

Collective-subspace requantization for sub-barrier fusion reactions: Inertial functions for collective motions

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Abstract. The adiabatic self-consistent collective coordinate (ASCC) method is used to determine the optimum reaction path and to calculate the potential and the inertial functions of the reaction model. The properties of the inertial functions are investigated with the ASCC method, in comparison with those of the cranking formulae. In addition, the properties of the pair rotation are investigated in the BCS pair model. The moments of inertia for rotation in both the real and the gauge spaces may decrease as the deformation develops.

1 Introduction

Time-dependent density functional theory (TDDFT) is a standard tool for studies of a variety of heavy-ion reactions [1–3], such as nuclear fusion above the Coulomb barrier energy [4–6], induced fission reaction [7], quasi-fission reaction [8], and multi-nucleon transfer reactions [9, 10]. It also provides an important method in studies of nuclear response, namely the (quasiparticle) random-phase approximation ((Q)RPA) in the linear regime. In addition, the properties of the giant resonances have been extensively investigated with TDDFT real-time simulations [11–14]. A universal description of nuclei in the entire mass region and a unified microscopic description of nuclear structure and reaction are great features of the TDDFT method.

On the other hand, the current TDDFT models of nuclei have a problem in a proper account of fluctuation effects. The problems are especially serious in transitional regions where the nuclear shape fluctuates and is not well-defined. In nuclear reaction studies, a prominent weak point is evident for the sub-barrier fusion and the spontaneous fission reactions, which never takes place in the straightforward TDDFT calculations. The theory lacks a part of important quantum fluctuation associated with the nuclear shape. In order to recover the missing quantum fluctuation, theories beyond the mean field are required.

The most popular method of improving the mean-field theory is the generator coordinate method (GCM) [15, 16]. The GCM is a quantum mechanical approach and is capable of describing the quantum fluctuations along the chosen generator coordinates. Increasing the number of generator coordinates, in principle, the solution converges to the exact eigenstates of the Hamiltonian. However, this is not the case for the energy density functionals. Al-

though many of the nuclear energy density functionals are based on density-dependent effective interactions, the exact ground state of the Hamiltonian is not physical. Therefore, we must carefully choose a small number of generator coordinates to avoid such unphysical states. This also prevents us from utilizing a variational method to determine the generator coordinates [17, 18]. The GCM has both numerical and theoretical problems [3], especially when we use the effective interactions which depend on a fractional power of density [19–21].

Our strategy for a solution to these problems is the requantization of collective degrees of freedom which are selected according to the TDDFT dynamics. Similar approaches have been adopted in studies of low-lying excitation spectra and in the fission dynamics, e.g., the five-dimensional collective Hamiltonian (5DCH) method instead of the GCM on the (β, γ) plane [3, 22, 23] and the collective model of spontaneous fission [24]. However, in these models, the shape variables are chosen by hand and the inertia parameters are approximated by the cranking formula [25, 26]. We aim to improve the models in terms of the microscopic point of view.

We determine a collective subspace which is decoupled from the other intrinsic degrees of freedom. For this purpose, we use the adiabatic self-consistent collective coordinate (ASCC) method [3, 27–30]. The solution of the ASCC equations provides a set of canonical variables (q, p) to specify the one-body density $\hat{\rho}(q, p)$, and the generators of collective variables $(\hat{Q}(q), \hat{P}(q))$. The collective potential is given by the energy values at $p = 0$, $V(q) = E[\rho(q, p = 0)]$, and the expansion with respect to the p provides the kinetic energy with the inertial masses, $M^{-1}(q) = \partial^2 E / \partial p^2|_{p=0}$. This leads to the collective Hamil-

tonian

$$H = \frac{p^2}{2M(q)} + V(q). \quad (1)$$

Since the scale of the coordinate q is arbitrary, we can adjust it so as to make the collective inertia constant, $M(q) = \mu$. In the study of the sub-barrier nuclear fusion, we expect that the coordinate q should be proportional to the distance between the projectile and the target nuclei, r , when two nuclei are far apart. Thus, it is intuitive to write down the collective Hamiltonian in the relative coordinate r and its conjugate momentum $p_r = p(dq/dr)$. It should be noted that the collective inertia $M(r)$, given by $\{M(r)\}^{-1} = (dr/dq)^2 \mu^{-1}$, is no longer constant, especially at $r \lesssim R_{\text{touch}}$ where R_{touch} is a touching distance of two nuclei.

