Diabatic Hamiltonian matrix elements made simple

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With a view to applying the generator coordinate method to large configuration spaces, we propose a simple approximate formula to compute diabatic many-body matrix elements without having to evaluate two-body interaction matrix elements. The method is illustrated with two analytically solvable Hamiltonians based on the harmonic oscillator.

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I. INTRODUCTION

In nuclear physics we use transparent models not only to understand the observed characteristics of nuclear spectra and dynamics but also to provide checks and guidance on the complex computer codes that produce the quantitative theory of their properties. The Lipkin model is a typical example [1].

In this spirit we derive and apply a simple formula, Eq. (10) below, for calculating matrix elements between configurations in the generator coordinate method (GCM). In GCM, many Slater determinants are linearly superposed to describe low-energy dynamics of many-body systems [1–3]. Since those Slater determinants are not orthogonal, one needs to calculate their overlaps and Hamiltonian matrix elements. To this end, the Hamiltonian matrix elements are computed using the generalized Wick's theorem (GWT) [4] as was first done in Ref. [5].

However, the GWT requires a full knowledge of the Hamiltonian in a Fock-space representation. In contrast, Eq. (10) below only needs the overlap matrix elements of the orbitals and the orbital energies calculated from the single-particle Hamiltonian. It is an approximate formula that can be used with any of the theories in which an effective single-particle Hamiltonian can be defined. This includes theories based on energy functionals such as Skyrme, Gogny, and Barcelona-Catania-Paris-Madrid (BCPM) [6], as well as those making use of the Strutinsky treatment of the total energy. In this paper, we shall apply the formula to two simple models, namely, the translational motion in a harmonic oscillator potential and a simplified Nilsson model.

II. ORBITAL ENERGY FORMULA

We first summarize the usual computational procedure. The starting point is a configuration space of many-particle wave functions that have the form of Slater determinants of orbitals in some common basis.[1] The Hartree-Fock method reduces a Hamiltonian with two-particle interactions to a one-particle Hamiltonian with the orbitals as its eigenstates.[2] The orbitals are obtained by minimizing the single-particle Hamiltonian or energy functional. The space of configurations in the GCM is expanded by introducing a collective coordinate. This is often implemented by adding a term in the Hamiltonian to constrain the expectation value of some single-particle operator, but the coordinate can also be defined in other ways. In the examples below, it is convenient to introduce the coordinate directly into the orbital wave functions.

Assuming that the constraint is described by a single parameter q, the task is to calculate the Hamiltonian matrix element between a configuration $|\Psi_q\rangle$ and some other configuration $|\Psi_{q'}\rangle$. The GWT method can be derived from Thouless's theorem [8] which is used to express the second wave function in the orbital basis of the first one. That is,

$$|\Psi_{q'}\rangle = \mathcal{N}\prod_h \left(1 + \sum_p c_{ph} a_p^\dagger a_h\right)|\Psi_q\rangle. \tag{1}$$

Here h and p are occupied and unoccupied orbitals in the basis of $|\Psi_q\rangle = \prod_h a_h^\dagger|\rangle$. The Fock-space operators are expressed in the q orbital basis and $\mathcal{N}$ is a normalization constant given by

$$\mathcal{N} = (\det M)^{-1/2} \tag{2}$$

where $M_{h,h'} = \delta_{h,h'} + \sum_p c_{ph}c_{ph'}$. With all of the operators expressed in the same basis it is easy to apply the ordinary Wick's theorem to calculate arbitrary many-body matrix elements.

[1]The extension to include pairing by the Hartree-Fock-Bogoliubov equation is beyond the scope of this paper.

[2]The method can easily be extended to Hamiltonians with three-particle and higher terms by the same reduction of the higher-order density matrices [7] as in the Hartree-Fock approximation.

To derive the orbital energy formula we place the reference configuration midway between the two states $|\Psi_q\rangle$ and $|\Psi_{q'}\rangle$. Changing the notation somewhat, the many-particle configurations can be written

$$|\Psi_{\pm q}\rangle = \mathcal{N}^{\pm}\prod_h\left(1+\sum_p c^{\pm}_{ph}a^{\dagger}_p a_h\right)|\Psi_0\rangle, \tag{3}$$

where $|\Psi_0\rangle$ is the reference configuration and $|\Psi_{\pm q}\rangle$ are the end configurations. The overlap between the two end configurations is given by

$$\langle\Psi_{-q}|\Psi_{+q}\rangle = \mathcal{N}^{-}\mathcal{N}^{+}\det\left|\delta_{h,h'}+\sum_p c^{+}_{ph}c^{-}_{ph'}\right|. \tag{4}$$

The object is to calculate the matrix element of the Hamiltonian between them.

