\rho(x) = \gamma_F(x, y)|_{y=x}. \tag{5}$$

Our interest in this Letter is to compare and contrast properties of the fermion density matrix given in Eq. (1) with those of its impenetrable boson counterpart $\gamma_{IB}(x, y)$, to be defined immediately below. The momentum distribution (see Eq. (14)) will prove an important focus. Our starting point is the explicit result of Forrester et al. [3] for $\gamma_{IB}(x, y)$ in their equation (78).

* Corresponding author.
E-mail address: capuzzi@sns.it (P. Capuzzi).

0375-9601/$ – see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.physleta.2006.08.089

This takes the form

$$\gamma_{\mathrm{IB}}(x,y)=\frac{2^{N-1}}{\sqrt{\pi}\Gamma(N)}\exp\left(-\frac{x^2+y^2}{2}\right)\times\det\left[\frac{2^{(j+k)/2}}{2\sqrt{\pi\Gamma(j)\Gamma(k)}}b_{j,k}(x,y)\right]_{j,k=1,\dots,N-1}. \quad (6)$$

The elements of the determinant are fixed by

$$b_{j,k}(x,y)=\int_{-\infty}^{\infty}dt\exp\left(-t^2\right)|x-t||y-t|t^{j+k-2},\quad j\geqslant 1,\ k\leqslant N-1. \quad (7)$$

Suffice it to say here that Forrester et al. [3] obtained the density matrix (6) from the ground-state wave function Ψ_{IB} simply by taking the modulus of the Slater determinant Ψ_{F} which must lead according to [1] to the Dirac density matrix in Eq. (1). Forrester et al. noted that when $b_{j,k}$ appearing in (6) above is replaced by $f_{j,k}$ given by

$$f_{j,k}(x,y)=\int_{-\infty}^{\infty}dt\exp\left(-t^2\right)(x-t)(y-t)t^{j+k-2} \quad (8)$$

(evaluated in turn in terms of Gamma functions), $\gamma_{\mathrm{IB}}(x,y)$ becomes the fermion density matrix, which must then equal that given in Eq. (1) above.

We turn next to the explicit evaluation of $\gamma_{\mathrm{IB}}(x,y)$ for a number of small values of N. Using MATHEMATICA, we have evaluated the difference

$$\Delta(x,y)=\gamma_{\mathrm{IB}}(x,y)-\gamma_{\mathrm{F}}(x,y) \quad (9)$$

for 2, 3 and 4 particles. The explicit results for 2 and 3 particles are quoted below. The interested reader may obtain the (now very lengthy) expression for 4 particles on request. First of all, for 2 particles

$$\Delta^{(2)}(x,y)=\frac{\mathrm{sign}(x-y)}{\pi}\mathrm{e}^{-\frac{3}{2}(x^2+y^2)}\left(2x\mathrm{e}^{x^2}-2y\mathrm{e}^{y^2}+\mathrm{e}^{x^2+y^2}\sqrt{\pi}(1+xy)\left(\mathrm{erf}(y)-\mathrm{erf}(x)\right)\right). \quad (10)$$

If one needs $\gamma_{\mathrm{IB}}(x,y)$ the operator $\mathcal{L}$ can readily be used on the harmonic oscillator wave function $\psi_1(x)=2^{1/2}\pi^{-1/4}x\times\exp(-x^2/2)$ to find

$$\gamma_{\mathrm{F}}^{(2)}(x,y)=\frac{1+2xy}{\sqrt{\pi}}\exp\left(-\frac{x^2+y^2}{2}\right). \quad (11)$$

One immediate check on Eq. (10) is to put $y=x$: this yields $\Delta(x,x)=0$, which must be so since the particle density is identical for spinless fermions and impenetrable bosons.

Analogous, though inevitably more lengthy expressions for 3 particles are given below:

$$\Delta^{(3)}(x,y)=\frac{\mathrm{e}^{-\frac{5}{2}(x^2+y^2)}}{2\pi^{3/2}}\Big\{\mathrm{e}^{2x^2}\left(8x^2-4xy-8\right)+\mathrm{e}^{2y^2}\left(8y^2-4xy-8\right)+4\mathrm{e}^{x^2+y^2}\left(x^2+y^2-4xy+4\right)-2\sqrt{2}\mathrm{e}^{x^2+y^2}\left[\mathrm{erf}(x)-\mathrm{erf}(y)-\mathrm{sign}(x-y)\right]\times\Big[\mathrm{e}^{x^2}\left(x-5y+6x^2y-2xy^2\right)-\mathrm{e}^{y^2}\left(y-5x+6xy^2-2yx^2\right)+\mathrm{e}^{x^2+y^2}\frac{\sqrt{\pi}}{2}\left(3+4xy-2y^2-2x^2+4x^2y^2\right)\times\left(\mathrm{erf}(x)-\mathrm{erf}(y)\right)\Big]\Big\}. \quad (12)$$