Assuming the axial symmetry with respect to the axis of the relative coordinate \mathbf{r} between the projectile and the target, two angles to fix the direction of \mathbf{r} describe the rotational motion, and their moments of inertia are calculated solving the Thouless-Valatin equation [31] at each point on the collective subspace r . Eventually, the following collective Hamiltonian is obtained.

$$H = \frac{p_r^2}{2M(r)} + \frac{L^2}{2\mathcal{I}(r)} + V(r), \quad (2)$$

where L^2 is the square of the angular momentum produced by the rotation of the coordinate \mathbf{r} . In the end, the canonical quantization is performed, replacing p_r by $-i\partial/\partial q$ ($\hbar = 1$) with the Pauli's prescription and L^2 by the angular momentum operator \hat{L}^2 . It should be noted that the point transformation from q to r does not change the physics, as far as the inertial functions and the conjugate momentum are properly defined.

In this paper, we focus our discussion on the inertial functions for various collective motions. In Sec. 2, we briefly review the ASCC method and present methods of calculating the inertial functions in Sec. 3. We especially, describe the derivation of the cranking formulae based on the TDDFT equation of motion, which can clarify the missing correlations in the cranking formulae. In Sec. 5, we show a somewhat surprising property of the moment of inertia for the pair rotation. The conclusion and the perspectives are given in Sec. 6.

2 Collective subspace

Using the energy density functional $E[\rho]$ and the local (normal-mode) generator $Q(q)$, the collective subspace for the low-energy collective motion is defined by

$$\left[h[\rho(q)] - \lambda Q(q), \rho(q) \right] = 0, \quad (3)$$

where $h_{ij} \equiv \delta E / \delta \rho_{ji}$. The Lagrange multiplier λ corresponds to the gradient of the energy, $\lambda = \partial E[\rho(q)] / \partial q$. The generators, $(Q(q), P(q))$, are given by a solution of the moving-frame random-phase approximation (MF-RPA).

$$\begin{aligned} \{A(q) + B(q)\} \{A(q) - B(q)\} Q(q) &= \omega^2 Q(q), \\ P(q) &= M(q) \{A(q) - B(q)\} Q(q), \end{aligned} \quad (4)$$

where the matrices $A(q)$ and $B(q)$ are given by

$$\begin{aligned} A_{php'h'}(q) &= (\epsilon_p - \epsilon_h) \delta_{pp'} \delta_{hh'} + \frac{\partial h_{ph}}{\partial \rho_{p'h'}}, \\ B_{php'h'}(q) &= \frac{\partial h_{ph}}{\partial \rho_{h'p'}}. \end{aligned} \quad (5)$$

The MF-RPA equation determines only the particle-hole and hole-particle matrix elements of the generators, $(Q(q), P(q))$. In this paper, we assume that their particle-particle and hole-hole matrix elements vanish. The single-particle energies ϵ_i in Eq. (5) are the eigenvalues of $h - \lambda Q(q)$. The derivatives in Eq. (5) are calculated according to the finite-amplitude method (FAM) [32–34], especially using the m-FAM scheme in Ref. [35].