We write the effective Hamiltonian in Fock space as

$$\hat{H} = E_0+\sum_p \varepsilon_p a^{\dagger}_p a_p-\sum_h \varepsilon_h a_h a^{\dagger}_h + \sum_{i\neq j}H_{ij}a^{\dagger}_i a_j+\sum_{ij,k\ell}v_{ij,k\ell}a^{\dagger}_i a^{\dagger}_j a_\ell a_k. \tag{5}$$

Here $E_0=\langle\Psi_0|\hat{H}|\Psi_0\rangle$ is the expectation value of the Hamiltonian in the reference configuration. The effective single-particle Hamilton H_{ij} has been split into diagonal contributions $H_{ii}=\varepsilon_i$ and off-diagonal ones appearing on the second line. The last term is the effective two-particle interaction. It contains all the interaction matrix elements not present in the other terms. We will argue that its contribution is small when the matrix elements are calculated between states related by a diabatic transformation.

In a diabatic evolution, each orbit is transformed independently according to a local single-particle operator such as the quadrupole operator $\hat{Q}=z^2-(x^2+y^2)/2$. Under those conditions the transition density $\langle\Psi_q|\hat{\rho}|\Psi_{q'}\rangle=\delta\rho$ is collective with a strong local component proportional to $d\rho(\boldsymbol{r})/dq$ in the coordinate space representation. The mean field V_0 behaves similarly. The interaction can then be parametrized in the separable form

$$v_{ij,k\ell}=\frac{\kappa}{2}\sum_{\lambda\mu}O^{\lambda\mu *}_{ik}O^{\lambda\mu}_{j\ell} \tag{6}$$

with single-particle matrix elements

$$O^{\lambda\mu}_{ij}=\int d^3r\,\phi^*_i(\boldsymbol{r})\phi_j(\boldsymbol{r})\frac{dV_0}{dr}Y_{\lambda\mu}(\hat{\boldsymbol{r}}). \tag{7}$$

The strength κ is determined by the self-consistency condition [9,10]

$$\kappa^{-1}=\int_0^{\infty}r^2dr\,\frac{d\rho_0(r)}{dr}\frac{dV_0(r)}{dr}. \tag{8}$$

In calculating the interaction between many-particle configurations, one includes only the direct term in the interaction; exchange effects are implicit in the single-particle potential V_0. Except for E_0, the resulting Hamiltonian can be generated entirely in terms of the effective single-particle mean field and its variation under the diabatic transformation. Interactions of this form have been applied not only to collective excitations [11,12] but even to treat nuclear spectra as a whole [13].

We now estimate many-body Hamiltonian matrix elements using Eqs. (5)–(8). Several assumptions in the derivation are justified by considering the limit of a large number N_h of particles together with small displacements in the collective coordinate. This leads to a simplification of the Löwdin formula [14,15] for matrix elements requiring the minors of the normalization determinant $\det(M)$. The off-diagonal minors are much smaller than the diagonal ones when the c_{ph} amplitudes are small. Also, the diagonal ones are approximately equal to $\det(M)$. The Hamiltonian matrix element can then be evaluated as

$$\begin{aligned}\frac{\langle\Psi_{-q}|\hat{H}|\Psi_{+q}\rangle}{\langle\Psi_{-q}|\Psi_{+q}\rangle} &\approx E_0+\sum_{ph}c^{+}_{ph}c^{-}_{ph}(\varepsilon_p-\varepsilon_h)+\sum_{ph}H_{ph}(c^{+}_{ph}+c^{-}_{ph})\\ &+\frac{\kappa}{2}\sum_{ph,p'h'}(c^{+}_{ph}c^{-}_{p'h'}+c^{-}_{ph}c^{+}_{p'h'}+c^{+}_{ph}c^{+}_{p'h'}+c^{-}_{ph}c^{-}_{ph})\\ &\times\sum_{\lambda\mu}O^{\lambda\mu *}_{ph}O^{\lambda\mu}_{p'h'}.\end{aligned} \tag{9}$$

