Quantum corrections to the potential energy for large amplitude collective motion

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We discuss the problem of inclusion of quantum corrections in the semiclassical theory of adiabatic large amplitude collective motion for many-fermion systems. We concentrate on deriving a formula for the leading quantum correction to the classical collective potential energy function in this theory. This is an extension of the usual calculation of the quantum corrections to the static Hartree-Fock energy using the random phase approximation. The answer can be expressed in terms of those solutions of a local random phase approximation that describe oscillations orthogonal to the collective surface. Because of the strict enforcement of the Pauli principle, however, the answer differs from the usual quasiboson approximation, yielding the correct ground-state correlation energy for a static solution to the Hartree-Fock equations. The result is applied, approximately, to help improve a previous treatment of the low energy spectrum of ^{28}Si.

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I. INTRODUCTION

In recent years, we have developed a theory of large amplitude collective motion (LACM) in the adiabatic limit and begun a program of applications to nuclear physics. (For a review of this theory and extensive references to previous work in the field, the reader can consult Ref. [1], for applications of our work other than to nuclear physics Refs. [2–5], and for applications to nuclear physics Refs. [6–8].) In almost all work in this subject, the approach is to construct a classical Hamiltonian and subsequently to requantize it. The justification for starting from the classical limit, equivalent to mean-field theory, is that it represents the leading term in the solution of the many-body problem in powers of $(1/N)$, where N is the number of degrees of freedom that participate in the collective motion.

In the theory of large amplitude adiabatic collective motion, the largest contribution to the classsical collective Hamiltonian is the potential energy. By comparison, the kinetic energy is of relative order $(1/N)$. The aim of this paper is to take a further step in the development of the theory, namely, to compute the first quantum correction to the potential energy. This goal is to be distinguished from much previous work in this field involving a quantum theory of collective motion, where the goal was to derive a classical description of large amplitude collective motion from some approximate quantum many-body theory. There one finds derivations based on the method of generator coordinates [9, 10], the Born-Oppenheimer method [11], a generalized coherent state method [12,13], and the equations of motion method [14, 15]. The point at issue is that none of the aforementioned work provided a *systematic* expansion in $(1/N)$.

The basic problem is that of computing quantum corrections about mean-field solutions describing *nonequilibrium* configurations. Thus in the simplest case of one collective coordinate, that we choose as an example, the fluctuations must be studied at an arbitrary point on a "collective path" that interpolates between equilibrium configurations.

The interest of studying quantum fluctuations about nonequilibrium mean fields has certainly not escaped the attention of previous workers in the field, including an extensive study of rotating nuclei [16] using a boson expansion method, a preliminary study of quantum fluctuations about an *arbitrary* time-dependent mean field [17], and semiclassical quantization of periodic solutions [18] using a path integral method. In the last work it is implied that the adiabatic case of interest to us had been disposed of earlier [19], but a study of this last reference does not sustain the claim. It appears that Reinhard and Goeke and their co-workers are the only authors who have evaluated and included a part of the correction in their calculations (see Ref. [10], and references therein). They have not evaluated the full $(1/N)$ corrections, however.

In this paper we present a method for studying quantum fluctuations that contains essential elements from previous work. In Sec. II, for example, we develop a formal theory of the collective potential energy based on the idea of a moment expansion of matrix elements of operators taken between localized collective states; this is a general method of defining an adiabatic expansion [20]. In Sec. III, we then describe the core of the microscopic theory, consisting of three elements.

(i) The first task is the perfectly standard one of decomposing the Hamiltonian into a sum of a (nonequilibrium) mean-field part and of a residual quantum part. The mean field is chosen by application of the (classical) self-consistent theory of large amplitude collective motion [1] that is taken to underlie the present developments. The discussion given in Sec. II leads to the

noncovariant (conventional) form of the random phase approximation (RPA) matrix. The changes necessary to obtain the covariant RPA (as defined in Ref. [1]) are given in Appendix C. A feature distinguishing our discussion from much previous work is that we do not resort to the Hartree approximation, so that direct and exchange terms are treated on an equal footing.

(ii) The analysis of the quantum part is carried out in terms of particle-hole (density fluctuation) creation and annihilation operators. Particle-particle and hole-hole operators are eliminated in favor of the particle-hole operators by means of a technique called the number-operator method [21, 22] that is technically elementary and enforces the Pauli principle.