The MF-RPA equation (3) cannot fix the magnitude of $Q(q)$. Since these equations are scale invariant concerning $Q(q) \rightarrow \alpha Q(q)$, $P(q) \rightarrow \alpha^{-1} P(q)$, and $M(q) \rightarrow \alpha^{-2} M(q)$, we can arbitrarily normalize $Q(q)$. In actual calculations, we set $M(q)$ a constant value, $M(q) = \mu$, to determine the normalization of $Q(q)$ according to the weakly canonicity condition, $\text{Tr}(\{[Q(q), P(q)] \rho(q)\}) = i$.

The ASCC equations consist of Eqs. (3) and (4) which should be solved self-consistently. Among solutions of Eq. (4), we select a normal mode of the lowest energy keeping the axial symmetry. Note that ω^2 can be negative. The numerical computation produces a series of density $\{\rho(q_0), \rho(q_1), \dots\}$ on the discretized collective coordinate $q_n = q_0 + n \times \Delta q$. This defines the collective subspace, namely the reaction path in the present study. The potential in Eq. (1), $V(q) = E[\rho(q)]$, then, transformed into $V(r) = V(q(r))$ in Eq. (2).

3 Inertial functions

In this paper, we focus our discussion on the properties of collective inertias and their effect on the nuclear dynamics.

3.1 ASCC inertial functions

Since the ASCC method provides a decoupled collective subspace, the inertial mass tensor should be block-diagonal: no off-diagonal elements between the collective subspace and the rest. The value of the constant mass μ determines the scale of the coordinate q , then, the inertial function $M(r)$ in Eq. (2) is given by

$$M(r) = \mu \left(\frac{dq}{dr} \right)^2, \quad \left(M_{ij}(r) = \sum_{kl} \frac{\partial q^k}{\partial r_i} \mu_{kl} \frac{\partial q^l}{\partial r_j} \right). \quad (6)$$

The second equation in the bracket corresponds to the case that the collective subspace is multi-dimensional, in general.

The rotational modes correspond to the zero-frequency solutions of Eq. (4). For the axially symmetric states, we should obtain two independent solutions corresponding to the rotation around the axes perpendicular to the symmetry axis. Since these modes violate the axial symmetry ($K \neq 0$), they are exactly decoupled from the adopted axially symmetric mode ($K = 0$), $(Q(q), P(q))$ in Sec. 2.

Although the rotational moments of inertia can be deduced from the zero-frequency solutions of Eq. (4), they can be even more easily obtained from the calculation of the strength function at the zero frequency [36]. We use this method to calculate the moments of inertia $\mathcal{I}(r)$ in Eq. (2). This is equivalent to solutions of the Thouless-Valatin equations [15, 31] with the moving-frame Hamiltonian.

3.2 Cranking mass

The most popular method to estimate the collective masses is the cranking formula [25, 26]. It has been utilized in a variety of applications. However, it has been known for many years that the collective masses of the cranking formula have serious problems with missing dynamical residual effects.

3.2.1 Translational motion

In this section, first, we present a derivation of the cranking formula for the translational motion, and demonstrate the importance of the residual effects.

In the TDDFT, a nucleus in the ground state is given by the stationary condition for the density ρ .

$$[h_0, \rho_0] = 0, \quad (7)$$

where ρ_0 is the one-body density of the ground state. h_0 is the Kohn-Sham (KS) Hamiltonian at the density ρ_0 which is represented by the KS orbitals $|\phi_i\rangle$, defined by the KS equation $h_0 |\phi_i\rangle = \epsilon_i |\phi_i\rangle$, as

$$\rho_0 = \sum_{h=1}^A |\phi_h\rangle \langle \phi_h|. \quad (8)$$

The center of mass of ρ_0 is arbitrary and chosen at the origin. Let us consider a nucleus in the ground state, moving in the x direction with a constant velocity v . The density is given as

$$\rho = e^{imv\hat{x}} e^{-ix(t)\hat{p}} \rho_0 e^{ix(t)\hat{p}} e^{-imv\hat{x}}, \quad (9)$$

where m is the nucleon mass. The expectation values of the center of mass X and the total momentum P are

$$X = \frac{1}{A} \text{Tr}(\hat{x}\rho) = \frac{1}{A} \text{Tr}(\hat{x}\rho_0) + \frac{x(t)}{A} \text{Tr}(\rho_0) = x(t), \quad (10)$$

$$P = \text{Tr}(\hat{p}\rho) = \text{Tr}(\hat{p}\rho_0) + mv \text{Tr}(\rho_0) = Amv. \quad (11)$$

