Time-dependent Hartree-Fock calculations for multi-nucleon transfer processes

Effects of particle evaporation on production cross sections

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Abstract. We present a microscopic calculation of multi-nucleon transfer reactions employing the time-dependent Hartree-Fock (TDHF) theory. In our previous publication [Phys. Rev. C **88**, 014614 (2013)], we reported our analysis for the multi-nucleon transfer processes for several systems. Here we discuss effects of particle evaporation processes on the production cross sections. Since particle evaporation processes may not be described adequately by the TDHF calculations, we evaluate them using a statistical model. As an input of the statistical model, excitation energies of the final fragments are necessary. We evaluate them from the TDHF wave function after collisions, extending the particle number projection technique. From the calculation, the particle evaporation effects are found to improve descriptions of the production cross sections. However, the production cross sections are still underestimated for processes where a number of protons are transferred. Possible origins of the discrepancy are discussed.

1 Introduction

In low-energy nuclear reactions at around the Coulomb barrier, multi-nucleon transfer (MNT) reactions are commonly observed at an impact parameter region slightly outside that corresponding to fusion reactions. The MNT reaction at around the Coulomb barrier contains rich physics related to both structural properties and time-dependent dynamics of colliding nuclei, and has been attracting much interests in a number of aspects. Properties of a neck formed at the distance of closest approach reflect structural and excitation properties of the colliding nuclei [1]. Exchanges of a number of nucleons caused by the neck formation can induce an energy dissipation, a transfer of energy from translational relative motion to that of internal excitations. This provides an opportunity to study correlation effects in nuclear dynamics [2]. MNT reactions have also been expected to be a new means to produce unstable nuclei whose production is difficult by other methods [3–5].

To uncover microscopic reaction mechanisms of MNT reactions and to predict preferable conditions to produce objective nuclei, we have undertaken microscopic calculations of the MNT reactions employing the time-dependent Hartree-Fock (TDHF) theory. We presented results of the TDHF calculations for MNT processes in ^{40,48}Ca+^{124}Sn, ^{40}Ca+^{208}Pb, and ^{58}Ni+^{208}Pb reactions, for which extensive measurements are available [6]. To calculate transfer probabilities and cross sections, we used a particle number projection technique which was recently proposed by C. Simenel [7]. From the results, we found that the TDHF calculations can reproduce measured cross sections quantitatively, when the number of transferred nucleons is small. However, as the number of transferred nucleons increases, a peak position of the calculated cross sections shifts towards larger neutron and proton number sides compared with measurements. One of possible origins of the discrepancy may be an insufficient description of particle evaporation processes in our TDHF calculations. Because we calculated the transfer probabilities and the cross sections from a TDHF wave function just after two nuclei separates (typically, order of 10^{-21} s after the reseparation), effects of secondary evaporation processes which occur in much longer time scale have not been taken into account in the calculated cross sections.

In the present article, we will show an outline of our recent attempt to evaluate effects of particle evaporation processes on the production cross sections based on the TDHF theory [8]. To estimate how many nucleons are to be evaporated from the produced fragment, we need to calculate excitation energy of the fragment in each transfer channel. We calculate the excitation energy extending the particle number projection technique which was originally used to calculate transfer probabilities from a TDHF wave function after collision. We then evaluate evaporation probabilities by employing a statistical model [9] in which the excitation energy obtained from the projection analysis will be used as an input. We finally calculate the production cross sections including evaporation effects.

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It is certainly true that correlation effects included in the TDHF theory is rather limited. For example, isoscalar and isovector pair transfers, α-cluster transfer are not treated adequately. We consider that MNT cross sections with improved treatment of evaporation processes will help to uncover what is lacking and what is needed in the TDHF calculation for the MNT processes. One of the aims of this work is to clarify to what extent the TDHF theory can describe MNT cross sections quantitatively if we include the effects of particle evaporation processes.

This article is organized as follows. In Sec. 2, we present an outline of our formalism to include the effect of the particle evaporation processes in the calculation of the production cross sections. In Sec. 3, we show calculated production cross sections for ^{58}Ni+^{208}Pb reaction with and without particle evaporation effects. In Sec. 4, a summary and a future prospect are presented.