(iii) Matrix elements of the linearized equations of motion are taken between suitably chosen superpositions of eigenstates of the Hamiltonian, leading to equations that reduce to the random phase approximation in lowest approximation. It is observed that the lowest-energy collective mode, that plays an essential role in the self-consistent classical theory, also plays a role similar to the one played by the spurious modes associated with broken symmetries.

Finally in Sec. IV we pull together the results of the previous sections, and by a method that respects the Pauli principle, derive a formula for the leading quantum corrections to the potential energy. In this way we obtain a result that disagrees with that obtained from the quasiboson approximation, but coincides with the correct result for the ground-state correlation energy at an equilibrium configuration [23]. In Appendixes A and B, we supply some technical details omitted from the body of the text.

In Sec. V, we show how application of an approximate form of the theory improves the results found previously [8] for the low-energy spectrum of ^{28}Si.

II. PHENOMENOLOGY

The computation of the quantum corrections to the collective potential energy will be carried out in Sec. IV, based on amplitudes defined in Sec. III. The present discussion is designed to lay a basis for our rigorous treatment. Perhaps the most important new result that emerges from the considerations that follow is that a well-defined meaning is assigned to the concept of excitation energy measured with respect to a nonequilibrium configuration.

A. Moment expansion and collective motion

Let us first introduce the concepts necessary to give a quantum foundation to collective motion. For simplicity of exposition, we shall develop the following argument for one "collective" coordinate, but the extension to any number is straightforward. We assume the existence of a set of states $|n\rangle$, labeled by an integer, n, and constituting a decoupled or approximately decoupled set in the Hilbert space. Let H be the many-body Hamiltonian. We introduce a complete set of states $|X\rangle$, localized in the coordinate X and related to the states $|n\rangle$ by the unitary transformation

$$|n\rangle = \int dX |X\rangle\langle X|n\rangle \ , \tag{2.1}$$

together with the Hermitian operator that characterizes these collective states,

$$\hat{Q}|X\rangle = X|X\rangle \ . \tag{2.2}$$

We can, formally, calculate the Hamiltonian matrix within the decoupled subspace by means of the expression

$$\begin{aligned}\langle n|H|n'\rangle &= W_n \delta_{n,n'} \\ &= \int \langle n|X\rangle dX \langle X|H|X'\rangle dX' \langle X'|n'\rangle \ .\end{aligned} \tag{2.3}$$

We now identify the many-body wave amplitudes $\langle X|n\rangle$ with a set of one-body collective wave functions

$$\langle X|n\rangle \equiv (X|n) \ . \tag{2.4}$$

This is the basic tenet of the quantum version of collective motion, and expresses the fact that collective motion is the *effective* behavior of a many-body system as a few-body system. Consequently, we identify $\langle X|H|X'\rangle$ as the collective Hamiltonian. The problem is that we have carried out a purely formal transformation, and except under very special circumstances, where the collective motion is associated with a symmetry operation of the Hamiltonian, we do not know either the wave functions (2.4) or the collective Hamiltonian. In order to make any progress, we must add some physics, i.e., make some special assumptions concerning the properties of the matrix elements of operators in the coordinate representation, that reflect the fact that we are describing adiabatic large amplitude collective motion.

To formulate the required assumptions, we first introduce the sum and difference coordinates

$$Q = \tfrac{1}{2}(X + X') \ , \tag{2.5}$$

$$\xi = X - X' \ , \tag{2.6}$$

and the notation

$$\langle X|H|X'\rangle \equiv \tilde{H}(Q, \xi) \ . \tag{2.7}$$

Our minimal assumption is that $\tilde{H}(Q, \xi)$ is always strongly peaked around the origin of the difference coordinate. It is also slowly varying in the average coordinate. This minimal assumption is reexpressed in terms of the Wigner transform $\bar{H}$ of $\tilde{H}$,

$$\bar{H}(Q, P) = \int d\xi \exp(-iP\xi)\tilde{H}(Q, \xi) \ , \tag{2.8}$$

which is now required to be a slowly varying function of P.

