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PROPRIETY OF APPROXIMATION FOR
CALCULATIONS OF NUCLEAR MATRIX
ELEMENTS BY WOODS–SAXON WAVE
FUNCTIONS

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Утамуратов Р. К., Муминов А. И., Насиров А. К. E7-2005-157
Правильность приближения для вычисления матричных элементов
с помощью волновых функций Вудса–Саксона

Одночастичные матричные элементы нуклонного перехода вычислены с волновыми функциями потенциала Вудса–Саксона, полученные результаты сравниваются с результатами, вычисленными с помощью аппроксимации со сферической ямой. Показано, что аппроксимация среднего поля ядер при столкновениях тяжелых ионов со сферической ямой широко применяется в модели, основанной на концепции двойной ядерной системы.

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Utamuratov R. K., Muminov A. I., Nasirov A. K. E7-2005-157
Propriety of Approximation for Calculations of Nuclear Matrix Elements
by Woods–Saxon Wave Functions

Single-particle matrix elements of nucleon transfer were calculated by Woods–Saxon potential wave functions and results are compared with ones calculated by spherical well approximation. The application of the approximation of the mean-field of nuclei at heavy-ion collisions by the spherical well, which is widely used in the model based on dinuclear concept, is proved.

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INTRODUCTION

The role of the shell structure of colliding nuclei in the reaction mechanism at low energies was demonstrated in theoretical analysis of the nonequilibrium share of the excitation energy (nonproportional to the masses of fragments) between reaction fragments at heavy-ion collisions [1–3] and of the observed fine structure in the mass distribution of the fission products [4]. These phenomena indicate that the nuclear shell structure plays an important role in nuclear reaction and in formation of the reaction fragments [5, 6]. So, the theoretical methods used to describe and analyze the above-mentioned phenomena should contain the realistic schemes of single-particle states, nucleon separation energy and single-particle matrix elements of the particle-hole excitations in nuclei caused by influence of field of projectile and matrix elements of nucleon exchange between interacting nuclei. One of these models was developed and applied to describe and interpret the experimental data [2–4, 7–11]. The calculations were performed based on dinuclear system concept [6, 8] which implies conservation of shell structure of the interacting nuclei. To simplify calculations of the matrix elements of nucleon transfer, the authors of the above-mentioned model used the wave functions of the spherical symmetric well in internal part of nuclei [9] instead of the Woods–Saxon wave functions. But the effect of shell structure was taken into account due to using of the eigenvalues of the Woods–Saxon potential as single-particle energies in the interacting nuclei. Nevertheless, the results obtained in the framework of this model for the observable quantities are in good agreement with the experimental data and allowed one to explain nonequilibrium distribution of excitation energy between the reaction products. The matrix elements calculated by the above-mentioned method were used in calculations of the collective transition coefficients of the master equation describing the yield of the fission [4] and quasifission [10, 11] products. In this paper, we compare the results which were obtained by the above-mentioned approximation and by using of the Woods–Saxon energy eigenvalues and wave functions for the single-particle states in both of the interacting nuclei. Our aim is to show that calculation of the matrix elements g_{PT} of nucleon transfer by the wave functions of the spherical symmetric well in internal part of nuclei [9] is appropriate to calculate the relevant physical quantities. The necessity of using this method is caused by the fact that the calculation of the matrix elements g_{PT} by the realistic Woods–Saxon wave functions of the interacting nuclei is a laborious task. This way of calculations to explore heavy-ion collision dynamics is cumbersome even using modern computer resources.

The method of calculation of the matrix elements describing nucleon transfer

between nuclei is presented in Sec. 1. In Sec. 2, we compared the matrix elements calculated by the former method [8] and ones obtained in this work. It is reasonable to compare the observable physical quantities being determined by the matrix elements calculated by two methods under discussion. Therefore, widths of the charge distributions of the reaction products and a friction coefficient for the radial motion of colliding nuclei obtained by making use of the matrix elements of both ways of calculation are discussed and compared with the experimental data. The conclusions of paper are in Sec. 3.