2 Formulation

2.1 Particle number projection technique

In the TDHF theory, a many-body wave function of the system is described by a single Slater determinant composed of single-particle wave functions of nucleons. We denote the number of neutrons and protons in the projectile (target) as $N_{\mathrm{P}}^{(n)}$ ($N_{\mathrm{T}}^{(n)}$) and $N_{\mathrm{P}}^{(p)}$ ($N_{\mathrm{T}}^{(p)}$), respectively. The total numbers of neutrons and protons are then given by $N^{(n)} = N_{\mathrm{P}}^{(n)} + N_{\mathrm{T}}^{(n)}$ and $N^{(p)} = N_{\mathrm{P}}^{(p)} + N_{\mathrm{T}}^{(p)}$, respectively. We denote the total number of nucleons as $A = N^{(n)} + N^{(p)}$. In the TDHF theory, the many-body wave function of the system is expressed as a direct product of Slater determinants for neutrons and protons,

$$\Psi(x_1, \cdots, x_A) = \Psi^{(n)}(x_1, \cdots, x_{N^{(n)}}) \otimes \Psi^{(p)}(x_1, \cdots, x_{N^{(p)}}),$$ (1)

where

$$\Psi^{(q)}(x_1, \cdots, x_{N^{(q)}}) = \frac{1}{\sqrt{N^{(q)}!}} \det\{\psi_i^{(q)}(x_j)\}$$ (2)

denotes the many-body wave function for neutrons ($q = n$) or protons ($q = p$). $\psi_i^{(q)}(x)$ is the single-particle wave function of a nucleon having an isospin q, where x denotes a set of spatial and spin coordinates, $x \equiv (\mathbf{r}, \sigma)$.

During the collision, single-particle wave functions which originally belong to either projectile or target region extend to a whole spatial region where a mean-field potential of the collision partner exists. After the collision, the whole system separates into two fragments, a projectile-like fragment (PLF) and a target-like fragment (TLF). We divide the whole space into two regions, a projectile region V_{P} which includes the PLF and a target region V_{T} which includes the TLF. Each single-particle wave function extends in both V_{P} and V_{T}. Then, the TDHF wave function after collision is not an eigenstate of the number operator in respective regions, $\hat{N}_{\mathrm{P}}^{(q)}$ and $\hat{N}_{\mathrm{T}}^{(q)}$ ($q = n$ for neutrons, $q = p$ for protons), but a superposition of states with different particle number distributions.

To calculate the particle number distributions, a particle number projection technique was recently proposed

by C. Simenel [7]. A particle number projection operator which projects out a particle number eigenstate of the number operators, $\hat{N}_{\mathrm{P}}^{(q)}$ and $\hat{N}_{\mathrm{T}}^{(q)}$, with eigenvalues, n and $N^{(q)} - n$, respectively, can be expressed as

$$\hat{P}_n^{(q)} = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, e^{\mathrm{i}(n - \hat{N}_{\mathrm{P}}^{(q)})\theta}.$$ (3)

The probability to find a nucleus composed of n neutrons and z protons in the spatial region V_{P} is given by

$$P_{n,z} = P_n^{(n)} P_z^{(p)},$$ (4)

where

$$P_n^{(q)} \equiv \langle \Psi^{(q)} | \hat{P}_n^{(q)} | \Psi^{(q)} \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \, e^{\mathrm{i}n\theta} \det \mathcal{B}^{(q)}(\theta)$$ (5)

and

$$\left(\mathcal{B}^{(q)}(\theta)\right)_{ij} \equiv \langle \psi_i^{(q)} | \psi_j^{(q)} \rangle_{V_{\mathrm{T}}} + e^{-\mathrm{i}\theta} \langle \psi_i^{(q)} | \psi_j^{(q)} \rangle_{V_{\mathrm{P}}}.$$ (6)

We have introduced a shorthand notation, $\langle \psi_i^{(q)} | \psi_j^{(q)} \rangle_\tau \equiv \sum_\sigma \int_\tau d\mathbf{r} \, \psi_i^{(q)*}(\mathbf{r}, \sigma) \psi_j^{(q)}(\mathbf{r}, \sigma)$ ($\tau = V_{\mathrm{P}}$ or V_{T}). Because the TDHF wave function is a direct product of wave functions for neutrons and protons, the probability is also given by a product of probabilities for neutrons and protons as Eq. (4).