We consequently assume that we may expand in a power series in P,

$$\bar{H}(Q, P) = \sum_{\nu=0} \frac{1}{\nu!} H^{(\nu)}(Q) P^{\nu} \ , \tag{2.9}$$

and by the inversion of (2.8) find the sum of distributions,

$$\tilde{H}(Q,\xi)=\sum_{\nu}H^{(\nu)}(Q)\frac{1}{\nu!}(-i\partial/\partial\xi)^{\nu}\delta(\xi)\ , \tag{2.10}$$

where

$$H^{(\nu)}(Q)=\int d\xi(-i\xi)^{\nu}\tilde{H}(Q,\xi)\ . \tag{2.11}$$

Substituting (2.10) into Eq. (2.3), we obtain the results

$$\langle n|H|n'\rangle=\int dQ(n|Q)\mathcal{H}_{\rm col}(Q,P_Q)(Q|n)\ , \tag{2.12}$$

$$\mathcal{H}_{\rm col}(Q,P)=\sum_{\nu}\frac{1}{\nu!2^{\nu}}\{H^{(\nu)}(Q),P\}^{(\nu)}\ , \tag{2.13}$$

$$\{H^{(\nu)}(Q),P\}^{(\nu)}\equiv\{\cdots\{H^{(\nu)},\underbrace{P\},\ldots P\}}_{\nu\text{ times}}\ , \tag{2.14}$$

where

$$P_Q=-i\frac{d}{dQ}\ . \tag{2.15}$$

In Eqs. (2.12)–(2.14), we have thus identified a possibly useful form of the collective Hamiltonian as a power series in the collective momentum, provided we can calculate the moment functions, $H^{(\nu)}$, independently of the wave functions (2.4). In particular, in this paper we shall address the problem of computing the potential energy, $V(Q)$,

$$V(Q)\equiv H^{(0)}(Q)\ . \tag{2.16}$$

It is now possible to state the physical underpinnings of our minimal assumption: It means that the power series (2.9) is dominated by the lowest term.

We can choose the scale of the coordinates and momenta consistently with the Poisson bracket such that $Q\propto N^{1/2}$ and $P\propto N^{-1/2}$, which is the typical scale for the low-energy matrix elements. Here N is the number of degrees of freedom that participate in the collective motion. For this choice of length scale the successive moments can be shown to be of the same order of magnitude, so that the convergence of the moment expansion is thus determined by the size of P. However, because of the scale of Q, each derivative with respect to Q brings in a factor of $N^{-1/2}$; this observation plays an essential role in terminating expansions at low order.

We study the equations of motion for an arbitrary operator, θ, first within the collective subspace,

$$\langle n|[\theta,H]|n'\rangle=(W_{n'}-W_n)\langle n|\theta|n'\rangle\ . \tag{2.17}$$

Transforming to the localized states $|X\rangle$, we have, as discussed in detail in Appendix A,

$$\begin{aligned}\langle X|[\theta,H]|X'\rangle&=\langle X|[\theta,\mathcal{H}_{\rm col}]|X'\rangle\\&\cong(dV/dQ)i\delta(\xi)\theta^{(1)}(Q)\\&\quad+\delta'(\xi)\bar{B}(Q)(d/dQ)\theta^{(0)}(Q)\ ,\end{aligned} \tag{2.18}$$

where the zeroth and first moments of θ occur, and

$$\bar{B}\equiv M^{-1}\equiv H^{(2)} \tag{2.19}$$

is the inverse collective mass. Using the operator $\hat{Q}$, defined in (2.2), Eq. (2.18) can be cast in the form

$$\langle X|[\theta,H-(dV/dQ)\hat{Q}]|X'\rangle\cong\delta'(\xi)\bar{B}(Q)(d/dQ)\theta^{(0)}(Q)\ . \tag{2.20}$$

Here we have made the adiabatic approximation, and have ignored all moments of higher than second order in the expansion of $\mathcal{H}_{\rm col}$.

B. Fluctuations orthogonal to the collective path

In order to study the quantum corrections to collective motion, we introduce a class of eigenstates of the Hamiltonian $|n,\omega_{n\mu}\rangle$, $\mu=1,2,\ldots$, where we have a noncollective excitation on top of a collective excitation. For each value of μ, we assume existence of a set of excited localized states, $|X,\mu\rangle$, where, in analogy to Eq. (2.1),

$$|X,\mu\rangle=\sum_{n}|n,\omega_{n\mu}\rangle\langle n,\omega_{n\mu}|X,\mu\rangle\ , \tag{2.21}$$

$$\langle X,\mu|X',\mu'\rangle=\delta_{\mu\mu'}\delta(X-X')\ , \tag{2.22}$$

$$\langle X,\mu|X'\rangle=0\ , \tag{2.23}$$

and, independently of μ,

$$\hat{Q}|X,\mu\rangle=X|X,\mu\rangle\ . \tag{2.24}$$

In order to make these assumptions we must be able to identify the states of the same μ but different n. Furthermore, for the latter relations we need the fact that the operator creating the state $|X,\mu\rangle$ from $|X\rangle$ commutes with $\hat{Q}$ as well as that those operators commute among themselves. These conditions are closely related to the adiabatic limit, where we can expect X to remain constant during a fast noncollective excitation.