Here, we use the commutation relation $[\hat{x}, \hat{p}] = i$ and the fact that the trace of a product is commutable. Equation (11) indicates that the mass for the translational motion is nothing but the total mass Am . These equations, (10) and (11), are valid at any values of x and $v = \dot{x}$. Assuming x and v are small, we may linearize the density variation as $\delta\rho = x\delta\rho^{(x)} + v\delta\rho^{(v)}$ with $\delta\rho^{(x)} = -i[\hat{p}, \rho_0]$ and $\delta\rho^{(v)} = im[\hat{x}, \rho_0]$. It is easy to verify that $\rho = \rho_0 + \delta\rho$ produces the same results as Eqs. (10) and (11). Note that the particle-particle and hole-hole matrix elements of $\delta\rho$ vanish, $\langle \phi_p | \delta\rho | \phi_{p'} \rangle = \langle \phi_h | \delta\rho | \phi_{h'} \rangle = 0$.

The density of Eq. (9) should satisfy the TDDFT equation $i\dot{\rho} = [h[\rho], \rho]$. Now, we linearize the equation as

$$i \frac{\partial}{\partial t} (x\delta\rho^{(x)} + v\delta\rho^{(v)}) = [h_0, x\delta\rho^{(x)} + v\delta\rho^{(v)}] + [x\delta h^{(x)} + v\delta h^{(v)}, \rho_0], \quad (12)$$

where $\delta h = x\delta h^{(x)} + v\delta h^{(v)}$ is the residual field induced by the density variation, $\delta h^{(i)} = \partial h / \partial \rho |_{\rho_0} \cdot \delta\rho^{(i)}$ with $i = x, v$. The term proportional to x , $x\delta h^{(x)}$, represents a change in the KS potential for a shift of the center of mass, that is present when the translational symmetry is violated in h_0 . The term proportional to v , $v\delta h^{(v)}$, is induced by the velocity of the nucleus, which appears when the KS potential has the velocity dependence. The left-hand side of Eq. (12) is

$$\text{LHS} = i \frac{\partial}{\partial t} (x\delta\rho^{(x)} + v\delta\rho^{(v)}) = iv\delta\rho^{(x)} = v[\hat{p}, \rho_0], \quad (13)$$

and the right-hand side is

$$\text{RHS} = [h_0, \delta\rho] + [\delta h, \rho_0] = v[h_0, \delta\rho^{(v)}] + v[\delta h^{(v)}, \rho_0]. \quad (14)$$

Here, we use the condition that the density (9) at any center-of-mass coordinate with $v = 0$ must satisfy the stationary equation (7). The particle-hole and hole-particle matrix elements of Eq. (12) lead to

$$\begin{aligned} \langle \phi_p | \hat{p} | \phi_h \rangle &= (\epsilon_p - \epsilon_h) \langle \phi_p | \delta\rho^{(v)} | \phi_h \rangle + \langle \phi_p | \delta h^{(v)} | \phi_h \rangle, \\ \langle \phi_h | \hat{p} | \phi_p \rangle &= (\epsilon_p - \epsilon_h) \langle \phi_h | \delta\rho^{(v)} | \phi_p \rangle + \langle \phi_h | \delta h^{(v)} | \phi_p \rangle. \end{aligned} \quad (15)$$

The expectation value of the total momentum is calculated as

$$\begin{aligned} P &= \text{Tr}(\hat{p}\delta\rho) = v \text{Tr}(\hat{p}\delta\rho^{(v)}) \\ &= v \sum_{p,h} \frac{\langle \phi_p | \hat{p} | \phi_h \rangle \langle \phi_h | (\hat{p} - \delta h^{(v)}) | \phi_p \rangle + \text{c.c.}}{\epsilon_p - \epsilon_h}, \end{aligned} \quad (16)$$

which should be equal to Amv , as we have shown in Eq. (11).

