Adiabatic hyperspherical potentials with localized correlated Gaussians

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The adiabatic hyperspherical approach is a natural extension of the well-known three-dimensional polar coordinate method to solving a Schrödinger equation of a few-body system. To evaluate the matrix element of an adiabatic Hamiltonian at a fixed hyper-radius is crucially important in that approach, but due to the difficulty of its calculation real applications have been limited mostly up to four-body systems. To resolve this limitation I introduce a localized hyper-radial function and show that the matrix element needed for N-body system can be obtained using correlated Gaussians with arbitrary angular momentum. I demonstrate its feasibility in the systems of $N = 3$–6 α particles. It is pointed out that an extension into correlated Gaussians with double global vectors is desirable for further realistic descriptions of the hyperangular motion.

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I. INTRODUCTION

The hyperspherical (HS) method attempts to solve an N-particle Schrödinger equation by expressing the total wave function as a sum of the product of hyper-radial and hyper-angular parts. It provides a unified framework to describe quantum dynamics involving a variety of recombinations of the constituent particles. Two realizations of the HS approach are widely used. In one approach the total wave function is expanded in terms of the HS harmonics that are eigenfunctions of the hyperangular kinetic-energy operator [1,2]. In another approach, often called the adiabatic HS approach [3], the adiabatic Hamiltonian involving the hyperangular kinetic-energy and the interaction potential is first diagonalized to obtain the adiabatic potentials (or the adiabatic channel energies) and channel wave functions.

The advantage of the first approach is that the HS harmonics are known, thereby making it applicable beyond three-body systems [4–10]. However, its applicability is hindered in some cases by the fact that the convergence of the HS harmonics expansion is slow especially when a long-range potential, e.g., the Coulomb coupling potential, acts at large hyper-radial distances. This slowness is due to the fact that the hyperangular kinetic-energy and the interaction potential do not commute [11]. The triple-α reaction rate obtained by both types of HS calculations [12,13] clearly indicates this delicate problem of large distance dynamics. The reaction rate obtained in the second approach [13] is found to be consistent with a Faddeev calculation [14].

The second approach has a great merit in that it also gives an intuitive picture for the underlying physics. Applying it to $N(>3)$-particle system is, however, confronted with two things. One, common to all *ab initio* type calculations, is a question of what type of basis functions are used. The other, more serious, is that the matrix element of an operator $\mathcal{O}$ of type

$$\langle \Phi' | \mathcal{O} | \Phi \rangle_{\rho=R}, \tag{1}$$

essential in the second approach, is very hard to calculate. Here, $\langle \ldots \rangle_{\rho=R}$ indicates that the matrix element is to be calculated by integrating over all the coordinates but the hyper-radius ρ, which is fixed to R.

The adiabatic potential plays a decisive role in determining not only bound-state structure but also continuum dynamics relevant to decay and fusion. It is a very useful quantity to give an insight into important processes involved. Its significant role in few-body systems is exemplified in, e.g., a recent review [15]. The competitive contribution of three-α continuum and ^{8}Be $+\alpha$ quasi-two-body continuum to forming the adiabatic potential is carefully examined [13,16]. To assess the effect of couplings of different configurations, it is desirable that one has a universal scale to measure the size of the system and that the adiabatic potential is given as a function of that scale. For example, in nuclear fusion initially the relative distance between the nuclei might be the most important coordinate, but later other coordinates will be more suitable and necessary. Thus the relative distance is not always a satisfactory scale for the adiabatic potential of the fusion, but the hyper-radius used in the HS method is an unambiguous scale. Also the total orbital angular momentum L is naturally taken into account in the HS method. The potential barriers for different shapes of multi-α particles were calculated using a generalized liquid-drop model [17,18]. The α-particle clustering of self-conjugate nuclei was studied by the Hartree-Fock-Bogoliubov approach with their radii constrained [19]. Since taking care of the angular momentum and removing spurious center of mass (c.m.) motion may not be easily done in those studies, it is interesting to apply the HS framework free from those problems to calculate the adiabatic potentials of multi-α particles.

The purpose of this paper is twofold. First is to show that the matrix element (1) can be evaluated for arbitrary N and arbitrary L using correlated Gaussians (CG) as the basis functions. Second is to test its feasibility by applying to the adiabatic potentials of multi-α-particle systems. The

CG proposed many years ago [20,21] is extended to describe motion with nonzero L, especially with the help of global-vector representation [22,23]. Together with the stochastic variational method [22–24] to select efficiently CG parameters, many problems have accurately been solved with the CG. See, e.g., Refs. [25–27] for its recent applications. In fact the CG basis functions have been applied to the HS calculation for few-body systems with $L = 0$ and 1 [28–31]. Fourier integration is attempted to evaluate Eq. (1) [31], but there are still several problems to overcome for its real applications [32]. In view of this situation, we have very recently proposed an approach to constrain the CG basis functions according to the expectation value of ρ^2 and its variance [33]. A new recipe developed in this paper further extends its idea, making it possible to compute Eq. (1) for arbitrary L values by localizing the hyper-radial part of the CG completely at $\rho = R$.

I recapitulate basic elements of the HS method in Sec. II. I introduce the localized CG and discuss a general prescription to calculate the matrix element (1) in Sec. III. Basic formulas to calculate the matrix element of the adiabatic Hamiltonian are presented in Sec. IV. I apply its method to the adiabatic potentials of multi-α-particle systems in Sec. V. Conclusion is drawn in Sec. VI. Details of the calculation method are given in Appendices A, B, and C.

II. BASIS OF HYPERSPHERICAL METHOD

A. Hyperspherical coordinates

Let us consider a system of N particles, and assume all the particles to have a common mass m. The case of unequal mass can be treated by defining mass-scaled coordinates. Let $\boldsymbol{r}_i$ $(i = 1, \ldots, N)$ denote the position coordinate of the ith particle, and let $\boldsymbol{x}_i$ stand for the relative (or Jacobi) coordinate,

$$\boldsymbol{x}_i = \sqrt{\frac{i}{i+1}}\left(\boldsymbol{r}_{i+1} - \frac{1}{i}\sum_{j=1}^{i}\boldsymbol{r}_j\right) \quad (i = 1, \ldots, \mathcal{N}), \tag{2}$$

where $\mathcal{N} = N - 1$. The set $\{\boldsymbol{x}_i\}$ together with the c.m. coordinate, $\boldsymbol{x}_N \equiv \boldsymbol{R}_{\rm c.m.} = \sum_{i=1}^{N}\boldsymbol{r}_i/N$, define a transformation matrix U from the single-particle coordinates to the relative and c.m. coordinates:

$$\boldsymbol{x}_i = \sum_{j=1}^{N} U_{ij}\boldsymbol{r}_j \quad (i = 1, \ldots, N). \tag{3}$$

Conversely, $\boldsymbol{r}_i$ is expressed as a combination of $\boldsymbol{x}_j$'s:

$$\boldsymbol{r}_i = \sum_{j=1}^{N} {U^{-1}}_{ij}\boldsymbol{x}_j. \tag{4}$$

The definition (3) implies $\det U = (-1)^{N-1}/\sqrt{N}$. The matrix U^{-1} reads as ${U^{-1}}_{ij} = U_{ji}$ $(i = 1, 2, \ldots, N;\ j = 1, 2, \ldots, \mathcal{N})$ and ${U^{-1}}_{iN} = 1$ $(i = 1, 2, \ldots, N)$.

The hyper-radius ρ is defined by

$$\rho^2 \equiv \sum_{i=1}^{N}(\boldsymbol{r}_i - \boldsymbol{R}_{\rm c.m.})^2 = \frac{1}{N}\sum_{i<j}^{N}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = \sum_{i=1}^{\mathcal{N}}\boldsymbol{x}_i^2. \tag{5}$$

Physically ρ^2 is N times the mean square radius of the system. Let Ω denote a set of hyperangles constructed from the dimensionless coordinates, $\boldsymbol{\xi}_i = \boldsymbol{x}_i/\rho$ $(i = 1, \ldots, \mathcal{N})$. They are constrained to be $\sum_{i=1}^{\mathcal{N}}\boldsymbol{\xi}_i^2 = 1$. A way of expressing Ω in terms of $\boldsymbol{\xi}_i$'s is not unique. Only ρ has the dimension of length, and the volume element for integration excluding $\boldsymbol{R}_{\rm c.m.}$ is

$$d\boldsymbol{x} \equiv \prod_{i=1}^{\mathcal{N}} d\boldsymbol{x}_i = \rho^{d-1} d\rho d\Omega, \tag{6}$$

where d is the degrees of freedom of the intrinsic motion,

$$d = 3(N-1) = 3\mathcal{N}. \tag{7}$$

B. Schrödinger equation in hyperspherical method

A Schrödinger equation for the N-particle system is expressed in terms of the HS coordinates. The Hamiltonian H of the system consists of the total kinetic energy $T_{\rm in}$ with the c.m. kinetic energy being subtracted and the potential energy V that is assumed to contain no derivative of ρ. $T_{\rm in}$ is separated into the hyper-radial (T_ρ) and hyperangular (T_Ω) parts:

$$T_{\rm in} \equiv -\frac{\hbar^2}{2m}\sum_{i=1}^{\mathcal{N}}\frac{\partial^2}{\partial \boldsymbol{x}_i^2} = T_\rho + T_\Omega \tag{8}$$

with

$$T_\rho = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial\rho^2} + \frac{d-1}{\rho}\frac{\partial}{\partial\rho}\right), \quad T_\Omega = \frac{\hbar^2\Lambda^2}{2m\rho^2}, \tag{9}$$

where Λ^2 is called the generalized angular momentum [34]. By writing the total wave function Ψ of the system as $\Psi = \rho^{-\frac{d-1}{2}}\psi(\rho, \Omega)$, the Schrödinger equation $H\Psi = E\Psi$ reduces to that for $\psi(\rho, \Omega)$:

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\rho^2} + H_{\rm ad}(\rho, \Omega)\right]\psi(\rho, \Omega) = E\psi(\rho, \Omega), \tag{10}$$

where $H_{\rm ad}(\rho, \Omega)$ is the adiabatic Hamiltonian,

$$H_{\rm ad}(\rho, \Omega) = \frac{\hbar^2}{2m\rho^2}\left(\Lambda^2 + \frac{(d-1)(d-3)}{4}\right) + V. \tag{11}$$

$H_{\rm ad}(\rho, \Omega)$ contains ρ just as a parameter.