To reach the result that we are after, we need one more assumption, namely, that just as the spectrum of the states $|n\rangle$ can be reproduced by a collective Hamiltonian, $\mathcal{H}_{\rm col}(X,P_X)$, dominated by its potential energy $V(X)$, so also can the additional energies, $\omega_{n\mu}$, be reproduced by an operator, $\tilde{\omega}_{\mu}(X,P_X)$ that is dominated by its local part, $\omega_{\mu}(X)$. In other words, the intrinsic excitations are assumed to vary slowly with X. In analogy to Eq. (2.20), we find, with the help of definitions and assumptions just made, that

$$\langle X,\mu|[\theta,H-(dV/dQ)\hat{Q}]|X'\rangle\cong-\omega_{\mu}(X)\langle X,\mu|\theta|X'\rangle\ . \tag{2.25}$$

Later, we shall only need the zeroth moment of matrix elements connecting the collective and noncollective spaces, for which purpose Eq. (2.25) will prove sufficiently accurate.

Both (2.20) and (2.25) show that in adiabatic limit the relevant Hamiltonian for study of the equations of motions at general points of the collective path is $H-(dV/dQ)\hat{Q}$. In the following we shall elaborate on the structure of the quantum corrections for such a constrained Hamiltonian.

III. QUANTUM CORRECTIONS TO THE POTENTIAL ENERGY

A. Transformation of the Hamiltonian: Normal form and number-operator method

In order to utilize the formalism that has just been described, we must express H as a function of operators whose matrix elements can themselves be studied by the moment expansion.

We work with a Hamiltonian of the form

$$H = \int \psi^\dagger(x) h(x|x') \psi(x') + \frac{1}{4} \int U(x,y|x',y') \psi^\dagger(x) \psi^\dagger(y) \psi(y') \psi(x') \ , \quad (3.1)$$

where the interaction, U, is Hermitian and antisymmetric,

$$U(x,y|x',y') = -U(y,x|x',y') = -U(x,y|y',x') \ . \quad (3.2)$$

We transform the Hamiltonian (3.1) by substituting the mode expansion (where we use the summation convention)

$$\psi(x) = \psi_\alpha(Q) f_\alpha(x,Q) \ , \quad (3.3)$$

where the $f_\alpha(x,Q)$ are a set of localized modes (i.e., they describe the local single-particle orbits), referring to the point Q along a collective path; these modes are determined by applying the self-consistent theory of large amplitude collective motion [1, 8]. They are thus solutions of the constrained Hartree-Fock equations

$$\mathcal{H}_{\rm ph} = \lambda q_{\rm ph} \ . \quad (3.4)$$

(It is not necessary to introduce any special assumptions concerning the matrix elements $\mathcal{H}_{\rm pp'}$ or $\mathcal{H}_{\rm hh'}$.) Here $\mathcal{H}_{\alpha\beta}$ are the matrix elements of

$$\mathcal{H} = h + \mathcal{V} \ , \quad (3.5)$$

where

$$\mathcal{V}(x|x') = \int U(x,y|x',y') \rho(y'|y) \ , \quad (3.6)$$

$$\rho(y'|y) = \sum_{\rm h} f_{\rm h}(y') f_{\rm h}^*(y) \ . \quad (3.7)$$

Furthermore, λ has the value

$$\lambda = dV(Q)/dQ \ , \quad (3.8)$$

and $q_{\rm ph}$ is a suitably chosen time-even solution of the random phase approximation (RPA) determined by the basis (3.3). [More precisely, it is a solution of an iterated local RPA equation whose eigenvalues are the squares of the usual ones; this equation must, in general, be solved in conjunction with Eq. (3.4).] The solutions of interest are real, and we choose the eigenvector with the smallest, often negative, eigenvalue. The solution procedure, the practical definition of the collective coordinate, Q, and other such matters of fundamental importance have been described in Refs. [1, 8] and earlier work cited there. We do not wish to cover this familiar ground again; it suffices for present purposes that a suitable algorithm has been established, the same algorithm that we shall apply in Sec. V.

