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Time-dependent generator coordinate method for many-particle tunneling

N. Hasegawa^a, K. Hagino^{b,*}, Y. Tanimura^{a,c}

^a Department of physics, Tohoku University, Sendai 980-8578, Japan

^b Department of physics, Kyoto University, Kyoto 606-8502, Japan

^c Graduate Program on Physics for the Universe, Tohoku University, Sendai 980-8578, Japan

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ABSTRACT

It has been known that the time-dependent Hartree-Fock (TDHF) method, or the time-dependent density functional theory (TDDFT), fails to describe many-body quantum tunneling. We overcome this problem by superposing a few time-dependent Slater determinants with the time-dependent generator coordinate method (TDGCM). We apply this method to scattering of two α particles in one dimension, and demonstrate that the TDGCM method yields a finite tunneling probability even at energies below the Coulomb barrier, at which the tunneling probability is exactly zero in the TDHF. This is the first case in which a many-particle tunneling is simulated with a microscopic real-time approach.

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1. Introduction

One of the primary goals of nuclear reaction theory is to develop a microscopic framework for nuclear reactions, starting from the nucleonic degrees of freedom. Such a framework will describe several complicated reaction processes in a unified way, not specialized in a certain reaction system. Ideally, such a framework will not contain any empirical parameter for reactions, once static nuclear properties or the nucleon-nucleon interaction are well investigated. This feature will be particularly important in applying the framework to unknown regions, in which experimental studies are difficult, e.g., reactions of neutron-rich nuclei and those for superheavy nuclei.

The time-dependent Hartree-Fock (TDHF) method is one of the promising microscopic frameworks for nuclear reactions, in which a many-body wave function is approximated by a single Slater determinant [1–5]. The TDHF has been successful in describing average behaviors of nuclear reactions, such as the energy-angle correlation in heavy-ion deep inelastic collisions [6]. In recent years, many TDHF calculations have been successfully carried out with current powerful computers, in order to discuss the main process of reaction for a given initial condition [7–15].

However, it has been well known that the TDHF has a serious drawback, that is, it considerably underestimates quantum fluc-

tuations and fails to describe minor processes, such as quantum many-body tunneling at energies below the potential barrier [3–5]. Notice that the TDHF can be formulated using the stationary phase approximation to the path integral representation of a many-body dynamics [3], and in this sense the collective path in the TDHF is classical. A tunneling probability in the TDHF therefore changes abruptly from 0 to 1 at a certain threshold energy. For this reason, the TDHF method fails to describe fusion reactions at energies below the barrier [4] and fission dynamics before a saddle point [16].

Several schemes have been considered so far in order to go beyond the TDHF approximation [17–28]. Nevertheless none of them has been applied to the problem of quantum tunneling. For instance, in the stochastic mean-field theory (SMF) [16,20,21], quantum fluctuations are simulated as an ensemble of TDHF trajectories, but it is still difficult to describe many-body tunneling with this framework.

Since a TDHF trajectory shows a classical behavior, to describe quantum tunneling based on the TDHF and its extension has a common feature to a problem of how to simulate quantum tunneling using classical trajectories. This problem has been actually discussed also in the field of quantum chemistry, in which the entangled trajectory molecular dynamics (ETMD) has been developed [29–32]. In this method, the Wigner function of a one particle wave function is represented as an ensemble of classical test particles. Those classical test particles are treated in a collective manner, rather than independently. By taking into account such

* Corresponding author.

E-mail address: hagino.kouichi.5m@kyoto-u.ac.jp (K. Hagino).

entanglement of test particles, that is, the influence of other test particles during the time evolution of a test particle, it has been demonstrated that the ETMD can simulate well quantum tunneling phenomena, despite that each test particle follows the classical equation of motion [29–32].

The success of ETMD would imply that quantum tunneling may be simulated by taking into account an entanglement of many TDHF trajectories. This would be equivalent to construct a many-body wave function as a superposition of many Slater determinants. This is nothing but the time-dependent generator coordinate method (TDGCM) [23,33]. The aim of this paper is to investigate whether the TDGCM method can describe in principle quantum tunneling phenomena. For such a proof of principle study, it would be ideal to choose a system which is as simple as possible. To this end, we consider a collision of two ${}^4\text{He}$ particles in the one dimensional space. Based on the idea of ETMD, we superpose a few Slater determinants, which have different initial relative distances and relative momenta between the two ${}^4\text{He}$ particles. During the time evolution, the trajectory of each Slater determinant is affected by the presence of other Slater determinants, and they are thus entangled as in the entangled classical trajectories in the ETMD method. We shall investigate in this paper whether such entanglement of Slater determinants improves the failure of the TDHF method.