Equation (10) takes exactly the same form as the one familiar in the spherical polar coordinate. Note, however, that $H_{\rm ad}(\rho, \Omega)$ is a Hermitian operator depending on $d-1$ hyperangle coordinates. In the adiabatic HS approach one attempts to solve the equation of motion (10) by first solving the eigenvalue problem of $H_{\rm ad}(\rho, \Omega)$,

$$H_{\rm ad}(\rho, \Omega)\Phi_\nu(\rho, \Omega) = U_\nu(\rho)\Phi_\nu(\rho, \Omega), \tag{12}$$

where ν labels the adiabatic channel energy or adiabatic potential $U_\nu(\rho)$ and the eigenfunction or the channel wave function $\Phi_\nu(\rho, \Omega)$. Next one expands $\psi(\rho, \Omega)$ in terms of those solutions as

$$\psi(\rho, \Omega) = \sum_\nu f_\nu(\rho)\Phi_\nu(\rho, \Omega), \tag{13}$$

where $f_\nu(\rho)$'s are determined from coupled equations derived from Eq. (10). Apparently $U_\nu(\rho)$ plays a crucial role in determining the solution.

Since the HS harmonics are eigenfunctions of Λ^2 [34], they are often conveniently used to solve the eigenvalue problem (12). However, Λ^2 does not commute with V in general [11], and thus other basis functions may become advantageous to solve Eq. (12), especially when the HS harmonics expansion leads to slow convergence. See, e.g., Ref. [13] concerning this issue. If other basis functions are used, the matrix element of type (1) has to be evaluated to solve Eq. (12).

III. LOCALIZED CORRELATED-GAUSSIANS

Fixing ρ at R defines the surface of a d-dimensional ball of radius R [see Eq. (5)]. The matrix element (1) demands an integration over the surface. Although such integration can be formulated by parametrizing the hyperangles as in, e.g., Refs. [29,30], its practice is hard beyond $N = 4$ because multiple numerical integrations have to be done. To bypass the difficulty I introduce a function localized at $\rho = R$, which allows performing the integration over the whole space of d dimension.

A. Localized hyper-radial function

Let us define a hyper-radial function,

$$S_{R\kappa}(\rho) = \sqrt{\frac{2E(\kappa)}{R^d}}\left(\frac{\rho}{R}\right)^\kappa e^{-\frac{\kappa}{2}(\frac{\rho}{R})^2}, \tag{14}$$

where R is an arbitrarily fixed positive parameter and κ is a positive integer. $E(\kappa)$ is defined by

$$E(\kappa) = \frac{\kappa^{\kappa+\frac{d}{2}}}{\Gamma\left(\kappa+\frac{d}{2}\right)} \tag{15}$$

with the Gamma function Γ, and approaches $\sqrt{\kappa/2\pi}e^\kappa$ when $\kappa \to \infty$.

$S_{R\kappa}(\rho)$ is normalized as $\int_0^\infty d\rho\, \rho^{d-1}[S_{R\kappa}(\rho)]^2 = 1$ consistently with the volume element (6), has a peak at $\rho = R$ independent of κ, and for $\kappa \to \infty$ approaches

$$\begin{aligned} S_{R\kappa}(\rho) &\to \left(\frac{2}{\pi R^{2d}}\right)^{\frac{1}{4}} \kappa^{\frac{1}{4}} e^{-\frac{\kappa}{2}\tau(\frac{\rho}{R})} \\ &\approx \left(\frac{2}{\pi R^{2d}}\right)^{\frac{1}{4}} \kappa^{\frac{1}{4}} e^{-\kappa(\frac{\rho-R}{R})^2}, \end{aligned} \tag{16}$$

where $\tau(x) = x^2 - \ln x^2 - 1$. The second line of Eq. (16) is valid because $\tau(x) \approx 2(x-1)^2$ at $x \approx 1$, where $\tau(x)$ reaches a minimum. The squared peak height, $[S_{R\kappa}(R)]^2$, increases in proportion to $\sqrt{\kappa}$. With increasing κ, $S_{R\kappa}(\rho)$ becomes more and more sharply localized at $\rho = R$.

The matrix element $\langle S_{R'\kappa}|f|S_{R\kappa}\rangle$ of a function $f(\rho)$ is evaluated for large κ with the saddle-point method:

$$\begin{aligned} \langle S_{R'\kappa}|f|S_{R\kappa}\rangle &= \int_0^\infty d\rho\, \rho^{d-1} S_{R'\kappa}(\rho) f(\rho) S_{R\kappa}(\rho) \\ &\approx \chi^{\kappa+\frac{d}{2}} f(\sqrt{\chi RR'}), \end{aligned} \tag{17}$$

where $\chi = 2RR'/(R^2 + R'^2)$. Since χ is equal to 1 if and only if $R = R'$ and less than 1 otherwise, one obtains $\lim_{\kappa\to\infty}\langle S_{R'\kappa}|f|S_{R\kappa}\rangle = f(R)\delta_{R,R'}$, where $\delta_{R,R'}$ is 1 for $R = R'$ or 0 for $R \neq R'$. The set $\{S_{R\kappa}\}$ is orthonormal when $\kappa \to \infty$, i.e., $\langle S_{R'\kappa}|S_{R\kappa}\rangle \to \delta_{R,R'}$.

B. Basic procedure to evaluate matrix elements

I define a function $\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x})$ by multiplying $S_{R\kappa}(\rho)$ by the simplest CG [22,23], $f^{uA}_{LM}(\boldsymbol{y})$,

$$\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x}) = S_{R\kappa}(\rho) f^{uA}_{LM}(\boldsymbol{y}), \tag{18}$$

$$f^{uA}_{LM}(\boldsymbol{y}) = \mathcal{Y}_{LM}(\widetilde{u}\boldsymbol{y}) e^{-\frac{1}{2}\widetilde{\boldsymbol{y}}A\boldsymbol{y}}, \tag{19}$$

where $\boldsymbol{y} = \boldsymbol{x}/R$ is a dimensionless coordinate. $\mathcal{Y}_{LM}(\boldsymbol{r}) = r^L Y_{LM}(\hat{\boldsymbol{r}})$ is a solid spherical harmonics, where $\hat{\boldsymbol{r}}$ stands for the polar and azimuthal angles of $\boldsymbol{r}$. u and A are parameters to characterize the CG: $u = (u_i)$ is a column vector of dimension $\mathcal{N}$, and $A = (A_{ij})$ is an $\mathcal{N}\times\mathcal{N}$ symmetric, positive-definite matrix. A tilde symbol $\widetilde{\ }$ stands for a transpose of a vector or a matrix. The exponential $e^{-\frac{1}{2}\widetilde{\boldsymbol{y}}A\boldsymbol{y}}$, where $\widetilde{\boldsymbol{y}}A\boldsymbol{y} = \sum_{i,j=1}^{\mathcal{N}} A_{ij}\boldsymbol{y}_i\cdot\boldsymbol{y}_j$, is invariant under a rotation, while $\mathcal{Y}_{LM}(\widetilde{u}\boldsymbol{y})$ describes rotational motion through a global vector, $\widetilde{u}\boldsymbol{y} = \sum_{i=1}^{\mathcal{N}} u_i\boldsymbol{y}_i$ [22,23,35,36]. A scalar product of three-dimensional vectors, e.g., $\boldsymbol{y}_i\cdot\boldsymbol{y}_j$, is abbreviated as $\boldsymbol{y}_i\boldsymbol{y}_j$ in what follows, and thus $\widetilde{\boldsymbol{y}}\boldsymbol{y} = (\rho/R)^2$. $\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x})$ has the total orbital angular momentum L and its z component M. The parity π of $\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x})$ is $(-1)^L$, so that unnatural parity states such as $L^\pi = 1^+, 2^-, \ldots$, cannot be represented by the simplest CG. I use it, however, to illustrate a method of calculating the matrix element.

Thanks to $S_{R\kappa}(\rho)$, $\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x})$ is localized at $\rho = R$ when $\kappa \to \infty$. The matrix element of $\mathcal{O}$ with $\Phi^{uA}_{R\kappa,LM}$ satisfies the orthogonality relation [see Eq. (17)]

$$\begin{aligned} &\lim_{\kappa\to\infty}\left\langle \Phi^{u'A'}_{R'\kappa,LM}\middle|\mathcal{O}\middle|\Phi^{uA}_{R\kappa,LM}\right\rangle \\ &\quad = \delta_{R,R'}\lim_{\kappa\to\infty}\left\langle \Phi^{u'A'}_{R\kappa,LM}\middle|\mathcal{O}\middle|\Phi^{uA}_{R\kappa,LM}\right\rangle. \end{aligned} \tag{20}$$

This confirms that the matrix element evaluated in the whole space of d dimension approaches the one (1) in the $\kappa \to \infty$ limit.