Next we arrange the Hamiltonian into normal form with respect to the Slater determinant constructed from the $f_{\rm h}$. We thus obtain the result

$$H = V_0(Q) + \lambda \hat{Q}_1 + H_{11} + H_{22} + (H_{40} + \text{H.c.}) + (H_{31} + \text{H.c.}) + H'_{22} \ , \quad (3.9)$$

where $V_0(Q)$ is the Hartree-Fock energy $W_{\rm HF}$ determined from the Q-dependent modes,

$$W_{\rm HF} = \text{tr}(h\rho + \tfrac{1}{2}\mathcal{V}\rho) = h_{\rm hh} + \tfrac{1}{2} V_{\rm hh'hh'} \ , \quad (3.10)$$

and

$$\hat{Q}_1 \equiv q_{\rm ph} \psi_{\rm p}^\dagger \psi_{\rm h} + q_{\rm hp} \psi_{\rm h}^\dagger \psi_{\rm p} \ , \quad (3.11)$$

$$H_{11} = \mathcal{H}_{\rm pp'} \psi_{\rm p}^\dagger \psi_{\rm p'} - \mathcal{H}_{\rm hh'} \psi_{\rm h} \psi_{\rm h'}^\dagger , \quad (3.12)$$

$$H_{22} = V_{\rm ph'hp'} (\psi_{\rm p}^\dagger \psi_{\rm h})(\psi_{\rm h'}^\dagger \psi_{\rm p'}) , \quad (3.13)$$

$$H_{40} = \tfrac{1}{4} V_{\rm pp'hh'} \psi_{\rm p}^\dagger \psi_{\rm p'}^\dagger \psi_{\rm h'} \psi_{\rm h} \ , \quad (3.14)$$

$$H_{31} = \tfrac{1}{2} V_{\rm pp'hp''} \psi_{\rm p}^\dagger \psi_{\rm h} \psi_{\rm p'}^\dagger \psi_{\rm p''} + \tfrac{1}{2} V_{\rm phh'h''} \psi_{\rm p}^\dagger \psi_{\rm h''} \psi_{\rm h'} \psi_{\rm h}^\dagger \ , \quad (3.15)$$

$$H'_{22} = \tfrac{1}{4} V_{\rm pp'p''p'''} \psi_{\rm p}^\dagger \psi_{\rm p'}^\dagger \psi_{\rm p'''} \psi_{\rm p''} + \tfrac{1}{4} V_{\rm hh'h''h'''} \psi_{\rm h'''} \psi_{\rm h''} \psi_{\rm h}^\dagger \psi_{\rm h'}^\dagger \ . \quad (3.16)$$

When deriving the equations of motion, as we have seen in Sec. II B, we must subtract from H the quantity $(dV/dQ)\hat{Q}$. We shall, as a practical expedient, approximate the operator $\hat{Q}$ by the one-body operator $\hat{Q}_1$, defined in Eq. (3.11). The difference between these two operators is of theoretical importance in guaranteeing the covariance of the description of the geometrical structure of our collective subspace, but has so far proved to be of no practical importance in numerical applications [1, 8]. In any event, the extension necessary to obtain these extra terms is described in Appendix C. The following derivations remain largely the same, apart from modifications to the detailed form of some terms.

As in previous, related, work on quantum fluctuations about an equilibrium mean-field configuration [22–24], we shall analyze this Hamiltonian by the combination of two techniques.

(i) By means of the so-called number-operator method, we shall rewrite the Hamiltonian as a formal series in the particle-hole (density fluctuation) operators $\psi_{\rm p}^\dagger \psi_{\rm h}$ and $\psi_{\rm h}^\dagger \psi_{\rm p}$. This method is used in place of the usual boson mapping; relative to the latter, it has the advantage that the Pauli principle is automatically taken care of, but the disadvantage that the algebra of particle-hole operators is nonlinear. Below, we shall give a brief review of the basic elements of this method. This analysis shows that H_{11} is second order in the density fluctuations, with higher-order corrections, H_{22} and H_{40} and Hermitian conjugate

are exactly second order, H_{31} and Hermitian conjugate are at least third order in these operators, and H'_{22} is at least fourth order.

(ii) Further analysis of the resulting Hamiltonian will be carried out with the help of equations of motion in which the basic dynamical entities are all possible matrix elements of density-fluctuation operators, with matrix elements of a product analyzed by means of the completeness relation. The simplest way of reaching the final form of the equations of motion is to use the original form of the Hamiltonian and of the commutation relations for all $\psi^\dagger\psi$ pairs, and to subsequently apply the number-operator method. But the correct equations of motion can also be obtained after first carrying out the number-operator transformation on the Hamiltonian and on the algebra [22]. In the latter case, one is led to the concept of effective Hamiltonian described below. (Similar ideas in another context have been applied previously with some success to the low-energy spectra of semimagic nuclei [25].)