1. CALCULATIONS OF MATRIX ELEMENTS OF NUCLEON TRANSFER BETWEEN INTERACTING NUCLEI

The colliding nuclei are suggested to be spherical, and wave functions are found by solving of the Schrödinger equation with the Woods–Saxon potential

$$\left(-\frac{\hbar^2}{2m}\Delta + U_{P(T)}(\mathbf{r})\right)\Psi_{P(T)}(\mathbf{r}) = \varepsilon_{P(T)}\Psi_{P(T)}(\mathbf{r}), \quad (1)$$

where

$$U_i(r) = V_i(r) + \mathbf{ls} \frac{1}{r} \frac{dV_i(r)}{dr}; \quad V_i(r) = -V_0^{N_i, Z_i} \left\{ 1 + \exp\left[\frac{r - R_i}{a}\right] \right\}^{-1}.$$

The Woods–Saxon potentials for neutrons and protons have different depths $V_0^{(N)} = V_0 \left[1 - 0.63 \frac{N - Z}{A} \right]$ and $V_0^{(Z)} = V_0 \left[1 + 0.63 \frac{N - Z}{A} \right]$, respectively; $V_0 = 53 \text{ MeV}$, $r_0 = 1.24 \text{ fm}$, $a = 0.63 \text{ fm}$. So, the spin-orbital part of the potential is proportional to derivation of the central part $V(r)$. The Woods–Saxon wave functions are presented in the well-known form:

$$\Psi_{nlj}(\mathbf{r}) = R_{n_i}(r) \cdot Y_{j_i m_i}^{l_i 1/2}(\mathbf{r}/r), \quad (2)$$

where

$$R_n(r) = \frac{N_n}{r} H_n(S(r)) \cdot \exp\left(-\frac{S(r)^2}{2}\right), \quad S(r) = \begin{cases} b_1 \cdot \ln\left(\frac{r}{a}\right), & r \leq a \\ b \cdot \ln\left(\frac{r}{a}\right), & r > a \end{cases},$$

H_n is the Hermitian polynomial and $Y_{j_i m_i}^{l_i 1/2}(\mathbf{r}/r)$ is the spherical function. The coefficients N_n, b, b_1, a , and energies of single-particle states are found by numerical solving of the Schrödinger equation with the Woods–Saxon potential [12]. These wave functions describe single-particle states of the mediate and heavy nuclei better than other approximated wave functions such as harmonic oscillator's

wave functions or wave functions of the symmetric rectangular potential well, particularly at the periphery of nuclei.

In the model of the dinuclear system concept, the friction coefficient and dynamical changes of nucleus–nucleus interaction potential for calculation of relative motion of interacting nuclei [2, 3] as well as the collective transition coefficients of the master equation describing the yield of the reaction fragments [4, 7] are calculated making use of the single-particle matrix elements of nucleon transitions between nuclei (nucleon exchange) $g_{PT}(\mathbf{R})$. In the coordinate presentation, these matrix elements describing the nucleon transfer from projectile-like to the target-like nuclei of a dinuclear system (DNS) are presented by the following form [8, 9]:

$$g_{PT}(\mathbf{R}) = \int d^3\mathbf{r} \cdot \Psi_T^*(\mathbf{r}) \left[\frac{1}{2} \{U_T(\mathbf{r}) + U_P(\mathbf{r} - \mathbf{R})\} \right] \Psi_P(\mathbf{r} - \mathbf{R}), \quad (3)$$

where $\{U_T(\mathbf{r}) + U_P(\mathbf{r} - \mathbf{R})\}$ is a total single-particle potential of DNS, R is a distance between centers of DNS nuclei; the single-particle states are characterized by set of quantum numbers $P = (n_p j_p l_p m_p)$ and $T = (n_t j_t l_t m_t)$ in projectile- and target-like nuclei, respectively. Using Fourier images of wave functions

$$\Psi_{nlj}(\mathbf{p}) = \varphi_{n_i}(p) \cdot Y_{j_i m_i}^{l_i 1/2}(\mathbf{p}/p) \quad (4)$$

and the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m} \Delta + U_{P(T)}(\mathbf{r}) \right) \Psi_{P(T)}(\mathbf{r}) = \varepsilon_{P(T)} \Psi_{P(T)}(\mathbf{r}), \quad (5)$$

we can get the following expression for matrix elements of nucleon transfer:

$$g_{PT}(R) = \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{p} \cdot \exp(i\mathbf{p}\mathbf{R}) \varphi_T^*(p) \left[\frac{1}{2} \left(\left\{ \varepsilon_P - \frac{\hbar^2}{2m} p^2 \right\} + \left\{ \varepsilon_T - \frac{\hbar^2}{2m} p^2 \right\} \right) \right] \varphi_P(p). \quad (6)$$