2. Time-dependent generator coordinate method

In the TDGCM, one assumes that a many-body wave function is given as a superposition of many Slater determinants,

$$\Psi(t) = \sum_a f_a(t) \Phi_a(t), \quad (1)$$

where f_a is a weight function and Φ_a is a Slater determinant with single-particle wave functions $\{\phi_{ai}\}$. The index a distinguishes each Slater determinant to one another, and is referred to as a generator coordinate. In nuclear structure calculations, multipole moments are often taken as a generator coordinate, for which the Slater determinant Φ_a is obtained with the constrained Hartree-Fock method [1]. In the calculation shown below, we take the initial values of the relative distance and the relative momentum between two α particles as the generator coordinates.

The time evolution of the weight functions $f_a(t)$ and the Slater determinants $\Phi_a(t)$ can be determined by the time-dependent variational principle,

$$\delta \int dt \frac{\langle \Psi | i\hbar \frac{\partial}{\partial t} - H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0, \quad (2)$$

where H is the total Hamiltonian of the system. In Refs. [23,33,34], the time evolution of the Slater determinants is replaced by TDHF trajectories, while the time evolution of the weight function is solved according to the variational principle. However, in an application to quantum tunneling, it would be essential to take into account a deviation from TDHF in the evolution of the Slater determinants. We therefore do not use TDHF trajectories, but determine the time-evolution of the Slater determinants under the influence of the other Slater determinants using the variational principle.

Notice that our method is conceptually different from the method developed in Refs. [35–39], even though the latter has often been called the time-dependent generator coordinate method. In Refs. [35–39], the Slater determinants Φ_a are prefixed by nuclear structure calculations, often taken as the ground state for a given value of multipole moments, whereas the time evolution of the weight functions is determined by solving the time-dependent Hill-Wheeler equation. Since the Slater determinants are static in these calculations, it may be more appropriate to call such

method as the time-dependent Hill-Wheeler method, rather than the time-dependent generator coordinate method. Even though non-adiabatic effects can in principle be taken into account in this method [37], the computational cost considerably increases when the number of configurations increases. In contrast, the non-adiabatic effects are automatically taken into account in our method by using time-dependent Slater determinants. This would be an important aspect of our method, especially in applications to nuclear reactions of heavy systems, in which excitations of colliding nuclei during reaction play an important role [40].

3. Application to $\alpha+\alpha$ scattering in one dimension

Let us now apply the TDGCM to the ${}^4\text{He}+{}^4\text{He}$ scattering in one dimension. In order to simplify the calculation, we parameterize the single-particle wave functions with a Gaussian function with a fixed width, as in the anti-symmetrized molecular dynamics (AMD) [41,42]. That is, we take the single-particle wave function ϕ_{ai} as,

$$\phi_{ai}(x, t) = e^{-v \left(x - \frac{Z_{ai}(t)}{\sqrt{v}} \right)^2} \chi_\sigma \chi_\tau, \quad (3)$$

where χ_σ and χ_τ are the spin and the isospin wave functions, respectively. The Gaussian center, Z_{ai} , is a complex quantity, whose real and imaginary parts are related to the mean position and the mean momentum of the Gaussian wave function, respectively.

In this paper, we fix the spin and isospin wave functions and assume that the Gaussian center is identical for all the four nucleons in each ${}^4\text{He}$ particle. That is, we take $Z_{p\uparrow} = Z_{p\downarrow} = Z_{n\uparrow} = Z_{n\downarrow}$ in each ${}^4\text{He}$ particle. Moreover, we assume that there is no transfer of nucleons during a reaction, and the two ${}^4\text{He}$ move symmetrically with respect to $x = 0$. That is, when one ${}^4\text{He}$ particle has a Gaussian center of $Z(t)$, the other ${}^4\text{He}$ particle has a Gaussian center of $-Z(t)$. With these approximations, there is only one single variational parameter, $Z_a(t)$, in each Slater determinant, $\Phi_a(t)$.

At $t = 0$, we construct each Slater determinant, $\Phi_a(t)$, by putting the two ${}^4\text{He}$ particles at $x = x_{a0}$ and $x = -x_{a0}$, with the momentum of $p = -p_{a0}$ and $p = p_{a0}$, respectively. This is equivalent to take

$$Z_a(t=0) = x_{a0} \sqrt{v} - i \frac{p_{a0}}{2\sqrt{v}\hbar}, \quad (4)$$

for a given Gaussian width, v .