It is convenient to change the integration variable, $\boldsymbol{x} \to \boldsymbol{y}$, in Eq. (20). Assume that $\mathcal{O}$ satisfies $\mathcal{O}\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x}) = \mathcal{O}(\boldsymbol{x})\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x})$, where $\mathcal{O}(\boldsymbol{x})$ is a function of $\boldsymbol{x}$ that contains no derivative operator of $\boldsymbol{x}$. It follows that

$$\left\langle \Phi^{u'A'}_{R\kappa,LM}\middle|\mathcal{O}\middle|\Phi^{uA}_{R\kappa,LM}\right\rangle = 2D^{(\kappa)}(t\to\kappa) M_{\mathcal{O}}(t), \tag{21}$$

where

$$M_{\mathcal{O}}(t) = \left\langle f^{u'A'_t}_{LM}\middle|\mathcal{O}(R\boldsymbol{y})\middle|f^{uA_t}_{LM}\right\rangle, \tag{22}$$

and $D^{(\kappa)}(t\to\kappa)$ stands for the operation

$$D^{(\kappa)}(t\to\kappa) = E(\kappa)\left(-\frac{d}{dt}\right)^\kappa\Bigg|_{t=\kappa}. \tag{23}$$

Note that I use $(\widetilde{\boldsymbol{y}}\boldsymbol{y})^\kappa e^{-\kappa\widetilde{\boldsymbol{y}}\boldsymbol{y}} = (-\frac{d}{dt})^\kappa|_{t=\kappa} e^{-t\widetilde{\boldsymbol{y}}\boldsymbol{y}}$ in Eq. (21) and define a matrix A_t to denote A plus t times $\mathcal{N}\times\mathcal{N}$ unit matrix $I_{\mathcal{N}}$,

$$A_t = A + tI_{\mathcal{N}}. \tag{24}$$

When $\kappa \to \infty$, $\rho \to R$ and $\sqrt{\widetilde{\boldsymbol{y}}\boldsymbol{y}} = y \to 1$. The matrix element (1) is thus obtained through $M_{\mathcal{O}}(t)$ evaluated by the integration over all $\boldsymbol{y}$ coordinates as follows:

$$\left\langle f^{u'A'}_{LM} \middle| \mathcal{O}(R\boldsymbol{y}) \middle| f^{uA}_{LM} \right\rangle_{y=1} = 2 \lim_{\kappa\to\infty} D^{(\kappa)}(t \to \kappa) M_{\mathcal{O}}(t). \quad (25)$$

To sum up, I obtain the desired matrix element in three steps. First is to calculate $M_{\mathcal{O}}(t)$, which is aided by generating $\mathcal{Y}_{LM}(\widetilde{\boldsymbol{u}}\boldsymbol{y})$ in Eq. (19) through (see Refs. [22,23,33])

$$\mathcal{Y}_{LM}(\widetilde{\boldsymbol{u}}\boldsymbol{y}) = \frac{(2L+1)!!}{4\pi L!} \int d\boldsymbol{e}\, Y_{LM}(\boldsymbol{e}) \left[\frac{\partial^L}{\partial \alpha^L} e^{\widetilde{\boldsymbol{s}}\boldsymbol{y}} \right]_{\alpha=0}, \quad (26)$$

where $\boldsymbol{s} = \alpha \boldsymbol{e} u$ with $\boldsymbol{e}$ being a three-dimensional unit vector. Next is to operate $D^{(\kappa)}(t \to \kappa)$ on $M_{\mathcal{O}}(t)$, which is performed by expanding $M_{\mathcal{O}}(t)$ in a power series of t^{-1}. Finally the $\kappa \to \infty$ limit is taken. See Appendix A for details of the second and third steps.

An example shown here is the overlap matrix element,

$$M_1(t) = f_0^L P^{B_t} \left(\widetilde{u} B_t^{-1} u \right)^L, \quad (27)$$

where the matrix B_t is defined by $B + tI_{\mathcal{N}}$ with

$$B = \tfrac{1}{2}(A + A'), \quad (28)$$

and

$$f_l^L = \frac{L!(2L+1)!!}{2^{L-l+2}(L-l)!} \sqrt{\pi}^{d-2}, \quad (29)$$

$$P^{B_t} = (\det B_t)^{-\frac{3}{2}}. \quad (30)$$

Since $M_1(t)$ does not depend on R, $\langle f^{u'A'}_{LM} | f^{uA}_{LM} \rangle_{y=1}$ turns out to be R-independent.

$M_{\mathcal{O}}(t)$ of interest usually takes the form

$$M_{\mathcal{O}}(t) = P^{B_t} Q_{\mathcal{O}}(t),$$

$$Q_{\mathcal{O}}(t) = \sum_{l=0}^{L} f_l^L T^{uA,u'A'}_{\mathcal{O},l}(t) \left(\widetilde{u} B_t^{-1} u \right)^{L-l}. \quad (31)$$

To determine $T^{uA,u'A'}_{\mathcal{O},l}(t)$ is of prime importance. See Ref. [33] for details. Although $T^{uA,u'A'}_{\mathcal{O},l}(t)$ may in general depend on R and $Q_{\mathcal{O}}(t)$ depends on L, they are suppressed for the sake of simplicity. $M_{\mathcal{O}}(t)$ depends on t through $\det B_t$ and B_t^{-1}.

C. Permutation symmetry

To impose the exchange symmetry of identical particles, one acts a permutation P on $\Phi^{uA}_{R\kappa,LM}(\boldsymbol{x})$. Since $S_{R\kappa}(\rho)$ is totally symmetric, the action actually applies on $f^{uA}_{LM}(\boldsymbol{y})$, which results in simply renaming the CG parameters as follows [22,23,27]:

$$P f^{uA}_{LM}(\boldsymbol{y}) = f^{u_P A_P}_{LM}(\boldsymbol{y}),$$
$$u_P = \widetilde{T}_P u, \quad A_P = \widetilde{T}_P A T_P, \quad (32)$$

where T_P is an $\mathcal{N} \times \mathcal{N}$ matrix defined by $U\mathcal{P}U^{-1}$. Here, $\mathcal{P}$ is the $N \times N$ permutation matrix whose (ij) element is given by $\mathcal{P}_{ij} = \delta_{j,p_i}$ corresponding to the well-known two-row symbol $P = \left(\begin{smallmatrix} 1 & 2 & \dots & N \\ p_1 & p_2 & \dots & p_N \end{smallmatrix}\right)$.

IV. MATRIX ELEMENTS OF ADIABATIC HAMILTONIAN

A. Potential energy

The relative distance vector, $\boldsymbol{r}_i - \boldsymbol{r}_j$, is expressed in terms of $\boldsymbol{x}$ as [see Eq. (4)]

$$\boldsymbol{r}_i - \boldsymbol{r}_j = \sum_{k=1}^{\mathcal{N}} \left(U^{-1}{}_{ik} - U^{-1}{}_{jk} \right) \boldsymbol{x}_k \equiv \widetilde{\omega^{(ij)}} \boldsymbol{x}, \quad (33)$$

where $\omega^{(ij)}$ is a column vector of dimension $\mathcal{N}$. The relative distance squared is

$$(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = \widetilde{\boldsymbol{x}} T^{(ij)} \boldsymbol{x}, \quad (34)$$

where $T^{(ij)} = T^{(ji)} = \omega^{(ij)} \widetilde{\omega^{(ij)}}$ $(i \neq j)$ is an $\mathcal{N} \times \mathcal{N}$ symmetric matrix that satisfies $\mathrm{Tr}\, T^{(ij)} = \widetilde{\omega^{(ij)}} \omega^{(ij)} = 2$ and $\sum_{i<j}^{N} T^{(ij)} = N I_{\mathcal{N}}$. A Gaussian potential, V_{ij}, is expressed as $V_{ij} = e^{-\nu(\boldsymbol{r}_i - \boldsymbol{r}_j)^2} = e^{-\nu R^2 \widetilde{\boldsymbol{y}} T^{(ij)} \boldsymbol{y}}$.

The matrix element of V_{ij} reduces to that of the overlap, that is, $M_{V_{ij}}(t)$ is given by Eq. (27) with B replaced by $G^{(ij)} = B + \nu R^2 T^{(ij)}$. One of the eigenvalues of $T^{(ij)}$ is 2 and others are all zero. As R increases, the matrix $G^{(ij)}$ therefore contains a large eigenvalue, which makes the $\kappa \to \infty$ limit calculation hard because the power-series expansion does not converge fast. See Appendix A.

A simple recipe to alleviate that difficulty is to shift $T^{(ij)}$ to $\Delta^{(ij)}$ by using the ansatz

$$\left\langle f^{u'A'}_{LM} \middle| \sum_{i<j}^{N} V_{ij} \middle| f^{uA}_{LM} \right\rangle_{y=1}$$
$$= e^{-\nu R^2 \tau} \left\langle f^{u'A'}_{LM} \middle| \sum_{i<j}^{N} e^{-\nu R^2 \widetilde{\boldsymbol{y}} \Delta^{(ij)} \boldsymbol{y}} \middle| f^{uA}_{LM} \right\rangle_{y=1}, \quad (35)$$

where $\Delta^{(ij)} = T^{(ij)} - \tau I_{\mathcal{N}}$. A choice for τ is

$$\tau I_{\mathcal{N}} = \frac{\sum_{i<j}^{N} T^{(ij)}}{\sum_{i<j}^{N} 1} = \frac{2}{N-1} I_{\mathcal{N}}. \quad (36)$$

A more elaborate recipe is discussed also in Appendix A.

A three- or more-body potential of Gaussian form factor can be evaluated similarly. It is possible to calculate the matrix element of a potential if it is approximated as a sum of Gaussians.

It is useful to note that the matrix element of a central potential $V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)$ with an arbitrary form factor is obtained by using Eq. (A.133) [23] as follows ($\omega^{(ij)}$ is abbreviated as ω):

$$M_{V(|\boldsymbol{r}_i - \boldsymbol{r}_j|)}(t) = P^{B_t} \sum_{l=0}^{L} g_l^L J_l(t) \mathcal{T}(t)^l \left(\widetilde{u} B_t^{-1} u - \mathcal{T}(t) \right)^{L-l}, \quad (37)$$

where

$$g_l^L = \frac{4}{\sqrt{\pi}} \frac{f_l^L}{l!\,(2l+1)!!}, \quad \mathcal{T}(t) = \frac{\left(\widetilde{u} B_t^{-1} \omega \right) \left(\widetilde{\omega} B_t^{-1} u \right)}{\widetilde{\omega} B_t^{-1} \omega},$$
$$J_l(t) = \int_0^{\infty} dx V\left(R \left(\widetilde{\omega} B_t^{-1} \omega \right)^{\frac{1}{2}} x \right) x^{2l+2} e^{-x^2}. \quad (38)$$