After integrating (5) over angular variables, we get

$$g_{PT}(R) = \frac{(-1)^{m_r-1/2}}{16\pi^3} [(2j_P + 1)(2j_T + 1)]^{1/2} \sum_L i^L (j_T - \frac{1}{2}, j_P \frac{1}{2} | L0) \times \\ \times (j_T - m_T, j_P m_P | L0) \int_0^{\infty} dp \cdot p^2 j_L(pR) \left[\left\{ \varepsilon_P - \frac{\hbar^2}{2m} p^2 \right\} + \left\{ \varepsilon_T - \frac{\hbar^2}{2m} p^2 \right\} \right] \varphi_{l_T}^*(p) \varphi_{l_P}(p). \quad (7)$$

The integral (6) cannot be integrated analytically because of complexity of the Woods–Saxon wave functions (2), and results of numerical calculations of (7) are presented in Sec. 2. Note that these numerical calculations at determination of the dynamical trajectories of heavy-ion collisions are time consuming even with modern computers. In the case of spherical symmetric well approximation, the integral (7) was analytically calculated in Ref. [9].

In this paper, the obtained values of g_{PT} are used to calculate the mean square fluctuation of the fragments proton number at deep inelastic collisions of heavy ions

$$\sigma_Z^2(t) = 2 \sum_{PT} \frac{|g_{PT}(R(t))|^2}{(\varepsilon_T - \varepsilon_P)^2} \left[1 - \cos \frac{t}{\hbar} (\varepsilon_T - \varepsilon_P) \right] [n_P(1 - n_T) + n_T(1 - n_P)], \quad (8)$$

and friction coefficient for the radial motion of nuclei

$$\gamma_R(R(t)) = \sum_{PT} \left| \frac{\partial g_{PT}(R)}{\partial R} \right|^2 B_{PT}(t), \quad (9)$$

where

$$B_{PT}(t) = \frac{2}{\hbar} \int_0^t (t - t') \exp \left(\frac{t - t'}{\tau_{PT}} \right) \sin [(\varepsilon_P - \varepsilon_T)(t - t')/\hbar] [n_T(t') - n_P(t')] dt' \quad (10)$$

and

$$n_{P(T)} = \left[1 + \exp \left(\frac{\varepsilon_{P(T)} - \lambda_{P(T)}}{\theta} \right) \right]^{-1} \quad (11)$$

is the proton occupation number in the single-particle states; λ_K is the chemical potential of nucleons in nuclei ($K = P, T$); θ is the effective temperature of nuclei which is determined by the total kinetic energy loss E_{loss} during collision

$$\theta = 3.46 \sqrt{\frac{E_{\text{loss}}}{(A_P + A_T)}}, \quad (12)$$

where A_P and A_T are mass numbers of the projectile and target nuclei, respectively; $\tau_{PT} = \tau_P \tau_T / (\tau_P + \tau_T)$, where $\tau_{i_K} = \hbar / \Gamma_{i_K}$, τ_{i_K} and Γ_{i_K} are the lifetime and width of the single-particle states, respectively. Γ_{i_K} is calculated by using the results of the theory of quantum liquids [13] and the effective nucleon–nucleon forces from [14]:

$$\Gamma_{i_K} = \frac{\sqrt{2\pi}}{32\varepsilon_{F_K}} \left[(f_K - g)^2 + \frac{1}{2}(f_K + g)^2 \right] [(\pi\theta)^2 + (\varepsilon_i - \lambda_K)^2] \left[1 + \exp\left(\frac{\lambda_K - \varepsilon_i}{T}\right) \right]^{-1}, \quad (13)$$

where ε_{F_F} is the isospin-dependent Fermi energy. For protons and neutrons, it is determined by

$$\varepsilon_{F_K} = \varepsilon_F \left[1 - \frac{2}{3}(1 + 2f'_K) \frac{N_K - Z_K}{N_K + Z_K} \right]$$

and

$$\varepsilon_{F_K} = \varepsilon_F \left[1 + \frac{2}{3}(1 + 2f'_K) \frac{N_K - Z_K}{N_K + Z_K} \right],$$

respectively, $\varepsilon_F = 37$ MeV; N_K and Z_K are neutron and proton numbers in nuclei ($K = P, T$), respectively.