We next review briefly the elements of the number-operator method. We write the number operator, $\hat{N}$, in the form applicable to a system with N particles,

$$\hat{N} - N = \psi_{\rm p}^\dagger\psi_{\rm p} - \psi_{\rm h}\psi_{\rm h}^\dagger \ . \tag{3.17}$$

This equation describes the only independent Casimir invariant of the algebra of particle-hole operators in the space of antisymmetric wave functions for N particles, and as such is an expression of the Pauli principle. If O_n is any operator that diminishes the particle number by n, and $|\alpha\rangle$ is any state with N particles, we can derive the two following identities from (3.17):

$$O_n|\alpha\rangle = n^{-1}(\psi_{\rm h}\psi_{\rm h}^\dagger - \psi_{\rm p}^\dagger\psi_{\rm p})O_n|\alpha\rangle \ , \tag{3.18}$$

$$O_n^\dagger|\alpha\rangle = n^{-1}(\psi_{\rm p}^\dagger\psi_{\rm p} - \psi_{\rm h}\psi_{\rm h}^\dagger)O_n^\dagger|\alpha\rangle \ . \tag{3.19}$$

As an example of the successive application of (3.18), we have

$$\begin{aligned}\langle\alpha'|\psi_{\rm p}^\dagger\psi_{\rm p'}|\alpha\rangle &= \langle\alpha'|\psi_{\rm p}^\dagger\psi_{\rm h}\psi_{\rm h}^\dagger\psi_{\rm p'}|\alpha\rangle - \langle\alpha'|\psi_{\rm p}^\dagger\psi_{\rm p''}^\dagger\psi_{\rm p''}\psi_{\rm p'}|\alpha\rangle \\ &\cong \langle\alpha'|\psi_{\rm p}^\dagger\psi_{\rm h}\psi_{\rm h}^\dagger\psi_{\rm p'}|\alpha\rangle - \tfrac{1}{2}\langle\alpha'|\psi_{\rm p}^\dagger\psi_{\rm p''}^\dagger\psi_{\rm h}\psi_{\rm h'}\psi_{\rm h'}^\dagger\psi_{\rm h}^\dagger\psi_{\rm p''}\psi_{\rm p'}|\alpha\rangle \ .\end{aligned} \tag{3.20}$$

Here, in the first transformation, we have $O_n = \psi_{\rm p}$, and in the second line two additional applications of (3.18), to other, equally obvious choices of O_n, with $n = 2$ and $n = 1$, respectively, have been used, giving an approximate result where the first omitted term involves six density-fluctuation operators. Of course the sums go over all indices except p. The operator $\psi_{\rm h}\psi_{\rm h}^\dagger$ is given by a similar expression with summation over all indices except h. The operators in H_{31} and $H_{22'}$ may be transformed in like fashion, and it is then seen that one obtains series that start with terms that are cubic and quartic, respectively, in the density fluctuations. The utility of the transformation just described is not at all obvious. In general, we shall discover that when matrix elements are evaluated by sum-rule methods to be described, each matrix element of a density-fluctuation operator contributes an amount of order $N^{-1/2}$, because this is the average size of RPA amplitudes as long as the quantum fluctuations are about a stable mean-field solution. In most cases, we encounter incoherent sums over such quantities, where the size of the individual matrix element then determines the size of the associated sum. Nevertheless, the matter of counting orders is more subtle than we have so far indicated, but further elaboration of this point will be more meaningful within the context of the arguments developed in Sec. IV.

The number-operator transformation may also be applied to the exact commutation relations

$$[\psi_{\rm p'}^\dagger\psi_{\rm p''}, \psi_{\rm p}^\dagger\psi_{\rm h}] = \delta_{\rm pp''}\psi_{\rm p'}^\dagger\psi_{\rm h}, \tag{3.21}$$

$$[\psi_{\rm h}^\dagger\psi_{\rm p}, \psi_{\rm p'}^\dagger\psi_{\rm h'}] = \delta_{\rm hh'}\delta_{\rm pp'} - \delta_{\rm hh'}\psi_{\rm p'}^\dagger\psi_{\rm p} - \delta_{\rm pp'}\psi_{\rm h'}\psi_{\rm h}^\dagger \ . \tag{3.22}$$

We then see that the second term on the right-hand side of Eq. (3.22) is at least second order in the density fluctuations. For our purposes, we can thus replace this equation by the quasiboson commutator,

$$[A_{\rm ph}, A_{\rm p'h'}^\dagger] = \delta_{\rm hh'}\delta_{\rm pp'} \ , \tag{3.23}$$

where we have introduced a notation for the particle-hole destruction and creation operators,

$$A_{\rm ph}^\dagger = (A_{\rm ph})^\dagger = \psi_{\rm p}^\dagger\psi_{\rm h} \ . \tag{3.24}$$

We are now in possession of all the elementary tools needed to calculate the potential energy defined by Eq. (2.16). The value of the leading quantum corrections that we seek will be seen to be determined by solutions of the equations of motion at the RPA level of accuracy. We therefore turn to the problem of studying these equations.