The cranking formula is obtained by the approximation to neglect the residual field $\delta h^{(v)}$ in Eq. (16), that results in the mass of the translational motion,

$$M = \frac{dP}{dv} = 2 \sum_{p,h} \frac{|\langle \phi_p | \hat{p} | \phi_h \rangle|^2}{\epsilon_p - \epsilon_h}. \quad (17)$$

In general, the cranking formula (17) produces $M \neq Am$. This is due to the violation of the Galilean invariance of the static KS Hamiltonian h_0 . In fact, if h_0 satisfies the relation,

$$i[h_0, \hat{x}] = \frac{\hat{p}}{m}, \quad (18)$$

then, we can rewrite the quantity

$$[\hat{p}, \rho_0] = im[[h_0, \hat{x}], \rho_0] = im[h_0, [\hat{x}, \rho_0]] = [h_0, \delta\rho^{(v)}], \quad (19)$$

where we use Eq. (7). This guarantees that the second term on the right-hand side of the TDDFT equation (14) vanishes. See Eqs. (13) and (14). Thus, the cranking formula gives the exact total mass, $M = Am$. In other words, when Eq. (18) is violated for h_0 , the residual field $\delta h^{(v)}$ is necessary to restore the Galilean invariance of the energy density functional $E[\rho]$.

3.2.2 Rotational motion

The arguments for the translational motion can be directly applicable to the motion of the uniform rotation. When the ground-state solution of the KS equation violates the rotational symmetry, the rotational degrees of freedom emerge from the orientation of the deformed intrinsic state. Assuming the rotation around the x axis with a constant angular velocity $\omega = \dot{\theta}$, the density is given, similar to Eq. (9), by

$$\rho = e^{iI\omega\hat{\theta}} e^{-i\theta(t)\hat{j}_x} \rho_0 e^{i\theta(t)\hat{j}_x} e^{-iI\omega\hat{\theta}}, \quad (20)$$

where the angle operator $\hat{\theta}$ is a conjugate variable to the angular momentum \hat{j}_x , namely $[\hat{\theta}, \hat{j}_x] = i$. $I = \mathcal{I}_x/A$ is linked to the moment of inertia of the nucleus, \mathcal{I}_x . Here, we only assume the existence of the angle operator $\hat{\theta}$ and the moment of inertia \mathcal{I} , but do not need the exact expression of those quantities¹. In addition, in contrast to the translational case in Sec. 3.2.1, the decoupling between the rotational and the intrinsic motions is not exact. Therefore, strictly speaking, Eq. (20) is true only when $\omega = 0$, and the density ρ_0 in Eq. (20) should change at a non-zero value of ω . In this section, we assume a small value of ω and neglect the ω -dependence of the intrinsic structure.

The rest of the derivation is the same as those in Sec. 3.2.1. Neglecting the residual fields, $\delta h^{(\omega)}$, the cranking formula for the moment of inertia is given by

$$\mathcal{I}_x = \frac{dJ}{d\omega} = 2 \sum_{p,h} \frac{|\langle \phi_p | \hat{j}_x | \phi_h \rangle|^2}{\epsilon_p - \epsilon_h}. \quad (21)$$

In the rotational case, there is no exact relation analogous to the Galilean invariance. Nevertheless, the condition in analogy to Eq. (18) results in the justification of the neglect of the residual effect. Therefore, the cranking formula (17) is valid (only) when the KS potential has no velocity dependence. In general, the residual terms associated with $\delta h^{(\omega)}$ proportional to ω (terms of $\delta h^{(v)}$ in Eq. (16)) is necessary to give a proper value for the moment of inertia.