We employ the same one dimensional Hamiltonian as the one in Ref. [23], to which we also add a soft-core Coulomb interaction between two protons in a form of [43–47]

$$v_C(x, x') = \frac{e^2}{\sqrt{\alpha^2 + (x - x')^2}}. \quad (5)$$

With this Hamiltonian, one obtains [48],

$$\begin{aligned} & \langle \Phi_a | H | \Phi_{a'} \rangle \\ &= \langle \Phi_a | \Phi_{a'} \rangle \int dx \left\{ \frac{\hbar}{2m} \tilde{\tau}(x) + \frac{t_3}{3} \tilde{\rho}^3(x) \right. \\ &+ \frac{t_0}{2} \tilde{\rho}(x) \int dx' \tilde{\rho}(x') \frac{b}{\sqrt{\pi}} e^{-\frac{(x-x')^2}{b^2}} \\ &+ \left. \frac{e^2}{2} \tilde{\rho}_p(x) \int dx' \tilde{\rho}_p(x') \frac{1}{\sqrt{\alpha^2 + (x - x')^2}} \right\}, \end{aligned} \quad (6)$$

with

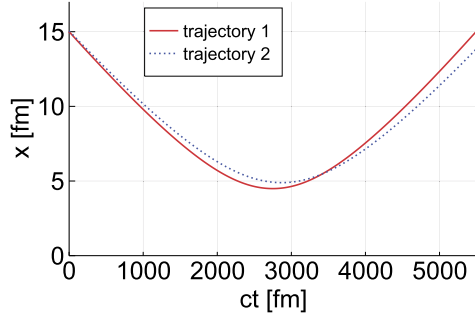


Fig. 1. The trajectory of the right α particle in $\alpha + \alpha$ scattering in one dimension obtained with the time-dependent Hartree-Fock with two different initial conditions. The two α particles are assumed to move symmetrically with respect to $x = 0$. The solid line is obtained with the initial condition of $x_0 = 30.0/2$ fm and $E = 0.113$ MeV, while the dashed line is obtained with $x_0 = 30.1/2$ fm and $E = 0.100$ MeV. The interaction is based on a Gaussian + density-dependent zero-range nuclear interaction together with a soft-core Coulomb interaction. The Coulomb barrier between the two α particles is located at $x = 3.84$ fm with the height of 0.13 MeV.

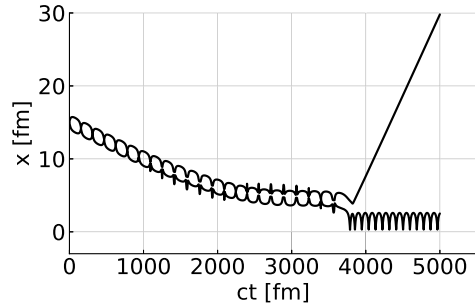


Fig. 2. Same as Fig. 1, but obtained with the time-dependent generator coordinate method with the same initial conditions.

$$\tilde{\tau}(x) = \sum_{i,j} \left(\frac{\partial}{\partial x} \phi_{ai}^*(x) \right) \left(\frac{\partial}{\partial x} \phi_{a'j}(x) \right) (B^{-1})_{ji} \quad (7)$$

$$\tilde{\rho}(x) = \sum_{i,j} \phi_{ai}^*(x) \phi_{a'j}(x) (B^{-1})_{ji}, \quad (8)$$

where the matrix B is defined as $B_{ij} = \langle \phi_{ai} | \phi_{a'j} \rangle$. The overlap kernel $\langle \Phi_a | \Phi_{a'} \rangle$ in Eq. (6) is given as $\langle \Phi_a | \Phi_{a'} \rangle = \det(B)$. We follow Refs. [23,49] and use the parameters of $t_0 = -12.5$ MeV fm $^{-1}$, $t_3 = 8.8$ MeV fm $^{-2}$, and $b = 2.0$ fm. For the Coulomb interaction, we arbitrarily set $\alpha = 1.0$ fm.

In order to derive the time-dependent equation for $Z_a(t)$ according to the variational principle, Eq. (2), one needs to evaluate the derivative of $\langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle$ with respect to $Z_a^*(t)$. We carry it out numerically, that is, we calculate a change of this quantity when $Z_a^*(t)$ is shifted to $Z_a^*(t) + \delta Z_a^*(t)$ and divide it by $\delta Z_a^*(t)$. Notice that the derivative does not depend on the direction of $\delta Z_a^*(t)$ in the complex plane, as long as the absolute value of $\delta Z_a^*(t)$ is small.