Again, using the harmonic oscillator wave function $\psi_2(x)$ and the operator $\mathcal{L}(x,y)$ the analogue of Eq. (11) is readily found to be

$$\gamma_{\mathrm{F}}^{(3)}(x,y)=\frac{1}{2\sqrt{\pi}}\left(3+4xy-2y^2-2x^2+4x^2y^2\right)\times\exp\left(-\frac{x^2+y^2}{2}\right). \quad (13)$$

This is identical to the result given by Forrester et al.

We consider next a simpler (in principle!) characterization of the density matrices $\gamma_{\mathrm{F}}(x,y)$ and $\gamma_{\mathrm{IB}}(x,y)$ by the momentum density $n(p)$, defined (with $\hbar=1$ throughout) by

$$n(p)=\frac{1}{2\pi}\int\gamma(x,y)\mathrm{e}^{ip(x-y)}\,dx\,dy. \quad (14)$$

For the fermion case, use of $\gamma_{\mathrm{F}}(x,y)$ plus properties of the fermion operator $\mathcal{L}(x,y)$ allow $n_{\mathrm{F}}(p)$ to be obtained for an arbitrary number of particles as

$$n_{\mathrm{F}}(p)=\frac{1}{2}\phi_{\mathcal{N}}^2(p)+\int_p^{\infty}k\phi_{\mathcal{N}}^2(k)\,dk, \quad (15)$$

where $\mathcal{N}$ is the number of nodes in the momentum wave function $\phi_{\mathcal{N}}(p)$, i.e. $\mathcal{N}=1$ for 2 particles, $\mathcal{N}=2$ for 3 particles, etc. Eq. (15) was obtained from Eq. (1) by calculating separately the contribution originating from the constant $1/2$ and that from the differential operator $\mathcal{L}$. Integration of the first is straightforward and yields $n_1(p)=\frac{1}{2}\phi_{\mathcal{N}}^2(p)$, whereas to obtain the second term we first differentiated Eq. (14) with respect to p to eliminate the denominator $(x-y)$ and then integrated by parts on spatial coordinates. Integration over momentum finally yields the second term on the RHS of Eq. (15), $n_2(p)=\int_p^{\infty}k\phi_{\mathcal{N}}^2(k)\,dk$. It is worth noticing that $n_1(p)$ contributes to $n_{\mathrm{F}}(p)$ a total probability $1/2$ irrespectively of the number of particles, from the normalization of $\phi_{\mathcal{N}}(p)$: the contribution $n_2(p)$ will therefore be progressively more important as N increases. We have used Eq. (15) to obtain $n_{\mathrm{F}}(p)$ for 10 particles, the two separate terms on the RHS of Eq. (15) also being displayed in Fig. 1. Evidently, $n_2(p)$ is the dominant contribution to $n_{\mathrm{F}}(p)$ as N gets larger.

To date, we have no simple analytical counterpart of Eq. (15) for the density matrix difference $\Delta(x,y)$ defined in Eq. (9) above. However, we can progress somewhat beyond the results of Minguzzi et al. [4] on the high momentum tail of the momentum density $n_{\mathrm{IB}}(p)$ for impenetrable bosons. Using our analytical results for $\gamma_{\mathrm{IB}}(x,y)$ plus MATHEMATICA, we find

$$n_{\mathrm{IB}}^{(N)}(p)\big|_{p\to\infty}=\frac{A_N}{p^4}+\frac{B_N}{p^6}+\mathrm{O}\left(p^{-8}\right). \quad (16)$$