2.2 Excitation energies of produced fragments

We have extended the particle number projection technique to calculate an expectation value of an arbitrary operator, using the particle number projected wave function [8]. The energy expectation value of the PLF composed of n neutrons and z protons is given by

$$E_{n,z}^{\mathrm{PLF}} \equiv \frac{\langle \Psi | \hat{H}_{V_{\mathrm{P}}} \hat{P}_n^{(n)} \hat{P}_z^{(p)} | \Psi \rangle}{\langle \Psi | \hat{P}_n^{(n)} \hat{P}_z^{(p)} | \Psi \rangle}.$$ (7)

$\hat{H}_{V_{\mathrm{P}}} \equiv \hat{T}_{V_{\mathrm{P}}} + \hat{V}_{V_{\mathrm{P}}} = \sum_i \Theta_{V_{\mathrm{P}}}(\mathbf{r}_i) \hat{t}_i + \sum_{i<j} \Theta_{V_{\mathrm{P}}}(\mathbf{r}_i) \Theta_{V_{\mathrm{P}}}(\mathbf{r}_j) \hat{v}_{ij}$ denotes a Hamiltonian acting only for the PLF, where we have introduced a space division function, $\Theta_{V_{\mathrm{P}}}(\mathbf{r}) \equiv 1$ for $\mathbf{r} \in V_{\mathrm{P}}$ and 0 for $\mathbf{r} \notin V_{\mathrm{P}}$.

In practice, we need to remove an energy associated with the center-of-mass motion of the fragment. For this purpose, we move to the rest frame of the PLF before calculating the energy expectation value. Denoting the mass and coordinates of the PLF at the final stage of the calculation as M_{PLF} and $\mathbf{R}_{\mathrm{PLF}}(t_f)$, respectively, the wave vector of the fragment is evaluated as $\mathbf{K}_{\mathrm{PLF}} = M_{\mathrm{PLF}} \dot{\mathbf{R}}_{\mathrm{PLF}}(t_f)/\hbar$, where $\dot{\mathbf{R}}_{\mathrm{PLF}}(t_f) \equiv [\mathbf{R}_{\mathrm{PLF}}(t_f + \Delta t) - \mathbf{R}_{\mathrm{PLF}}(t_f - \Delta t)]/(2\Delta t)$. We multiply the plane wave $e^{-\mathrm{i}\mathbf{K}_{\mathrm{PLF}} \cdot \mathbf{r}}$ to the wave function in the spatial region V_{P}.

After the removal of the center-of-mass motion of the fragment, we evaluate the energy expectation value using Eq. (7). The kinetic energy term for the PLF composed of n neutrons and z protons can be calculated as

$$\mathcal{E}_{n,z,\mathrm{kin}}^{\mathrm{PLF}} = \mathcal{E}_{n,\mathrm{kin}}^{(n)\,\mathrm{PLF}} + \mathcal{E}_{z,\mathrm{kin}}^{(p)\,\mathrm{PLF}},$$ (8)

where

$$\mathcal{E}_{n,\text{kin}}^{(q)\,\text{PLF}} \equiv \frac{1}{2\pi P_n^{(q)}} \int_0^{2\pi} d\theta\, e^{\text{i}n\theta} \det \mathcal{B}^{(q)}(\theta)$$

$$\times \frac{\hbar^2}{2m} \sum_{i=1}^{N^{(q)}} \sum_\sigma \int_{V_P} d\mathbf{r}\, \boldsymbol{\nabla}\psi_i^{(q)*}(\mathbf{r},\sigma) \cdot \boldsymbol{\nabla}\tilde{\psi}_i^{(q)}(\mathbf{r},\sigma,\theta). \quad (9)$$

$\tilde{\psi}_i^{(q)}(\mathbf{r},\sigma,\theta)$ is defined by $\sum_{k\in q}\left(\mathcal{B}^{(q)}(\theta)\right)_{ik}^{-1}\psi_k^{(q)}(\mathbf{r},\sigma)$. The center-of-mass correction is simply taken into account by considering the one-body term, replacing the coefficient of the kinetic energy operator $\frac{\hbar^2}{2m}$ with $\frac{\hbar^2}{2m}(1-\frac{1}{a})$, where $a = n + z$ denotes the mass number of the PLF. The interaction part is calculated using transition densities, (e.g. the transition proton density is given by $\tilde{\rho}^{(p)}(\mathbf{r},\theta) \equiv \sum_{i\in p,\sigma}\psi_i^*(\mathbf{r},\sigma)\tilde{\psi}_i(\mathbf{r},\sigma,\theta)$). The two-body and three-body interaction terms for the fragment composed of n neutrons and z protons are calculated as