3.2.3 Collective motion on the reaction path

Instead of determining the collective subspace by solving Eq. (3), the generator $\hat{Q}(q)$ is most commonly replaced by a constraining one-body operator given by hand, \hat{C} . The constrained KS density is obtained by

$$[h_\lambda, \rho_\lambda] = 0, \quad h_\lambda \equiv h[\rho_\lambda] - \lambda \hat{C} \quad (22)$$

¹This is different from the case of translational motion. We explicitly know both the center-of-mass coordinate, the total linear momentum, and the exact value of the total mass in Sec. 3.2.1.

where λ is the Lagrange multiplier. We may change the label λ into the collective coordinate, for instance, the distance between two colliding nuclei r . The relation between λ and R is given by $r = \text{Tr}(\hat{r}\rho_\lambda)$. The choice of the operator \hat{r} may not be unique, but a possible choice is given in Ref. [37]. The density is represented by the KS orbitals $|\phi_i(r)\rangle$ which are solutions of $h_\lambda |\phi_i(r)\rangle = \epsilon_i(r) |\phi_i(r)\rangle$.

The cranking formula of the inertial mass for the collective motion with respect to the coordinate r can be given, in analogy to Eqs. (17) and (21), as

$$M^{\text{np}}(r) = 2 \sum_{p,h} \frac{|\langle \phi_p(r) | \partial/\partial r | \phi_h(r) \rangle|^2}{\epsilon_p(r) - \epsilon_h(r)}. \quad (23)$$

The formula (23) is often called ‘‘non-perturbative cranking formula.’’ This is why we put the superscript for M^{np} . A further approximation can give ‘‘perturbative cranking formula’’ [37], denoted as M^{p} in this paper,

$$M^{\text{p}} = \frac{1}{2} S_3(\hat{C}, \hat{C}) \{S_1(\hat{r}, \hat{C})\}^{-2}, \quad (24)$$

with

$$S_k(\hat{A}, \hat{B}) \equiv \frac{1}{2} \sum_{p,h} \frac{\langle \phi_h | \hat{A} | \phi_p \rangle \langle \phi_p | \hat{B} | \phi_h \rangle + \text{c.c.}}{(\epsilon_p - \epsilon_h)^k} = S_k(\hat{B}, \hat{A}), \quad (25)$$

where \hat{A} and \hat{B} are the one-body operators. In the case of $\hat{A} = \hat{B}$, $S_k(\hat{A}, \hat{A})$ corresponds to the k th inverse energy-weighted sum-rule value, $m_k(\hat{A}) \equiv S_k(\hat{A}, \hat{A})$. In the case of $\hat{C} = \hat{r}$, the perturbative cranking formula has become an even simpler form

$$M^{\text{p}} = \frac{1}{2} m_3(\hat{r}) \{m_1(\hat{r})\}^{-2}, \quad (26)$$

which has been extensively utilized in the literature.

4 Results

4.1 Inertial functions for sub-barrier nuclear reactions

The energy density functional is slightly modified from $E_{\text{BKN}}[\rho]$ of Ref. [38] to allow the KS potential to be velocity-dependent.

$$E[\rho] = E_{\text{BKN}}[\rho] + B_3 \int d\mathbf{r} \{ \rho(\mathbf{r}) \tau(\mathbf{r}) - \mathbf{j}^2(\mathbf{r}) \}, \quad (27)$$

where $\rho(\mathbf{r})$ is the isoscalar density, $\tau(\mathbf{r})$ is the isoscalar kinetic density, and $\mathbf{j}(\mathbf{r})$ is the isoscalar current density. The positive value of the parameter B_3 produces the effective mass smaller than the bare nucleon mass, $m^*/m < 1$.

