Small-amplitude limit of the nuclear Born-Oppenheimer method

Nouredine Zettili
Department of Physics, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia and Institut de Physique, Universite de Blida, Blida, Algeria
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We examine here how the nuclear Born-Oppenheimer (NBO) method describes the collective dynamics of nuclei undergoing small-amplitude oscillations around the equilibrium state. After specifying the NBO trial wave function, and assuming that the intrinsic state is not very different from the Hartree-Fock (HF) ground state, we show that the NBO method yields the random phase approximation (RPA) equations. We then derive an expression for the ground state energy. This expression, which contains zero-point energy correction terms, is smaller than the static HF energy. Next, we derive the correlated ground state energy and then show that it is identical with the corresponding expressions obtained from the generator-coordinate method, from the properly quantized adiabatic time-dependent Hartree-Fock approach, and from the RPA.

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I. INTRODUCTION

Nuclear collective motion and the dynamics of molecular rotations and vibrations present many striking similarities. This idea received strong consolidation when the Born-Oppenheimer approximation (BOA) [1] of molecular physics was shown to be very useful in the study of nuclear collective motion [2–6]. This approximation yielded accurate results when used in the phenomenological calculations of nuclear multiple moments and charge radii [7].

The essence of the molecular BOA consists in the approximate decoupling of the nuclear and the electronic states using the fact that electrons are so much faster (and lighter) than molecular nuclei. The model calculations of Moshinsky-Kittel [8] have revealed that this approximation is very accurate for the calculation of both the energy and the wave function. In these calculations, the accuracy of the energy and of the wave function was found to be of the order of the ratio of the electronic and nucleonic masses (i.e., $m_e/M \simeq 10^{-4}$).

The nuclear analogy to the molecular BOA consists in the approximate decoupling of the intrinsic and collective dynamics. This approximation finds its justification — in the nuclear case — in the fact that the time evolution of the nuclear collective variables is slow on the scale of the single-particle or intrinsic motion. Villars carried out the formal implementation of the atomic BOA for the study of nuclear collective motion [2,3]. Villars' method, to be called here the nuclear Born-Oppenheimer (NBO) method, has two main appealing features: it is quantum mechanical, and the collective variables are not chosen by hand, but are determined from the dynamics of the system.

Using an exactly solvable model [4], we have shown, in a previous work [5], that the NBO method is very accurate for the calculation of the energy. From these model calculations, we have asserted that this method is more accurate than the time-dependent Hartree-Fock (TDHF) approximation in the adiabatic domain.

In this paper, we study the small-amplitude limit of the NBO method and its connection with the random phase approximation (RPA) method. In particular, we focus on the derivation of an expression for the NBO ground state energy for small-amplitude collective oscillations and then compare it with the RPA energy.

In Sec. II, we give a brief presentation of the NBO formalism. We work out the formalism of the small-amplitude limit of the method in Sec. III. We focus on the derivation of an expression for the ground state energy of harmonically oscillating rigid nuclei, and then discuss the contribution of the zero-point fluctuations to the ground state energy. In Sec. IV, we derive the NBO correlated ground state energy and then compare it, in Sec. V, with the corresponding expressions obtained from the generator-coordinate method (GCM), the correctly quantized adiabatic time-dependent Hartree-Fock (ATDHF) approach, and the particle-hole RPA.

II. THE NUCLEAR BORN-OPPENHEIMER METHOD

To describe collective dynamics (nuclear rotations and vibrations), we introduce an operator $\hat{Q}$ which depends on the nuclear coordinates x (x consists of all nucleonic degrees of freedom: positions, momenta, spins, and isospins). We assume here that $\hat{Q}$ is a one-body operator which is even under time reversal and nonlocal, and that $\hat{Q}$ has a continuous eigenvalue spectrum (to be designated by q).

In analogy to the atomic Born-Oppenheimer ansatz, we introduce a trial function $\langle x \mid \psi \rangle$ of the form

$$\langle x \mid \psi \rangle = \int dq \langle x \mid \delta(q - \hat{Q}) \mid \phi(q) \rangle f(q), \qquad (2.1)$$

where the state $\mid \phi(q)\rangle$ is used to describe the intrinsic structure of the nucleus, and where $f(q)$ is a collective amplitude. We will use a constrained variational principle to determine $\mid \phi(q)\rangle$, so that $\langle \phi(q) \mid \hat{Q} \mid \phi(q)\rangle$ is equal to q. As for $f(q)$, it will be determined variationally by minimizing $\langle \psi \mid \hat{H} \mid \psi\rangle$.

