TEST OF THE VALIDITY OF THE DENSITY MATRIX EXPANSION METHOD FOR ION–ION COLLISION PROCESS

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(Received January 18, 1996)

In the present work, we test the validity of replacing the nondiagonal densities $\rho(\vec{r},\vec{r}')$ appearing in the exchange part of the nucleus-nucleus optical potential by an approximation based on the density matrix expansion (DME) used frequently in nuclear structure calculations. This procedure has been used recently by many authors in driving the real nucleus-nucleus potential. We have found that for M3Y-Paris nucleon-nucleon interaction the use of DME may produce a maximum error of 12% in the nucleus-nucleus potential.

PACS numbers: 24.10.-i, 25.90.+k

1. Introduction

Recently successful trials have been performed to determine the nuclear equation of state which is important in both nuclear physics and astrophysics from nucleus-nucleus elastic scattering [1]. The heavy ion (HI) processes are described successfully using the optical model potential. During the last decade, the double-folding model [2] has been widely used by many groups [1–7] in deriving the real part of HI potential. Besides the computational simplicity of the double-folding model, it is very appealing because it emerges naturally from a nuclear many body approach. The simple double-folding model [2] which reproduce correctly the tail region of the real optical model potential failed to give a good description to the experimental data in certain cases such as nuclear rainbow scattering observed in α-particles [3] and latter on for other light HI systems [4]. In these cases the data are sensitive to the real optical model potential over a wider radial domain and not only to the tail region of the HI potential [5]. Moreover, a more realistic shape of the real part of the HI potential is needed to study

the equation of state for cold nuclear matter and consequently to determine its nuclear incompressibility [1]. Therefore, many further developments of the simple-folding model have been made to obtain a correct HI real potential over the whole radial domain. The most important approach in this direction is to treat the exchange term (U_E) of the real HI potential correctly. Instead of approximating it by a zero-range force [6], several authors [5, 7, 8] suggested to keep U_E as it is and to approximate the nuclear densities $\rho(\vec{r}, \vec{r}')$ appearing in U_E using an expression derived from the density matrix expansion (DME) of Negele and Vautherin [9]. Since the accuracy of replacing $\rho(\vec{r}, \vec{r}')$ by a DME expression has been examined in nuclear structure calculation [10], a test of this procedure in deriving the ion-ion potential is needed.

The aim of the present paper is to test the validity of approximating the non-diagonal densities $\rho(\vec{r}, \vec{r}')$ appearing in U_E by an expression based on the DME approximation. This approximation has been used recently by many authors [5, 7, 8] in calculating the real optical potential. To test its validity in HI scattering we consider the two nuclear interacting pairs O^{16}–O^{16} and Ca^{40}–Ca^{40} and we calculate the real part of the interaction potential (U) for each pair at different incident energies. For each case, we first calculate U_E using harmonic oscillator wave functions to construct $\rho(\vec{r}, \vec{r}')$. We compare the HI potential derived by this method with that calculated using DME method to approximate $\rho(\vec{r}, \vec{r}')$. In the present study, we shall use the so-called M3Y nucleon-nucleon (NN) interaction based on the G-matrix elements of the Paris [11] (M3Y-Paris) potential.

The next section briefly present the derivation of the HI real potential using an approximation based on the DME method. Our results are given in Section 3.

2. Formalism

The direct part of the nucleus-nucleus potential is obtained by the usual folding procedure [2, 7]

$$U_D(R) = \int \rho_1(\vec{r}_1)\rho_2(\vec{r}_2)\nu_D(S)dr_1dr_2, \qquad \vec{S} = \vec{r}_2 - \vec{r}_1 + \vec{R}, \qquad (1)$$

where $\nu_D(S)$ is the direct part of the effective N-N interaction, ρ_i $(i = 1, 2)$ are the densities of the two colliding nuclei and R is the distance between the centers of the two interacting nuclei.

