Wigner function and the one-sided flux

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We calculate the Wigner function of the one-body density of a system of 32 independent particles moving in two adjacent cubic boxes communicating through a window. We discuss the applicability of the currently used definition of the classical analog of the one-sided flux obtained from the Wigner function.

[NUCLEAR REACTIONS Wigner function for a simple quantum mechanical model, nucleon exchange, static one-sided flux.]

The static one-sided current is used as a measure of the dissipation rate produced by nucleon exchange between colliding nuclei.[1–3] In the simplest form of his model Swiatecki[1] assumes that the nucleons are exchanged via a sharply defined window. Randrup[3] has taken into account the diffuseness of the nuclear surface in the Thomas-Fermi model and applied the proximity concept to derive the one-sided current as a function of the separation distance between nuclei. Within the same concept penetrability effects[4–6] and temperature dependence[4] have been considered.

Recently attempts to derive the one-sided current on a more microscopic basis have been made.[7,8] These calculations have a quantum-mechanical input. They are based on the knowledge of the wave functions given by time-dependent[7] or adiabatic time-dependent[8] Hartree-Fock calculations, from which the Wigner distribution function $f(\vec{r},\vec{k},t)$ of the one-body density can be constructed. Then the classical analog of the one-sided flux in the z direction is defined as

$$j_+(\vec{r},t)=\frac{\hbar}{m}\int_{k_z\geq 0} d^3k\, k_z f(\vec{r},\vec{k},t) . \tag{1}$$

Feldmeier[9] has also defined a quantum mechanical operator for the one-sided current. If the flux is oriented in the z direction, the expectation value of this operator amounts to expression (1).

In the present work we want to discuss the applicability of Eq. (1). This is related to the fact that, contrary to the classical distribution function, the Wigner function can have regions of negative values and make the quantity (1) negative. In such cases some care must be taken.

We limit our discussion to the static case by using the simple three-dimensional quantum mechanical model introduced in Ref. 10. This model can be briefly described as follows. We consider two adjacent hard-walled cubes of length L on each edge. They communicate through a window situated in the plane $z=0$ and which extends from $x=-w$ to $x=w$ and from $y=-(L/2)$ to $y=L/2$. The system is therefore symmetric with respect to reflections through each coordinate. As the parity $\pi_i=\pm 1$ $(i=x,y,z)$ is conserved, the basis functions are

$$\begin{aligned} u_{n_i}^{\pi_i}(i) &= \left[\frac{2}{L_i}\right]^{1/2} \cos\frac{n_i\pi}{L_i}i\ ;\quad \pi_i=+1\ ,\quad n_i \text{ odd} \\ &= \left[\frac{2}{L_i}\right]^{1/2} \sin\frac{n_i\pi}{L_i}i\ ;\quad \pi_i=-1\ ,\quad n_i \text{ even} \end{aligned} \tag{2}$$

with $L_x=L_y=L$ and $L_z=2L$. The total parity is $\pi=\pi_x\pi_y\pi_z$ and the wave functions ψ_α^π defined inside the volume occupied by the two cubes can be expanded in terms of the basis set (2)

$$\psi_\alpha^\pi=u_{n_y}^{\pi_y}(y)\sum_n C_{\alpha n}^p u_{n_x}^{\pi_x}(x)u_{n_z}^{\pi_z}(z) , \tag{3}$$

where $n=(n_x,n_z)$ and $p=\pi_x\pi_z$.

The intermediate wall in which the window has been created can be simulated by the following potential:

$$V=\lambda\delta(z)\theta(|x|-w) . \tag{4}$$

An alternative description has been given in Ref. 10. The Schrödinger equation with the potential (4) becomes the following matrix equation:

$$\sum_{n'}[(E_n^p-E_\alpha^p)\delta_{nn'}+V_{nn'}^p]C_{\alpha n'}^p=0 , \tag{5}$$

where

$$E_n^p=\frac{\hbar^2}{2m}\frac{\pi^2}{L^2}(n_x^2+\tfrac{1}{4}n_z^2) \tag{6}$$

and

$$V^p_{nn'}=\lambda\left[\frac{2}{L}\right]^2\left[-\frac{L}{\pi}\left[\frac{\sin\frac{\pi}{L}(n_x+n_x')w}{n_x+n_x'}+p\frac{\sin\frac{\pi}{L}(n_x-n_x')w}{n_x-n_x'}\right]\right]\ ;\ n_x\neq n_x'$$

$$=\lambda\left[\frac{2}{L}\right]^2\left[\frac{L}{2}-w-p\frac{L}{2\pi n_x}\sin\frac{2\pi n_x}{L}w\right]\ ;\ n_x=n_x'\ . \tag{7}$$