Using the relation

$$\delta(q-\hat{Q})\delta(q'-\hat{Q}) = \delta(q'-q)\delta(q-\hat{Q}), \tag{2.2}$$

we can show that the norm $\langle \psi \mid \psi\rangle$ reduces to

$$\langle \psi \mid \psi\rangle = \int dq W(q) f^*(q) f(q), \tag{2.3}$$

where the notation $W(q)$ stands for $\langle \phi(q)|\delta(q-\hat{Q})|\phi(q)\rangle$.

Now, we need to derive an expression for the mean energy $\langle \psi \mid \hat{H} \mid \psi\rangle$. Upon substitution of the wave function (2.1) into $\langle \psi|\hat{H}|\psi\rangle$, the term $\delta(q'-\hat{Q})\hat{H}\delta(q-\hat{Q})$ is obtained. In dealing with this term, we can pull $\hat{H}$ either to the right of $\delta(q-\hat{Q})$ or to the left of $\delta(q'-\hat{Q})$. The two expressions of $\langle \psi|\hat{H}|\psi\rangle$ thus obtained are adjoint to each other. Their average gives rise to a Hermitized expression for the energy. In what follows, we are going to work out the derivation of $\langle \psi|\hat{H}|\psi\rangle$ only for the case where $\hat{H}$ is pulled to the right.

Using the Fourier transform of the δ function, we can show that

$$\hat{H}\delta(q-\hat{Q}) = \delta(q-\hat{Q})\hat{H} + \frac{i\partial}{\partial q}\left[\delta(q-\hat{Q})\right]\hat{H}_Q + \frac{i^2}{2!}\frac{\partial^2}{\partial q^2}\left[\delta(q-\hat{Q})\right]\hat{H}_{2Q} + \cdots, \tag{2.4}$$

where $\hat{H}_Q$ and $\hat{H}_{2Q}$ are given, respectively, by the commutators $[\hat{H}, i\hat{Q}]$ and $[[\hat{H}, i\hat{Q}], i\hat{Q}]$.

In the calculation of $\hat{H} \mid \psi\rangle$, we can transfer, by means of partial integrations, the q derivatives from $\delta(q-\hat{Q})$ to the product $\mid \phi(q)\rangle f(q)$:

$$\hat{H} \mid \psi\rangle = \int dq \delta(q-\hat{Q})\left\{\hat{H} + \hat{H}_Q(p-\hat{G}) + \frac{1}{2!}\hat{H}_{2Q}(p-\hat{G})(p-\hat{G}) + \cdots\right\}\mid \phi(q)\rangle f(q), \tag{2.5}$$

where $\hat{G}$ operates only on $\mid \phi(q)\rangle$, whereas p acts only on the amplitude $f(q)$ as follows:

$$\hat{G}\mid \phi(q)\rangle = i\frac{\partial}{\partial q}\mid \phi(q) >, \qquad pf(q) = i\frac{\partial f(q)}{\partial q}. \tag{2.6}$$

Now, using the relations (2.2) and (2.5), we can ascertain that $\langle \psi \mid \hat{H} \mid \psi\rangle$ reduces to

$$\langle \psi \mid \hat{H} \mid \psi\rangle = \int dq f^*(q)\left\{\frac{1}{2}\langle \phi(q)|\delta(q-\hat{Q})\hat{H}_{2Q}|\phi(q)\rangle p^2 + \langle \phi(q)|\delta(q-\hat{Q})\left[\hat{H}_Q - \hat{H}_{2Q}\hat{G}\right]|\phi(q)\rangle p + \langle \phi(q)|\delta(q-\hat{Q})\left[\hat{H} - \hat{H}_Q\hat{G} + \frac{1}{2!}\hat{H}_{2Q}\hat{G}^2\right]|\phi(q)\rangle\right\} f(q). \tag{2.7}$$

In deriving this expression, we have neglected the terms beyond the second powers of the momenta p and $\hat{G}$ (or beyond the double commutator $[[\hat{H}, i\hat{Q}],\ i\hat{Q}]$), since we will be dealing in this work only with small-amplitude collective motion. The justification for this will become transparent later on.

At this level, we need to introduce an approximation, which consists in replacing the projected mean value $\langle \delta(q-\hat{Q})\hat{A}\rangle_q$ of every operator $\hat{A}$ by

$$\langle \delta(q-\hat{Q})\hat{A}\rangle_q \simeq \langle \delta(q-\hat{Q})\rangle_q \langle \hat{A}\rangle_q, \tag{2.8}$$

where the notation $\langle \hat{A}\rangle_q$ is used here and throughout the rest of this work to abbreviate $\langle \phi(q) \mid \hat{A} \mid \phi(q)\rangle$. Implementing this approximation on the energy expression (2.7), we obtain