Equation (9) can be further simplified in several ways. First, we limit the scope to axially symmetric diabatic transformations. Then the last sum can be restricted to $\mu=0$ operators, and the amplitudes can be treated as real quantities. Next, we can assume that $c^{-}=-c^{+}$ if q is not too large. Then the last term vanishes. Note that the cancellation requires that the separable terms in the interaction are even under the time-reversal transformation. Finally, if the state $|0\rangle$ is a self-consistent solution of the mean-field equation, the off-diagonal elements H_{ph} vanish as well.

Changing the notation back to the original, the resulting formula reads

$$\frac{\langle\Psi_{q_1}|\hat{H}|\Psi_{q_2}\rangle}{\langle\Psi_{q_1}|\Psi_{q_2}\rangle}\approx E_0-\sum_{ph}c^2_{ph}(\varepsilon_p-\varepsilon_h), \tag{10}$$

where the particle-hole amplitudes have been determined with respect to a reference configuration at $q=(q_1+q_2)/2$. It is remarkable that all dependence on the residual interaction has disappeared.

The formula can be easily applied to calculate the inertial parameter associated with the collective coordinate q. For small q the amplitudes may be expanded as a power series with the leading term $c_{ph}=\frac{1}{2}(q_1-q_2)\,dc_{ph}/dq$ to give

$$\frac{\langle\Psi_{q_1}|\hat{H}|\Psi_{q_2}\rangle}{\langle\Psi_{q_1}|\Psi_{q_2}\rangle}\approx E_0-\frac{1}{4}\sum_{ph}\left(\frac{dc_{ph}}{dq}\right)^2(q_1-q_2)^2(\varepsilon_p-\varepsilon_h). \tag{11}$$

Finally, one can calculate the collective inertial parameter B by applying the formula to the plane-wave state

$$|k\rangle=\int dq|\Psi_q\rangle e^{ikq}. \tag{12}$$

Writing the derivative as $dc_{ph}/dq = c'_{ph}$, one has

$$\langle \Psi_q | \Psi_{q'} \rangle \sim e^{-\sum_{ph}(c'_{ph})^2 (q-q')^2/2} \tag{13}$$

for small $(q - q')$. One thus obtains

$$\frac{\langle k|\hat{H}|\Psi_q\rangle}{\langle k|\Psi_q\rangle} \approx E_0 - \frac{\sum_{ph}(c'_{ph})^2(\varepsilon_p - \varepsilon_h)}{4\sum_{ph}(c'_{ph})^2} + \frac{\sum_{ph}(c'_{ph})^2(\varepsilon_p - \varepsilon_h)}{4(\sum_{ph}(c'_{ph})^2)^2} k^2. \tag{14}$$

The third term is the collective kinetic energy $k^2/2B$ with B given by

$$B = \frac{2\left(\sum_{ph}(c'_{ph})^2\right)^2}{\sum_{ph}(c'_{ph})^2(\varepsilon_p - \varepsilon_h)}. \tag{15}$$

This agrees with the inertia derived from GCM with Gaussian overlap approximation (GOA) using sum rules of a constraining field [16, Eq. (22)].

III. MODEL 1: TRANSLATIONAL MOTION

Here we consider a Hamiltonian of N distinguishable particles interacting through a translationally invariant quadratic potential in one dimension,

$$H = T + v_2 \ = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{m\omega_v^2}{2} \sum_{i<j} (x_i - x_j)^2. \tag{16}$$

The GCM algebra below generalizes the discussion of the harmonic oscillator model in Ref. [1, Sec. 10.5].