B. Modified RPA analysis

A typical element needed in the analysis of $\langle Y|H|X\rangle$, the quantity that enters into the evaluation of the quantum corrections to the potential, is the matrix element of a product of fluctuation operators. As an example, we consider a contribution from H_{22},

$$\langle Y|A_{\rm p'h'}^\dagger A_{\rm ph}|X\rangle = \sum_I \langle Y|A_{\rm p'h'}^\dagger|I\rangle\langle I|A_{\rm ph}|X\rangle \ . \tag{3.25}$$

Accuracy to relative order N^{-1} is maintained by choosing the intermediate states to comprise two sets: the elementary fluctuation operators induce transitions primarily either to a range of localized collective states $|Z\rangle$ or to states, $|Z,\omega_\mu(Z)\rangle$, with additional intrinsic excitation energies $\omega_\mu(Z)$, that we shall soon identify with local RPA states. Thus to evaluate sums such as (3.25), we must calculate the following matrix elements:

$$\langle Y,\mu|A^\dagger_{\rm ph}|X\rangle \equiv \mathcal{X}_\mu({\rm ph}|XY) \ , \tag{3.26}$$

$$\langle Y,\mu|A_{\rm ph}|X\rangle \equiv \mathcal{Y}_\mu({\rm ph}|XY) \ , \tag{3.27}$$

$$\langle Y|A^\dagger_{\rm ph}|X\rangle \equiv \mathcal{X}({\rm ph}|XY) \ , \tag{3.28}$$

$$\langle Y|A_{\rm ph}|X\rangle \equiv \mathcal{Y}({\rm ph}|XY) \ . \tag{3.29}$$

We remind the reader that we are after moment expansions for these matrix elements, since it is simple to verify that integrals over products of moment expansions of the individual operators will generate the required moments of the Hamiltonian (convolution theorem). It will turn out to be sufficient to calculate the zeroth moments of (3.26) and of (3.27), whereas we shall require up to the first moments of the recoil amplitudes (3.28) and (3.29). In other words it is sufficient to consider the approximation

$$\langle Y,\mu|A^\dagger_{\rm ph}|X\rangle \cong \delta(\xi)\mathcal{X}_\mu({\rm ph}|Q) \ , \tag{3.30}$$

$$\langle Y,\mu|A_{\rm ph}|X\rangle \cong \delta(\xi)\mathcal{Y}_\mu({\rm ph}|Q) \ , \tag{3.31}$$

$$\langle Y|A^\dagger_{\rm ph}|X\rangle \cong \delta(\xi)\mathcal{X}^{(0)}({\rm ph}|Q) + (-i\partial/\partial\xi)\delta(\xi)\mathcal{X}^{(1)}({\rm ph}|Q) \ , \tag{3.32}$$

$$\langle Y|A_{\rm ph}|X\rangle \cong \delta(\xi)\mathcal{Y}^{(0)}({\rm ph}|Q) + (-i\partial/\partial\xi)\delta(\xi)\mathcal{Y}^{(1)}({\rm ph}|Q) \ . \tag{3.33}$$

(The reason that we can ignore higher moments, despite our assertion in the introduction that the moments are all of the same order of magnitude, is that the corrections to the contribution of a given moment involve derivatives with respect to the collective coordinate Q of higher moments, and each such derivative introduces a factor of $N^{-1/2}$.)

To derive equations for these moments, the cleanest procedure is to use the Hamiltonian in the form (3.9) before application of the number-operator transformation, together with the exact commutation relations (3.21) and (3.22). Subsequent application of the number-operator relations (3.17)–(3.20) then allows us to identify the linear approximation

$$-[A^\dagger_{\rm ph},H] = \mathcal{A}_{{\rm php'h'}}A^\dagger_{\rm p'h'} + \mathcal{B}_{{\rm php'h'}}A_{\rm p'h'} + \lambda q_{\rm hp} \ , \tag{3.34}$$