$$\langle \psi \mid \hat{H} \mid \psi\rangle = \int dq f^*(q) W(q)\left\{-\frac{1}{2}\langle \hat{H}_{2Q}\rangle_q \frac{\partial^2 f(q)}{\partial q^2} - ib(q)\frac{\partial f(q)}{\partial q} + V(q)f(q)\right\}, \tag{2.9}$$

where $b(q)$ and $V(q)$ are given by

$$b(q) = \langle \phi(q) \mid \hat{H}_Q - \hat{H}_{2Q}\hat{G} \mid \phi(q)\rangle, \tag{2.10}$$

$$V(q) = \langle \phi(q) \mid \hat{H} - \hat{H}_Q\hat{G} + \tfrac{1}{2}\hat{H}_{2Q}\hat{G}^2 \mid \phi(q)\rangle. \tag{2.11}$$

We should mention now that, due to time reversal (TR) symmetry, $b(q)$ is identically zero. To see this, the mean values of the operators $\hat{H}_Q$ and $\hat{H}_{2Q}\hat{G}$ when sandwiched between $\mid \phi(q)\rangle$ vanish, because $\mid \phi(q)\rangle$ is even under TR and both $\hat{H}_Q$ and $\hat{H}_{2Q}\hat{G}$ are odd.

As mentioned above, the adjoint expression for the total energy (2.9) can be easily obtained; by pulling $\hat{H}$ to the left of $\delta(q'-\hat{Q})$ in the calculation of $\langle \psi \mid \hat{H} \mid \psi\rangle$, we can ascertain that

$$\langle \psi \mid \hat{H} \mid \psi\rangle = \int dq f^*(q) W(q)\left\{-\frac{1}{2}\frac{\partial^2}{\partial q^2}\left[\langle \hat{H}_{2Q}\rangle_q f(q)\right] + V(q)f(q)\right\}, \tag{2.12}$$

where we have neglected the derivatives of $W(q)$. The Hermitized expression for the total energy is equal to half the sum of (2.9) and (2.12):

$$\langle \psi \mid \hat{H} \mid \psi\rangle = \int dq f^*(q) W(q)\left\{-\frac{1}{4}\langle \hat{H}_{2Q}\rangle_q \frac{\partial^2 f(q)}{\partial q^2} - \frac{1}{4}\frac{\partial^2}{\partial q^2}\left[\langle \hat{H}_{2Q}\rangle_q f(q)\right] + V(q)f(q)\right\}. \tag{2.13}$$

Taking the variation of this Hermitized energy expression with respect to $f^*(q)$ (i.e., $\delta\langle\psi \mid \hat{H} \mid \psi\rangle/\delta f^*\langle\psi \mid \psi\rangle = 0$), we obtain the equation of collective motion

$$-\frac{1}{4}\frac{\partial^2}{\partial q^2}\left[\langle\hat{H}_{2Q}\rangle_q f_n(q)\right] - \frac{1}{4}\langle\hat{H}_{2Q}\rangle_q \frac{\partial^2 f_n(q)}{\partial q^2}$$

$$+V(q)f_n(q) = E_n^{\mathrm{NBO}} f_n(q). \quad (2.14)$$

This expression has the form of a Schrödinger equation. Hence collective motion emerges naturally quantized within the framework of the NBO method. To solve this equation, we need to determine the terms $\langle H_{2Q}\rangle_q$ and $V(q)$, which, in turn, require the specification of the intrinsic state $\mid \phi(q)\rangle$ and of the operators $\hat{Q}$ and $\hat{G}$.

In the determination of $\mid \phi(q)\rangle$, we proceed in such a way that the mean value $\langle\phi(q) \mid \hat{Q} \mid \phi(q)\rangle$ of the operator $\hat{Q}$ is equal to q. We can enforce this property by means of a constrained variational principle:

$$\delta\langle\phi(q) \mid \hat{H} - \lambda\hat{Q} \mid \phi(q)\rangle = 0. \quad (2.15)$$

The state $\mid \phi(q)\rangle$ thus obtained is a mean field.

As for the determination of $\hat{Q}$ and $\hat{G}$, we need to make use of the relations (2.10) and (2.15). We should note that $b(q)$, as given by Eq. (2.10), is identically zero, but not necessarily variationally stable, because terms like $\langle\phi_{\mathrm{ph}} \mid \hat{H}_Q - \hat{H}_{2Q}\hat{G}\mid\phi\rangle$ are not equal to zero. Since Eq. (3.2) provides only a partial determination of the operators $\hat{Q}$ and $\hat{G}$, we are going to tailor their choice so that Eq. (3.2) is satisfied and, at the same time, $b(q)$ is variationally stable

$$\delta b(q) = \delta\langle\phi(q) \mid \hat{H}_Q - \hat{H}_{2Q}\hat{G} \mid \phi(q)\rangle = 0. \quad (2.16)$$

This stability condition along with Eq. (3.2) is sufficient to determine all the particle-hole (ph) elements of the operators $\hat{Q}$ and $\hat{G}$.