The exchange part, in general, must be nonlocal [8]. Since the exact treatment of nonlocal exchange term is too complicated in numerical calculations, one usually obtains the equivalent local potential by representing the relative-motion wave function of nucleons by a plane wave. In such an assumption the exchange potential is the following fully antisymmetrized matrix element of the exchange part, $\nu_E(S)$, of the effective N-N interaction (see Ref. [7])

$$U_E(R) = \sum_{\substack{i\in A_P \\ j\in A_T}} \langle ij|\nu_E|ji\rangle \,, \tag{2}$$

where $|i\rangle$ and $|j\rangle$ refer to the single particle wave functions of the projectile (A_P) and target (A_T), respectively. By introducing the one-body density $\rho(r, r')$, one can explicitly write equation (2) as [7]

$$U_E(R) = \int \rho_1(\vec{r}_1, \vec{r}_1 + \vec{S})\rho_2(\vec{r}_2, \vec{r}_2 - \vec{S})\nu_E(S) \exp\left[i\vec{K}(R)\frac{\vec{S}}{M}\right] d\vec{r}_1 d\vec{r}_2 \,, \tag{3}$$

where $|K(R)|$ is the relative-motion momentum given by [8]

$$K^2(R) = \frac{2mM}{\hbar^2}[E_{\text{C.M.}} - U(R) - V_C(R)] \tag{4}$$

with $M[= A_P A_T/(A_P + A_T)]$ and $E_{\text{C.M.}}$ are the reduced mass and the relative energy in the center-of-mass system, respectively and m is the nucleon mass. In equation (4), $U(R) = U_D(R) + U_E(R)$ and $V_C(R)$ are the total nuclear and Coulomb potentials, respectively. In order to simplify the numerical calculation of U_E, many authors [5, 7, 8] have used an approximation for the density matrix [10] derived from DME of Negele and Vautherin [9]. This approximation is

$$\rho(\vec{R}, \vec{R} + \vec{S}) = \rho\left(\vec{R} + \frac{\vec{S}}{2}\right)\hat{j}_1\left[K_{\text{eff}}\left(\left|\vec{R} + \frac{\vec{S}}{2}\right|\right)S\right] , \tag{5}$$

where

$$K^2_{\text{eff}}(r) = \frac{5}{3\rho(r)}\left[\tau(r) - \frac{1}{4}\nabla^2\rho(r)\right] ,$$

and

$$\hat{j}_1(x) = \frac{3}{x}j_1(x) = 3\frac{\sin x - x\cos x}{x^2} \,.$$

In the present work we shall consider three different approximations for $\tau(r)$. They are used by many authors and are given by the following equations

$$\tau(r) = \frac{3}{5}K_f^2\rho(r) + \frac{1}{3}V^2\rho(r) + \frac{1}{36}\frac{|\nabla\rho(r)|^2}{\rho(r)}, \tag{6a}$$

$$\tau(r) = \frac{3}{5}K_f^2\rho(r) + \frac{1}{2}\nabla^2\rho(r), \tag{6b}$$

and

$$\tau(r) = \frac{3}{5}K_f^2\rho(r) + \frac{1}{3}\nabla^2\rho(r) + \frac{1}{4}\frac{|\nabla\rho(r)|^2}{\rho(r)}, \tag{6c}$$

where the first term in each equation is the Thomas–Fermi term with

$$K_f^2 = \left[\frac{3}{2}\pi^2\rho(r)\right]^{2/3}.$$

Equations (6a) and (6c) have been used to calculate the ion-ion potential in Refs. (7) and (13), respectively, while equation (6b) have been used in Ref. (12).

After some transformations one can obtain the exchange potential in the following form

$$U_E(R) = 4\pi\int_0^\infty \nu_E(S)S^2dS\int f_1(\vec{r},S)f_2(\vec{r}-R,S)j_0\left[K(R)\frac{S}{M}\right]d\vec{r}, \tag{7}$$

where

$$f_{1,2}(\vec{r},S) = \rho_{1,2}(r)\hat{j}_1[K_{\text{eff}_{1,2}}(r)S],$$

and

$$j_0(x) = \frac{\sin x}{x}.$$

The total ion-ion potential $U(R)$ is obtained from equations (1) and (7) either by using the Bessel function expansion approximation described in Ref. (7) or by the iteration procedure (13). For M3Y-Paris [11] NN force, the direct $\nu_D(S)$ and the exchange $\nu_E(S)$ components are respectively

$$\nu_D(S) = 11061.625\frac{\exp(-4S)}{4S} - 2537.5\frac{\exp(-2.5S)}{2.5S}, \tag{8}$$

$$\nu_E(S) = 1524.25\frac{\exp(-4S)}{4S} - 518.75\frac{\exp(-2.5S)}{2.5S} - 7.8474\frac{\exp(-0.7072S)}{0.7072S}. \tag{9}$$