The first task is to find a mean-field ground-state wave function Ψ_0. Since the particles are distinguishable, all the orbitals ϕ_i are the same and the many-body ground-state configuration has the form

$$\Psi_0 = \prod_{i=1}^{N} \phi(x_i). \tag{17}$$

We may assume that the orbitals are Gaussian functions centered at $x = 0$,

$$\phi(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}, \tag{18}$$

with a common size parameter α. It can be verified later that the Gaussian form allows a self-consistent solution of the mean-field equations. The expectation value of the Hamiltonian is

$$\langle \Psi_0 | H | \Psi_0 \rangle = N\frac{\alpha\hbar^2}{4m} + N(N-1)\frac{m\omega_v^2}{4\alpha}. \tag{19}$$

The first term is from the kinetic energy operator T and the second is from the interaction v_2. Minimizing this expression with respect to α yields

$$\alpha = (N-1)^{1/2}\omega_v m/\hbar \tag{20}$$

giving a total energy

$$E_0 = \langle \Psi_0 | H | \Psi_0 \rangle = N\frac{(N-1)^{1/2}}{2}\hbar\omega_v. \tag{21}$$

The next GCM task is to define a generator coordinate; we take it to be a displacement of the ground-state configuration by an amount z,

$$\Psi_z = \left(\frac{\alpha}{\pi}\right)^{N/4} \prod_{i=1}^{N} e^{-\alpha(x_i - z)^2/2} \equiv \prod_{i=1}^{N} \phi_z(x_i). \tag{22}$$

Applications of the GCM require the overlap matrix elements $\langle \Psi_z | \Psi_{z'} \rangle$ and the Hamiltonian matrix elements $\langle \Psi_z | H | \Psi_{z'} \rangle$. The overlaps are given by

$$\langle \Psi_z | \Psi_{z'} \rangle = \exp\left(-N\frac{\alpha}{4}(z - z')^2 \right). \tag{23}$$

Decomposing the matrix elements of the Hamiltonian into the kinetic term and the interaction term, we have

$$\langle \Psi_z | T | \Psi_{z'} \rangle = \left(N\frac{\alpha\hbar^2}{4m} - N\frac{\alpha^2\hbar^2}{8m}(z - z')^2 \right) \langle \Psi_z | \Psi_{z'} \rangle \tag{24}$$

for the kinetic term and

$$\langle \Psi_z | v_2 | \Psi_{z'} \rangle = N(N-1)\frac{m\omega_v^2}{4\alpha} \langle \Psi_z | \Psi_{z'} \rangle, \tag{25}$$

for the interaction term. Note that it is the same as the expectation value in the ground state except for the overlap factor. Combining the two terms, the Hamiltonian matrix element can be expressed

$$\langle \Psi_z | H | \Psi_{z'} \rangle = \langle \Psi_z | \Psi_{z'} \rangle (E_0 - h_2 (z - z')^2) \tag{26}$$

where

$$h_2 = N\frac{\alpha^2\hbar^2}{8m}. \tag{27}$$

This is identical to [1, Eq. 10.51] except for the N dependence.

One can derive the effective mass associated with the collective coordinate from Eq. (23) and (26). It will be shown below that it is just the value for translational motion, namely Nm.

Before that, we verify the orbital energy formula, Eq. (10), choosing end configurations at $\pm z$ and the reference configuration at $z = 0$. The Ψ_z particle-hole amplitudes in the basis of Ψ_0 are calculated by taking orbital overlaps. We only need orbitals up to the second excited state for our purposes. The amplitudes are

$$\phi_z(x) = \psi_0(x - z) = e^{-\alpha z^2/4} \left(\phi_0(x) + z\left(\frac{\alpha}{2}\right)^{1/2} \phi_1(x) + z^2 \frac{\alpha}{8^{1/2}} \phi_2(x) + \ldots \right). \tag{28}$$

Next we need the orbital excitation energies, obtained from the spectrum as $\varepsilon_n = n\alpha\hbar^2/m$. Then the orbital excitation formula gives

$$\sum c_{10}^{+} c_{10}^{-} (\varepsilon_1 - \varepsilon_0) = N\frac{\alpha}{2}\frac{\alpha}{m}\hbar^2 \cdot \frac{1}{4}(z - z')^2, \tag{29}$$

in agreement with Eq. (26) with Eq. (27).

Let us now discuss the associated mass term in the collective Hamiltonian. We can construct a plane-wave state from

the GCM configurations according to Eq. (12). The overlap with Ψ_0 is

$$\langle\Psi_0|k\rangle = \left(\frac{4\pi}{\alpha N}\right)^{1/2} e^{-k^2/\alpha N} \tag{30}$$

and the Hamiltonian matrix element reduces to

$$\langle\Psi_0|H|k\rangle = \langle\Psi_0|k\rangle\left(\frac{k^2}{2Nm} - \frac{\alpha}{4m}\right). \tag{31}$$

The first term in parenthesis $k^2/2Nm$ is just what we expected for a free particle of mass m [17, Eq. (43)]. The other term is the zero point kinetic energy associated with the center-of-mass coordinate in the original GCM configuration composed of Gaussian orbitals.