B. Hyperangular kinetic-energy

To obtain the matrix element of Λ^2 in Eq. (9), I follow the indirect way [28–30] that does not require an explicit construction of Λ^2 but makes use of the relation (8). I show how to determine $\Lambda^2(R\boldsymbol{y})$ and $M_{\Lambda^2}(t)$ in Appendix B. $M_{\Lambda^2}(t)$ is found to be

$$M_{\Lambda^2}(t) = P^{B_t} \sum_{l=0}^{\min(L,2)} f_l^L T^{uA,u'A'}_{\Lambda^2,l}(t)\left(\widetilde{u'}B_t^{-1}u\right)^{L-l}, \tag{39}$$

where, with $C = \frac{1}{2}(A - A')$, $T^{uA,u'A'}_{\Lambda^2,l}(t)$'s are given by

$$\begin{aligned} T^{uA,u'A'}_{\Lambda^2,0}(t) &= -\tfrac{1}{4}d(d-2) + \tfrac{3}{2}\mathrm{Tr}B_t - \tfrac{3}{2}(t^2+2t)\,\mathrm{Tr}B_t^{-1} \\ &\quad + \tfrac{9}{4}t^2\left(\mathrm{Tr}B_t^{-1}\right)^2 + \tfrac{3}{2}t^2\,\mathrm{Tr}B_t^{-2} - \tfrac{3}{2}\mathrm{Tr}B_t^{-1}C^2 \\ &\quad + \tfrac{9}{4}\left(\mathrm{Tr}B_t^{-1}C\right)^2 + \tfrac{3}{2}\mathrm{Tr}\left(B_t^{-1}C\right)^2, \end{aligned} \tag{40}$$

$$\begin{aligned} T^{uA,u'A'}_{\Lambda^2,1}(t) &= \tfrac{1}{2}\widetilde{u'}u - \tfrac{1}{2}\widetilde{u'}B_t^{-1}u - \tfrac{1}{2}(t^2+2t)\widetilde{u'}B_t^{-2}u \\ &\quad + t^2\widetilde{u'}B_t^{-3}u + \tfrac{3}{2}t^2\left(\mathrm{Tr}B_t^{-1}\right)\widetilde{u'}B_t^{-2}u \\ &\quad + \tfrac{1}{2}\widetilde{u'}\left(B_t^{-1}C - CB_t^{-1}\right)u - \tfrac{1}{2}\widetilde{u'}B_t^{-1}C^2B_t^{-1}u \\ &\quad + \widetilde{u'}\left(B_t^{-1}C\right)^2B_t^{-1}u + \tfrac{3}{2}\left(\mathrm{Tr}B_t^{-1}C\right)\widetilde{u'}B_t^{-1}CB_t^{-1}u, \end{aligned} \tag{41}$$

$$T^{uA,u'A'}_{\Lambda^2,2}(t) = \tfrac{1}{4}t^2\left(\widetilde{u'}B_t^{-2}u\right)^2 + \tfrac{1}{4}\left(\widetilde{u'}B_t^{-1}CB_t^{-1}u\right)^2. \tag{42}$$

V. APPLICATION TO MULTI α-PARTICLE SYSTEMS

I apply the present method to the system of α particles to demonstrate its feasibility. The emphasis is not placed on obtaining accurate adiabatic potentials. I will not take care of the asymptotics of the potentials nor perform configuration interaction calculations, but simply vary the parameters of a single CG basis.

The Hamiltonian used here is the same as that of Refs. [13,16]. In units of fm and MeV for the length and energy, the two-body $\alpha\alpha$ potential consisting of the nuclear (V_{2B}) and Coulomb (V_C) potentials reads

$$V(r) = 125e^{-\frac{r^2}{1.53^2}} - 30.18e^{-\frac{r^2}{2.85^2}} + \frac{4e^2}{r}\mathrm{erf}(0.60141r). \tag{43}$$

The last term is approximated by a sum of Gaussians. The three-body potential (V_{3B}), $v_3\exp(-\nu F_3(\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{r}_k))$, is also included, where $F_3(\boldsymbol{r}_i,\boldsymbol{r}_j,\boldsymbol{r}_k) = 3\sum_{l=i,j,k}(\boldsymbol{r}_l - \boldsymbol{R}_{ijk})^2$ with $\boldsymbol{R}_{ijk} = (\boldsymbol{r}_i+\boldsymbol{r}_j+\boldsymbol{r}_k)/3$. The range parameter ν is $(2.58^2\sqrt{3})^{-1}$ and the potential strength v_3 is -151.737 for $L=0$ and -179.463 for $L=2$, respectively. The contribution of V_{3B} is evaluated by taking a sum over $\binom{N}{3}$ different combinations of three particles.

I specify the matrix A of Eq. (19) via a set of $\{d_{ij}\}$, a measure of the relative distance of particles i and j:

$$\widetilde{\boldsymbol{x}}A\boldsymbol{x} = \sum_{i<j}^{N}\frac{1}{d_{ij}^2}(\boldsymbol{r}_i - \boldsymbol{r}_j)^2 = R^2\widetilde{\boldsymbol{y}}\sum_{i<j}^{N}\frac{T^{(ij)}}{d_{ij}^2}\boldsymbol{y}. \tag{44}$$

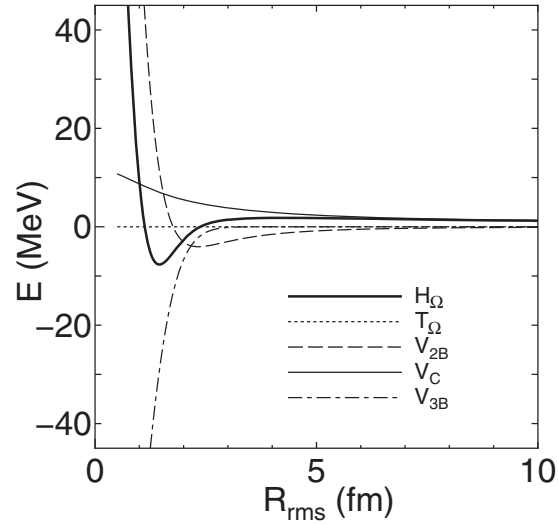

FIG. 1. The minimum energy of $\langle H_\Omega\rangle$ as a function of $R_{\rm rms}$ obtained by a single 3α configuration with $L=0$. The contribution of each piece of the adiabatic Hamiltonian is also displayed. Note that $\langle H_\Omega\rangle$ includes the term, $\hbar^2/(2m\rho^2)[(d-1)(d-3)/4]$. See Eq. (11).

Replacing R^2 with $\sum_{i<j}^N d_{ij}^2/N$ [see Eq. (5)], A is written, independent of R, as follows:

$$A = c_A\frac{1}{N}\left(\sum_{i<j}^{N}d_{ij}^2\right)\sum_{i<j}^{N}\frac{T^{(ij)}}{d_{ij}^2}, \tag{45}$$

where c_A is a variational parameter. When all d_{ij}'s are equal, A becomes $c_A(N(N-1)/2)I_{\mathcal{N}}$. In the following cases the expectation value of H_Ω turns out to be insensitive to c_A, and I set it to $(N(N-1)/2)^{-1}$ mostly.

Any intrinsic shape of the three-body system is specified by two angles, α and β, [37]:

$$\begin{aligned} d_{12}^2 &= \cos^2\alpha\cos^2\beta + \sin^2\alpha\sin^2\beta, \\ d_{13}^2 &= \cos^2\alpha\cos^2\left(\beta+\frac{\pi}{3}\right) + \sin^2\alpha\sin^2\left(\beta+\frac{\pi}{3}\right), \\ d_{23}^2 &= \cos^2\alpha\left(\cos\beta - \cos\left(\beta+\frac{\pi}{3}\right)\right)^2 \\ &\quad + \sin^2\alpha\left(\sin\beta - \sin\left(\beta+\frac{\pi}{3}\right)\right)^2. \end{aligned} \tag{46}$$

The parameter u in Eq. (19) is redundant for $L=0$. For $L=2$ it is set to $u_1 = \sin\theta$ and $u_2 = \cos\theta$. α, β, and θ are varied to find a minimum of $\langle H_\Omega\rangle$ for each R. In what follows, I use the point-α root-mean-square (rms) radius $R_{\rm rms}$ instead of R:

$$R_{\rm rms} = \frac{1}{\sqrt{N}}R. \tag{47}$$

Figure 1 plots the minimum of $\langle H_\Omega\rangle$ for 3α system with $L=0$ as a function of $R_{\rm rms}$. The minimum occurs at a regular triangle configuration for all $R_{\rm rms}$'s. A global minimum is -7.17 MeV at $R_{\rm rms} = 1.45$ fm. This minimum value appears quite reasonable in comparison to the K dependence of Fig. 1 [33]. However, it is considerably high compared

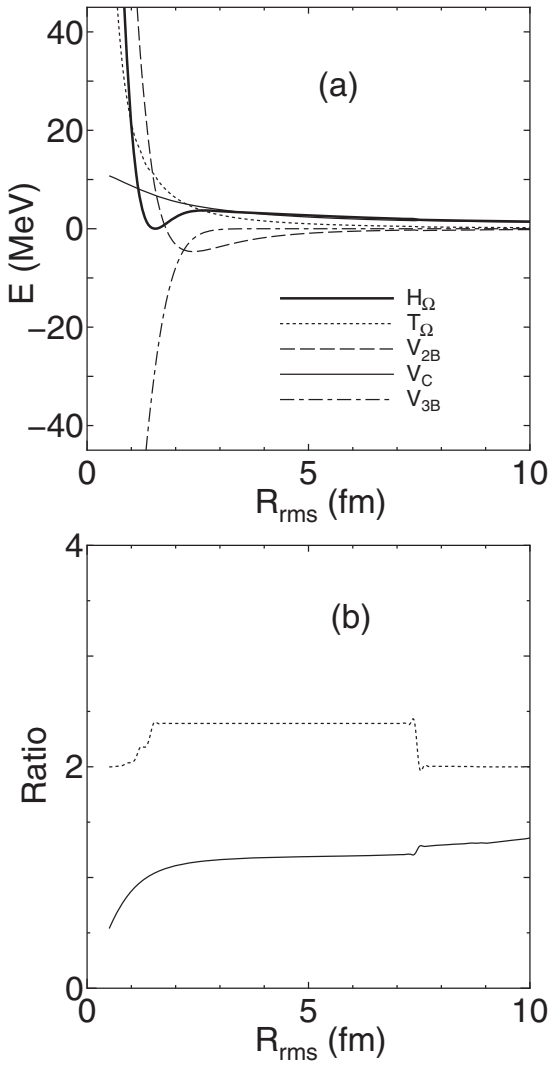

FIG. 2. (a) The same as Fig. 1 but for $L = 2$. (b) $R_{\rm rms}$ dependence of $\langle T_\Omega \rangle$ and $\langle V_{\rm C} \rangle$ contributions. They are, respectively, given in ratio to the centrifugal potential barrier, $\hbar^2 L(L+1)/(2mR^2)$ ($L = 2$) (dotted line), and to the Coulomb potential of point α-particles forming a regular triangle, $12e^2/R$ (solid line).

to the minimum (-17.8 MeV) [13], which clearly indicates that configuration interaction calculations are needed to gain the energy. As seen from the contribution of each operator to $\langle H_\Omega \rangle$, the Coulomb potential makes a dominant contribution beyond 2 fm. The contribution of T_Ω is negligible at all $R_{\rm rms}$ values, which is probably because the basis function (19) is too simple to represent the hyperangular dependence of $L = 0$ states.