$$f_K = f_{\text{in}} - \frac{2}{A_K^{1/3}}(f_{\text{in}} - f_{\text{ex}}) \quad \text{and} \quad f'_K = f'_{\text{in}} - \frac{2}{A_K^{1/3}}(f'_{\text{in}} - f'_{\text{ex}}),$$

where $f_{\text{in}} = 0.09$, $f'_{\text{in}} = 0.42$, $f_{\text{ex}} = -2.59$, $f'_{\text{ex}} = 0.54$ and $g=0.7$ are the constants of the effective nucleon–nucleon interaction [14].

2. RESULTS OF CALCULATIONS AND THEIR ANALYSIS

In Fig. 1, matrix element g_{PT} of the transition of nucleon from the state $P = 1f_{7/2}$ of the projectile-nucleus to the state $T = 1p_{3/2}$ of target-nucleus calculated by Eq. (6) and one calculated by the corresponding equation of Ref. [9] (dashed line) are compared. The matrix element calculated by realistic wave functions of the spherical Woods–Saxon potential (solid line) has no depression at the relative distance corresponding to the sum of radii of the half nucleon density in nuclei. The depression of the matrix elements calculated according to the method of Ref. [9] is caused at the cross-linking of solutions of the Schrödinger equation obtained for the internal and external parts of nucleus for the spherical well. This depression does not affect the calculated relevant physical quantities such as friction coefficient or width of the charge and mass distributions due to two reasons: at first, the nucleus–nucleus interaction potential used in the models of the DNS concept has a repulsive core at the internuclear distance corresponding to the sum of radii of the half nucleon density in nuclei. The repulsive core is caused by the effective nucleon–nucleon (Migdal) forces [14], which change its sign by the change of nucleon density on the nuclear surface. The second

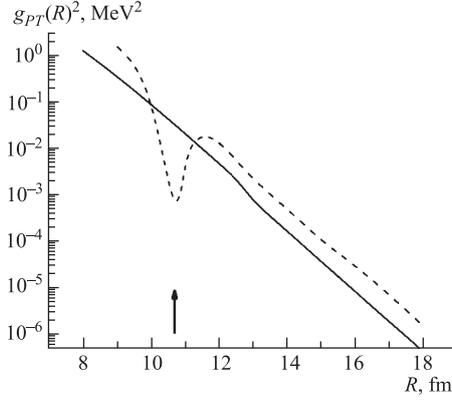


Fig. 1. Comparison of matrix elements calculated as a function of distance between nuclear centers by the spherical well (dashed line) and Woods–Saxon potential wave functions (solid line)

reason is that the cross-linking point and depth of depression are different for the different single-particle states, consequently, at summing the resulting curve is smoothed. The difference between absolute values of g_{PT} calculated by the two methods under discussion is explained by the fact that different wave functions were used.

In Fig. 2, the curves of the dispersion of the charge distribution of reaction products in $^{40}\text{Ar} + ^{100}\text{Mo}$ calculated as a function of the total energy loss (reaction time) by two methods under discussion are compared with the experimental data [15]. As seen from Fig. 2 the agreement of our results obtained by both methods for the dependence of the dispersion of the charge distribution of reaction products in $^{40}\text{Ar} + ^{100}\text{Mo}$ on interaction time with the corresponding experimental data is good. The experimental interaction time is estimated from the angular distribution of the reaction products and it is connected with total energy loss during reaction time.

