

A new semiclassical approach for the spatial density of nuclear systems

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Abstract We show that a new decomposition of the many-body Wigner function in the squeezed states basis set of the quantum phase-space associated to bound states allows one to separate the spatial density of the many-body system into a semiclassical part plus its quantum complement.

1. Introduction

A description of quantum mechanical properties of many-body systems bearing some resemblance to the usual classical phase-space has been long known, at least in an approximate form, since the work by Wigner¹.

From the mathematical point of view, the scheme of generating a pair of labels closely paralleling the well known classical one, (q, p) , was first proposed by Weyl² and the connection with that treatment by Wigner was extensively studied by several authors³. Since then the Weyl-Wigner approach has been studied and its applications have greatly increased. In particular, the interest in using Wigner functions⁴ for nuclear systems received a new boost from the phase-space-like treatment of the Time-Dependent Hartree-Fock mean-field approximation⁵. In that case the semiclassical features of the nuclear systems became much more conspicuous⁵ and the expected connections with other well established treatments were studied⁶.

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Nowadays one encounters a vast literature referring to the use of Weyl-Wigner transformations for the description of the Boltzmann-Vlasov - like equation governing the time evolution of a one-body mean field density function⁷ - sometimes also including ad hoc collision effects. However, it is not so common to find discussions about the semiclassical behavior already embodied in the original many-body Wigner functions. Besides the work by Balazs and Zipfel⁸, Prakash et al⁹ have studied this problem from the interesting point of view of an *a priori* smearing of the occupation numbers related to the single particle wave functions used in defining the one-body mean-field Wigner functions. Two alternative ways were discussed: the usual Strutinskii's prescription of blurring the occupation numbers by means of an average over the energy spectrum, and by introducing an effective temperature **dependence** in the quantum statistical expression for the fermion occupation number of a nuclear system. The results are conclusive: they do show, in fact, that the smooth behavior of the resultant Wigner function gives origin to a semiclassical spatial density akin to the usual well-known ones⁸.

In this paper we show how one can extract a semiclassical component from a complete mean field Wigner function using a procedure different from those already mentioned.

Our starting goal here is to **separate** the full Wigner function into two pieces, one behaving as a semiclassical component and the other as its quantum complement. This, as we will show, can be achieved by a very simple decomposition of the full original Wigner function into an infinite set of basis functions defined on a suitable quantum phase space. More precisely, the harmonic oscillator Wigner functions, in which the harmonic oscillator width is taken as a free parameter, will be considered as our basis functions. This is, however, nothing but a phase space version based on the squeezed states¹⁰. Another approach closely related to the present one is that proposed by Mizrahi¹¹ which was also shown to constitute a squeezed-states phase-space representation¹².

In order to show details of our scheme we apply our method to the simple case of a fixed width harmonic oscillator many-body Wigner function. The ratio

between the free width (associated to the basis functions) and the fixed one (characterizing the function one wants to decompose) now stands as a new parameter which, as we are going to show, brings to light a semiclassical component in the decomposition process. We determine, at least in this particular case, the existence of a **critical** value for that parameter beyond which a semiclassical contribution can always be extracted. This critical value is interpreted in terms of the usual uncertainty principle.

This work is organized as follows: in section 2 we present our decomposition scheme and apply it to a one-dimensional system; section 3 is devoted to the extension to three-dimensional nuclear systems and the study of approximations for the spatial densities. Finally, conclusions are presented in section 4.

2. A particular representation of the one-dimensional Wigner function

In order to illustrate the main features of our scheme we restrict ourselves in this section to the one-dimensional case. Extension to three-dimensional calculations is straightforward and is will be presented in the next sections.

Let us begin by writing the following identity for the Wigner functions

$$W(q, p) \equiv \int dq' dp' W(q', p') \delta(q - q') \delta(p - p') \quad (2.1)$$

Whenever we are treating Wigner functions (Wf) associated to bound states, it is more convenient to take advantage of a particular representation of the delta functions which makes use of wave functions belonging to the square-integrable Hilbert space. In this connection we recall the closure relations associated to the space state bases for coordinates and momenta, respectively. As is well known, those relations may be expressed by means of the harmonic oscillator wave functions. Therefore, they depend on a width parameter b , which will be considered here as a free parameter. We then write

$$\delta(q - q') = \frac{1}{\gamma_1} \exp \left[-\frac{1}{2\gamma_1^2} \frac{(q^2 + q'^2)}{b_0^2} \right] \sum_{n=0}^{\infty} \mathcal{N}_n^2 H_n \left(\frac{q}{b_0 \gamma_1} \right) H_n \left(\frac{q'}{b_0 \gamma_1} \right) \quad (2.2a)$$