The minimum energy of 3α system with $L = 2$ is exhibited in Fig. 2(a). The intrinsic shape reaching the minimum changes depending on $R_{\rm rms}$: For $1.5 \leqslant R_{\rm rms} \leqslant 7.4$ fm, $d_{12} \approx 0.24$, $d_{13} \approx 0.76$, $d_{23} \approx 0.93$, and $u_1 = 1.0$, $u_2 = 0.0$. For $7.8 \leqslant R_{\rm rms} \leqslant 8.3$ fm, $d_{12} \approx 0.37$, $d_{13} \approx 0.65$, $d_{23} \approx 0.97$, and $u_1 = 0.5$, $u_2 = 0.866$. For $R_{\rm rms} \geqslant 9.5$ fm an isosceles configuration with its apex angle less than 60° is formed and $u_1 = 0.0$, $u_2 = 1.0$. A global minimum is considerably lower than that of Fig. 2 of Ref. [33], but a comparison with

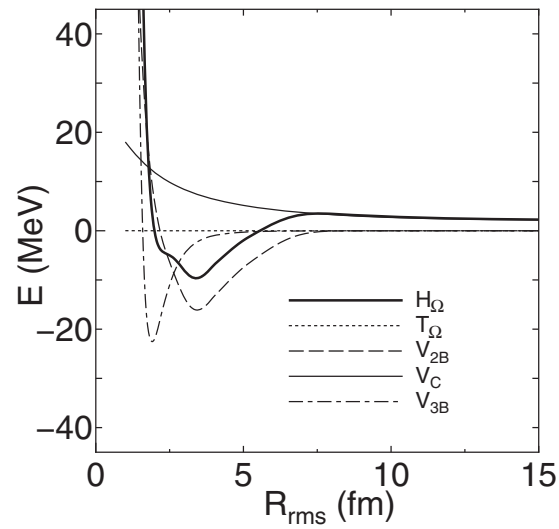

FIG. 3. The same as Fig. 1 but for 4α system with $L = 0$. The adiabatic potential is calculated by a single configuration covering various shapes of tetrahedron, square, rhombus, rectangle, linear-chain, and hypersphere. The lowest one among them is plotted together with the contribution of each piece of the adiabatic Hamiltonian.

the adiabatic HS potential curve [13] clearly indicates the importance of configuration interaction calculations.

The contribution of the operator $\mathcal{O}$ to $\langle H_\Omega \rangle$ is drawn in Fig. 2(a). The Coulomb potential contribution becomes largest beyond $R_{\rm rms} = 2.8$ fm. A careful look shows that discontinuous contributions occur at $R_{\rm rms} = 7.4$ to 7.5 fm. Although the sum of the potentials, $V_{\rm 2B} + V_{\rm C}$, gives a decreasing contribution with increasing $R_{\rm rms}$, each of them does not follow a monotonous change. This can be shown conveniently in ratio to some standard values: For T_Ω and $V_{\rm C}$ contributions I take the standards to be the centrifugal potential, $6\hbar^2/(2mR^2)$, and the Coulomb potential, $12e^2/R$, respectively. Figure 2(b) displays the contributions of T_Ω and $V_{\rm C}$ in ratio to these standards. As expected, both of them approximately follow constant curves but still vary. The discontinuous behavior as well as the deviation from the constant may be attributed to that T_Ω and the potentials do not commute.

Next I present results of four-α system. The 2B and 3B potentials defined above predict the rms radius of ^{12}C slightly smaller than the empirical value [13]. To fit the radius of ^{12}C I add a repulsive 3B potential with $v_3 = 2000$ and $\nu = (1.41^2\sqrt{3})^{-1}$. With this addition the 3α minimum of $\langle H_\Omega \rangle$ for $L = 0$ changes to -4.9 MeV at $R_{\rm rms} = 1.7$ fm. I compare $\langle H_\Omega \rangle$ values calculated from various shapes of 4 α-particles: tetrahedron, square and rhombus, rectangle, linear-chain, hypersphere. It is meant by the hypersphere that the matrix A is proportional to $I_{\mathcal{N}}$. In the cases of tetrahedron, rectangle, and linear-chain some configurations slightly deviated from the respective highest symmetric shape are also tested. In all the cases the $\alpha\alpha$ relative distances are taken to increase with increasing $R_{\rm rms}$. The $\langle H_\Omega \rangle$ value is therefore the one relative to the 4α threshold. The ground state of ^{16}O is 14.43 MeV below the 4α threshold. The $\langle H_\Omega \rangle$ values predicted by the various shapes are found to be close to each other. In Fig. 3

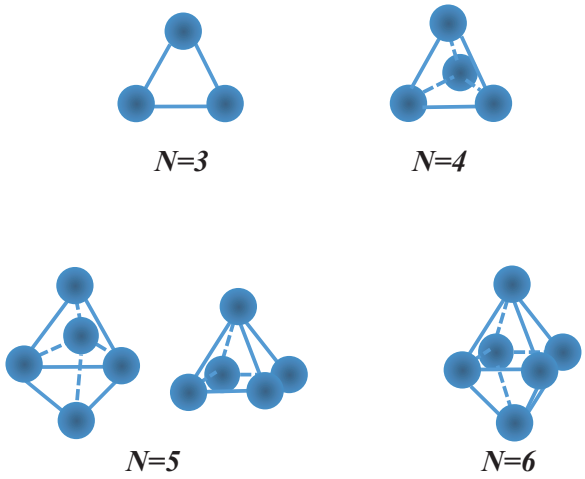

FIG. 4. Schematic diagram of $N\alpha$ configuration: regular triangle ($N = 3$), regular tetrahedron ($N = 4$), regular triangular bipyramid ($N = 5$, left) or regular quadrangular pyramid ($N = 5$, right), and regular square bipyramid ($N = 6$).

I plot the lowest one among them as a function of $R_{\rm rms}$. The minimum reaches about -9.7 MeV at $R_{\rm rms} = 3.4$ fm, which corresponds to the rms radius of ^{16}O, $r_{\rm rms} = 3.7$ fm. The minimum energy is considerably higher than experiment and the rms radius is too large compared to the empirical radius (2.7 fm) of ^{16}O. Again the importance of configuration interaction calculation is suggested.

Finally I test the method by increasing the number of α particles up to $N = 6$. Only the 2B force is included in this calculation. The matrix A for N-body system is fixed according to the shape shown in Fig. 4. In the same way as Fig. 3, all of the $\alpha\alpha$ distances are taken to get larger as $R_{\rm rms}$ increases. In the case of $L = 2$, a minimum of $\langle H_\Omega \rangle$ is searched for by changing the u parameter according to $u_i = \delta_{i,j}$ ($i = 1, \ldots, \mathcal{N}$), where j runs from 1 to $\mathcal{N}$. Two configurations of $N = 5$ give almost the same energy, so that I show the case of regular triangular bipyramid. Results of calculation are drawn in Figs. 5(a) and 5(b). No difficulty in the calculation arises with increasing N. Note that $E = 0$ horizontal axis corresponds to the $N\alpha$ threshold. Experimentally the ground states of ^{20}Ne and ^{24}Mg are respectively -19.2 and -28.5 MeV below the 5α and 6α thresholds. To predict realistic adiabatic potential curves one has to mix other configurations. In particular, it would be interesting to study the effects of clustering of 6α system into $3\alpha + 3\alpha$, $2\alpha + 4\alpha$, and $\alpha + 5\alpha$, where each subsystem may form some compact configurations. See, e.g., Ref. [18]. As stressed in Introduction, the potential curve is obtained as a function of the universal scale, the hyper-radius or the rms radius of the system. Because of this reason the present formulation has no ambiguity in evaluating various coupling effects. In addition no spurious c.m. motion is involved, assuring that the threshold is correctly treated. An extensive study of these issues based on configuration interaction calculations will be interesting.

I comment on a choice of the matrix A in relation to the asymptotic behavior of the adiabatic potential. As R increases,

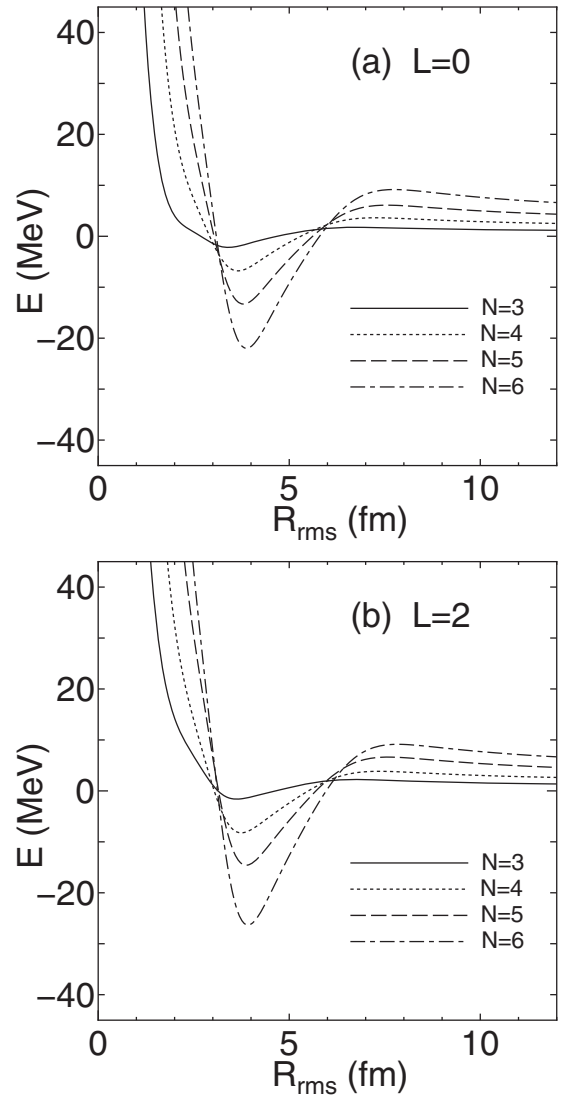

FIG. 5. (a) The minimum energy of $N\alpha$ system with $L = 0$ obtained by a single configuration drawn in Fig. 4. Two configurations of $N = 5$ case give almost the same energy, so that the energy calculated by the regular triangular bypyamid is shown. (b) The same as (a) but for $L = 2$.

the system expands and tends to break into some fragments. It is useful to note that ρ^2 of Eq. (5) is always separated into a sum of two parts, internal and relative, as discussed in, e.g., [32]. The internal part is a sum of the squared hyper-radius of each fragment, while the relative part is the squared hyper-radius defined by the c.m. coordinates of the fragments. It is then natural to choose a set of $\{d_{ij}\}$ in such a way that the relative distances of the particles inside each fragment remain finite, whereas the relative distances connecting the fragments increase with R. For example, in the case of two-fragment decomposition consisting of $N - 1$ particles and one particle, a reasonable and simplest choice for A is diagonal, $A_{ij} = (1/d_i^2)\delta_{i,j}$, with the constraint $\sum_{i=1}^{\mathcal{N}-1} d_i^2 = D^2$ and $d_{\mathcal{N}}^2 = R^2 - D^2$, where D^2 is $\mathcal{N} - 1$ times the squared mean radius of the fragment. Off-diagonal elements of A take account of the

coupling of the different coordinates. A combination of the CGs whose parameters are selected with some optimization procedure is expected to give a refined description of the asymptotic behavior of the adiabatic potential. A study along this line with specific cases is important to corroborate the present formalism.