$$\mathcal{E}_{n,z,\text{int}}^{\text{PLF}} \equiv \frac{1}{(2\pi)^2 P_n^{(n)} P_z^{(p)}} \int_0^{2\pi} d\theta \int_0^{2\pi} d\varphi\, e^{\text{i}(n\theta+z\varphi)}$$

$$\times \det \mathcal{B}(\theta,\varphi) \int_{V_P} d\mathbf{r}\, \tilde{\mathcal{V}}[\mathbf{r},\theta,\varphi], \quad (10)$$

where $\det \mathcal{B}(\theta,\varphi) \equiv \det \mathcal{B}^{(n)}(\theta) \det \mathcal{B}^{(p)}(\varphi)$. The Coulomb energy is evaluated using the transition proton density, $\tilde{\rho}^{(p)}(\mathbf{r},\theta)$.

We then define the excitation energy of the PLF composed of n neutrons and z protons as

$$E_{n,z}^{*\,\text{PLF}}(E,b) \equiv \mathcal{E}_{n,z}^{\text{PLF}}(E,b) - E_{n,z}^{\text{g.s.}}, \quad (11)$$

where

$$\mathcal{E}_{n,z}^{\text{PLF}} \equiv \mathcal{E}_{n,z,\text{kin}}^{\text{PLF}} + \mathcal{E}_{n,z,\text{int}}^{\text{PLF}} + \mathcal{E}_{z,\text{Coulomb}}^{\text{PLF}} \quad (12)$$

denotes the energy expectation value of the PLF. $E_{n,z}^{\text{g.s.}}$ is the ground state energy of the nucleus composed of n neutrons and z protons. We can also evaluate excitation energy of the TLF in a similar way.

2.3 Particle evaporation probabilities

We evaluate the particle evaporation employing a statistical model developed by I. Dostrovsky and his coworkers [9]. In this model, evaporation of neutrons, protons, deuterons, tritons, ^{3}He, and α particles are taken into account. An input of the model is the excitation energy of a nucleus to be disintegrate. For more detail explanation of the model, see Ref. [9] and references therein.

Putting as an input the excitation energy evaluated from the TDHF wave function after collision using Eq. (11), we evaluate evaporation processes. Starting with the excited fragment, all possible decay sequences reaching to the final state at which any emissions of a particle are energetically prohibited are considered. Each series of the evaporation is called as the evaporation cascade. In each evaporation cascade, the kind of emitted particles and its kinetic energy are selected stochastically.

As an example, let us consider a case that we calculate evaporation processes from an excited PLF composed of

N neutrons and Z protons with excitation energy of $E_{N,Z}^{*\,\text{PLF}}$. If a nucleus composed of N' neutrons and Z' protons is formed at the end of an evaporation cascade, the total number of evaporated neutrons and protons are given by $N-N'$ and $Z-Z'$, respectively. We count the number of cases in which n neutrons and z protons are evaporated until the end of an evaporation cascade among all of the evaporation cascades examined. Then, we calculate the evaporation probability of n neutrons and z protons as

$$P_{n,z}^{\text{evap.}}[E_{N,Z}^{*\,\text{PLF}}(b)] = N_{n,z}/N_{\text{cascade}}, \quad (13)$$

where $N_{n,z}$ denotes the total number of processes in which n neutrons and z protons are emitted until the end among all of the evaporation cascades. N_{cascade} denotes the total number of evaporation cascades examined. Because the excitation energy, $E_{N,Z}^{*\,\text{PLF}}$, depends on the impact parameter, resulting evaporation probabilities, $P_{n,z}^{\text{evap.}}$, also depend on the impact parameter.