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and

$$\delta(p - p') = \frac{b_0^2}{\gamma^2} \exp \left[-\frac{b_0^2}{2\gamma^2} (p^2 + p'^2) \right] \sum_{m=0}^{\infty} \mathcal{N}_m^2 H_m \left(\frac{b_0 p}{\gamma} \right) H_m \left(\frac{b_0 p'}{\gamma} \right) \quad (2.2b)$$

where $H_n(x)$ are the usual Hermite polynomials, and $\gamma_1 = b_1/b_0$ and $\gamma_2 = b_0/b_2$ are dimensionless parameters introduced in order to scale the width b_0 appearing in the two wave functions. Here b_0 plays the central role of a **reference** width to be fixed later. Furthermore, since the 6-functions are related to the same point in the quantum phase space characterized by q and p , we take $\gamma_1 = \gamma_2 = 7$. It is important to note that with this choice we are clearly **allowing** deformations in the unitary cell in phase-space while preserving the uncertainty relation connecting q and p .

Using those expressions, the identity (2.1) is now written as

$$W(q, p) \equiv \frac{b_0^2}{\gamma^2} \exp \left[-\frac{1}{2\gamma^2} \left(\frac{q^2}{b_0^2} + b_0^2 p^2 \right) \right] \sum_{n,m=0}^{\infty} (\mathcal{N}_n \mathcal{N}_m)^2 H_n \left(\frac{q}{b_0 \gamma} \right) H_m \left(\frac{b_0 p}{\gamma} \right) \\ \int dq' dp' \exp \left[-\frac{1}{2\gamma^2} \left(\frac{q'^2}{b_0^2} + b_0^2 p'^2 \right) \right] H_n \left(\frac{q'}{b_0 \gamma} \right) H_m \left(\frac{b_0 p'}{\gamma} \right) W(q', p') \quad (2.3)$$

Now, as is well known¹², the harmonic oscillator Wigner functions form a complete orthonormal set in this quantum phase space. This fact suggests us to immediately particularize our study to this set of functions since any other one can be expressed in terms of them. With this in mind we only have to work out the general expression (2.3) by considering $W(q', p')$ as the ℓ -th state harmonic oscillator Wigner functions. We then write¹²

$$W^{(\ell)}(q', p') = \frac{2}{h} (-)^{\ell} e^{-\tilde{\epsilon}} L_{\ell}(2\tilde{\epsilon}) \quad (2.4)$$

where

$$\tilde{\epsilon} = \frac{b_0^2}{\hbar^2} p'^2 + \frac{q'^2}{b_0^2}, \quad (2.5)$$

and, as usual

$$b_0^2 = \frac{\hbar}{mw} \quad (2.6)$$

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$L_\ell(x)$ stands for the Laguerre polynomials. Note that for the sake of convenience we have taken the parameter b_0 for the width of the functions under consideration.

Using the relations¹³

$$L_\ell^{\alpha+\beta+1}(x+y) = \sum_{k=0}^{\ell} L_k^\alpha(x) L_{\ell-k}^\beta(y) \quad (2.7)$$

$$H_{2n}(ax) = (-)^n 2^{2n} n! L_n^{-1/2}(a^2 x^2) \quad (2.8)$$

and

$$H_m(bx) = \sum_{\ell=0}^m A_{m\ell}(b, a) H_\ell(\sqrt{a}x), \quad (2.9)$$

where the sum in this last expression is restricted to even (odd) values if m is even (odd), and with

$$A_{m\ell}(b, a) = \frac{m!}{\ell! \left(\frac{m-\ell}{2}\right)!} \left[\left(\frac{b}{\sqrt{a}}\right)^2 - 1 \right]^{\frac{m-\ell}{2}} \left(\frac{b}{\sqrt{a}}\right)^\ell, \quad (2.10)$$

we get the general expression for our identity:

$$\begin{aligned} W^{(\ell)}(q, p) &= \frac{2}{h} \frac{(-)^\ell e^{-\epsilon/2}}{2^{2\ell-1}} \sum_{m,n=0}^{\infty} \sum_{k=0}^{\ell} \sum_{j=0}^1 \sum_{r=0}^t (-)^{\frac{r+j}{2}} \gamma^{r+j} \\ &\frac{H_n\left(\frac{q}{b_0}\right) H_m\left(\frac{b_0 p}{h}\right)}{(1+2\gamma^2)^{r+j+1}} \left(\frac{1-2\gamma^2}{1+2\gamma^2}\right)^{\ell-r-j+m+n} I_{m,n,k,j,r} \end{aligned} \quad (2.11)$$

