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ABSTRACT

Using a coherent states phase space representation the distribution function corresponding to many-particles harmonic oscillator wavefunctions is obtained in explicit analytic expressions form. A density matrix expansion is performed and found to produce good approximations to the exact results.

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The idea of a phase-space probability distribution function in quantum mechanics has attracted a lot of interest since the work of Wigner(1). However, as is well known, the Wigner function is not a true probability distribution over the phase-space, since it is not pointwise nonnegative in general. In order to overcome this apparent difficulty, various rather artificial smoothing procedures of Wigner function have been performed(2-4).

In parallel to the Wigner formalism another formulation has been developed in terms of the overcomplete gaussian wave-packets or coherent states basis(5), $|\mathbb{p}\mathbb{q}\rangle$, where the pair $\mathbb{p}$-$\mathbb{q}$, the label space, defines the Wave-Packet Phase Space Representation (WPPSR). The representation of the density matrix $\hat{\rho} = |\psi\rangle\langle\psi|$, leads to a nonnegative distribution function $P(\mathbb{p},\mathbb{q})$, that allows for interpretation as a probability density distribution function. This function was first introduced by Husimi(2) as a convoluted Wigner function and can be interpreted as a dynamical map in the sense of Sudarshan(5-6).

Given the density matrix $\rho(\mathbb{r},\mathbb{r}')$ the corresponding WPPSR $P(\mathbb{p},\mathbb{q})$, is defined by(5)

$$P(\mathbb{p},\mathbb{q}) = \int d^3r\, d^3r'\, K(\mathbb{p},\mathbb{q};\mathbb{r}',\mathbb{r})\, \rho(\mathbb{r},\mathbb{r}') \tag{1}$$

where the kernel of the transformation is

$$K(\mathbf{p},\mathbf{q};\mathbf{r},\mathbf{r}') = \left(\frac{a_0^2}{\pi\hbar}\right)^{3/2} \exp\left[-(\mathbf{r}-\mathbf{q})^2\frac{a_0^2}{2\hbar} - (\mathbf{r}'-\mathbf{q})^2\frac{a_0^2}{2\hbar} - i\,\mathbf{p}\cdot\frac{(\mathbf{r}-\mathbf{r}')}{\hbar}\right] \tag{2}$$

a_0 is a constant with dimensions $M^{\frac{1}{2}}T^{-\frac{1}{2}}$ that leads to the sharp momentum (coordinate) representation when the limit $a_0 \to 0$ ($a_0 \to \infty$) is taken.

We will consider the WPPSR of the one body density matrix of a pure state of independent fermions. In this case, $\rho(\mathbf{r},\mathbf{r}')$, is given by

$$\rho(\mathbf{r},\mathbf{r}') = \sum_n{}' \, \psi_n^*(\mathbf{r})\, \psi_n(\mathbf{r}') \tag{3}$$

where the sum is over all occupied single-particle states. Hereafter, for analytical simplicity, we will take the ψ_i to be the single-particle eigenfunctions of the spherical H.O. Hamiltonian.

In the one-dimensional case, the eigenfunction is given by

$$\psi_n(x) = \left(\frac{m\omega}{\hbar}\right)^{1/4}\left(\sqrt{\pi}\, 2^n n!\right)^{-1/2} H_n(\xi)\, e^{-\xi^2/2} \tag{4}$$

where $\xi = (m\omega/\hbar)^{\frac{1}{2}}x$ and $H_n(\xi)$ is a Hermite polynomial[7].

The WPPSR of eq. (3) for a particle in a state n is

$$\rho_n(p,q) = \int dx\, dx'\, K(p,q;x',x)\,\psi_n^*(x')\,\psi_n(x) \tag{5}$$

The integration in eq. (5) is easily done if we use the generating function of the Hermite polynomials. When $a_0^2 = m\omega$ we get

$$\rho_n(p,q) = \rho_n(\varepsilon) = e^{-\varepsilon/2}\,\frac{\varepsilon^n}{2^n n!} \tag{6}$$

where ε is the energy parameter as introduced by Shlomo and Prakash[8]

$$\varepsilon = \frac{p^2}{m\omega\hbar} + \frac{m\omega}{\hbar}q^2 \tag{7}$$

The generalization to higher dimensions is easy, and following (8) we have

$$\rho(\mathbf{p},\mathbf{q}) = \rho(\varepsilon) = 4\, e^{-\varepsilon/2}\sum_{n=0}^{F}\frac{\varepsilon^n}{2^n n!} \tag{8}$$

for the tridimensional case $\varepsilon = \sum_{i=1}^{3}\left(\frac{p_i^2}{m\omega\hbar} + \frac{m\omega}{\hbar}q_i^2\right)$.

