QUANTUM MECHANICAL MODEL FOR THE ONE-SIDED FLUX IN HEAVY ION COLLISIONS

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We construct a three-dimensional quantum mechanical model relevant for nucleon transfer in heavy ion collisions. It consists of two adjacent cubic boxes with a rectangular window in the wall which separates them. We calculate the one-sided flux as a function of the window size and compare it with previous results.

In heavy ion collisions the flow of particles through the region of contact between interacting nuclei is an important source of dissipation. The classical window formula of Swiatecki [1] gives a simple method [2] for deriving the friction force in terms of the static one-way mass current. Randrup [3,4] has used the proximity approach to calculate the particle flow during a nucleus–nucleus collision. As it will be later discussed the technique was semi-classical inasmuch as it utilizes the Thomas–Fermi model for the density and momentum distribution. The flux was evaluated at the window plane from the product p^3v where p and v are the local Fermi momentum and velocity related through a space dependent effective mass.

In the present work we construct a simple three-dimensional quantum mechanical independent particle model for the interacting nuclei. The wave functions are obtained numerically and the one-sided flux is calculated from the associated Wigner function. We obtain the total flux as a function of the window size for a composite system of 32 particles and make a comparison with Randrup's proximity results [3].

Our model consists of two adjacent hard-walled cubes having a length L on each edge, communicating through a window. The geometry is shown in fig. 1. The window plane is $z = 0$. The window extends from

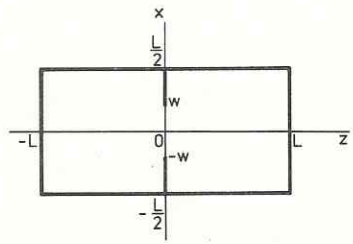

Fig. 1. The geometry of the model in the plane y = const.

$x = -w$ to $x = w$, independent of y. Hence the y-dependence of the wave function clearly factorizes while the x- and z-dependence does not.

With the center-of-coordinates at the middle of the window the hamiltonian possesses symmetry with respect to reflection through each of the coordinate axes. We specify the reflectional quantum numbers by π_x, π_y and π_z, each assuming the possible values ±1. We choose the basis functions ($i = x, y$ or z)

$$u^{\pi_i}_{n_i}(i) = (2/L_i)^{1/2} \times \cos(n_i\pi/L_i)i\,, \quad \pi_i = +1\,, \quad n_i \text{ odd}\,,$$

$$u^{\pi_i}_{n_i}(i) = (2/L_i)^{1/2} \times \sin(n_i\pi/L_i)i\,, \quad \pi_i = -1\,, \quad n_i \text{ even}\,, \qquad (1)$$

with $L_x = L_y = L$ and $L_z = 2L$. These functions vanish on the planes $i = \pm L_i/2$; $u^-_{n_z}$ vanishes also at $z = 0$ but $u^+_{n_z}$ does not. If we denote $\pi_x\pi_y\pi_x = \pi$ the system is described by the functions ψ^π_α defined only inside the volume occupied by the two cubes. We expand them in terms of the complete basis states

$$\psi^\pi_\alpha(r) = u^{\pi y}_{n_y}(y) \sum_{n_x n_z} C^{\pi x \pi z}_{\alpha, n_x n_z} u^{\pi x}_{n_x}(x) u^{\pi z}_{n_z}(z) . \qquad (2)$$

Each term satisfies the outside boundary conditions and continuity across the window. The vanishing of the wave function on the separating wall ($z = 0$, $w < |x| < L/2$) is automatic for $\pi_z = -1$ states where

$$C^{\pi x -}_{\alpha, n_x n_z} = \delta_{\alpha, n_x n_z},$$

but because in practical calculations the summation in (2) must be truncated this boundary condition is achieved only approximately for $\pi_z = +1$ states.

In order to impose the interface condition we introduce the quantity

$$I^\pi_\alpha = \int_{w<|x|<L/2} |\psi^\pi_\alpha(x, y, 0)|^2 \, dx \, dy , \qquad (3)$$

which we minimize with respect to $C^{\pi x \pi z}_{\alpha, n_x n_z}$ in a manner similar to the method of Lagrange multipliers, i.e. we minimize the expression

$$\langle \psi^\pi_\alpha | T - E^\pi_\alpha | \psi^\pi_\alpha \rangle + \lambda I^\pi_\alpha , \qquad (4)$$

where T is the kinetic energy operator, E^π_α is the Lagrange multiplier for the normalization condition and λ is a positive parameter. The minimization procedure leads to the matrix equation

$$\sum_{n'} [(\epsilon^\pi_n - E^\pi_\alpha)\delta_{nn'} + V^\pi_{nn'}] C^\pi_{\alpha n'} = 0 , \qquad (5)$$

where ϵ^π_n are the kinetic energy eigenvalues of the basis states and $V^\pi_{nn'}$ is the matrix element of the "potential"

$$V = \lambda\delta(z)\theta(|x| - w) , \qquad (6)$$

with $n = (n_x, n_z)$. Trivially $V^\pi_{nn'} = 0$ for $\pi_z = -1$. As the number of terms in the basis set increases the dependence on λ of the physical results should decrease. This is indeed verified below.