2.4 Transfer cross sections with evaporation effects

In our previous article [6], we calculated a transfer cross section for the channel in which a PLF is composed of N neutrons and Z protons by integrating the probability $P_{N,Z}(b)$ over the impact parameter, as

$$\sigma_{\text{tr}}(N,Z) = 2\pi \int_{b_{\min}}^{\infty} b\, P_{N,Z}(b)\, db. \quad (14)$$

The minimum impact parameter of the integration was taken to be a border dividing fusion and binary reactions. Here, we have assumed that both projectile and target nuclei are spherical, so that the reaction is specified by the incident energy E and the impact parameter b. In practice, we first examined the maximum impact parameter, b_{f}, in which fusion reactions take place for a given incident energy. We then repeated reaction calculations at various impact parameters for the region, $b > b_{\text{f}}$, and calculated the cross section by numerical quadrature according to Eq. (14).

To include effects of particle evaporation into the cross section, we simply extend the expression of the cross section by using the evaporation probabilities obtained from the statistical calculation. Let us denote the evaporation probability of n neutrons and z protons from the PLF composed of $N + n$ neutrons and $Z + z$ protons having excitation energy of $E_{N+n,Z+z}^{*\,\text{PLF}}$ as $P_{n,z}^{\text{evap.}}[E_{N+n,Z+z}^{*\,\text{PLF}}]$. The residual nucleus after the particle evaporation is composed of N neutrons and Z protons. We calculate the cross section for the channel where the PLF is composed of N neutrons and Z protons including effects of particle evaporation as

$$\sigma_{\text{tr}}^{\text{evap.}}(N,Z) = 2\pi \int_{b_{\min}}^{\infty} b \sum_{n,z} P_{N+n,Z+z}(b)$$

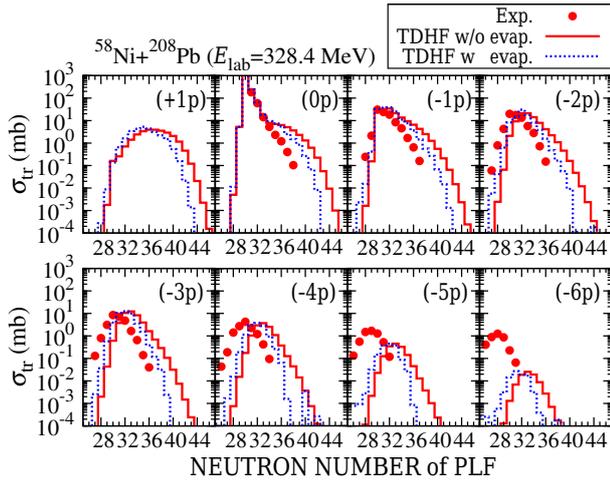$$\times P_{n,z}^{\text{evap.}}[E_{N+n,Z+z}^{*\,\text{PLF}}(b)]\, db. \quad (15)$$

Figure 1. (Color online) Production cross sections of the projectile (^{58}Ni) like fragments in ^{58}Ni+^{208}Pb reaction at E_{lab} = 328.4 MeV. Solid (dotted) Line shows cross sections calculated by the TDHF theory without (with) evaporation effects. Measured cross sections [10] are also shown by filled circles.

3 Results

We consider ^{58}Ni+^{208}Pb reaction, which was also studied in Ref. [6]. In Fig. 1, we show cross sections classified according to the change of the proton number of the PLF from ^{58}Ni, as functions of the neutron number of the PLF. Red filled circles denote measured cross sections [10] and red solid (blue dotted) lines denote results of the TDHF calculations without (with) effects of particle evaporation. As the figure shows, the TDHF theory describes surprisingly well the measured cross sections when the number of transferred nucleons is small. We note that there is no empirical parameter in our calculations, since we employ a standard Skyrme effective interaction (SLy5 [11]). As the number of transferred nucleons increases, there appear discrepancies even when we include evaporation effects. This fact may indicate significance of correlation effects which are not included in the framework of the TDHF theory. A more detail investigation will be presented in the forthcoming paper [8].

4 Summary

In the article, we have presented an outline of our attempt to include effects of particle evaporation in the description of multi-nucleon transfer processes based on the microscopic TDHF theory. We evaluate excitation energy of a produced fragment in each transfer channel extending the particle number projection technique. We calculated multi-nucleon transfer cross sections for ^{58}Ni+^{208}Pb reaction in the TDHF theory with and without evaporation effects, and compared with measured cross sections. We have found that the inclusion of evaporation effects improves the cross section towards the measurements. However, calculations still underestimate measured cross sections when a number of protons are transferred.

Acknowledgements

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