The factor 4 in eq. (8) has been included because of spin-isospin degeneracy and F is the Fermi level.

The result of a numerical evaluation of eq. (8) is shown in fig. 1. While the corresponding Wigner function exhibits strong oscillations and is negative in some regions[9] this function looks like a difuse Fermi function.

We want now to perform a density matrix expansion[10] on $P(\varepsilon)$, eq. (8). Toward this we first return to eq. (1), and perform there the change of variables, $\mathbb{r} = \mathbb{R} + \vec{s}/2$ and $\mathbb{r}' = \mathbb{R} - \vec{s}/2$:

$$P(\mathbb{p},\mathbb{q}) = \int d^3R \int d^3s\, K(\mathbb{p},\mathbb{q};\mathbb{R}-\vec{s}/2,\mathbb{R}+\vec{s}/2)\,\rho(\mathbb{R}+\vec{s}/2,\mathbb{R}-\vec{s}/2) \tag{9}$$

If we now write

$$\rho(\mathbb{R}+\vec{s}/2,\mathbb{R}-\vec{s}/2) = e^{\vec{s}\cdot\frac{(\nabla_1-\nabla_2)}{2}}\,\rho(\mathbb{R}_1,\mathbb{R}_2)\Big|_{\mathbb{R}_1=\mathbb{R}_2=\mathbb{R}} \tag{10}$$

and angle-average by performing the angular integration over the direction of $\mathbb{p}$ we approximate $P(\mathbb{p},\mathbb{q})$ by

$$P(p,q) = 4\pi\left(\frac{m\omega}{\pi\hbar}\right)^{3/2}\int d^3R\int_0^\infty ds\Big\{s^2 j_0\left(\frac{ps}{\hbar}\right)\exp\Big[-\frac{m\omega}{2\hbar}\Big(2(\mathbb{R}-q)^2+\frac{s^2}{2}\Big)\Big]\, j_0\left(\frac{s|\nabla_1-\nabla_2|}{2}\right)\rho(\mathbb{R}_1,\mathbb{R}_2)\Big|_{\mathbb{R}_1=\mathbb{R}_2=\mathbb{R}}\Big\} \tag{11}$$

Following Negele and Vautherin we make use of the identity

$$j_0(xy) = \frac{1}{x}\sum_{m=0}^{\infty}(4m+3)\, j_{2m+1}(x)\, Q_m(y^2) \tag{12}$$

where
$$Q_m(y^2) = \frac{P_{2m+1}(iy)}{iy} = \frac{1}{2^{2m+1}}\sum_{\ell=0}^{m}\frac{(4m+2-2\ell)!\; y^{2(m-\ell)}}{\ell!\,(2m+1-\ell)!\,(2m+1-2\ell)!} \tag{13}$$

thus

$$P(p,q) = 4\pi\left(\frac{m\omega}{\pi\hbar}\right)^{3/2}\int d^3R\, e^{-\frac{m\omega}{\hbar}(\mathbb{R}-q)^2}\sum_{m=0}^{\infty}(4m+3)\int_0^\infty ds\, s^2 j_0\left(\frac{ps}{\hbar}\right)\cdot e^{-\frac{m\omega}{4\hbar}s^2}\,\frac{j_{2m+1}(sk_0)}{sk_0}\, Q_m\left(\left(\frac{\nabla_1-\nabla_2}{2k_0}\right)^2\right)\rho(\mathbb{R}_1,\mathbb{R}_2)\Big|_{\mathbb{R}_1=\mathbb{R}_2=\mathbb{R}} \tag{14}$$

It was shown in ref. (10) that the first term of this expansion alone reproduces the exact result for nuclear matter. If we keep the first two terms of expansion (14) we get

$$P_{DME}(p,q) = 4\pi\left(\frac{m\omega}{\pi\hbar}\right)^{3/2}\int d^3R\, e^{-\frac{m\omega}{\hbar}(\mathbb{R}-q)^2}\int_0^\infty ds\, s^2 j_0\left(\frac{ps}{\hbar}\right)\cdot e^{-\frac{m\omega}{4\hbar}s^2}\Big[\frac{3\, j_1(sk_0)}{sk_0}\rho(\mathbb{R}) - \frac{7}{2}\frac{j_3(sk_0)}{sk_0}\Big(\frac{5\,\tau(\mathbb{R})}{k_0^2} - \frac{5}{4}\frac{\nabla^2\rho(\mathbb{R})}{k_0^2} + -3\rho(\mathbb{R})\Big)\Big] \tag{15}$$

where we use the local density approximations

$$\rho(\mathbb{R}) = \frac{2}{3\pi^2}\, k_F^3(\mathbb{R}) \quad (16) \quad , \quad \tau(\mathbb{R}) = \sum_k |\nabla \psi_k(\mathbb{R})|^2 = \frac{2}{5\pi^2}\, k_F^5(\mathbb{R}) \tag{17}$$