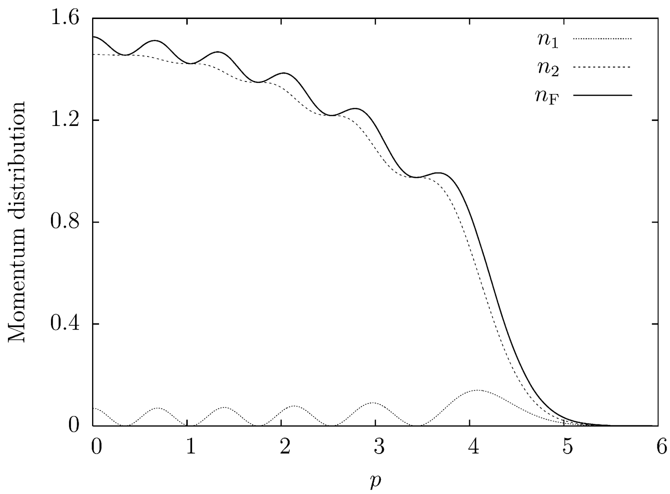

Fig. 1. Momentum distribution $n_{\mathrm{F}}(p)$ for 10 harmonically confined fermions as function of momentum p (arbitrary units). The dotted and dashed lines refer to the two contributions $n_1(p)$ and $n_2(p)$ to the total momentum distribution n_{F} (solid line).

Table 1
Coefficients of the large-p expansion of $n_{\mathrm{IB}}(p)$, Eq. (16), for $N = 2$ to 5

	$N=2$	$N=3$	$N=4$	$N=5$
A_N	$(\frac{2}{\pi})^{3/2}$	$\frac{27}{8}(\frac{2}{\pi})^{3/2}$	$\frac{475}{64}(\frac{2}{\pi})^{3/2}$	$\frac{13715}{1024}(\frac{2}{\pi})^{3/2}$
B_N	$\frac{11}{2}(\frac{2}{\pi})^{3/2}$	$\frac{429}{16}(\frac{2}{\pi})^{3/2}$	$\frac{9889}{128}(\frac{2}{\pi})^{3/2}$	$\frac{353485}{2048}(\frac{2}{\pi})^{3/2}$

The coefficients A_N and B_N are collected in Table 1 for $N =$ 2–5 inclusive. Additionally, Fig. 2 shows plots of A_N and B_N vs N, demonstrating that both A_N and B_N approximately follow power laws in this range of N with exponents 3 and 4, respectively. Though we have not achieved an analytic result for the low-momentum limit $n_{\mathrm{IB}}(p \to 0)$, Papenbrock's finding [5] from his numerical studies is that this is proportional to N.

We shall conclude this Letter by enquiring as to the relation between $\gamma_{\mathrm{IB}}(x, y)$ and $\gamma_{\mathrm{F}}(x, y)$, using the formalism of density functional theory. This theory tells us (formally, because presently we do not know the relevant functionals) that both density matrices are functionals of their diagonal elements, which as already stressed are equal to the particle density $\rho(x)$. From the symmetry between x and p space for γ_{F} and then the use of the x coordinate analogue of Eq. (15) we have

$$\rho(x) = \rho\left[\psi_{\mathcal{N}}(x)\right], \tag{17}$$

where again $\mathcal{N}$ is the number of nodes. Since $\rho(x)$ is also the diagonal element $\gamma_{\mathrm{IB}}(x, x)$ we have, with $\gamma_{\mathrm{F}}(x, y) \equiv \gamma_{\mathrm{F}}[\rho]$, the formal result

$$\gamma_{\mathrm{IB}}(x, y) \equiv \gamma_{\mathrm{IB}}\left[\gamma_{\mathrm{F}}(x, y); \rho; \psi_{\mathcal{N}}\right]. \tag{18}$$

Though we cannot proceed generally from Eq. (18) for an arbitrary number of particles $\mathcal{N} + 1$, we have for 2 particles utilized the explicit Eqs. (9)–(11) to write $\gamma_{\mathrm{IB}}(x, y = 0)$ in the form (18). Since from Eq. (11) at $y = 0$ we have $\gamma_{\mathrm{F}}(x, 0) = \pi^{-1/2}\exp(-x^2/2)$, it is straightforward from Eq. (10) to show

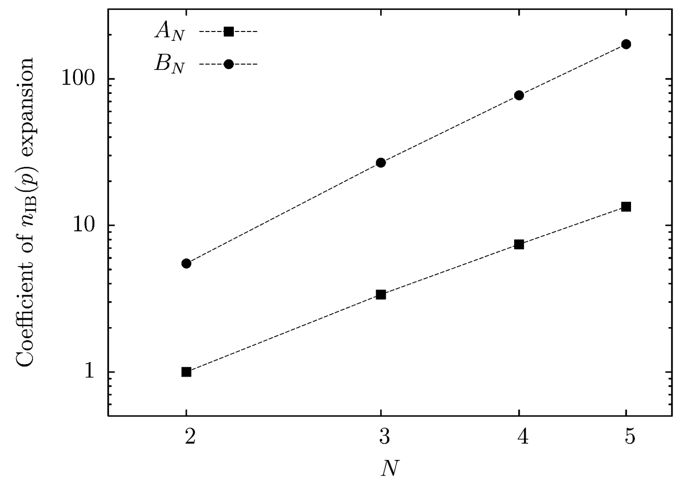

Fig. 2. Coefficients A_N and B_N (in log scale) of the large-p expansion of $n_{\mathrm{IB}}(p)$ as function of N (in log scale). The lines are guides to the eyes.