Let us now define the total averaged one-sided flux as:

$$j(w) = \sum_{\pi, \alpha(\mathrm{occ})} j^\pi_\alpha(w) , \qquad (7)$$

where the contribution of each single particle state ψ^π_α is given by

$$j^\pi_\alpha(w) = \frac{1}{2wL} \int_{-L/2}^{L/2} dy \int_{-w}^{w} dx \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \int_{0}^{\infty} dp_z \frac{p_z}{m}$$

$$\times f^\pi_\alpha(x, y, 0, p_x, p_y, p_z) . \qquad (8)$$

In the above expression the one-sided flux perpendicular to the window has been integrated over the window and divided by its area $2wL$; the integrand contains the Wigner function

$$f^\pi_\alpha(r, p) = \frac{1}{(2\pi)^3} \int d^3s \exp[-(i/\hbar)p \cdot s]$$

$$\times \psi^\pi_\alpha(r + \tfrac{1}{2}s) \psi^\pi_\alpha(r - \tfrac{1}{2}s) , \qquad (9)$$

taken at $z = 0$. Its integration over p_x and p_y gives

$$\int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \, f^\pi_\alpha(r, p)\Big|_{z=0}$$

$$= [u^{\pi y}_{n_y}(y)]^2 \sum_{n, n'} C^{\pi x \pi z}_{\alpha n} C^{\pi x, \pi z}_{\alpha n'} u^{\pi x}_{n_x}(x) u^{\pi x}_{n'_x}(x)$$

$$\times \frac{1}{2\pi} \int_{-2L}^{2L} ds \exp[(-i/\hbar)p_z s] u^{\pi z}_{n_z}(\tfrac{1}{2}s) u^{\pi z}_{n'_z}(-\tfrac{1}{2}s) . \qquad (10)$$

The Wigner function can have regions of negative values which lead to negative j^π_α. This is not surprising because j^π_α is not an observable quantity [5,6]. However the summation over all occupied states in (7) turns out to be positive. The formula (8) is consistent with the quantum mechanical operator introduced by Feldmeier [7].

Calculations have been made for cubes of size $L = 4.548$ fm. The system contains 32 particles at density $\rho_0 = 0.17$ fm^{-3}. Spin and isospin degeneracy is assumed. A simple scaling relation permits reinterpretation of the results to other L-values and corresponding densities. The window size is varied with an increment $\Delta w = 0.2$ fm in the interval 0.8 fm to $L/2$. The region $w < 0.8$ fm has not been explored due to computational limitations.

In the limit $I^\pi_\alpha \to 0$ (infinite basis) the results should be independent on λ. Hence the spirit of the model is to find a region of λ where quantities of in-

Table 1
The eigenvalues of the lowest states $[\alpha = 1, \pi_x = \pi_z = 1]$ $[\alpha = 2, \pi_x = \pi_z = 1]$ and $[\alpha = 3, \pi_x = -1, \pi_z = +1]$ as a function of λ (MeV fm) and $N = \max(n_z)$. The term $(\hbar^2/2m) \times [(\pi/L)n_y]^2$ has not been included, as in eq. (5).

Eigenvalue	λ	N			
		19	23	27	31
E_1^+	10^4	17.66	17.49	17.37	17.28
	10^5	18.01	17.78	17.60	17.48
	10^6	18.23	17.99	17.82	17.69
E_2^+	10^4	40.80	40.36	40.05	39.82
	10^5	41.94	41.21	40.71	40.37
	10^6	42.71	41.90	41.39	41.01
E_3^-	10^4	49.49	49.38	49.30	49.24
	10^5	49.59	49.48	49.40	49.33
	10^6	49.68	49.55	49.45	49.38

terest vary very slowly with λ i.e. show the tendency of forming a plateau. Once this region is established we increase the basis set with the intent of reaching convergence. As a typical example we show results for $w = 1$ fm. First let us consider the lowest eigenvalues E_α^π for $\pi_z = \pi_y = +1$ since the states with $\pi_z = -1$ are exact and $\pi_y = -1$ gives equivalent information to $\pi_y = +1$. They are shown in table 1 as a function of λ and $N = \max(n_z)$ i.e. the maximum value taken by n_z in a fixed basis set. One can see very good stability with respect to λ and this stability increases as N increases. Second, in fig. 2 we plot the integrated probability