It is not generally recognized that the GCM/GOA methodology can deliver exact composite-particle masses for translational motion. It was noticed as an empirical finding in Ref. [18] that the translational masses of nuclei calculated with a Gogny functional were close to Am, the number of nucleons A times the nucleon mass m.

IV. MODEL 2: DYNAMICS IN A DEFORMATION COORDINATE

We next consider a simplified Nilsson model to illustrate the use of the self-consistent separable interaction Eq. (6) to generate a two-particle interaction from a diabatic treatment of the mean field. The single-particle potential is given by a deformed harmonic oscillator potential,

$$V(\boldsymbol{r}) = \tfrac{1}{2}m\omega_z^2 z^2 + \tfrac{1}{2}m\omega_\perp^2(x^2+y^2), \tag{32}$$

where $\omega_z^2 = \omega_0^2(1-4\delta/3)$ and $\omega_\perp^2 = \omega_0^2(1+2\delta/3)$, following the notation of Ref. [9, Eq. 5-5]. This potential can also be expressed as

$$V(\boldsymbol{r}) = \tfrac{1}{2}m\omega_0^2 r^2 - \tfrac{2}{3}\delta\, m\omega_0^2[z^2 - (x^2+y^2)/2]. \tag{33}$$

We take the parameter δ as the generator coordinate.[3]

The eigenstates of the Hamiltonian are specified by a set of quantum numbers (n_x, n_y, n_z) together with the z components of spin and isospin; their spatial distributions are determined by ω_0 and δ, combined to give oscillator length parameters $b_i = \sqrt{\hbar/m\omega_i}$ for $i = z, \perp, 0$.

For simplicity, we consider a harmonic oscillator model of the nucleus ^{16}O. Its eight neutrons and eight protons occupy the $1s$ state with $N_{osc} = n_x + n_y + n_z = 0$ and the three $1p$ states with $N_{osc} = 1$. The density distribution is given by

$$\rho(\boldsymbol{r}) = 4\sum_k |\phi_k(\boldsymbol{r})|^2 \tag{34}$$

$$= \frac{4}{\pi b_\perp^2\sqrt{\pi b_z^2}}\left[1 + 2\left(\frac{x^2+y^2}{b_\perp^2} + \frac{z^2}{b_z^2}\right)\right] \times e^{-z^2/b_z^2} e^{-(x^2+y^2)/b_\perp^2}, \tag{35}$$

where $k \equiv (n_x, n_y, n_z) = (0,0,0)$, $(0,0,1)$, $(0,1,0)$, and (1,0,0).

[3]Another parameter in common use is $\beta_2 \approx \frac{2}{3}\sqrt{\frac{4\pi}{5}}\,\delta$.

TABLE I. Overlaps $\langle nb|nb'\rangle \equiv \langle\phi_n(b)|\phi_n(b')\rangle$ and needed matrix elements for one-dimensional harmonic oscillator wave functions with oscillator lengths b and b'. The oscillator quanta are denoted by n.

n	$\langle nb\|nb'\rangle$	$\langle nb\|x^2\|nb'\rangle$	$\langle nb\|p^2\|nb'\rangle$
0	$\sqrt{\frac{2bb'}{b^2+b'^2}}$	$\frac{bb'}{2}\left(\frac{2bb'}{b^2+b'^2}\right)^{3/2}$	$\frac{\hbar^2}{b^2+b'^2}\left(\frac{2bb'}{b^2+b'^2}\right)^{1/2}$
1	$\left(\frac{2bb'}{b^2+b'^2}\right)^{3/2}$	$\frac{3bb'}{2}\left(\frac{2bb'}{b^2+b'^2}\right)^{5/2}$	$\frac{3\hbar^2}{b^2+b'^2}\left(\frac{2bb'}{b^2+b'^2}\right)^{3/2}$