This expression holds for n_z and n_z' odd only. Otherwise the basis set (2) implies automatically

$$V^p_{nn'}=0 \text{ for } \pi_z=-1\ , \tag{8}$$

equivalent to $C^p_{\alpha n}=\delta_{\alpha n}$. One can notice that the variable y plays no role in solving Eq. (5). This is due to the fact that the window has a constant width $2w$ along the y axis, which allowed the factorization (3). For solving numerically one must truncate the sum in Eq. (5). Let us call N the maximum value taken by n_z in the truncated space. The case $N+1$ even reduces to N odd due to (8). For N odd, n_x runs up to N for $p=+1$ and up to $N-1$ for $p=-1$. Then at fixed w the model has two parameters, N and λ. The choice of the range of λ and the convergence with respect to N has been studied in Ref. 10. As an example here we take $L=4.548$ fm and $w=1$ fm, i.e., a window about one third of the box size, and solve Eq. (5) for $\lambda=10^5$ MeV fm and $N=27$. According to Ref. 10 these values achieve the cancellation of the wave function at the intermediate wall to a very good approximation.

The Wigner transform of the one-body density is

$$f(\vec{r},\vec{k})=\sum_{\alpha,\pi} f^\pi_\alpha(\vec{r},\vec{k})\ , \tag{9}$$

where α runs over all occupied states of both parities π and

$$f^\pi_\alpha(\vec{r},\vec{k})=\frac{1}{(2\pi)^3}\int d^3s\, e^{-i\vec{k}\cdot\vec{s}}\left[\psi^\pi_\alpha\left[\vec{r}+\frac{\vec{s}}{2}\right]\right]^* \times\psi^\pi_\alpha\left[\vec{r}-\frac{\vec{s}}{2}\right]\ . \tag{10}$$