Here

$$\epsilon = \frac{p^2 b_0^2}{h^2 \gamma^2} + \frac{q^2}{b_0^2 \gamma^2}$$

and

$$I_{m,n,k,j,r} = \frac{(2k)! 2^{\frac{5}{2}(j+r)} [2(\ell-k)]!}{2^{2(m+n)} j! r! (n - \frac{i}{2})! \left(m - \frac{r}{2}\right)! k! (\ell-k)! \left(\ell-k - \frac{i}{2}\right)! \left(k - \frac{r}{2}\right)!} \quad (2.12)$$

where i and t stand for the smallest to the two numbers $(n, (\ell-k))$, or (m, k) , respectively.

The restriction in the sums now means that we must consider even values only.

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A first interesting aspect of this entangled manner of writing the harmonic oscillator Wigner function can be illustrated if we **separate** the $m = n = 0$ term from the remaining ones in the sum defining $W^{(\ell)}(q, p)$, namely

$$W^{(\ell)}(q, p) = W_s^{(\ell)}(q, p) + W_r^{(\ell)}(q, p) . \quad (2.13)$$

The contribution from the $m = n = 0$ term, here called $W_s^{(\ell)}(q, p)$, is easily calculated, giving

$$W_s^{(\ell)}(q, p) = \frac{2}{h} \frac{2}{1 + 2\gamma^2} \frac{e^{-\epsilon/2}}{2^{2\ell}} \left(\frac{2\gamma^2 - 1}{2\gamma^2 + 1} \right)^\ell \sum_{k=0}^{\ell} \frac{(2k)! [2(\ell - k)]!}{(k!)^2 [(\ell - k)!]^2} \quad (2.14)$$

which can be immediately seen to be strictly positive for $\gamma > \frac{1}{\sqrt{2}}$, while for $\gamma < \frac{1}{\sqrt{2}}$ its sign depends on the value of ℓ . From the above we observe that using an **appropriate** value of the parameter γ , we can **separate** a smooth positive contribution even in those cases when the full harmonic oscillator Wigner function oscillates **assuming negative** values. Let us now concentrate on the separation (2.13). We emphasize two points: i) the parameters γ plays a central role, i.e., whenever the width associated to the representation of the 6-functions is scaled such that it is greater than a certain minimum value defined by b_0 , we ensure the separation of a positive contribution from $W^{(\ell)}(q, p)$. The existence of this positive part suggests that we could treat it as a semiclassical **first** approximation to the full Wigner function as pointed out by Prakash et al⁸. In fact when we consider this kind of term only, we are implicitly performing an average over a broad region of a phase space sector (q or p) depending on **how** we select the value of γ . For $\gamma > \frac{1}{\sqrt{2}}$ we are smearing the Wigner function in its coordinate phase-space sector. (ii) we could as well have defined the smooth contribution $W_s^{(\ell)}(q, p)$ (not necessarily positive) by writing a truncated series with a few terms in (2.11), instead of that containing only the $m = n = 0$ term. The extent to which the basic characteristic properties of (2.14) are still preserved in doing so is going to be discussed in the next section. Here we only stress that of this contribution is expected to contain essentially the same basic physical meaning as (2.14). However, the truncation criterion is absolutely arbitrary, we must study the limit in which the separation (2.13) can

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still represent a sum of a semiclassical contribution plus a quantum correction for the Wigner function. For a given γ , as we sum more and more terms in the series defining $W_s^{(\ell)}(q, p)$, we expect that, at some point, this contribution will cease to represent a good semiclassical approximation. Nevertheless, the arbitrariness mentioned above is not necessarily a drawback since it can be conveniently handled, giving in the process a new way of treating the Wigner function.