3. Results and discussion

We use the generalized double-folding model discussed in the previous section to calculate the HI optical potential for O^{16}–O^{16} and Ca^{40}–Ca^{40} pairs. Let us denote the HI potential $U(R)$ calculated using equations (1) and (7) with $\tau(r)$ defined by equations (6a), (6b) and (6c) by $U_1(r)$, $U_2(r)$ and $U_3(R)$, respectively. Also we denote the HI potential calculated without using DME method to approximate $\rho(\vec{r}, \vec{r}')$ by $U_{\text{exact}}(R)$.

Before making the ion-ion calculations, we checked the validity of approximation (5) by comparing it with the exact density matrices built up from harmonic oscillator wave functions. In Fig. 1 the validity of approximation (5) is demonstrated. In this figure we compare the exact normalized density matrix $\rho\left(\vec{R} + \frac{\vec{S}}{2}\right)/\rho(\vec{R})$ with $\hat{j}_1(KS)$ for a range of values of the distance from the center of the nucleus R. In calculating the non-diagonal density we have considered the two cases $\vec{S}$ parallel to $\vec{R}$ and $\vec{S}$ perpendicular to $\vec{R}$. The three approximations with $\tau(r)$ given by equations (6a), (6b) and (6c) are shown on the figures by the curves labelled PW1, PW2 and PW3, respectively.

Figure 1 shows that the first approximation for $\tau(r)$, given by equation (6a), is the best one in the region of the nuclear surface. The second approximation for $\tau(r)$ (Eq. (6b)) is good in the inner region and satisfactory at the nuclear surface. The third approximation is bad before and after the nuclear surface. Since the exchange NN force has a very short range we expect that only the small S values contribute to the exchange HI real potential. For $S \leq 1$ fm the first and second approximations of $\tau(r)$ reproduce well the exact density matrix.

Before describing the effect of the choice of $\tau(r)$ on the real ion-ion potential we first investigated the accuracy of the Bessel function approximation [7]. For this purpose we calculated $U_{\text{exact}}(R)$ (using harmonic oscillator wave functions) by the iteration method then by using the Bessel function expansion approximation at two different values of the laboratory energy per projectile ($E_{\text{lab}}/A_P = 0$ and 46.6 MeV). Our results are displayed on Fig. 2 for the interacting nuclear pair Ca^{40}–Ca^{40}. This figure shows that at high incident energy ($E_{\text{lab}}/A_P = 46.6$ MeV) the Bessel function expansion approximation is not adequate both at the inner and surface regions of the ion-ion potential. As the projectile energy decreases it becomes correct to calculate the ion-ion potential. We conclude that the Bessel function expansion approximation can only be used to calculate the ion-ion potential at low incident energy.

To show the effect of choosing $\tau(r)$ on the real ion-ion potential we considered the two scattering pairs O^{16}–O^{16} and Ca^{40}–Ca^{40} and used the iteration method to calculate the HI potential $U(R)$ at three different values