that

$$\frac{\Delta^{(2)}(x, 0)}{\gamma_{\mathrm{F}}^{(2)}(x, 0)} = \frac{\operatorname{sign}(x)}{\pi^{1/2}}\left[2x - \pi^{1/2}\operatorname{erf}(x)\right]. \tag{19}$$

From $\psi_1(x)$ quoted above we can express the RHS of Eq. (19) solely in terms of $\psi_1(x)/\gamma_{\mathrm{F}}^{(2)}(x, 0)$. The result is

$$\frac{\Delta^{(2)}(x, 0)}{\gamma_{\mathrm{F}}^{(2)}(x, 0)} = \operatorname{sign}(x)\left[\frac{2^{1/2}\pi^{-3/4}\psi_1(x)}{\gamma_{\mathrm{F}}^{(2)}(x, 0)} - \operatorname{erf}\left\{\frac{2^{-1/2}\pi^{-1/4}\psi_1(x)}{\gamma_{\mathrm{F}}^{(2)}(x, 0)}\right\}\right]. \tag{20}$$

Eq. (20) for $N = 2$ exemplifies the functional relationship (18). At $y = 0$, Eq. (18) evidently reduces to $\gamma_{\mathrm{IB}}(x, 0) \equiv \gamma_{\mathrm{IB}}[\gamma_{\mathrm{F}}(x, 0); \psi_1(x)/\gamma_{\mathrm{F}}(x, 0)]$ and hence, for this admittedly simple case we can reconstruct $\gamma_{\mathrm{IB}}(x, 0)$ explicitly using solely harmonically confined fermion properties. In fact, the above argument is readily generalized for all $y \neq 0$ and again the functional form (18) is confirmed. However the detail proliferates and we shall not quote the y generalization.

In summary, the main achievements of the present Letter are as follows: (i) the construction of the explicit forms of the difference density matrix $\Delta(x, y)$ in Eq. (9) for 2–4 particles inclusive, with the evident demonstration that $\Delta(x, y)|_{y\to x}$ is identically zero for those three examples; (ii) the fermion momentum density $n_{\mathrm{F}}(p)$ given solely in terms of the momentum eigenfunction $\phi_{\mathcal{N}}(p)$ in Eq. (15), where $\mathcal{N}$ is the number of nodes in the momentum wave function; (iii) the high momentum tail of the impenetrable boson density $n_{\mathrm{IB}}(p) \to A_N p^{-4} + B_N p^{-6}$ where A_N is approximately proportional to N^3 and B_N to N^4 in a range of low particle numbers; and (iv) the formal density-functional-theory relation (18) between the one-body density matrix for impenetrable bosons and purely harmonically constrained fermion properties. However, in (iv) only for 2 particles has it proved possible to construct such a functional relationship quite explicitly, and this may prove a useful direction for future studies.

Acknowledgements

This work has been partially supported by an Advanced Research Initiative of Scuola Normale Superiore di Pisa (SNS). I.A.H. acknowledges support from IWT-Flemish region under grant No. IWT-161. N.H.M. wishes to acknowledge the stimulating atmosphere at SNS in which his contribution to this work was brought to fruition. He also thanks SNS for the generous hospitality during his visit to Pisa.

References

[1] I.A. Howard, I.V. Komarov, N.M. March, L.M. Nieto, J. Phys. A: Math. Gen. 36 (2003) 4757.
[2] Yu.N. Demkov, I.V. Komarov, Vestnik Leningradskogo Gosudarstvennogo Universiteta, Serija Fiziki i Khimii 10 (1965) 18.
[3] P.J. Forrester, N.E. Frankel, T.M. Garoni, N.S. Witte, Phys. Rev. A 67 (2003) 043607.
[4] A. Minguzzi, P. Vignolo, M.P. Tosi, Phys. Lett. A 294 (2002) 222.
[5] T. Papenbrock, Phys. Rev. A 67 (2003) 041601(R).