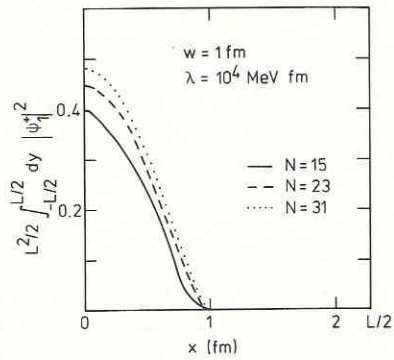

Fig. 2. The y-integrated probability for the lowest state $\alpha = 1$, $\pi_x = \pi_z = 1$ in the window plane $z = 0$ as a function of x at $N = 15$, 23 and 31 and $\lambda = 10^4$ MeV fm. The window size is $w = 1$ fm.

$$\frac{L^2}{2} \int_{-L/2}^{L/2} \mathrm{d}y |\psi_1^+(r)|^2 ,$$

for the lowest state $\alpha = 1, \pi_x = \pi_z = +1$ as a function of x in the window plane $z = 0$. The value of λ is 10^4 MeV fm and we take $N = 15$, 23 and 31 in order to show that by increasing the basis set the wave function becomes better localized in the window interval. The localization decreases with increasing the single particle energy E_α^π. An interesting quantity is Δx, the root mean square spread of the probability in the window plane. This is included in table 2 for the lowest three eigenstates $[\alpha = 1, \pi_x = \pi_z = 1]$, $[\alpha = 2, \pi_x = \pi_z = 1]$ and $[\alpha = 3, \pi_x = -1, \pi_z = 1]$. The range of val-

Table 2
The one-sided flux j and the root mean square probability spread Δx of the $\pi_z = 1$ occupied states as a function of w. The second column gives $N = \max(n_z)$ for the corresponding basis set used in the calculations, the third column gives the range of λ where the flux tends towards a plateau. The other columns indicate the values of Δx or j at the edges of the "plateau".

w (fm)	N	λ (MeV fm)	Δx (fm)			$j \times 10^3$ (c fm^{-3})
			$\alpha = 1$, $\pi_x = \pi_z = 1$	$\alpha = 2$, $\pi_x = \pi_z = 1$	$\alpha = 3$, $\pi_x = -1$, $\pi_z = 1$	
0.8	39	$10^4 - 10^6$	0.33 – 0.30	0.33 – 0.30	0.49 – 0.45	4.16 – 2.78
1.0	31	$10^4 - 10^6$	0.41 – 0.38	0.40 – 0.37	0.60 – 0.55	7.19 – 5.58
1.2	27	$10^4 - 10^6$	0.48 – 0.45	0.48 – 0.45	0.71 – 0.66	9.36 – 8.00
1.4	27	$10^4 - 10^6$	0.56 – 0.53	0.55 – 0.52	0.82 – 0.77	10.61 – 9.55
1.6	27	$10^3 - 10^6$	0.66 – 0.61	0.65 – 0.60	0.96 – 0.88	11.97 – 10.37
1.8	27	$10^3 - 10^6$	0.73 – 0.68	0.72 – 0.67	1.06 – 1.00	12.44 – 11.44
2.0	27	$10^3 - 10^6$	0.78 – 0.75	0.77 – 0.73	1.14 – 1.08	12.72 – 11.55
$L/2$	27		0.82	0.82	1.46	12.29

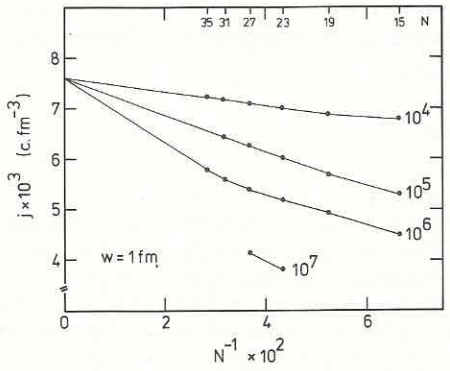

Fig. 3. The total averaged one-sided flux as a function of $1/N$ for $\lambda = 10^4, 10^5, 10^6$ and 10^7 MeV fm and $w = 1$ fm. The points are the calculated values. The lines are interpolations or extrapolations of the calculations. The upper scale gives the values of N.