Another physical quantity, which was calculated and compared with the values obtained by the previous method [8, 9], is the friction coefficient [16] for the relative motion of nuclei at deep inelastic heavy-ion collisions. The values of the friction coefficient obtained for ^{56}Fe (480 MeV) + ^{208}Pb and ^{64}Zn (440 MeV) + ^{196}Pt reactions are compared in Figs. 3 and 4, respectively. As seen from Figs. 3 and 4, the calculations of friction coefficient of the radial motion making use of the matrix elements by the wave functions of the symmetric spherical well and Woods–Saxon potential lead to nearly the same results. The noticeable difference at the large distances between nuclei is caused by the long tail of the wave

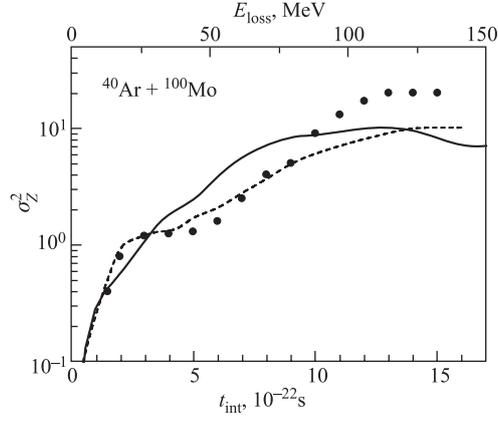


Fig. 2. Dependence of dispersion of measured and calculated charge distributions of the reaction products in deep inelastic collisions on the interaction time. Full circles are experimental data; lines are the same as in Fig. 1

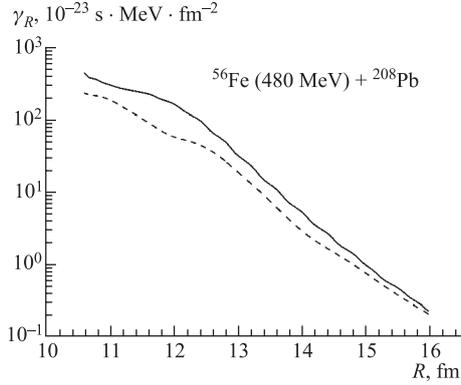


Fig. 3. Comparison of the values of friction coefficient calculated by the wave functions of the Woods-Saxon potential (solid line) and symmetrical spherical well (dashed line) for the $^{56}\text{Fe} (480 \text{ MeV}) + ^{208}\text{Pb}$ reaction

functions of the Woods-Saxon potential. It is clear that this difference appears at small values of friction coefficient which does not lead to sufficient difference for the total kinetic energy loss at initial stage of heavy-ion collisions.

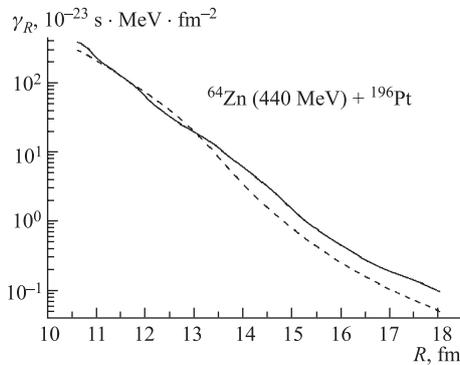


Fig. 4. The same as in Fig. 3 but for $^{64}\text{Zn} (440 \text{ MeV}) + ^{196}\text{Pt}$ reaction

3. CONCLUSIONS

The mean square fluctuations of the fragments proton numbers and radial friction coefficients at deep inelastic collisions of heavy ions were analyzed to study their dependence on the way of calculation of the used matrix elements describing of the multinucleon transfer between interacting nuclei. It was done to estimate the propriety of the approximation of the mean field of nuclei interacting at low-energy heavy-ion collisions by the spherical well which is widely used in the model based on dinuclear concept due to its simplicity. The estimation was performed by comparison of the matrix elements calculated by using the wave functions which were obtained by the numerical solution of the Schrödinger equation for the Woods–Saxon potential and those determined by analytical solution of the Schrödinger equation for the spherical potential well. The absolute values of the matrix elements calculated as a function of the relative distance between nucleus centers by the former method are several times lower than those obtained by wave functions of spherical well. The depression of the matrix elements of the method [9] arises due the cross-linking of the wave functions of the spherical well and free particles and its affect on the characteristic physical observables. Use of matrix elements calculated by both methods under discussion to calculate dispersion of the charge distribution of reaction products at deep inelastic collisions of heavy ions allowed us to reach a good agreement with the experimental data (see Fig.2). We conclude that in spite of its simplicity the approximation by spherical well of the mean fields of interacting nuclei in the dinuclear system concept is acceptable for the kinetic coefficients to study multinucleon transfer and fusion–fission reactions at heavy-ion collisions.

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