VI. CONCLUSION

The matrix element of the adiabatic Hamiltonian requires the integration over the surface of the d-dimensional ball of a fixed hyper-radius R. The integration becomes extremely hard beyond four-particle systems. I have proposed a simple prescription to resolve this difficulty by introducing the localized hyper-radial function. The function is combined with correlated Gaussians responsible for describing the hyperangular motion of the system. The prescription consists of the evaluation of usual matrix elements with all the coordinates and the limiting procedure to pin down the hyper-radius to R. All the details of the procedure are given considering that it is quite new to the best of the author's knowledge.

The system of α particles interacting via both two-body and three-body potentials is used to convince a reader of the feasibility of the proposed prescription. The number of α particles is increased up to $N = 6$. No difficulty is observed with increasing N. The convergence of the power-series expansion for $\kappa \to \infty$ is fairly fast with mild dependence on N. A noticeable problem arises in evaluating the matrix element of the interaction potentials at large R. The reason for that is elucidated and some recipes to alleviate the problem are adopted. It is still challenging, however, to calculate the potential matrix element at an extremely large hyper-radius.

Since the emphasis of the present work is to propose a new approach and to demonstrate its usefulness, no configuration interaction calculation is performed. No difficulty is expected to arise in combining a number of basis functions. It is a future work to examine what type of basis parameters are important to obtain accurate solutions of the eigenvalue problem of the adiabatic Hamiltonian including its asymptotics.

The correlated Gaussian used in the paper is the simplest one. The contribution of the hyperangular kinetic-energy to the adiabatic potential almost vanishes in the case of $L = 0$ orbital angular momentum, which appears to indicate the limitation of the simplest Gaussian. It is thus of particular interest to extend the correlated Gaussian $f_{LM}^{uA}(\mathbf{y})$ to the one including double global vectors, $[\mathcal{Y}_{L_1}(\widetilde{u}_1\mathbf{y}) \times \mathcal{Y}_{L_2}(\widetilde{u}_2\mathbf{y})]_{LM} e^{-\frac{1}{2}\widetilde{\mathbf{y}}A\mathbf{y}}$. This is because the basis function can accommodate a description of more complex hyperangular motion as well as unnatural parity states and because basic matrix elements needed with this basis function are already available in Refs. [35,36].

ACKNOWLEDGMENTS

The author is grateful to N. Itagaki, I. Shimamura, and K. Varga for useful communication and advice.

APPENDIX A: EVALUATION OF $\kappa \to \infty$ LIMIT

Here two things are discussed. One is to calculate $(-\frac{d}{dt})^\kappa P^{B_t} Q_\mathcal{O}(t)$ at $t = \kappa$ [see Eqs. (21), (23), and (31)] and the other is to take its $\kappa \to \infty$ limit. A basic idea is to expand $P^{B_t} Q_\mathcal{O}(t)$ in a power series of t^{-1}.

The t dependence appears as $\det B_t$ in P^{B_t} and as B_t^{-1} in $Q_\mathcal{O}(t)$, respectively. Let $(b_1, b_2, \ldots, b_\mathcal{N})$ be the eigenvalues of B, and T denote the orthogonal matrix that diagonalizes B: $B = T D \widetilde{T}$ with $D = (b_i \delta_{i,j})$. Thus $B_t = B + t I_\mathcal{N}$ and B_t^{-1} are expressed as

$$B_t = t T D_x \widetilde{T}, \quad B_t^{-1} = t^{-1} T (D_x)^{-1} \widetilde{T}, \tag{A1}$$

where D_x is a diagonal matrix

$$D_x = I_\mathcal{N} + xD, \quad x = t^{-1}. \tag{A2}$$

By using $\det B_t = t^\mathcal{N} \prod_{i=1}^\mathcal{N} (1 + b_i x)$, $P^{B_t} = (\det B_t)^{-\frac{3}{2}}$ is expanded as

$$P^{B_t} = t^{-\frac{d}{2}} \sum_{m=0}^\infty p_m^B x^m. \tag{A3}$$

It is easy to determine p_m^B's from b_i's. $Q_\mathcal{O}(t)$ in general comprises a number of scalar terms, each of which contains several, say N_0, B_t^{-1}'s. For instance, $Q_1(t)$ for the overlap is $(\widetilde{u'} B_t^{-1} u)^L$. By using the expansion $B_t^{-1} = t^{-1} \sum_{l=0}^\infty (-1)^l T D^l \widetilde{T} x^l$, the scalar term containing B_t^{-1} is expanded in a power series of x, e.g.,

$$\begin{aligned} \mathrm{Tr} B_t^{-1} &= t^{-1} \sum_{l=0}^\infty (-1)^l (\mathrm{Tr}\, D^l)\, x^l, \\ \widetilde{u'} B_t^{-1} u &= t^{-1} \sum_{l=0}^\infty (-1)^l (\widetilde{v'} D^l v)\, x^l, \end{aligned} \tag{A4}$$

where $v = \widetilde{T} u$, $v' = \widetilde{T} u'$. By replacing each B_t^{-1} in this way, $Q_\mathcal{O}(t)$ becomes a combination of expansions with appropriate coefficient $q_{\mathcal{O},n}^{uA,u'A'}$ as follows:

$$Q_\mathcal{O}(t) = \sum \left\{ t^{-N_0} \sum_{n=0}^\infty q_{\mathcal{O},n}^{uA,u'A'} x^n \right\}. \tag{A5}$$

The symbol $\sum \{\ \}$ is suppressed below.

Combining Eqs. (A3) and (A5), I obtain

$$\begin{aligned} \left(-\frac{d}{dt}\right)^\kappa \Big|_{t=\kappa} P^{B_t} Q_\mathcal{O}(t) &= \left(-\frac{d}{dt}\right)^\kappa \Big|_{t=\kappa} t^{-\lambda} \sum_{n=0}^\infty c_n t^{-n} \\ &= \sum_{n=0}^\infty \frac{c_n \Gamma(\kappa + n + \lambda)}{\Gamma(n + \lambda) \kappa^{\kappa+n+\lambda}}, \end{aligned} \tag{A6}$$

where

$$\lambda = N_0 + \frac{d}{2}, \quad c_n = \sum_{m=0}^n p_m^B q_{\mathcal{O},n-m}^{uA,u'A'}. \tag{A7}$$

By using the relation

$$\lim_{\kappa\to\infty} \frac{E(\kappa)\Gamma(\kappa + n + \lambda)}{\kappa^{\kappa+n+\lambda}} = 1, \tag{A8}$$

the limit of Eq. (A6) is found to be

$$\lim_{\kappa\to\infty} D^{(\kappa)}(t\to\kappa)P^{B_t}Q_{\mathcal{O}}(t) = \sum_{n=0}^{\infty}\frac{c_n}{\Gamma(n+\lambda)} = \frac{1}{\Gamma(\lambda)}\left\{c_0 + \frac{c_1 + \frac{c_2+\frac{c_3+\cdots}{\lambda+2}}{\lambda+1}}{\lambda}\right\}. \quad \text{(A9)}$$

The sum over n can be expressed in a continued fraction as above. The needed task is to determine the expansion coefficients c_n, which is not difficult but involves several steps for the hyperangular kinetic-energy.

How fast does the series converge? As a simple example, consider the norm, $\langle f^{uA}_{LM}|f^{uA}_{LM}\rangle_{y=1}$, assuming that $A = (a\delta_{i,j})$ $(a>0)$ and $\widetilde{u}u = 1$. Equation (27) gives $M_1(t) = f_0^L(a+t)^{-\lambda}$ $(\lambda = L+\frac{d}{2})$. The power-series expansion of $M_1(t)$ is easily done by using a formula

$$(ax+a_0)^{-\alpha} = a_0^{-\alpha}\sum_{n=0}^{\infty}\frac{(\alpha)_n}{n!}\left(-\frac{a}{a_0}x\right)^n, \quad \text{(A10)}$$

where $(\alpha)_n$ is the Pochhammer symbol, $\Gamma(\alpha+n)/\Gamma(\alpha)$. The nth term in the sum (A9) for this case is $c_n/\Gamma(n+\lambda) = (-a)^n/n!\Gamma(\lambda)$, and the $\kappa\to\infty$ limit is found to be

$$\langle f^{uA}_{LM}|f^{uA}_{LM}\rangle_{y=1} = 2f_0^L\frac{e^{-a}}{\Gamma(\lambda)}. \quad \text{(A11)}$$

When a is small, $|c_n|$ is sufficiently small to ensure the convergence. For large a, however, $|c_n|$ rapidly increases with n, which makes computing c_n itself hard and results in ill behavior of the alternating series.

In passing I note that the left-hand side of Eq. (A11) with $L=0$ is nothing but $e^{-a}/4\pi$ times S_d, the surface area of the d-dimensional ball of radius 1. One thus obtains $S_d = 2\pi^{\frac{d}{2}}/\Gamma(\frac{d}{2})$, which is indeed correct.