In the calculations shown below, we use the Gaussian width of $\nu = 0.5$ fm $^{-2}$. This value is determined so that the internucleus potential at $x = 0$ evaluated in the frozen density approximation with a single Slater determinant [12] becomes higher than the height of the Coulomb barrier. With the parameter set employed, the barrier in the frozen density approximation is located at 3.84 fm with the height of 0.13 MeV, while the potential at $x = 0$ is 7.1 MeV.

We first discuss the result of a superposition of two Slater determinants. For the first Slater determinant, the initial positions of the α particles are set to be $x_0 = \pm 30.0/2$ fm with the initial relative momentum of $p_0 = \mp \sqrt{2\mu E}$ with $E = 0.113$ MeV, where μ is the reduced mass evaluated with the static calculation

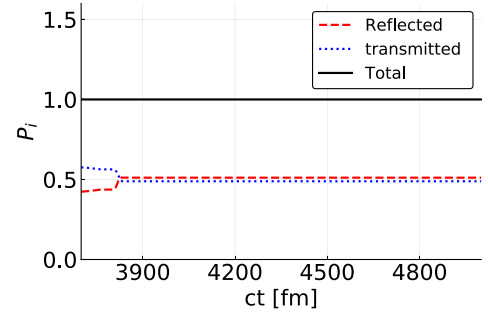


Fig. 3. The time-evolution of the fractions of each Slater determinant shown in Fig. 2. The dashed and the dotted lines show the reflected and the transmitted Slater determinant respectively.

for a single α particle, whereas for the second Slater determinant we take $x_0 = \pm 30.1/2$ fm and $p_0 = \mp \sqrt{2\mu E}$ with $E = 0.100$ MeV. Fig. 1 shows the position of each Gaussian wave packet, $x(t) = \text{Re}[Z(t)]/\sqrt{\nu}$, where $\text{Re}[Z]$ denotes the real part of Z , for the case where the Slater determinants are evolved independently to each other with the TDHF method. Since the initial energy is below the barrier for both the Slater determinants, they are both reflected at the barrier located at 3.84 fm.

Fig. 2 shows the result of the TDGCM with two Slater determinants, for which the initial conditions are taken to be the same as those in the independent TDHF calculations in Fig. 1. In this calculation, we initially take equal weights for the two Slater determinants, that is, $f_1 = f_2$.

The average initial relative energy, $E_{\text{rel}} \equiv \langle \Psi | H | \Psi \rangle / \langle \Psi | \Psi \rangle - 2E_{\text{g.s.}}$, where $E_{\text{g.s.}}$ is the ground state energy of the α particle, is calculated to be 0.099 MeV, which is still below the Coulomb barrier. Yet, one can clearly see that one of the trajectories overcomes the barrier and undergoes the fusion process, while the other trajectory is reflected at the barrier. This is in marked contrast to the TDHF case shown in Fig. 1, in which both of the trajectories are reflected at the barrier. That is, the tunneling probability of the Coulomb barrier is zero in the TDHF, but it is finite in the TDGCM, even though the exact value of the tunneling probability is difficult to evaluate only with two Slater determinants. Fig. 3 shows the time-evolution of the probabilities of each trajectory in the wave function. Here, the probabilities are defined as (see Eq. (1)),

$$P_i(t) = \frac{|f_i(t)|^2 \langle \Phi_i(t) | \Phi_i(t) \rangle}{\langle \Psi(t) | \Psi(t) \rangle}. \quad (9)$$

Notice that we only plot the long-time behavior, for which the overlap between the two Slater determinant is small, that is, $\langle \Phi_1(t) | \Phi_2(t) \rangle \sim 0$. The fraction for the transmitted trajectory becomes from 0.5 at $t = 0$ to 0.489 at $t = \infty$. This value might be identified with the tunneling probability.

In the case of ETMD, a finite tunneling probability is explained as that the energy of individual test particles is not conserved, and some of test particles can “borrow” an energy from an ensemble of the other test particles in order to overcome the barrier [29–32]. We anticipate that the same argument applies to the TDGCM as well, even though it is difficult to visualize the energy of each Slater determinant as a function of time due to the non-orthogonality of the Slater determinants.