To the linear order of δ, the density distribution (35) is expanded to

$$\rho(\boldsymbol{r}) = \rho_0(r) + \rho_2(r)P_2(\cos\theta) \tag{36}$$

with

$$\rho_0(r) = \frac{4}{(\pi b_0^2)^{3/2}}\left(1 + \frac{2r^2}{b_0^2}\right)e^{-r^2/b_0^2} \tag{37}$$

and

$$\rho_2(r) = \frac{\delta}{3(\pi b_0^2)^{3/2}}\left(\frac{4r^4}{b_0^4} - \frac{2r^2}{b_0^2}\right)e^{-r^2/b_0^2}. \tag{38}$$

Given the form of the potential (33), the many-body Hamiltonian with a separable interaction reads

$$H = \sum_i\left(\frac{\boldsymbol{p}_i^2}{2m} + \frac{1}{2}m\omega_0^2 r_i^2\right) + \frac{\kappa}{2}\left(\sum_i r_i^2 P_2(\cos\theta_i)\right)^2. \tag{39}$$

The strength κ evaluated with Eq. (8) is

$$\kappa = -\frac{2}{3}\delta m\omega_0^2\left(\frac{4\pi}{5}\int_0^\infty r^2 dr\, r^2\rho_2(r)\right)^{-1} = -\frac{m^2\omega_0^3}{18}. \tag{40}$$

Using orbital overlaps in Table I, it is easy to evaluate the many-body overlap and Hamiltonian matrix element,

$$\langle\Psi_\delta|\Psi_{\delta'}\rangle = \left(\frac{2b_\perp b'_\perp}{b_\perp^2 + b'^2_\perp}\right)^{24}\left(\frac{2b_z b'_z}{b_z^2 + b'^2_z}\right)^{12}, \tag{41}$$

$$\frac{\langle\Psi_\delta|H|\Psi_{\delta'}\rangle}{\langle\Psi_\delta|\Psi_{\delta'}\rangle} = \frac{24\hbar^2}{2m}\left(\frac{2}{b_\perp^2 + b'^2_\perp} + \frac{1}{b_z^2 + b'^2_z}\right) + \frac{1}{2}m\omega_0^2\left(\frac{48b_\perp^2 b'^2_\perp}{b_\perp^2 + b'^2_\perp} + \frac{24b_z^2 b'^2_z}{b_z^2 + b'^2_z}\right) + \frac{\kappa}{2}\left[24\left(\frac{b_\perp^2 b'^2_\perp}{b_\perp^2 + b'^2_\perp} - \frac{b_z^2 b'^2_z}{b_z^2 + b'^2_z}\right)\right]^2. \tag{42}$$

The result for the overlap can also be obtained as a special case of the general formula for many-particle harmonic oscillator configurations given in Ref. [19, Eq. 3.5].[4]

Finally we expand Eq. (42) to the quadratic order of δ and δ' to obtain

$$\frac{\langle\Psi_\delta|H|\Psi_{\delta'}\rangle}{\langle\Psi_\delta|\Psi_{\delta'}\rangle} = 18\hbar\omega_0 - \hbar\omega_0(\delta - \delta')^2 + \cdots. \tag{43}$$

[4]The variable ε in the notation of Ref. [19] is identical to $(\delta - \delta')/6$.

TABLE II. The contribution of each single-particle wave function ψ_k to the second order term in the energy overlap, $-\sum_{ph}|C_{ph}|^2(\epsilon_p-\epsilon_h)$. Here, the particle-hole energy is $\epsilon_p-\epsilon_h=2\hbar\omega_0$, and the spin degeneracy is also taken into account.

ψ_{000}	$-8\hbar\omega_0\left[2(a_2^{(\perp)})^2+(a_2^{(z)})^2\right]$
ψ_{001}	$-8\hbar\omega_0\left[2(a_2^{(\perp)})^2+(a_3^{(z)})^2\right]$
ψ_{100}	$-8\hbar\omega_0\left[(a_3^{(\perp)})^2+(a_2^{(\perp)})^2+\left(a_2^{(z)}\right)^2\right]$
ψ_{010}	$-8\hbar\omega_0\left[(a_3^{(\perp)})^2+(a_2^{(\perp)})^2+\left(a_2^{(z)}\right)^2\right]$