3. The three-dimensional harmonic oscillator nuclear system

The extension of the scheme presented in the previous section to the three-dimensional case is straightforward since it merely uses products of the delta-function representation in each direction. Furthermore, may to make use of the well known expression¹⁵

$$W^{(\ell)}(\vec{q}, \vec{p}) = \left(\frac{2}{h}\right)^3 (-)^{\ell} \exp \left[-\frac{q^2}{b_0^2} - \frac{p^2}{\hbar^2} \right] L_{\ell}^{(2)} \left[2 \left(\frac{q^2}{b_0^2} + \frac{p^2}{\hbar^2} \right) \right] \quad (3.1)$$

Let us now consider a more detailed example of how to write a semiclassical approximation for a three-dimensional Wigner function by using our previously described approach. First we take a nuclear system such that the six first shells of a shell-model harmonic oscillator potential are completely filled ($L = 0, 1, \dots, 5$). If we take into account the spin-isospin degeneracy we get

$$W(\vec{r}, \vec{p}) = 4 \sum_{\ell=0}^5 W^{(\ell)}(\vec{r}, \vec{p}) \quad (3.2)$$

which describes a system of 224 nucleons already studied in the literature^{6,16}. As we have assumed from the very beginning that the occupation number takes values 0 or 1, we ensure that the semiclassical behavior in our scheme will not arise from the blurring of the occupation numbers as is usual in the temperature or Strutinskii's method. Instead it comes from the smearing of the Wigner functions themselves.

Here we divide again $W(\vec{r}, \vec{p})$ in to two contributions, namely

$$W(\vec{r}, \vec{p}) = W_s(\vec{r}, \vec{p}) + W_r(\vec{r}, \vec{p}) , \quad (3.3)$$

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The results follow directly from the calculations of eq. (3.2) with expression (3.1). In order to illustrate how the truncation criterion works, we present plot of the full Wigner function (fig. 1) which should be compared to those of $W_s(r, p)$, for $7 = 1$ (fig. 2) and $7 = 2$ (fig. 3) for the same system. We took $\hbar\omega = 41A^{-1/3}$ in all cases, as usual. We note that when we use $7 = 2$, the Wigner function oscillations are for a same number of terms more damped for $7 = 1$. It is also clear that asymptotically both cases converge to the exact result for $7 = 2$ we need many more terms in the series in order to obtain the main characteristics of the full Wigner function than for $7 = 1$. The reason for this behavior is quite clear since the larger 7 the broader the are a in the q -sector of the quantum phase space over which the Wigner function is smeared. Thus, only including a considerable number of terms we can reconstruct the oscillations. It is also worth mentioning that for large ϵ the approximation to the Wigner function changes very little with the number of terms considered, for both values of 7 (figs. 1,2). This effect is related to the turning points of the potential well and has been discussed by Balazs and Zipfel⁸, so we do not comment further on it.

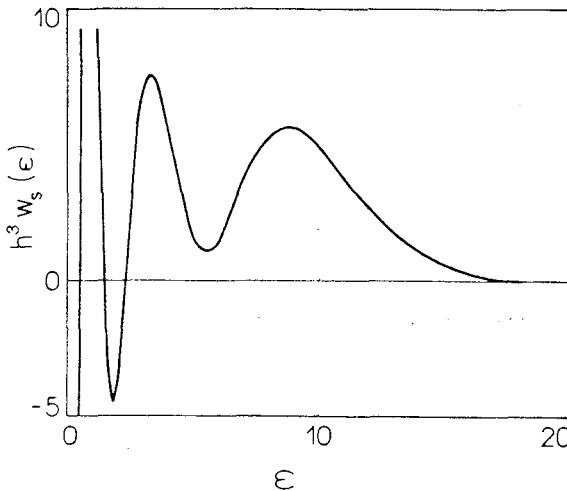


Fig. 1 - The exact Wigner function for 224 particles in a three dimensional isotropic harmonic oscillator.

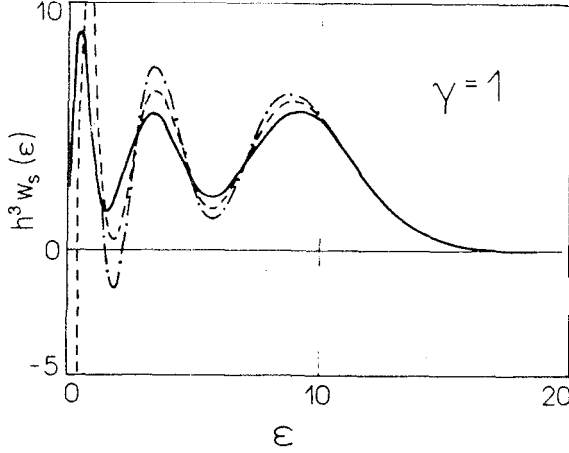


Fig. 2 - Smeared three-dimensional isotropic harmonic oscillator Wigner functions for 224 particles, $\gamma = 1$ and three truncation levels: solid line 9 terms, dashed line 10 terms and dot-dashed line 11 terms.