Fig. 4 shows the behavior of the energy of each trajectory after the overlap of the Slater determinants becomes appreciably small. At such t , we can define the energy of each trajectory as

$$E_a(t) = \frac{\langle \Phi_a(t) | H | \Phi_a(t) \rangle}{\langle \Phi_a(t) | \Phi_a(t) \rangle} \quad (10)$$

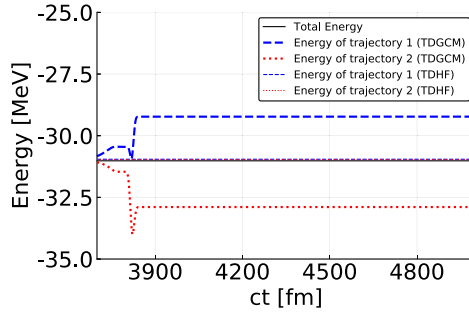


Fig. 4. The energy of each Slater determinant in the time-dependent generator coordinate method (the thick dashed and the dotted lines) and that for the TDHF trajectories (the thin dashed line (-30.95 MeV) and the dotted line (-30.96 MeV)). The total energy is also shown by the solid line. While the total energy is conserved, the energy of each trajectory changes as a function of time.

As compared to the energies for the independent Slater determinants (see the thin dashed and dotted lines), the energy of one of the trajectories (the trajectory 1; the thick dashed line) increases while that of the other trajectory (the trajectory 2; the thick dotted line) decreases, even though the total energy of the system,

$$E_{\text{tot}} = \frac{\sum_{ab} f_a(t)^* f_b(t) \langle \Phi_a(t) | H | \Phi_b(t) \rangle}{\sum_{ab} f_a(t)^* f_b(t) \langle \Phi_a(t) | \Phi_b(t) \rangle}, \quad (11)$$

remains a constant at any time (see the solid line). Notice that the trajectory 1 corresponds to the transmitted fraction in Fig. 3, while the trajectory 2 corresponds to the reflected fraction in Fig. 3. This indicates that the trajectory 1 borrows the energy from the trajectory 2 and passes the barrier.

We next discuss the result with 10 Slater determinants. To this end, we take the same weight factor f_a for each Slater determinant at $t = 0$ and randomly generate the initial conditions for x_{a0} and p_{a0} around a central value assuming a Gaussian distribution. For the initial distances, we take the central value of $30.0/2$ fm with the Gaussian width of 0.1 fm. On the other hand, for the initial energies, we take the central value of 0.1 MeV with the width of 0.02 MeV. We use a particular ensemble where all the 10 Slater determinants have an energy below the barrier so that they are all reflected at the barrier when they are evolved individually. The average energy of this ensemble is computed to be 0.11 MeV. By taking into account the entanglement among the Slater determinants with the TDGCM method, we find that 3 Slater determinants undergo fusion, whereas the other 7 Slater determinants are reflected at the barrier. As in the case of a superposition of 2 Slater determinants, it is remarkable that the tunneling phenomenon is simulated using “classical” TDHF trajectories. Evidently, the TDGCM provides a promising microscopic framework to describe many-particle tunneling phenomena.

4. Summary

In summary, we have applied the time-dependent generator coordinate method (TDGCM) to the ${}^4\text{He}+{}^4\text{He}$ scattering in one dimension at energies below the Coulomb barrier. To this end, we have used the initial relative distance and the initial relative momentum between the two ${}^4\text{He}$ particles as generator coordinates which characterize each Slater determinant. We have shown that, by superposing Slater determinants, a many-body tunneling can be simulated with this method, whereas the time-dependent Hartree-Fock (TDHF) method yields the tunneling probability of either 0 or 1. That is, even when individual TDHF trajectories are all reflected at the barrier, some of them undergo fusion in the TDGCM. It is thus evident that the TDGCM provides a promising means to microscopically describe many-body tunneling.

Since the aim of this paper was to carry out a proof-of-principle study of the TDGCM framework, for simplicity we have parameterized single-particle wave functions in a Gaussian form with a fixed width. Similar wave functions may be employed in applications of the TDGCM to scattering of heavier nuclei in the more realistic three-dimensional space. That is, if one assumes that the single-particle wave functions in the colliding nuclei are given by pre-fixed mean-field potentials, those single-particle wave functions are characterized only by the time-dependent centers of the mean-field potentials. TDGCM calculations can thus be carried out in the same way as what we have done in this paper for scattering of two α particle in one-dimension.

Of course, one can improve the performance of the TDGCM method by using less restricted single-particle wave functions, even though this would be numerically challenging, especially in applications to reactions in the three-dimensional space. Moreover, we remark that an application of the TDGCM is not restricted to nuclear reactions, but it can also be applied to several phenomena, such as a decay of unstable states, including nuclear fission, and chemical reactions. These will be interesting future works.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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