The above convergence problem does not occur for the overlap and the hyperangular kinetic-energy, but becomes serious in the Gaussian potential matrix element $M_{V_{ij}}(t)$ as R increases. As shown in Sec. IV A, $M_{V_{ij}}(t)$ is simply given by $M_1(t)$ with B replaced by $G^{(ij)} = B + \nu R^2 T^{(ij)}$. The ill behavior arises because $G^{(ij)}$ contains a large eigenvalue for large R. I propose another power-series expansion to resolve this difficulty. I keep B instead of $G^{(ij)}$ but assume that one of the eigenvalues of B, say, b_1 is much larger than the others.

With multinomial coefficients I obtain

$$P^{B_t}\left(\widetilde{u'}B_t^{-1}u\right)^L = \sum_{l_1+l_2+\ldots+l_{\mathcal{N}}=L}\binom{L}{l_1,l_2,\ldots,l_{\mathcal{N}}} \times\left(\prod_{i=1}^{\mathcal{N}}(v_i'v_i)^{l_i}\right)F_{l_1l_2\ldots l_{\mathcal{N}}}(t) \quad \text{(A12)}$$

with

$$F_{l_1l_2\ldots l_{\mathcal{N}}}(t) = t^{-\lambda}\prod_{i=1}^{\mathcal{N}}(b_ix+1)^{-l_i-\frac{3}{2}}, \quad \text{(A13)}$$

where $\lambda = L+\frac{d}{2}$ and l_i's are nonnegative integers. Using Eq. (A10), I expand $F_{l_1l_2\ldots l_{\mathcal{N}}}(t)$ in powers of t^{-1} as

$$F_{l_1l_2\ldots l_{\mathcal{N}}}(t) = \sum_{m=0}^{\infty}(-1)^m t^{-m-\lambda} \times\sum_{m_1+\ldots+m_{\mathcal{N}}=m} D(b_1,\ldots,b_{\mathcal{N}};m_1,\ldots,m_{\mathcal{N}}), \quad \text{(A14)}$$

where m_i's are nonnegative integers, and the function D is defined by

$$D(b_1,\ldots,b_{\mathcal{N}};m_1,\ldots,m_{\mathcal{N}}) = \prod_{i=1}^{\mathcal{N}}\frac{(l_i+\frac{3}{2})_{m_i}}{m_i!}b_i^{m_i}. \quad \text{(A15)}$$

Taking the $\lim_{\kappa\to\infty}$ leads to the desired limit

$$\lim_{\kappa\to\infty} D^{(\kappa)}(t\to\kappa)F_{l_1l_2\ldots l_{\mathcal{N}}}(t) = \sum_{m=0}^{\infty}\frac{(-1)^m}{\Gamma(m+\lambda)}\sum_{m_1+\ldots+m_{\mathcal{N}}=m} D(b_1,\ldots,b_{\mathcal{N}};m_1,\ldots,m_{\mathcal{N}}). \quad \text{(A16)}$$

Since the limit is already taken, a remaining task is to find an efficient way of making m_i sums to accelerate the evaluation of the limit. D is a kind of distribution function of the eigenvalues. Because b_1 is by far larger than the others, those with $m_1 = m, m-1, m-2$ etc. are expected to make dominant contributions. To focus on the contribution from $m_1 = m-p$, I rewrite the m_1-dependent factor of D as (see Appendix C)

$$\frac{(l_1+\frac{3}{2})_{m-p}}{(m-p)!} = \frac{1}{m!}\sum_{k=0}^{p}(-1)^k\binom{p}{k}\left(l_1+\frac{3}{2}-k\right)_m. \quad \text{(A17)}$$

By defining

$$\langle b^{(p)}\rangle = \frac{1}{b_1^p}\sum_{m_2+\ldots+m_{\mathcal{N}}=p} D(b_2,\ldots,b_{\mathcal{N}};m_2,\ldots,m_{\mathcal{N}}), \quad \text{(A18)}$$

the contribution to the limit of Eq. (A16) is given by

$$\frac{\langle b^{(p)}\rangle}{\Gamma(\lambda)}\sum_{k=0}^{p}(-1)^k\binom{p}{k}\left[M\left(l_1+\frac{3}{2}-k,\lambda,-b_1\right) - \sum_{n=0}^{p-1}\frac{(-b_1)^n}{n!(\lambda)_n}\left(l_1+\frac{3}{2}-k\right)_n\right], \quad \text{(A19)}$$

where $M(a,b,z)$ is the confluent hypergeometric function or Kummer's function [38]

$$M(a,b,z) = \sum_{n=0}^{\infty}\frac{(a)_n}{(b)_n n!}z^n. \quad \text{(A20)}$$

The Pochhammer symbol $(l_1+\frac{3}{2}-k)_n$ in Eq. (A19) is a polynomial of k of degree n. Since n takes 0 to $p-1$, $\sum_{k=0}^{p}(-1)^k\binom{p}{k}k^n$ vanishes. See Eq. (C4). As a result, I

conclude that

$$\lim_{\kappa\to\infty} D^{(\kappa)}(t\to\kappa)F_{l_1 l_2\ldots l_N}(t) = \frac{1}{\Gamma(\lambda)}\sum_{p=0}^{\infty}\langle b^{(p)}\rangle\sum_{k=0}^{p}(-1)^k\binom{p}{k}M\left(l_1+\frac{3}{2}-k,\lambda,-b_1\right). \tag{A21}$$

I find that the sum over p converges fast.

APPENDIX B: MATRIX ELEMENT OF Λ^2

I show how to determine $\Lambda^2(R\boldsymbol{y})$ needed to obtain the matrix element of Λ^2, Eq. (39). A simple way is to make use of the generating function g for $\Phi^{uA}_{R\kappa,LM}$ [22,23],

$$g = \left(\frac{\rho}{R}\right)^{\kappa} e^{-\frac{\kappa}{2}\left(\frac{\rho}{R}\right)^2-\frac{1}{2}\widetilde{\boldsymbol{y}}A\boldsymbol{y}+\widetilde{\boldsymbol{s}}\boldsymbol{y}}, \tag{B1}$$

where $\boldsymbol{s}=\alpha\boldsymbol{e}u$. See Eq. (26).

By using $\boldsymbol{y}=(\rho/R)\boldsymbol{\xi}$, the action of T_ρ on g reads

$$-\left(\frac{\partial^2}{\partial\rho^2}+\frac{d-1}{\rho}\frac{\partial}{\partial\rho}\right)g = \frac{1}{\rho^2}\mathcal{O}_\rho(\boldsymbol{x})g. \tag{B2}$$

$\mathcal{O}_\rho(\boldsymbol{x})$ consists of several terms depending on A and $\boldsymbol{s}$ as well as κ. In taking the limit of $\kappa\to\infty$, ρ^2 in $\mathcal{O}_\rho(\boldsymbol{x})$ approaches R^2. This replacement in $\mathcal{O}_\rho(\boldsymbol{x})$ leads to

$$\mathcal{O}_\rho(R\boldsymbol{y}) = 2\kappa-(d-1)\widetilde{\boldsymbol{s}}\boldsymbol{y}-(\widetilde{\boldsymbol{s}}\boldsymbol{y})^2+d\widetilde{\boldsymbol{y}}A\boldsymbol{y} + 2\widetilde{\boldsymbol{s}}\boldsymbol{y}\widetilde{\boldsymbol{y}}A\boldsymbol{y}-(\widetilde{\boldsymbol{y}}A\boldsymbol{y})^2. \tag{B3}$$

Similarly, the action of $T_{\rm in}$ on g is obtained by noting $\boldsymbol{y}=\boldsymbol{x}/R$ and using, e.g., $\partial\rho/\partial x_{iz}=x_{iz}/\rho$:

$$-\sum_{i=1}^{\mathcal{N}}\frac{\partial^2}{\partial\boldsymbol{x}_i^2}g = \frac{1}{\rho^2}\mathcal{O}_{\rm in}(\boldsymbol{x})g. \tag{B4}$$

The same replacement of ρ^2 by R^2 as above leads to

$$\mathcal{O}_{\rm in}(R\boldsymbol{y}) = 2\kappa+3{\rm Tr}A-\widetilde{\boldsymbol{s}}\boldsymbol{s}+2\widetilde{\boldsymbol{s}}A\boldsymbol{y}-\widetilde{\boldsymbol{y}}A^2\boldsymbol{y}. \tag{B5}$$

Thus $\Lambda^2 g$ is given by $[\mathcal{O}_{\rm in}(R\boldsymbol{y})-\mathcal{O}_\rho(R\boldsymbol{y})]g$:

$$\Lambda^2 g = [3{\rm Tr}A-\widetilde{\boldsymbol{s}}\boldsymbol{s}+(d-1)\widetilde{\boldsymbol{s}}\boldsymbol{y}+2\widetilde{\boldsymbol{s}}A\boldsymbol{y}+(\widetilde{\boldsymbol{s}}\boldsymbol{y})^2 - d\widetilde{\boldsymbol{y}}A\boldsymbol{y}-\widetilde{\boldsymbol{y}}A^2\boldsymbol{y}-2\widetilde{\boldsymbol{s}}\boldsymbol{y}\widetilde{\boldsymbol{y}}A\boldsymbol{y}+(\widetilde{\boldsymbol{y}}A\boldsymbol{y})^2]g. \tag{B6}$$

Both $\mathcal{O}_\rho(R\boldsymbol{y})$ and $\mathcal{O}_{\rm in}(R\boldsymbol{y})$ contain the diverging term, 2κ, but it disappears from $\Lambda^2 g$, as expected. Symmetrizing Eq. (B6) [28–30] with respect to the interchange of $(A,\boldsymbol{s})$ and $(A',\boldsymbol{s}')$, I obtain $\Lambda^2 g=\Lambda^2(R\boldsymbol{y})g$, where

$$\Lambda^2(R\boldsymbol{y}) = 3{\rm Tr}B-\tfrac{1}{2}(\widetilde{\boldsymbol{s}}\boldsymbol{s}+\widetilde{\boldsymbol{s}}'\boldsymbol{s}')+\tfrac{1}{2}(d-1)(\widetilde{\boldsymbol{s}}+\widetilde{\boldsymbol{s}}')\boldsymbol{y} + (\widetilde{\boldsymbol{s}}A\boldsymbol{y}+\widetilde{\boldsymbol{s}}'A'\boldsymbol{y})+\tfrac{1}{2}((\widetilde{\boldsymbol{s}}\boldsymbol{y})^2+(\widetilde{\boldsymbol{s}}'\boldsymbol{y})^2)-d\widetilde{\boldsymbol{y}}B\boldsymbol{y} - \tfrac{1}{2}(\widetilde{\boldsymbol{y}}A^2\boldsymbol{y}+\widetilde{\boldsymbol{y}}A'^2\boldsymbol{y})-((\widetilde{\boldsymbol{s}}\boldsymbol{y})\widetilde{\boldsymbol{y}}A\boldsymbol{y}+(\widetilde{\boldsymbol{s}}'\boldsymbol{y})\widetilde{\boldsymbol{y}}A'\boldsymbol{y}) + \tfrac{1}{2}(\widetilde{\boldsymbol{y}}A\boldsymbol{y})^2+(\widetilde{\boldsymbol{y}}A'\boldsymbol{y})^2). \tag{B7}$$

The matrix element $M_{\Lambda^2}(t)$ is derived by using the formulas in Appendix B of Ref. [33] and by performing the operations with respect to $\boldsymbol{s}$ and $\boldsymbol{s}'$ as indicated in Eq. (26). The result is given in Sec. IV B.