If we note that eq. (8) involves only powers of q^2 and p^2 we have a physical motivation to make the angular integration over the $\mathbf{q}$ direction. The results of numerical calculations to $P_{DME}(p,q)$ of eq. (15) and the exact distribution of eq. (8) are shown in fig. (2). It is evident from this figure that, in this case, DME yields an excellent approximation, unlike in the case of the Wigner distribution function studied by Martorell and Moya de Guerra[(11)].

As a further point we would like to analyze the dependence of eq. (15) on k_0. The results shown in fig. (2) were obtained with $k_0 = k_F(0)$ and fig. (3) shows P_{DME} as a function of p for $q = 0$ and for different values of k_0. We note a strong dependence of P_{DME} on k_0.

If we take the full expansion in eq. (14) the value of k_0 is, of course, irrelevant. However, as the expansion is truncated, there is a compromise between the values of k_0 that make the integral in the variable s (eq. (14)) small for large n, and the values of k_0 such that

$$-1 \leqslant \frac{|i(\nabla_1 - \nabla_2)|}{2k_0} \leqslant 1 \tag{18}$$

which is the valid formal condition to write eq. (11) in the form of eq. (14) (see ref. (11)).

As $\left(\frac{\nabla_1 - \nabla_2}{2k_0}\right)^{2k} \rho(\mathbb{R}_1, \mathbb{R}_2)$ (see eqs. (13) and (14)) can provide all values of the transferred momenta contained in ρ, for small k_0 $(k_0 < k_F(0))$ the range of these values will overshoot $2k_0$ and the condition (18) will not be satisfied. On the other hand, for large k_0 $(k_0 > k_F(0))$, there will be important contributions from $j_{2n+1}(sk_0)$, for large n, in the region where the gaussian in the integral of eq. (14) is still important. This may mean, as suggested by Martorell and Moya de Guerra, that in processes where high momentum components are important, an approximation like DME may be hazardous.

In conclusion, we have shown that the phase-space distribution obtained in the formalism of the gaussian wave-packets reveals a remarkable similarity with the diffuse Fermi function. At the same time, the DME yields an excellent agreement with the exact distribution unlike in the case of the Wigner distribution function.

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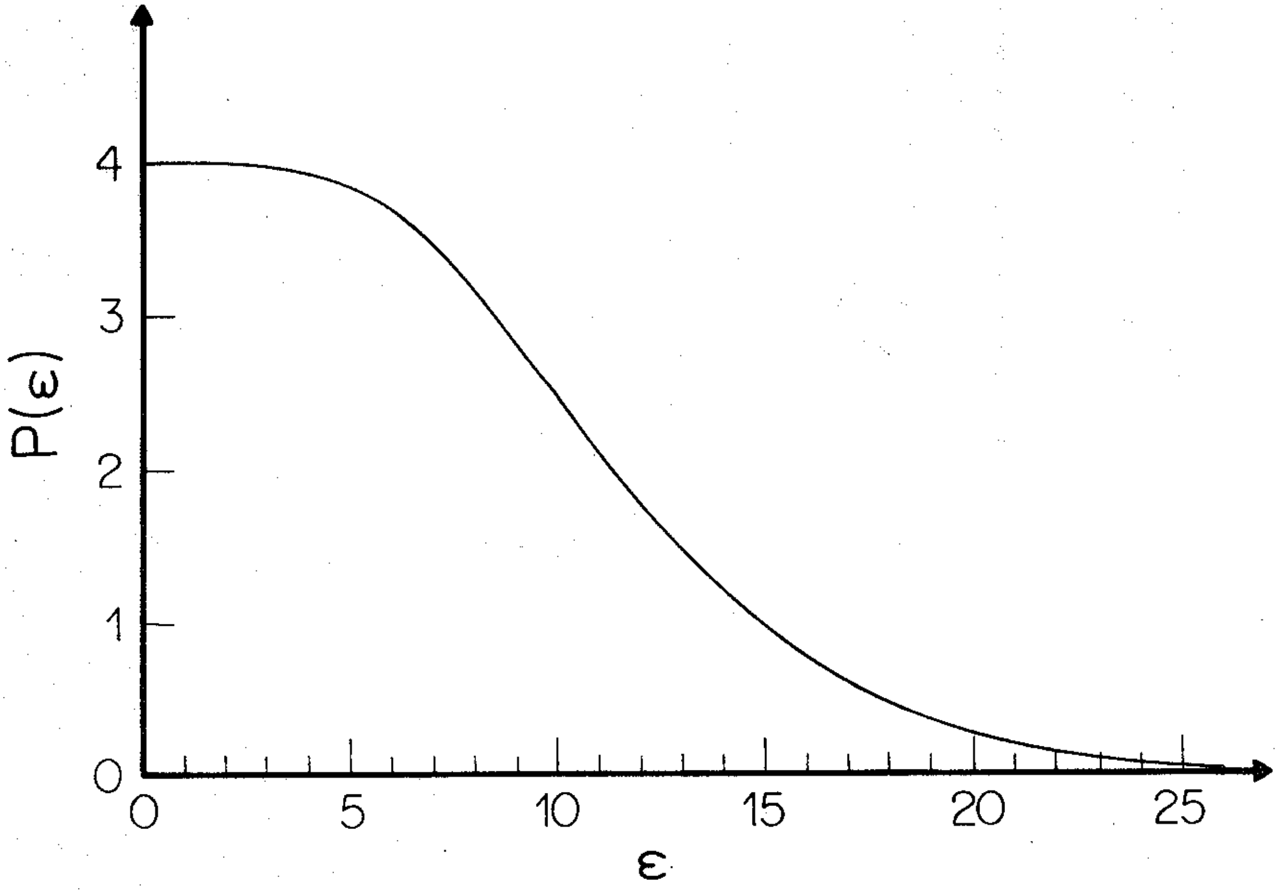
FIGURE CAPTIONS