Most of the numerical results are shown in the paper [37]. Here, we recapitulate the summary of the results. The ASCC inertial functions calculated according to Eq. (6) reproduce

1. the total mass Am for the translation,
2. the reduced mass, $\mu_{\text{red}} = A_1 A_2 m / (A_1 + A_2)$, for the relative motion at large r ($r \gg R_{\text{touch}}$),

3. the reduced value of the moment of inertia, $\mathcal{I}_{\text{red}} \equiv \mu_{\text{red}} r^2$, at large r .

On the other hand, the cranking formulae, Eqs. (17), (21), (23), and (24), fail to reproduce these quantities. Instead, the cranking formulae approximately produce

1. the total effective mass, $A\langle m^* \rangle$ for the translational motion,
2. the reduced effective mass $\mu_{\text{red}}^* = A_1 A_2 \langle m^* \rangle / (A_1 + A_2)$ at large r
3. the moments of inertia $\mu_{\text{red}}^* r^2$ at large r

These results apparently indicate the failure of the cranking formulae and the superiority of the ASCC masses over the cranking masses.

We have also found an interesting property of the moments of inertia, opposite to our naive intuition: the calculated values decrease in the vicinity of the ground state as a function of the relative distance r , or equivalently as a function of the nuclear deformation β .

$$\frac{d\mathcal{I}}{dr} < 0, \quad \frac{d\mathcal{I}}{d\beta} < 0. \quad (28)$$

This is due to the property that the moment of inertia is close to the rigid-body value at the ground state (without pairing), $\mathcal{I} \approx \mathcal{I}_{\text{rig}}$, then, immediately drops to the reduced value \mathcal{I}_{red} once two nuclei are apart, $r \gtrsim R_{\text{touch}}$. This is a consequence of the quantum mechanical requirement. The total moment of inertia for two separated nuclei can be decomposed as

$$\mathcal{I}(r) = \mathcal{I}_1 + \mathcal{I}_2 + \mathcal{I}_{\text{red}}(r), \quad (29)$$

where \mathcal{I}_i ($i = 1, 2$) is the moment of inertia of the nucleus i concerning its own center of mass. When the two nuclei are both spherical, the quantum mechanics requires $\mathcal{I}_1 = \mathcal{I}_2 = 0$ and produces the reduced value, $\mathcal{I}(r) = \mathcal{I}_{\text{red}}$ at $r \gtrsim R_{\text{touch}}$.

For more details and possible effects on the fusion cross sections, the reader is referred to Ref. [37].

5 Moments of inertia for pair rotation

In a somewhat different context, we have recently found a property, similar to Eq. (28), that the moments of inertia of the pair rotation decreases as a function of the pairing gap (deformation in the gauge space) Δ .

$$\frac{\partial \mathcal{I}_{\text{pair}}}{\partial \Delta} < 0, \quad (30)$$

where the moment of inertia is calculated, using the ground-state energies with different neutron (proton) numbers, as

$$\frac{1}{\mathcal{I}_{\text{pair}}} = \frac{E(N+2) - 2E(N) + E(N-2)}{4}. \quad (31)$$

This behavior can be qualitatively understood as follows, using the BCS treatment of the pair model. The particle number N is written as

$$N(\lambda, \Delta) = \int_{\lambda-\Delta}^{\lambda+\Delta} \rho(\epsilon) g(\epsilon - \lambda, \Delta) d\epsilon, \quad (32)$$

$$g(\tilde{\epsilon}, \Delta) \equiv \frac{1}{2} \left(1 - \frac{\tilde{\epsilon}}{\sqrt{\tilde{\epsilon}^2 + \Delta^2}} \right), \quad (33)$$

where $\rho(\epsilon)$ is the single-particle level density and λ is the chemical potential. We truncate the model space for the pairing correlations to include the single-particle levels in the section of 2Δ centered around the chemical potential. The moment of inertia is given by

$$\begin{aligned} \mathcal{I}_{\text{pair}} &= \frac{\partial N}{\partial \lambda} = \int_{\lambda-\Delta}^{\lambda+\Delta} \rho(\epsilon) \frac{\partial g(\epsilon - \lambda, \Delta)}{\partial \lambda} d\epsilon \\ &= - \int_{-\Delta}^{\Delta} \rho(\tilde{\epsilon} + \lambda) \frac{\partial g(\tilde{\epsilon}, \Delta)}{\partial \tilde{\epsilon}} d\tilde{\epsilon}. \end{aligned} \quad (34)$$