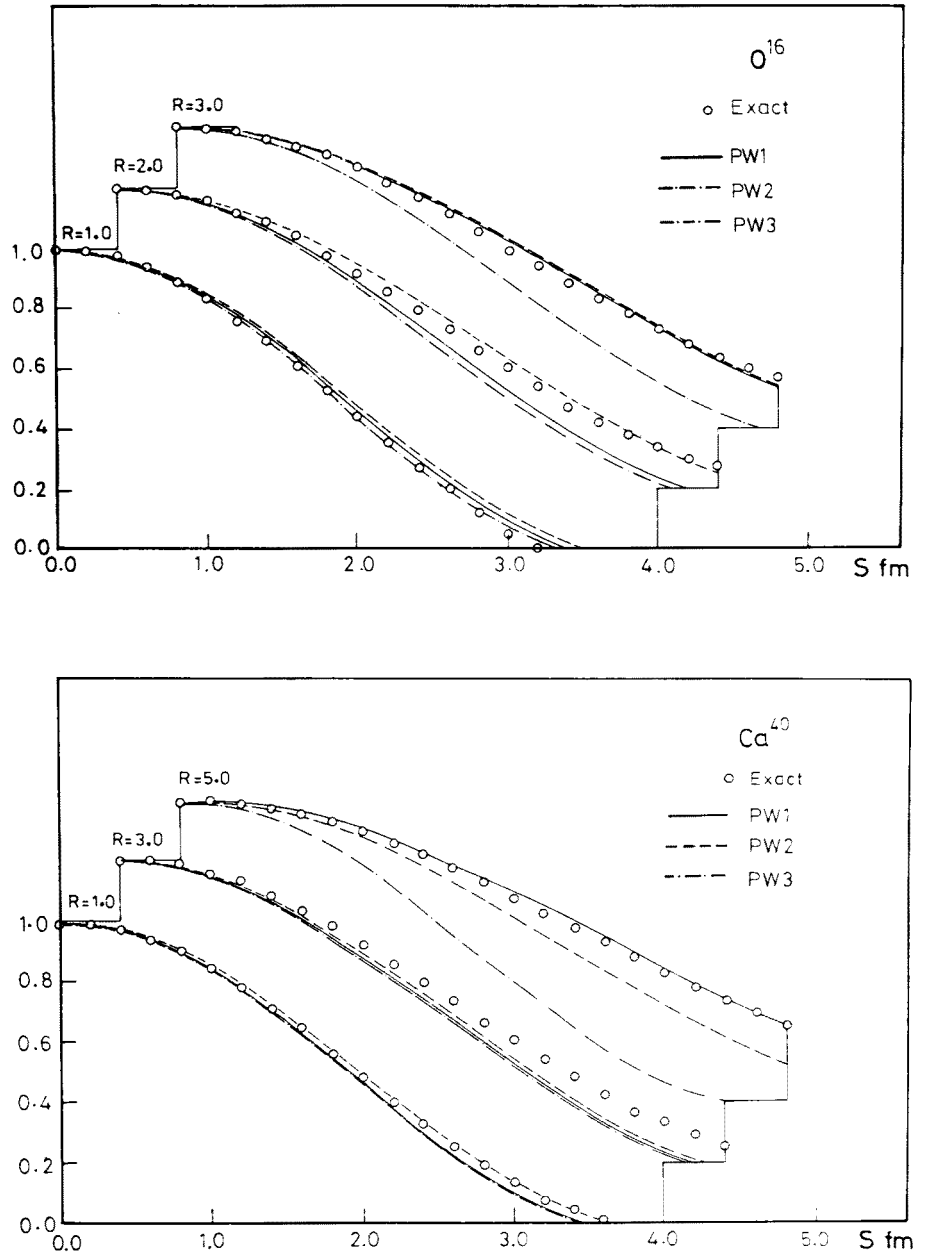

Fig. 1. (a) — Ratio off-diagonal to diagonal density matrix $\rho\left(\vec{R}+\frac{\vec{S}}{2}, \vec{R}-\frac{\vec{S}}{2}\right)/\rho(R)$ as a function of the interparticle distance S for various values of the distance from the center of the nucleus R for O^{16}; (b) — the same as in (a) for Ca^{40}.

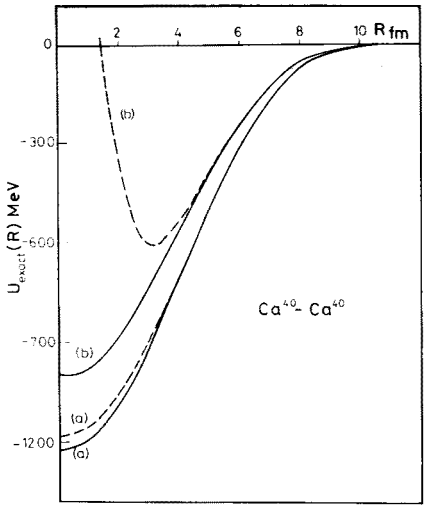

Fig. 2. Comparison between the real part of the ion-ion interaction potentials $U_{\text{exact}}(R)$ between two Ca^{40} nuclei calculated at: (a) — $E_{\text{lab}}/A_P = 0$ MeV and (b) — $E_{\text{lab}}/A_P = 46.6$ MeV using the iteration method (solid line) and the Bessel function approximation (dashed line).