Using these results we can now calculate the spatial density associated to the nuclear system. As usual the spatial density is given by

$$\rho(\vec{r}) = \int d\vec{p} W(\vec{r}, \vec{p}), \quad (3.4)$$

and it is clear that the separation (3.3), implies

$$\rho(\vec{r}) = \rho_s(\vec{r}) + \rho_r(\vec{r}). \quad (3.5)$$

In this case the density is a function of $r = |\vec{r}|$ only. We have performed calculations to show how the truncation (3.3) influences the behavior of the $\rho_s(r)$ contribution to the total spatial density. They were carried out for $\gamma = 1$ and $\gamma = 2$, again. Fig. 4 shows the full spatial density calculated from the exact wave function, and figs. 5 and 6 depict different truncation levels for the $\rho_s(r)$ contribution for the $\gamma = 1, 2$, respectively. It is immediately seen that the $\rho_s(r)$ contribution in fact resembles the well known semiclassical approximations to the spatial density^{9,16} both for $\gamma = 1$ and $\gamma = 2$. The depression appearing in the inner part of the spatial density

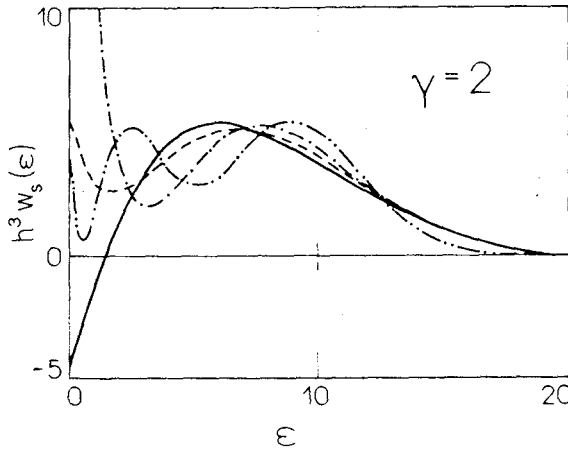


Fig. 3 - Smeared Wigner functions for the same system, $\gamma = 2$ and four truncation levels: solid line 7 terms, dashed line 8 terms and dot-dashed line 12 terms and double dot-dashed 25 terms.

is washed out and at the same time the tail becomes negative in a way similar to that observed in the Modified Thomas Fermi Approximation⁶. This small negative region vanishes when more terms are added to the $\rho_s(r)$ series. In fact it has been shown¹⁵ that one can always obtain the Modified Thomas Fermi Approximation results through a convenient choice of the value of γ and the number of terms in the series.

Those results are quite interesting because the point to the same characteristics already obtained by other methods while controlling the semiclassical contribution, to some extent at least, by means of the number of contributing terms.

Conclusions

In this paper we have shown how one can **separate** a semiclassical contribution for the spatial density of a nuclear system from a **full** many-body mean-field Wigner function. Our main point here is that the separation technique proposed does

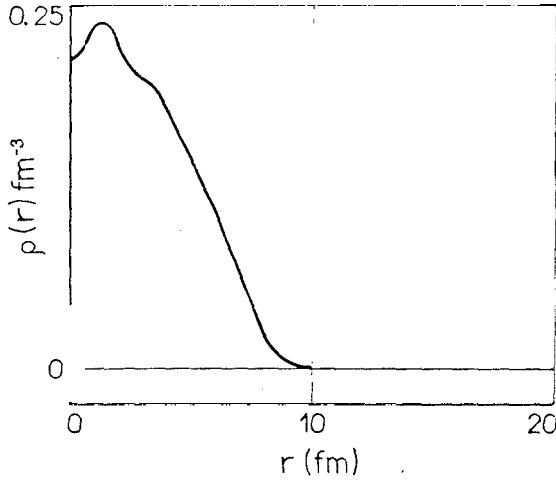


Fig. 4 - The exact spatial density for 224 particles in a three dimensional isotropic harmonic oscillator.