III. SMALL-AMPLITUDE LIMIT OF THE NBO METHOD

In this section, we are going to examine the small-amplitude limit of the NBO method, and then derive an expression for the ground state energy.

A. Derivation of the RPA equations

Let us study how the NBO method describes the small-amplitude oscillations of a system about its point of stable equilibrium. Let $q = q_0$ be the stable equilibrium point and $\mid \phi_0\rangle = \mid \phi(q_0)\rangle$ be the unconstrained equilibrium state. To simplify the formalism, we assume that $q_0 = 0$, otherwise terms like q^n will have to be replaced by $(q - q_0)^n$.

In this type of motion, the state $\mid \phi(q)\rangle$ undergoes small-amplitude fluctuations about the HF ground state $|\phi_0\rangle$. We can parametrize its q dependence by means of the Thouless parametrization of determinants:

$$\mid \phi(q)\rangle = e^{-iq\hat{G}} \mid \phi_0\rangle = \left[1 - iq\hat{G} - \frac{1}{2}\left(q\hat{G}\right)^2 + \cdots\right] \mid \phi_0\rangle. \quad (3.1)$$

Since q is small for all times, this expression need not be pushed beyond the second order in q, nor beyond $\hat{G}^2$; $\mid \phi(q)\rangle$ is not very different from $\mid \phi_0\rangle$. Here lies the underlying justification for having truncated the series (2.7) at the second power of $\hat{G}$.

We now focus on the derivation of the small-amplitude limits of the variational equations (2.15) and (2.16) and then discuss the resulting dynamics. Inserting the state (3.1) into (2.15) and (2.16) and keeping only the lowest order terms in q, we can show that these two variational conditions reduce, respectively, to

$$\delta\langle\phi_0 \mid [\hat{H}, i\hat{G}] + K\hat{Q} \mid \phi_0\rangle = 0, \quad (3.2)$$

$$\delta\langle\phi_0 \mid [\hat{H}, i\hat{Q}] - \frac{1}{M}\hat{G} \mid \phi_0\rangle = 0, \quad (3.3)$$

where $K = \frac{d\lambda(q)}{dq}\Big|_{q=0}$ and $M^{-1} = \langle\phi_0 \mid \hat{H}_{2Q} \mid \phi_0\rangle$. In deriving (3.3), we have approximated in (2.10) the term $\hat{H}_{2Q}\hat{G}$ by $\langle\hat{H}_{2Q}\rangle_q\hat{G}$ and then replaced $\langle\hat{H}_{2Q}\rangle_q$ by its small-q limit, $\langle\phi_0 \mid \hat{H}_{2Q} \mid \phi_0\rangle$, since q fluctuates around $q_0 = 0$. Note that the expressions of K and M can also be obtained from Eqs. (3.2) and (3.3) as follows. Since the operators $\hat{Q}$ and $\hat{G}$ satisfy the condition $\langle\phi_0|[\hat{G}, i\hat{Q}]|\phi_0\rangle = 1$, we can easily derive the expression of K from (3.2):

$$\langle\phi_0|[[\hat{H}, i\hat{G}], i\hat{G}]|\phi_0\rangle = K\langle\phi_0|[\hat{G}, i\hat{Q}]|\phi_0\rangle = K. \quad (3.4)$$

Similarly, we can ascertain from (3.3) that the expression of M is given by

$$\langle\phi_0|[[\hat{H}, i\hat{Q}], i\hat{Q}]|\phi_0\rangle = \frac{1}{M}\langle\phi_0|[\hat{G}, i\hat{Q}]|\phi_0\rangle = \frac{1}{M}. \quad (3.5)$$

The two expressions (3.2) and (3.3) are the RPA equations. Jointly, they determine self-consistently the particle-hole (ph) matrix elements of the operators $\hat{Q}$ and $\hat{G}$. Introducing the following transformations:

$$\hat{Q} = \frac{1}{\sqrt{2M\hbar\omega}}\left(\hat{F}^\dagger + \hat{F}\right), \quad (3.6)$$

$$\hat{G} = i\sqrt{\frac{M\hbar\omega}{2}}\left(\hat{F}^\dagger - \hat{F}\right), \quad (3.7)$$

we can recast Eqs. (3.2) and (3.3) into the more familiar form

$$\delta\langle\phi_0|\left[H, \hat{F}\right] + \omega\hat{F}|\phi_0\rangle = 0, \quad (3.8)$$

$$\delta\langle\phi_0|\left[H, \hat{F}^\dagger\right] - \omega\hat{F}^\dagger|\phi_0\rangle = 0, \quad (3.9)$$

with $\omega = \sqrt{K/M}$. These are the equations of motion of a system of coupled harmonic oscillators.