Fig. 1 - The WPPSR of the one body density matrix for a nucleus with $A = 224$ particles calculated for a spherical O.H. potential.

Fig. 2 - Comparison between WPPSR of the one body density matrix (broken line) and DME for a nucleus with $A = 224$ particles, calculated for a spherical H.O. potential. p and q are in units of $(m\omega\hbar)^{\frac{1}{2}}$ and $(\hbar/m\omega)^{\frac{1}{2}}$ respectively.

Fig. 3 - The DME to the WPPSR of the one body density matrix as a function of p (in units of $(m\omega\hbar)^{\frac{1}{2}}$) for different values of k_0 (in units of $(m\omega/\hbar)^{\frac{1}{2}}$). The broken line shows the exact function of eq. (8).

Fig. 1



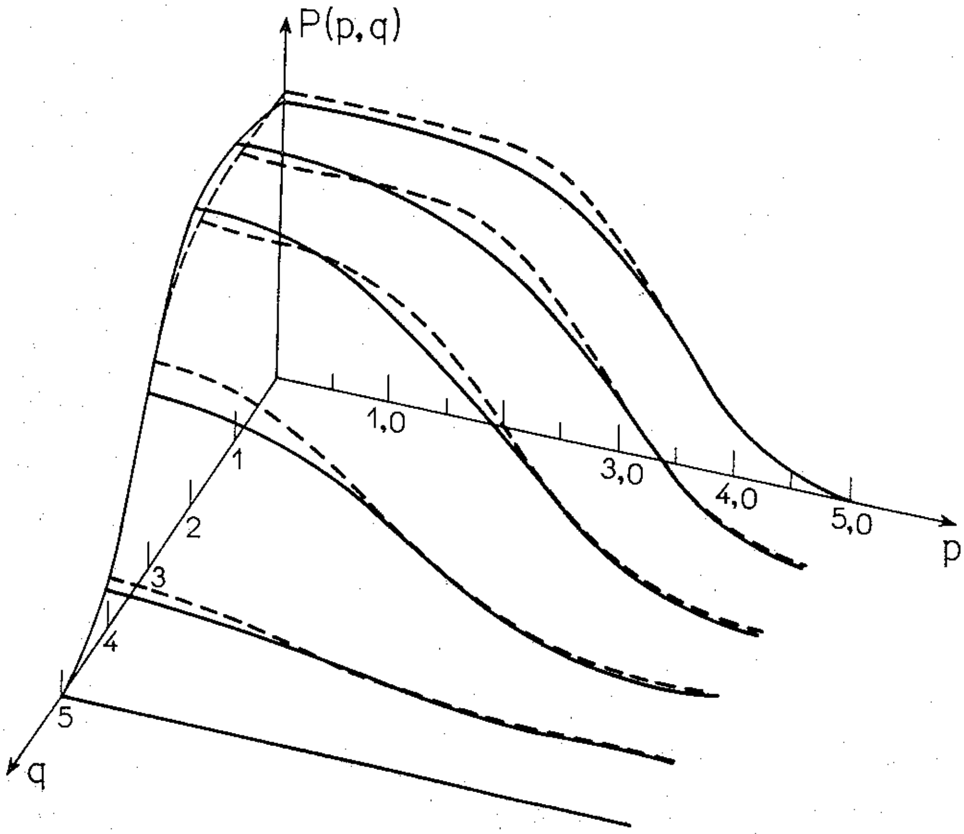


Fig. 2

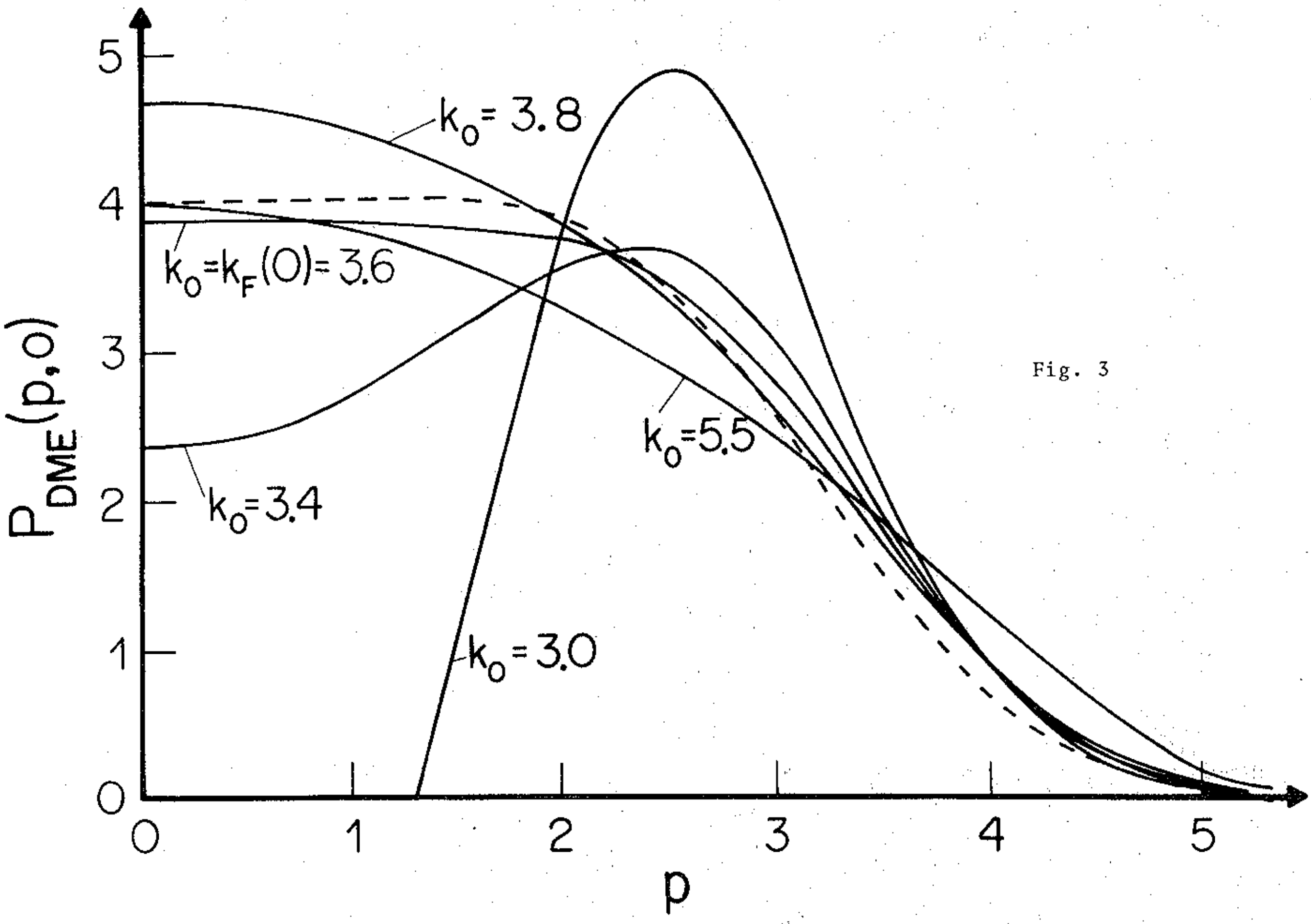


Fig. 3