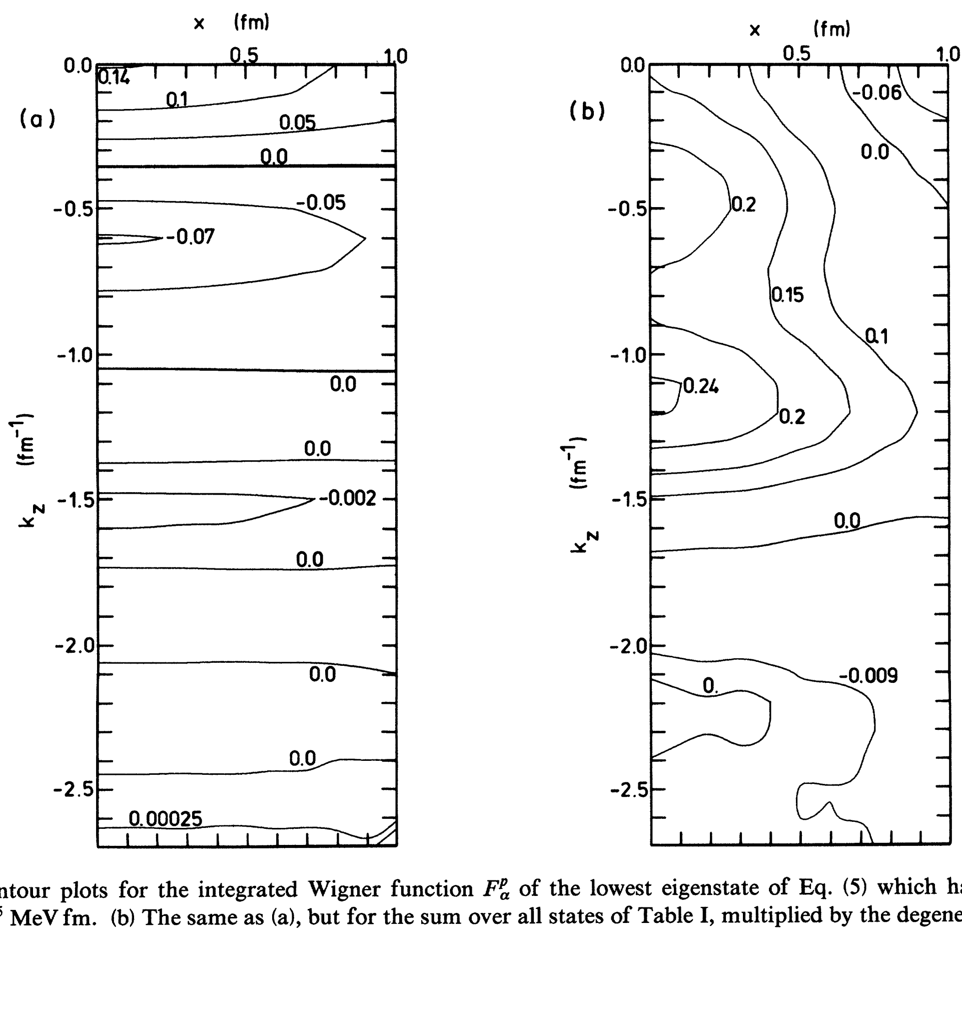

FIG. 1. (a) Contour plots for the integrated Wigner function F^p_α of the lowest eigenstate of Eq. (5) which has been solved for $N=27$ and $\lambda=10^5$ MeV fm. (b) The same as (a), but for the sum over all states of Table I, multiplied by the degeneracy factor 4.

Here we want to calculate the one-sided flux at and perpendicular to the window. Then the quantity of interest is the Wigner function evaluated at $z=0$ and integrated over the variables y, k_x, and k_y. For fixed α and p let us call it

$$F^p_\alpha(x,k_z)=\int_{-(L/2)}^{L/2} dy \int_{-\infty}^{\infty} dk_x \int_{-\infty}^{\infty} dk_y f^p_\alpha(\vec{r},\vec{k})\,|_{z=0}\;. \tag{11}$$

Carrying out the integrations we obtain:

$$F^p_\alpha(x,k_z)=\frac{1}{4\pi L}\sum_{n,n'} C^p_{\alpha n} C^p_{\alpha n'} u^{\pi_x}_{n_x}(x)\, u^{\pi_x}_{n'_x}(x) \left\{ \frac{\sin\left[k_z+\frac{\pi(n_z-n'_z)}{2L}\right]2L}{k_z+\frac{\pi(n_z-n'_z)}{2L}} + \frac{\sin\left[k_z-\frac{\pi(n_z-n'_z)}{2L}\right]2L}{k_z-\frac{\pi(n_z-n'_z)}{2L}} + \frac{\sin\left[k_z+\frac{\pi(n_z+n'_z)}{2L}\right]2L}{k_z+\frac{\pi(n_z+n'_z)}{2L}} + \frac{\sin\left[k_z-\frac{\pi(n_z+n'_z)}{2L}\right]2L}{k_z-\frac{\pi(n_z+n'_z)}{2L}} \right\}. \tag{12}$$

At the window we define an average one-sided flux for each state α,π

$$(j^\pi_{+,\alpha})^{\rm av}=\frac{\hbar}{m}\frac{1}{2wL}\int_{-w}^{w} dx \int_{k_z\geq 0} dk_z k_z F^p_\alpha(x,k_z)\;, \tag{13}$$

where $2wL$ is the window area.

In a plane (x,k_z) the function (12) has reflectional symmetry with respect to both variables. Therefore only one quarter of this plane needs to be used to represent it and we have chosen the half axes $x>0$ and $k_z<0$. Throughout the whole of this work the values of N and λ have been fixed as mentioned. Figure 1(a) shows contour plots of the function (12) for $\alpha=1$ and $p=1$, i.e., the lowest eigenvalue of Eq. (5). The variable x runs through the opening of the window of size $w=1$ fm, and $|k_z|$ extends up to 2.7 fm^{-1}, i.e., well beyond the region where the function is practically zero. The contour plots show a simple structure. The function is positive only for $|k_z|<0.35\ \text{fm}^{-1}$. The integration over x and $|k_z|$ gives roughly zero but the one-sided flux (1) results from the product

$$k_zF^p_\alpha(x,k_z)=k_zF^p_\alpha(x,-k_z)$$

with $k_z>0$, which gives large weight to the negative values of F^p_α so that the average flux (13) turns out to be negative. The result is shown in Fig. 2(a) and is associated with state (1) or (4) from Table I. One can also see that these are not the only states which produce a negative flux at $w<1$ fm. By taking four or five occupied states the total flux remains negative, but the situation changes at larger w or when more states are occupied. The box size under consideration can accommodate 32 particles at density $\rho=0.17\ \text{fm}^{-3}$. Then all eight states from Table I must be occupied, each being four times degenerate. Sum-