These equations are usually solved by writing $\hat{F}$ and $\hat{F}^\dagger$ in terms of the creation and annihilation operators a and $a^\dagger$:

$$\hat{F}^\dagger = \sum_{mi} \left(X_{mi} a_m^\dagger a_i \quad - \quad Y_{mi} a_i^\dagger a_m \right), \tag{3.10}$$

$$\hat{F} = (\hat{F}^\dagger)^\dagger = \sum_{mi} \left(X_{mi}^* a_i^\dagger a_m \quad - \quad Y_{mi}^* a_m^\dagger a_i \right), \tag{3.11}$$

where X_{mi} and Y_{mi} are complex numbers. They are the RPA amplitudes; X_{mi} are the particle-hole amplitudes and Y_{mi} are the ground state correlation amplitudes. The indices i, j refer to states below the Fermi sea (particle states), while m, n refer to states above (hole states).

Note that, using the transformations (3.6) and (3.7) along with (3.10) and (3.11), we can verify that $\langle \phi_0 | [\hat{G}, i\hat{Q}] | \phi_0 \rangle = 1$, i.e.,

$$\begin{aligned} \langle \phi_0 | [\hat{G}, i\hat{Q}] | \phi_0 \rangle &= \langle \phi_0 | [\hat{F}, \hat{F}^\dagger] | \phi_0 \rangle \\ &= \sum_{nj} \sum_{mi} \Big\{ X_{nj}^* X_{mi} \langle \phi_0 | a_j^\dagger a_n a_m^\dagger a_i | \phi_0 \rangle \\ &\quad - Y_{nj}^* Y_{mi} \langle \phi_0 | a_i^\dagger a_m a_n^\dagger a_j | \phi_0 \rangle \Big\} \\ &= \sum_{mi} \left(|X_{mi}|^2 - |Y_{mi}|^2 \right) \\ &= 1, \end{aligned} \tag{3.12}$$

since $\langle \phi_0 | a_j^\dagger a_n a_m^\dagger a_i | \phi_0 \rangle = \delta_{ji} \delta_{nm}$.

B. Ground state energy

To obtain the ground state energy, we need to derive the small-q limit for the equation of collective motion (2.14). For this, let us calculate the small-q limits for the coefficients that are involved in Eq. (2.14), $\langle \phi(q) | \hat{H}_{2Q} | \phi(q) \rangle$ and $V(q)$. The small-amplitude limit for $\langle \phi(q) | \hat{H}_{2Q} | \phi(q) \rangle$ is given simply by $\langle \phi_0 \mid \hat{H}_{2Q} \times \mid \phi_0 \rangle = M^{-1}$. As for the small-$q$ limit for $V(q)$, we need to find the small-q expressions of $\langle \phi(q) | \hat{H} | \phi(q) \rangle$, $\langle \phi(q) | \hat{H}_Q \hat{G} | \phi(q) \rangle$, and $\langle \phi(q) | \hat{H}_{2Q} \hat{G}^2 | \phi(q) \rangle$.

First, since $|\phi(q)\rangle$ is not an eigenstate of the collective operator $\hat{Q}$ but is a wave packet in the collective space, terms like $\langle \phi(q) | (\hat{Q} - q)^2 | \phi(q) \rangle$ do not vanish. Thus, the energy expectation value with this packet, $\langle \phi(q) | \hat{H} | \phi(q) \rangle$, must contain a contribution from the zero-point energy of the wave packet. Following the folding-unfolding procedure of Goeke and Reinhard [9], we can perform a Taylor expansion and obtain

$$\begin{aligned} \langle \hat{H} \rangle_q &= \langle \phi_0 | \hat{H} | \phi_0 \rangle - \frac{1}{2} \langle (\hat{Q} - q)^2 \rangle_q \frac{\partial^2 \langle \hat{H} \rangle_q}{\partial q^2} \\ &\simeq E_{\rm HF} + \frac{1}{2} K \left(q^2 - \langle \hat{Q}^2 \rangle_0 \right), \end{aligned} \tag{3.13}$$

where $E_{\rm HF} = \langle \phi_0 | \hat{H} | \phi_0 \rangle$ is the Hartree-Fock energy, and[1] $K = \langle \phi_0 \mid [[\hat{H}, i\hat{G}], i\hat{G}] \mid \phi_0 \rangle$. In deriving this expression, we have approximated $\langle \hat{Q}^2 \rangle_q$ with $\langle \hat{Q}^2 \rangle_0$, where the notation $\langle \hat{A} \rangle_0$ will be used to abbreviate $\langle \phi_0 | \hat{A} | \phi_0 \rangle$. The term $K \langle \hat{Q}^2 \rangle_0 / 2$ in (3.13) represents the potential zero-point energy of the collectively deformed wave packet.