ues given in table 2 for Δx and j correspond to the edge values of λ in the region where the flux is close to a plateau. This range of λ is also indicated in table 2 and one can see that it increases with the window size w. At each w we have given the results corresponding to the largest basis set, indicated by N, for which calculations have been performed. As w decreases it was necessary to increase N. The dimension of the matrix to be diagonalized is $(N+1)^2/4$ for $\pi_x = +1$ and $(N^2-1)/4$ for $\pi_x = -1$. The convergence at fixed $w = 1$ fm is best illustrated in fig. 3 where we have plotted the flux as a function of $1/N$. The lines connect values of the flux at fixed $\lambda = 10^4, 10^5, 10^6$ and 10^7 MeV fm. When N increases the lines get closer to each other. By assuming a linear dependence on $1/N$ we extrapolate the lines towards $N \to \infty$. The values obtained for the current $J(w) = 2wLj(w)$ from this extrapolation procedure are drawn in fig. 4 as a function of wk_F where $k_F = 1.36$ fm^{-1}. We can compare it with

$$J^{\text{open}} = 2wLj^{\text{open}} , \tag{11}$$

where j^{open} is the normal one-way flux of particles when the window is fully open. For a system of 32 particles in its ground state we have

$$j^{\text{open}} = \frac{\hbar}{m}\frac{1}{L^4}\sum_{n_z=1}^{4} n_z \,\mathrm{Si}(\pi n_z) = 12.29 \times 10^{-3}\, c\ \text{fm}^{-3} , \tag{12}$$

where $\mathrm{Si}(x)$ is the sine integral function [8]. In the

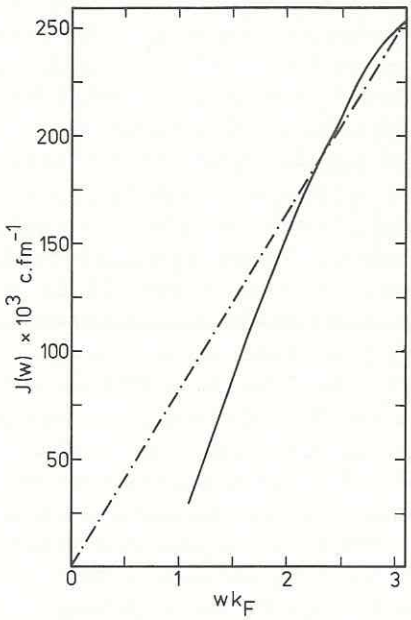

Fig. 4. The total current J as a function of wk_F with $k_F = 1.36$ fm^{-1}. Full line: our result as explained in the text. Dashed–dotted line: J^{open} of eqs. (11) and (12).

limit $L \to \infty$ this corresponds to the bulk flux n_0 considered by Randrup

$$j^{\text{open}} \xrightarrow[L\to\infty]{} j_0 = n_0/m = \tfrac{3}{16}(\hbar/m)k_F\rho_0$$

$$= 9.1 \times 10^{-3}\, c\ \text{fm}^{-3} , \tag{13}$$

for $k_F = 1.36$ fm^{-1} and $\rho_0 = 0.17$ fm^{-3}.

The variation with respect to w in $J(w)$ arises from wave effects. The vanishing of the wave function at the window edge reduces the effective window size and decreases the current. In fig. 4 we can distinguish two regions. For $wk_F \lesssim 2.3$, $J(w)$ is smaller and drops faster to zero than the classical value J^{open} when w decreases. By contrast at $wk_F > 2.3$, $J(w)$ is a few percent higher than J^{open}. Such a small difference between the classical and quantum mechanical values is not surprising at large window sizes.

The difference between j^{open} and j_0 is an expression of the finite size effects and is independent of w. The value of j_0 from eq. (13) can be used within proximity concept [3,4] where finite nuclei are replaced by semi-infinite slabs. At zero separation distance between the nuclear surfaces the proximity current is of

the order 3×10^{22} s^{-1} for $^{16}O + ^{16}O$. At maximum opening our result is closer to the maximum value (closest approach) of $\sim 8 \times 10^{22}$ s^{-1} of the one-way current derived [9] from time dependent Hartree–Fock calculations at 1.25 MeV/nucleon.

In order to make a detailed comparison between our results and Randrup's proximity current it is necessary to find a correspondence between w and the surface separation s. A possibility would be to identify [10] the window areas of both models. But in comparing our slit model with Randrup's proximity current we must emphasize the differences and complementarity of the models. In the slit model the current decreases with the window size due to wave mechanical effects; the flux "incident" on the window is characterized by the mean density of the box and each occupied state contributes. Randrup uses a semi-classical model (no diffraction) and only particles with an energy higher than the barrier top contribute to the flux in the window area. The current decreases with the increase of the barrier height i.e. with the separation distance.

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