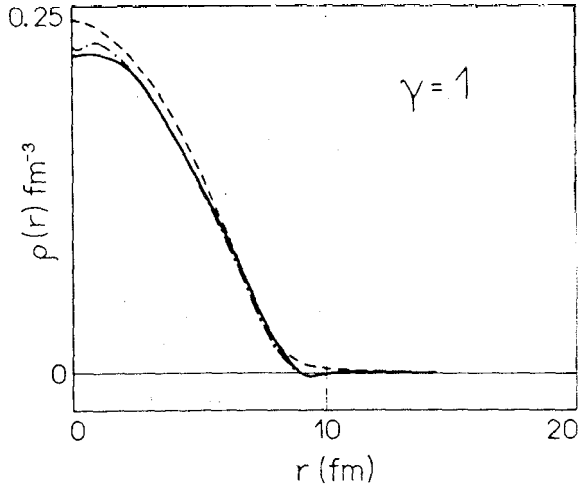


Fig. 5 - Semiclassical spatial density for the same system $\gamma = 1$ and three truncation levels: solid line 5 terms, dashed line 9 terms and dot-dashed line 10 terms.

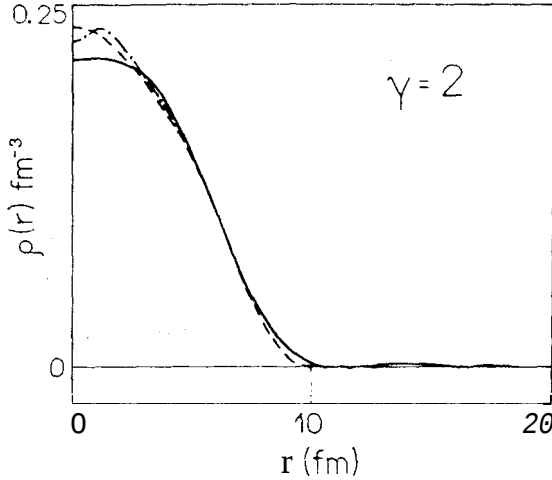


Fig. 6 - Semiclassical spatial density for the same system $\gamma = 2$ and three truncation levels: solid line 6 terms, dashed line 9 terms and dot-dashed line 22 terms.

not correspond to the usual ones, namely, the smearing of the the occupation numbers via the introduction of a temperature or Strutinskii's prescription. It is not equivalent, either, to the well known folding schemes in which the smeared Wigner function is obtained through integration of a distribution built from a coherent state or wave packet. Although akin to Strutinskii's method, the present approach differs from it in the way one constructs the separation. In our proposal we keep of the control relation of quantum corrections to the smooth part.

In writing the identity that permits the separation, a fundamental role is played by the characteristic width associated to the wave functions constituting the basis set. As we have developed our calculations for bound state systems, that width appeared naturally as the harmonic oscillator one. We raw that the ratio γ between the characteristic width of the basis states and that associated to the Wigner function, γ , plays the role of a control parameter for the separation of the semiclassical contribution. This parameter, in the harmonic oscillator case, exhibits a critical value, $\gamma_c = 1/\sqrt{2}$, above which one can always find a semiclassical part of the full Wigner functions. This effect can be easily understood as a coarse grainning in a

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chosen sector of the quantum phase space; if $\gamma > \gamma_c$, we are smearing the q-sector, while for $\gamma < \gamma_c$, we are smearing the p-sector. So, whenever we consider values of γ greater than γ_c , we are able to write a semiclassical density in the q-variable provided we use a convenient number of terms in the sum defining that contribution. The calculations completely confirm this interpretation; in particular, our results for the spatial density of a harmonic oscillator system can always be fitted to the results obtained with the Modified Thomas Fermi approach¹⁵.

As a final remark we observe that, since the harmonic oscillator Wigner functions constitute a basis set for the quantum phase space description of bound state systems, we can always decompose general bound state functions in that basis and then apply our approach.

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Resumo

Apresentamos uma descrição da densidade espacial de um sistema nuclear a partir da função de Wigner definida num espaço de fase quântico. Mostramos, num exemplo analítico, como médias no setor de momentos desse espaço de fase podem produzir uma descrição semiclássica da densidade espacial. Esses resultados indicam uma nova maneira de se entender dados para densidades espaciais de sistemas nucleares.