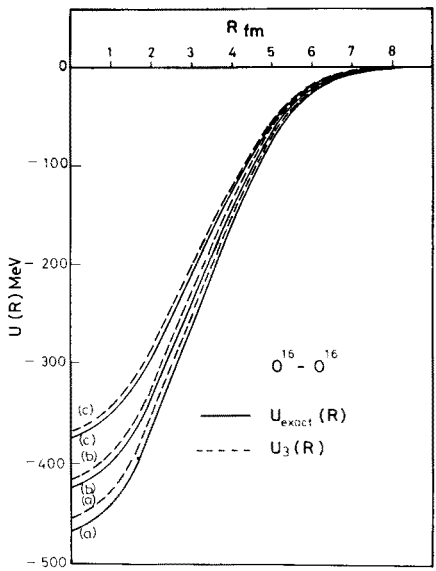

Fig. 3. The real part of the ion-ion interaction potentials $U_{\text{exact}}(R)$ (solid line) and $U_3(R)$ (dashed line) between two O^{16} nuclei calculated using the iteration method at: (a) — $E_{\text{lab}}/A_P = 0$ MeV, (b) — $E_{\text{lab}}/A_P = 20.7$ MeV and (c) — $E_{\text{lab}}.A_P = 46.6$ MeV.

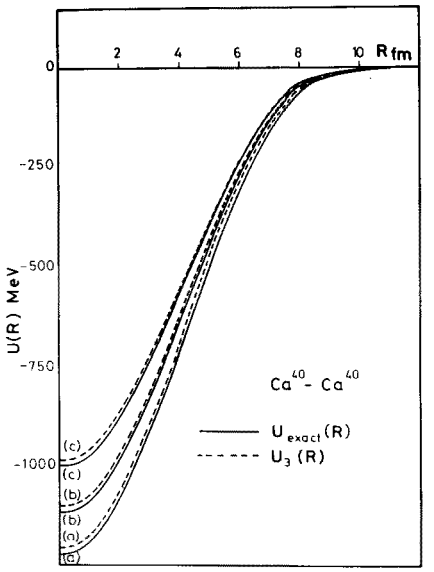

Fig. 4. The same as in Fig. 3 between two Ca^{40} nuclei.

of the projectile energy per nucleon in the laboratory frame. These values are $E_{\rm lab}/A_P = 0$, 20.7 and 46.6 MeV. We found that $U_1(R)$ and $U_2(R)$ are very good approximations to $U_{\rm exact}(R)$ at all projectile energies and $U_1(R)$ is better than $U_2(R)$. The maximum difference between $U_2(R)$ and $U_{\rm exact}(R)$ is about 1%. For $U_3(R)$ which is calculated using $\tau(r)$ given by equation (6c), the maximum difference between it and $U_{\rm exact}(R)$ for O^{16}–O^{16} nuclear pair is about 12% at $E_{\rm lab}/A_P = 0$ MeV and this difference is reduced to about 6% at $E_{\rm lab}/A_P = 46.6$ MeV. For Ca^{40}–Ca^{40} nuclear pair, the maximum error in $U_3(R)$ is reduced to about 5% at $E_{\rm lab}/A_P = 0$ MeV and about 2% at $E_{\rm lab}/A_P = 46.6$ MeV. Figures 3 and 4 show our results for O^{16}–O^{16} and Ca^{40}–Ca^{40}, respectively. In each figure, we compare between $U_3(R)$ and $U_{\rm exact}(R)$ at three different energies. These figures show that the error in using equation (6c) for $\tau(r)$ decreases as the energy increases and as the nuclei becomes heavier.

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