Here, we keep the model space invariant when we differentiate the equation with respect to λ . Then, its derivative with respect to Δ is

$$\begin{aligned} \frac{\partial \mathcal{I}_{\text{pair}}}{\partial \Delta} &= \frac{\partial^2 N}{\partial \lambda \partial \Delta} = - \int_{-\Delta}^{\Delta} d\tilde{\epsilon} \rho(\tilde{\epsilon} + \lambda) \frac{\partial^2 g(\tilde{\epsilon}, \Delta)}{\partial \tilde{\epsilon} \partial \Delta} \\ &= - \frac{1}{2\Delta} \int_{-\Delta/\Delta}^{\Delta/\Delta} \rho(\lambda + x\Delta) \frac{1 - 2x^2}{(x^2 + 1)^{5/2}} dx. \end{aligned} \quad (35)$$

In the energy interval of 2Δ , we approximate the level density in the linear order as

$$\rho(\lambda + x\Delta) \approx \rho(\lambda) + x\Delta \rho'(\lambda), \quad (36)$$

which is inserted into Eq. (35) to obtain

$$\frac{\partial \mathcal{I}_{\text{pair}}}{\partial \Delta} = - \frac{\rho(\lambda)}{\Delta} I(\Delta/\Delta), \quad (37)$$

and

$$I(\eta) \equiv \int_0^\eta dx \frac{1 - 2x^2}{(x^2 + 1)^{5/2}} = \frac{\eta}{(\eta^2 + 1)^{3/2}}. \quad (38)$$

For $\eta = \Delta/\Delta > 0$, it is trivial to have $I(\eta) > 0$. Thus, Eq. (30) is proved.

6 Conclusion and future perspectives

Using the ASCC method, we have microscopically derived a collective subspace (reaction path) for the sub-barrier fusion reaction. In addition, the method provides the potential and the inertial functions, which leads to the collective Hamiltonian of the reaction model. In this paper, we particularly focus our discussion on properties of the inertial functions.

The ASCC inertial functions perfectly agree with the correct values in the asymptotic region, such as the total mass for the translational motion, the reduced mass for the relative motion at large r , and the reduced moments of inertia at large r . On the other hand, the cranking formulae fail to reproduce these asymptotic values. This indicates the superiority of the ASCC method over the cranking formula.

The moment of inertia at the ground state is approximately equal to that of the rigid-body value, but surprisingly, it decreases as the deformation increases. We may expect that the isotropic velocity distribution at the equilibrium is distorted to be anisotropic, leading to a transition from the ‘‘rigid body’’ to the ‘‘irrotational flow.’’ Since the moment of inertia for the irrotational fluid vanishes for spherical systems, the two spherical nuclei, whose mass

numbers A_1 and A_2 , at distance r , produce the moment of inertia, $\mu_{\text{red}}r^2$. This is well reproduced by ASCC moments of inertia, but not for the cranking formula.

Further studies on the collective masses are desired, particularly effects of pairing and beyond the mean field. We have shown that the recovery of the Galilean invariance violated in the KS potential is essential to produce the collective inertia. Since the pair field is known to break the Galilean invariance [39], it is of great interest to investigate residual effects of the pair fields.

We have also studied properties of the pair rotation in the gauge space, then, have found that the moment of inertia also decreases as the pair deformation increases. This property can be explained by the BCS pair model. This may indicate a prominent difference in the effect of the deformation between the spatial rotation and the pair rotation. Further investigation is under progress.

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