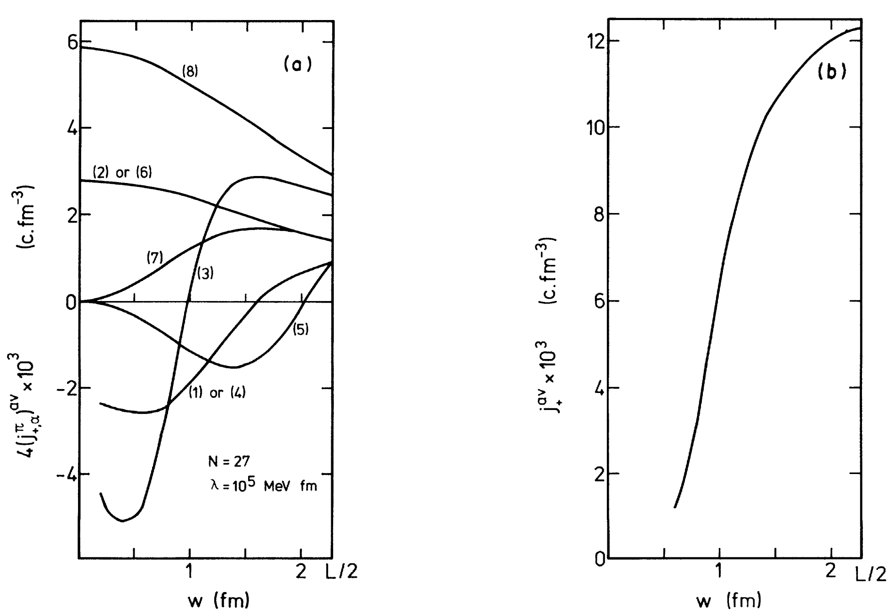

FIG. 2. (a) The partial average one-sided flux (13) as a function of w. Each curve gives four times the contribution of one of the states indicated in Table I. (b) The total average one-sided flux as a function of w for a system of 32 particles.

TABLE I. The lowest eight states in increasing order for E_α^π for a box of size $L=4.548$ fm and a window size $w=1$ fm. Equation (5) has been solved for $N=27$ and $\lambda=10^5$ MeV fm. The columns indicate the following: π_i—the parity for $i=x,y,z$; α—the eigenvalues E_α^p of Eq. (5) in increasing order,

$$\epsilon_{n_y}^{\pi_y}=\frac{\hbar^2}{2m}\left[\frac{\pi}{L}\right]^2 n_y^2$$

and

$$E_\alpha^\pi=E_\alpha^p+\epsilon_{n_y}^{\pi_y} .$$

State	π_x	π_y	π_z	α	E_α^p	$\epsilon_{n_y}^{\pi_y}$	E_α^π
1	+1	+1	+1	1	17.60	9.90	27.50
2	+1	+1	−1	2	19.80	9.90	29.70
3	+1	+1	+1	3	40.71	9.90	50.61
4	+1	−1	+1	1	17.60	39.60	57.20
5	−1	+1	+1	4	49.40	9.90	59.30
6	+1	−1	−1	2	19.80	39.60	59.40
7	−1	+1	−1	5	49.50	9.90	59.40
8	+1	+1	−1	5	49.50	9.90	59.40

ming up all the corresponding functions F_α^p we obtain the result of Fig. 1(b). The function has more structure and is positive in a large region, reaching a maximum at $|k_z|\sim 1.15\ \text{fm}^{-1}$. Altogether this produces a positive average flux shown in Fig. 2(b). In detail this happens as follows: The total average flux is the sum of all partial contributions from Fig. 2(a). The states with $\pi_z=-1$ give rise to a positive flux at any w. One can see that at small w there is almost a compensation for pairs of states, one with $\pi_z=+1$ and the other with $\pi_z=-1$, so that the flux remains small but positive. Around $w\simeq 1$ fm the rise in the flux is dominated by the third occupied state, and beyond $w=1$ fm the positive contributions dominate. We found that such a description holds for any N between 5 and 39 when λ takes a value in the range 10^3–10^6 MeV fm. In Fig. 2(b) the region $w<0.6$ fm has been omitted because $N=27$ is not yet large enough to give a satisfactory cancellation of the wave function at the intermediate wall. As mentioned in Ref. 10, at $w<0.8$ fm we must take $N>39$ for having such a condition fulfilled.

The conclusion we would like to draw is that some care must be taken in using the definition (1) of the one-sided flux for a quantum system. When the number of occupied states is not large enough the result might be negative and the result does not have a meaning. But when the system contains a sufficient number of particles the result can be interpreted as the classical analog of the one-sided flux. A detailed analysis of the one-sided current resulting from other quantum-mechanical models might bring more insight into the problem.

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