One thus finds

$$h_2=\hbar\omega_0. \tag{44}$$

We now evaluate h_2 in the orbital energy formula Eq. (11) to compare with Eq. (44). We apply the formula to the matrix elements between Ψ_δ and $\Psi_{-\delta}$ taking Ψ_0 as the reference configuration. The main task is to determine the coefficients c_{ph} of the deformed orbits in terms of the orbitals in the spherical basis. Since we are interested in the second-order behavior of the Hamiltonian overlap with respect to δ, it is sufficient to expand the wave functions up to $n=2$ and $n=3$ for $\phi_0(b,x)$ and $\phi_1(b,x)$, respectively. This leads to

$$\phi_0(b,x)\propto\phi_0(b_0,x)+a_2\phi_2(b_0,x)+\cdots, \tag{45}$$

$$\phi_1(b,x)\propto\phi_1(b_0,x)+a_3\phi_3(b_0,x)+\cdots \tag{46}$$

with the coefficients of

$$a_2=\frac{1}{\sqrt{2}}\frac{b^2-b_0^2}{b^2+b_0^2} \tag{47}$$

and

$$a_3=\sqrt{\frac{3}{2}}\frac{b^2-b_0^2}{b^2+b_0^2} \tag{48}$$

for the one-dimensional Gaussians in an orbital. The three-dimensional orbitals ϕ_{n_x,n_y,n_z} are expanded as

$$\phi_{000}\propto\phi_{000}^{(0)}+a_2^{(\perp)}\left(\phi_{200}^{(0)}+\phi_{020}^{(0)}\right)+a_2^{(z)}\phi_{002}^{(0)}+\cdots, \tag{49}$$

$$\phi_{001}\propto\phi_{001}^{(0)}+a_2^{(\perp)}\left(\phi_{201}^{(0)}+\phi_{021}^{(0)}\right)+a_3^{(z)}\phi_{003}^{(0)}+\cdots, \tag{50}$$

$$\phi_{100}\propto\phi_{100}^{(0)}+a_3^{(\perp)}\phi_{300}^{(0)}+a_2^{(\perp)}\phi_{120}^{(0)}+a_2^{(z)}\phi_{102}^{(0)}+\cdots, \tag{51}$$

where $\phi_k^{(0)}$ is a spherical orbital. The contribution of each single-particle state to the second-order term in the energy overlap, $-\sum_{ph}|C_{ph}|^2(\epsilon_p-\epsilon_h)$, is shown in Table II. From this table, one has

$$-\sum_{ph}|C_{ph}|^2(\epsilon_p-\epsilon_h)$$

$$=-8\hbar\omega_0\left[6(a_2^{(\perp)})^2+2(a_3^{(\perp)})^2+3\left(a_2^{(z)}\right)^2+\left(a_3^{(z)}\right)^2\right] \tag{52}$$

$$=-8\hbar\omega_0\left\{6\left(\frac{b_\perp^2-b_0^2}{b_\perp^2+b_0^2}\right)^2+3\left(\frac{b_z^2-b_0^2}{b_z^2+b_0^2}\right)^2\right\}. \tag{53}$$

Expanding this quantity up to the second order of δ, one finds

$$-\sum_{ph}|C_{ph}|^2(\epsilon_p-\epsilon_h)\sim-4\hbar\omega_0\delta^2. \tag{54}$$

This coincides with the second-order term in Eq. (43) with $\delta'=-\delta$. It is easy to confirm that the same relation holds also with a deformed reference configuration, with $b_0=b(\delta_{\rm ref})$ and $b=b(\delta_{\rm ref}+\delta)$.

V. SUMMARY

We have derived a simple formula for the Hamiltonian matrix elements by the generator coordinate method. The formula is based on a residual interaction of separable form, determined by a diabatic treatment of the generator coordinate. The formula was shown to be exact for the leading dependence on q_1-q_2 for two solvable models.

Although it is approximate, the formula has several attractive features. First, it does not require full details of the many-body Hamiltonian. Thus one can carry out GCM calculations even when only the mean-field potential is known. This is the case when using a phenomenological mean-field potential such as a Woods-Saxon potential. Second, the formula is much simpler than the original multistep procedure based on the generalized Wick theorem or the Löwdin formula. Third, by using a separable interaction, one can avoid the well-known difficulties of treating energy functionals as Hamiltonians.

We plan to report numerical calculations of more realistic models in a separate publication.

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