Second, we can replace $\langle \hat{H}_Q \hat{G} \rangle_q$ by its zero-q order term $\langle \phi_0 | \hat{H}_Q \hat{G} | \phi_0 \rangle$, which, in turn, when combined with (3.3) becomes equal to $\langle \hat{G}^2 \rangle_0 / M$:

$$\begin{aligned} \langle \phi(q) | \hat{H}_Q \hat{G} | \phi(q) \rangle &= \langle \phi_0 | \hat{H}_Q \hat{G} | \phi_0 \rangle \\ &= \frac{\langle \hat{G}^2 \rangle_0}{M}. \end{aligned} \tag{3.14}$$

Third, the term $\langle \hat{H}_{2Q} \hat{G}^2 \rangle_q$ in (2.11) can be approximated by the product $\langle \hat{H}_{2Q} \rangle_0 \langle \hat{G}^2 \rangle_0$:

$$\begin{aligned} \langle \hat{H}_{2Q} \hat{G}^2 \rangle_q &\simeq \langle \hat{H}_{2Q} \rangle_0 \langle \hat{G}^2 \rangle_0 \\ &= \frac{\langle \hat{G}^2 \rangle_0}{M}. \end{aligned} \tag{3.15}$$

Next, inserting (3.13), (3.14), and (3.15) into (2.11), we obtain

$$\begin{aligned} V(q) = E_{\rm HF} + \frac{1}{2} K q^2 - \frac{1}{2M} \langle \phi_0 \mid \hat{G}^2 \mid \phi_0 \rangle \\ - \frac{1}{2} K \langle \phi_0 \mid \hat{Q}^2 \mid \phi_0 \rangle. \end{aligned} \tag{3.16}$$

The term $\langle \hat{G}^2 \rangle_0 / 2M$ can be interpreted as the kinetic zero-point energy. It corresponds to the shape fluctuations of the nuclear ground state; that is, the mean kinetic collective oscillation energy about the HF state $\mid \phi_0 \rangle$. The operator $\hat{G}$ can be viewed as a generator of deformation. It accounts for tranformations from one nuclear shape to another (e.g., from oblate to prolate).

We see that the "NBO potential" (3.16) contains two subtractive zero-point energy terms, $\langle \hat{G}^2 \rangle_0 / 2M$ and $K \langle \hat{Q}^2 \rangle_0 / 2$, which are absent in the potential of HF theory. These quantum corrections, which are contained in $\mid \phi(q) \rangle$, are due to the wave packet nature of $\mid \phi(q) \rangle$ in the collective space, since the states $\mid \phi(q) \rangle$ are spread over some q values.

Now, using the relation $\langle \phi_0 | \hat{H}_{2Q} | \phi_0 \rangle = M^{-1}$ along with the fact that $\langle \phi_0 \mid \hat{H}_{2Q} \mid \phi_0 \rangle$ is q independent (since the operator $\hat{Q}$ is nonlocal), and substituting (3.16) into (2.14), we obtain

$$-\frac{1}{2M} \frac{d^2 f_n(q)}{dq^2} + \frac{K}{2} q^2 f_n(q) = E_n' f_n(q), \tag{3.17}$$

with

$$\begin{aligned} E_n' = E_n^{\rm NBO} - E_{\rm HF} + \frac{1}{2M} \langle \phi_0 \mid \hat{G}^2 \mid \phi_0 \rangle \\ + \frac{1}{2} K \langle \phi_0 \mid \hat{Q}^2 \mid \phi_0 \rangle. \end{aligned} \tag{3.18}$$

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[1] Using Eq. (3.1), it is easy to ascertain that the term $\partial^2 \langle \hat{H} \rangle_q / \partial q^2$ is equal to $\langle \phi_0 \mid [[\hat{H}, i\hat{G}], i\hat{G}] \mid \phi_0 \rangle$.

This is the NBO equation of collective motion for small-amplitude oscillations. This equation describes harmonic oscillations with frequeny $\hbar\omega = \sqrt{K/M}$; M and K represent, respectively, the mass and the restoring force parameters of the oscillations. Thus the collective vibrational energy is given by

$$E'_n = (n + \tfrac{1}{2})\hbar\omega \qquad (n = 0, 1, 2, 3, \ldots), \tag{3.19}$$

where n represents the number of phonons in the nth excited state.