Let us apply the above result to the diagonal matrix element $\langle f^{uA}_{LM}|\Lambda^2|f^{uA}_{LM}\rangle_{y=1}$, where $A=(a\delta_{i,j})$ and $\widetilde{\boldsymbol{u}}\boldsymbol{u}=1$. Note that for this A the hyperangular dependence of f^{uA}_{LM} comes only from $\mathcal{Y}_{LM}(\widetilde{\boldsymbol{u}}\boldsymbol{y})$ which is the homogeneous polynomial of degree L. $M_{\Lambda^2}(t)$ turns out to comprise of $(a+t)^{-\lambda-p}$ with $p=0,1,2$. See Eqs. (39)–(42). Taking the $\kappa\to\infty$ limit leads to

$$\frac{\langle f^{uA}_{LM}|\Lambda^2|f^{uA}_{LM}\rangle_{y=1}}{\langle f^{uA}_{LM}|f^{uA}_{LM}\rangle_{y=1}} = L(L+d-2). \tag{B8}$$

For $d=3$, the expectation value of Λ^2 reduces to $L(L+1)$ as expected. For larger d, the value is consistent with the fact that Λ^2 has the eigenvalue $K(K+d-2)$ [34] when it acts on the HS harmonics with the hypermomentum K. In a general case where A has off-diagonal elements, $A_{ij}\boldsymbol{y}_i\boldsymbol{y}_j$ terms of the exponential of the CG contribute to the hyperangular motion with larger K values.

APPENDIX C: STIRLING NUMBERS

Equation (A17) states that

$$\binom{m}{p}(x)_{m-p} = \frac{1}{p!}\sum_{k=0}^{p}(-1)^k\binom{p}{k}(x-k)_m, \tag{C1}$$

where $m\geqslant p$ are both non-negative integers, and $x=l_1+\frac{3}{2}$ may be extended to any real number. Although this equation has been numerically checked, I have no proof of it yet. Here, I point out that the problem is formulated using Stirling numbers [38].

I start from expanding a falling factorial $x^{\underline{n}}$ with the Stirling number of the first kind, $s_n^{(m)}$, as

$$x^{\underline{n}} \equiv x(x-1)\cdots(x-n+1) = \sum_{m=0}^{n}s_n^{(m)}x^m. \tag{C2}$$

The Stirling number of the second kind, $\boldsymbol{S}_n^{(m)}$, conversely relates x^n to the falling factorials,

$$x^n = \sum_{m=0}^{n}\boldsymbol{S}_n^{(m)}x^{\underline{m}}. \tag{C3}$$

Both $s_n^{(m)}$ and $\boldsymbol{S}_n^{(m)}$ vanish for $m>n$, and $s_n^{(n)}=\boldsymbol{S}_n^{(n)}=1$.

By differentiating both sides of the binomial relation, $\sum_{k=0}^{p}\binom{p}{k}a^{p-k}b^k=(a+b)^p$, n times with respect to b and by setting $a=1$, $b=-1$, one obtains a useful formula

$$\sum_{k=0}^{p}(-1)^k\binom{p}{k}k^{\underline{n}} = (-1)^p p!\delta_{n,p}. \tag{C4}$$

Note that the case of $n > p$ trivially holds true. It follows from Eqs. (C3) and (C4) that $\boldsymbol{S}_n^{(p)}$ is explicitly given by

$$\boldsymbol{S}_n^{(p)} = \frac{1}{p!}\sum_{k=0}^{p}(-1)^{p-k}\binom{p}{k}k^n. \tag{C5}$$

The use of $(x)_n = x(x+1)\cdots(x+n-1) = (-1)^n(-x)^{\underline{n}}$ and Eq. (C2) leads to

$$(x-k)_m = (-1)^m\sum_{n=0}^{m}s_m^{(n)}\sum_{l=0}^{n}\binom{n}{l}k^l(-x)^{n-l}. \tag{C6}$$

Substitution of this equation into Eq. (C1) and use of Eq. (C5) reduces the right-hand side of Eq. (C1) to

$$(-1)^{m+p}\sum_{n=0}^{m}s_m^{(n)}\sum_{l=0}^{n}\binom{n}{l}\boldsymbol{S}_l^{(p)}(-x)^{n-l}. \tag{C7}$$

Comparing the coefficient of $(-x)^i$ $(0 \leqslant i \leqslant m-p)$ on both sides of Eq. (C1), one finds that Eq. (C1) is equivalent to a set of equations,

$$\binom{m}{p}s_{m-p}^{(i)} = \sum_{n=p+i}^{m}\binom{n}{n-i}s_m^{(n)}\boldsymbol{S}_{n-i}^{(p)}. \tag{C8}$$

[1] M. V. Zhukov, B. V. Danilin, D. V. Fedorov, J. M. Bang, I. J. Thompson, and J. S. Vaagen, Phys. Rep. **231**, 151 (1993).
[2] R. Krivec, Few-Body Syst. **25**, 199 (1998).
[3] E. Nielsen, D. V. Fedorov, A. S. Jensen, and E. Garrido, Phys. Rep. **347**, 373 (2001).
[4] N. Barnea, W. Leidemann, and G. Orlandini, Phys. Rev. C **61**, 054001 (2000).
[5] N. Barnea, W. Leidemann, and G. Orlandini, Phys. Rev. C **67**, 054003 (2003).
[6] N. Barnea, W. Leidemann, and G. Orlandini, Phys. Rev. C **81**, 064001 (2010).
[7] S. Bacca, N. Barnea, and A. Schwenk, Phys. Rev. C **86**, 034321 (2012).
[8] N. K. Timofeyuk, Phys. Rev. C **65**, 064306 (2002).
[9] N. K. Timofeyuk, Phys. Rev. C **78**, 054314 (2008).
[10] M. Gattobigio, A. Kievsky, and M. Viviani, Phys. Rev. C **83**, 024001 (2011).
[11] J. Macek, J. Phys. B **1**, 831 (1968).
[12] N. B. Nguyen, F. M. Nunes, and I. J. Thompson, Phys. Rev. C **87**, 054615 (2013).
[13] H. Suno, Y. Suzuki, and P. Descouvemont, Phys. Rev. C **94**, 054607 (2016).
[14] S. Ishikawa, Phys. Rev. C **87**, 055804 (2013).
[15] C. H. Greene, P. Giannakeas, and J. Pérez-Ríos, Rev. Mod. Phys. **89**, 035006 (2017).
[16] H. Suno, Y. Suzuki, and P. Descouvemont, Phys. Rev. C **91**, 014004 (2015).
[17] G. Royer, A. Escudie, and B. Sublard, Phys. Rev. C **90**, 024607 (2014).
[18] G. Royer, G. Ramasamy, and P. Eudes, Phys. Rev. C **92**, 054308 (2015).
[19] M. Girod and P. Schuck, Phys. Rev. Lett. **111**, 132503 (2013).
[20] S. F. Boys, Proc. R. Soc. London, Ser. A **258**, 402 (1960).
[21] K. Singer, Proc. R. Soc. London, Ser. A **258**, 412 (1960).
[22] K. Varga and Y. Suzuki, Phys. Rev. C **52**, 2885 (1995).
[23] Y. Suzuki and K. Varga, *Stochastic Variational Approach to Quantum-Mechanical Few-Body Problems*, Lecture Notes in Physics, Vol. 54 (Springer, Berlin, 1998).
[24] K. Varga, Y. Suzuki, and R. G. Lovas, Nucl. Phys. A **571**, 447 (1994).
[25] J. Mitroy, S. Bubin, W. Horiuchi, Y. Suzuki, L. Adamowicz, W. Cencek, K. Szalewicz, J. Komasa, D. Blume, and K. Varga, Rev. Mod. Phys. **85**, 693 (2013).
[26] W. Horiuchi and Y. Suzuki, Phys. Rev. C **89**, 011304(R) (2014).
[27] Y. Suzuki and W. Horiuchi, Phys. Rev. C **95**, 044320 (2017).
[28] J. von Stecher and C. H. Greene, Phys. Rev. A **80**, 022504 (2009).
[29] S. T. Rittenhouse, J. von Stecher, J. P. D'Incao, N. P. Mehta, and C. H. Greene, J. Phys. B: At. Mol. Opt. Phys. **44**, 172001 (2011).
[30] D. Rakshit and D. Blume, Phys. Rev. A **86**, 062513 (2012).
[31] K. M. Daily and C. H. Greene, Phys. Rev. A **89**, 012503 (2014).
[32] Y. Suzuki, Prog. Theor. Exp. Phys. **2015**, 043D05 (2015).
[33] Y. Suzuki and K. Varga, Few-Body Syst. **60**, 3 (2019).
[34] See, for example, J. S. Avery, J. Comput. Appl. Math. **233**, 1366 (2010).
[35] Y. Suzuki, W. Horiuchi, M. Orabi, and K. Arai, Few-Body Syst. **42**, 33 (2008).
[36] S. Aoyama, K. Arai, Y. Suzuki, P. Descouvemont, and D. Baye, Few-Body Syst. **52**, 97 (2012).
[37] R. C. Whitten and F. T. Smith, J. Math. Phys. **9**, 1103 (1968).
[38] M. Abramowitz and I. A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables* (Dover, Mineola, NY, 1970).