The NBO energy spectrum, $E_n^{\rm NBO}$, can be inferred from the previous two expressions:

$$E_n^{\rm NBO} = E_0^{\rm NBO} + n\hbar\omega \qquad (n = 0, 1, 2, 3, \ldots), \tag{3.20}$$

where the NBO ground state energy $E_0^{\rm NBO}$ is given by

$$E_0^{\rm NBO} = E_{\rm HF} + \frac{1}{2}\hbar\omega - \frac{1}{2M}\langle\phi_0 \mid \hat{G}^2 \mid \phi_0\rangle$$

$$-\frac{1}{2}K\langle\phi_0 \mid \hat{Q}^2 \mid \phi_0\rangle. \tag{3.21}$$

This energy $E_0^{\rm NBO}$ contains zero-point energy subtractions because expectation values are taken with respect to a wave packet.

We need now to determine how the NBO ground state energy (3.21) compares with the HF and the RPA energies. We will deal with these issues in the next two sections. We can state, however, that the NBO energy (3.21) is expected to be lower than $E_{\rm HF}$, since the NBO trial function (2.1) is better than that of HF; it is richer and more general than a Slater determinant, and allows for zero-point oscillations around $|\phi_0\rangle$.

IV. CORRELATED GROUND STATE ENERGY

To calculate the correlated ground state energy, we need to express the energy (3.21) in terms of the RPA amplitudes X_{mi} and Y_{mi}. For this, we need simply to determine the expressions of $\langle\phi_0|\hat{Q}^2|\phi_0\rangle$ and $\langle\phi_0|\hat{G}^2|\phi_0\rangle$ in terms of X_{mi} and Y_{mi}. The operators $\hat{Q}$ and $\hat{G}$ can be written in terms of X_{mi} and Y_{mi} by substituting (3.10) and (3.11), respectively, into (3.6) and (3.7):

$$\hat{Q} = \frac{1}{\sqrt{2M\hbar\omega}}\sum_{mi}\left(\alpha_{mi}a_m^\dagger a_i + \alpha_{mi}^* a_i^\dagger a_m\right), \tag{4.1}$$

$$\hat{G} = i\sqrt{\frac{M\hbar\omega}{2}}\sum_{mi}\left(\beta_{mi}a_m^\dagger a_i - \beta_{mi}^* a_i^\dagger a_m\right), \tag{4.2}$$

with $\alpha_{mi} = X_{mi} - Y_{mi}^*$ and $\beta_{mi} = X_{mi} + Y_{mi}^*$. Now, since $a_m|\phi_0\rangle = 0$ and $\hbar\omega = \sqrt{K/M}$, we can easily show that Eqs. (4.1) and (4.2) lead to

$$\langle\phi_0|\hat{Q}^2|\phi_0\rangle = \frac{1}{2M\hbar\omega}\sum_{mi}|X_{mi} - Y_{mi}^*|^2$$

$$= \frac{\hbar\omega}{2K}\sum_{mi}\Big\{|X_{mi}|^2 + |Y_{mi}|^2 - 2\mathrm{Re}\,(X_{mi}Y_{mi})\Big\} \tag{4.3}$$

and

$$\langle\phi_0|\hat{G}^2|\phi_0\rangle = \frac{1}{2}M\hbar\omega\sum_{mi}|X_{mi} + Y_{mi}^*|^2$$

$$= \frac{1}{2}M\hbar\omega\sum_{mi}\Big\{|X_{mi}|^2 + |Y_{mi}|^2 + 2\mathrm{Re}\,(X_{mi}Y_{mi})\Big\}. \tag{4.4}$$

Thus we can write

$$\frac{1}{2}K\langle\hat{Q}^2\rangle_0 + \frac{1}{2M}\langle\hat{G}^2\rangle_0 = \frac{\hbar\omega}{2}\sum_{mi}\left(|X_{mi}|^2 + |Y_{mi}|^2\right)$$

$$= \frac{\hbar\omega}{2}\left(1 + 2\sum_{mi}|Y_{mi}|^2\right), \tag{4.5}$$

where we have used the normalization condition (3.12).

Now, inserting (4.5) into (3.21), we end up with the NBO correlated ground state energy

$$E_0^{\rm NBO} = E_{\rm HF} - \hbar\omega\sum_{mi}|Y_{mi}|^2. \tag{4.6}$$

This relation shows clearly that $E_0^{\rm NBO}$ is smaller than $E_{\rm HF}$. As mentioned above, this result was expected due to the use of a trial function (2.1) which is superior to the HF state. In addition, we should recall that in deriving the NBO ground state energy (3.21) we have made use of the approximation (2.8). By means of a model calculation, we have shown in a previous work [5] that, when corrections to approximation (2.8) are considered, they generate a subtractive term of the order of half the term $\langle\phi_0|\hat{G}^2|\phi_0\rangle/2M$. Hence, when corrections to this approximation are included, they would bring the entire NBO energy spectrum further down.

V. DISCUSSION AND CONCLUDING REMARKS

Let us now turn to the comparison of the NBO correlated energy expression (4.6) with those obtained from other approximation methods such as the generator-coordinate method (GCM), the adiabatic time-dependent Hartree-Fock (ATDHF) approach, and the RPA.

First, we should mention that the NBO method presents a significant amount of formal analogy with the GCM. For instance, the structure of the GCM trial function is similar to (2.1), but without the projection opera-

tor $\delta(q-\hat{Q})$. It is this term that allows the NBO method to avoid the kernel's nonlocality problem inherent in the GCM. In addition, the GCM and NBO methods are quantum mechanical prescriptions, for collective motion comes out naturally quantized within their contexts. In their small-amplitude limits, both of the GCM and NBO methods resort to the approximation which considers the intrinsic state not to be very different from the static Hartree-Fock state. In view of this, we would expect the NBO and the GCM correlated ground state energies to be equivalent. The GCM correlated energy is given, within the approximation of Jancovici and Shiff [10], by this relation [10–13]:

$$E_0^{\mathrm{GCM}} = E_{\mathrm{HF}} + \frac{1}{2}\hbar\omega - \frac{1}{2}\sum_{mi} A_{mimi} = E_{\mathrm{HF}} - \hbar\omega \sum_{mi} |Y_{mi}|^2 , \tag{5.1}$$

where A_{minj} is the RPA Hamiltonian submatrix, whose expression reads $A_{minj} = \langle\phi_0|[\hat{a}_i^\dagger \hat{a}_m, [\hat{H}, \hat{a}_n^\dagger \hat{a}_j]]|\phi_0\rangle$. We see that the correlated ground state energy (4.6) extracted from the NBO method is indeed the same as its GCM counterpart.

Second, the NBO energy (4.6) is also identical with the expression obtained by de Guerra [14] from a properly quantized ATDHF method. An essential difference between the NBO and ATDHF methods is that NBO is a quantum mechanical prescription, whereas ATDHF is a semiclassical approach. We may recall that de Guerra [14] has shown that, after a proper quantization of the collective variables, the ATDHF approach yields the same ground state energy as the GCM.

Third, the NBO method predicts the correct expression for the correlated ground state energy, and hence avoids the well-known problem encountered in the usual[2] RPA which consists in the overestimation of the ground state correlations [15–22]. It was pointed out [15–17] that a straightforward RPA calculation leads to a correlated energy that is in error by a factor of 2. Similarly, it was also noted [18–22] that the usual RPA overestimates the correlated occupation probabilities by a factor of 2. The origin of this factor was traced to a double counting of ground state correlations inherent in the quasiboson approximation [18–22]. Using a more reliable approach, the number-operator method, Rowe [18] has derived the correct expressions for the ground state densities; the expressions found are smaller by a factor of 2 than those obtained from the quasiboson prescription. The same result was found by Johnson *et al.* [21] from another method, the core-particle approach. It was then argued [17–22] that the quasiboson methods for extracting ground state correlations are unreliable whenever these correlations are large. However, when the double counting problem in the quasiboson approximation is avoided, the RPA is shown [12,15–22] to yield the correct expression for the correlated energy:

$$E_0^{\mathrm{RPA}} = E_{\mathrm{HF}} - \hbar\omega \sum_{mi} |Y_{mi}|^2 . \tag{5.2}$$

The correlated energy expression (5.2) was obtained by Rowe [18] from the equations-of-motion method. Parikh and Rowe [19] investigated the ground state correlations for the model Hamiltonian of Lipkin, Meshkov, and Glick. They showed that the correlated energies obtained from the equations-of-motion technique and from the GCM are equivalent and, in addition, are in very good agreement with the exact results. Similar conclusions have also been obtained by Ellis and Zamick [22] and Ullah and Rowe [20] from numerical comparisons of the RPA and exact calculations.

In summary, we have worked out the formalism of the small-amplitude limit of the NBO method. Taking the ansatz (2.1) as the wave function of the system and considering the intrinsic state $|\phi(q)\rangle$ to undergo small oscillations about the static HF state $|\phi_0\rangle$, we have shown that the NBO prescription gives back the RPA equations. This work contains essentially two main new results: the derivation of the NBO ground state energy (3.21) and the proof that it leads to a correlated energy expression, Eq. (4.6), that is identical with the expressions obtained from the GCM, the properly quantized ATDHF approach, and from the RPA.

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