$$[A_{\rm ph},H] = \mathcal{A}^*_{{\rm php'h'}}A_{\rm p'h'} + \mathcal{B}^*_{{\rm php'h'}}A^\dagger_{\rm p'h'} + \lambda q_{\rm ph} \ ,$$

where

$$\mathcal{A}_{{\rm php'h'}} = \mathcal{H}_{\rm pp'}\delta_{\rm hh'} - \mathcal{H}_{\rm hh'}\delta_{\rm pp'} + V_{\rm p'hh'p} \ , \tag{3.35}$$

$$\mathcal{B}_{{\rm php'h'}} = V_{\rm hh'pp'} \ , \tag{3.36}$$

and the asterisk indicates complex conjugation. Equations (3.34) are recognized as the RPA equations, except for the inhomogeneous terms that have their origin in our choice of nonequilibrium mean field as a starting point.

It is useful to observe that the same equations of motion follow by replacing the Hamiltonian H by an operator, $H_{\rm eff}$, where

$$H_{\rm eff} = \mathcal{A}_{{\rm php'h'}}A^\dagger_{\rm p'h'}A_{\rm ph} + \tfrac{1}{2}(\mathcal{B}_{{\rm php'h'}}A_{\rm ph}A_{\rm p'h'} + {\rm H.c.}) + \lambda\hat{Q}_1 \ , \tag{3.37}$$

and evaluating the commutator by using the quasiboson commutation relations (3.23). In this approximation, we may replace the Hamiltonian, Eq. (3.9), by the expression

$$H = C_0(Q) + H_{\rm eff} \ . \tag{3.38}$$

We cannot, however, obtain the value of the function $C_0(Q)$ except by computing the zeroth moment of the original Hamiltonian and comparing the corresponding result for $H_{\rm eff}$.

The procedure just described, that will be implemented below, can be generalized as follows: (i) Compute the exact equations of motion for particle-hole operators, using the exact commutation relations. (ii) Apply the number-operator method up to any desired order to both the equations of motion and to the algebra. The latter now becomes a nonlinear algebra of particle-hole operators. (iii) Define $H_{\rm eff}$ as a sum of contributions of different order so that its commutator with a particle-hole operator, computed by means of the nonlinear algebra, also carried to the appropriate order, yields the equations of motion to the desired accuracy. (iv) The function $C_0(Q)$ is to be computed as described above. The results of steps (i)–(iii) are somewhat surprising, and will be reported in a separate account.

Let us note that the only difference between (3.37) and the *quadratic* terms of H is that $H_{40}+H_{04}$ has been multiplied by a factor of two in the former.

The preliminary spadework necessary to derive matrix elements of the equations of motion has already been carried out in Sec. II B. We deal first with the excited states. The equation we need is simply the zeroth moment of the equation of motion, Eq. (2.25). This yields standard RPA equations, which we write in the matrix form

$$\omega_\mu\tau_3\mathcal{Z}_\mu({\rm ph}|Q) = \mathcal{M}_{{\rm php'h'}}\mathcal{Z}_\mu({\rm p'h'}|Q) \ , \tag{3.39}$$

where τ_3 is the usual generalized Pauli matrix $\left(\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix}\right)$,

$$\mathcal{Z}_\mu({\rm ph}|Q) \equiv \begin{pmatrix} \mathcal{X}_\mu({\rm ph}|Q) \\ \mathcal{Y}_\mu({\rm ph}|Q) \end{pmatrix} \ , \tag{3.40}$$

and

$$\mathcal{M} = \begin{pmatrix} \mathcal{A} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{A}^* \end{pmatrix} \ . \tag{3.41}$$

That the solutions satisfy the usual RPA orthonormality condition,

$$\sum_{\rm ph}\mathcal{X}_\mu({\rm ph})\mathcal{X}^*_\nu({\rm ph}) - \mathcal{Y}_\mu({\rm ph})\mathcal{Y}^*_\nu({\rm ph}) = \delta_{\mu\nu} \ , \tag{3.42}$$

follows from the equations themselves together with the completeness relations derived below.

As discussed in our previous work on adiabatic large amplitude collective motion, we use the eigenvector with lowest ω_μ^2 (which is always real) of the local RPA equation, Eq. (3.39), to determine the collective coordinate. This squared eigenvalue can be positive, corresponding to a stable mode, or negative when the local mode is unstable. (If there is more than one unstable mode we have to introduce more than one adiabatic collective coordinate.) The character of this eigenvalue will generally change as we change the point Q. According to the standard theory, as we have already remarked, the role of this solution is to determine the self-consistent cranking operator. In geometrical terms this solution specifies the direction of a path labeled by the variable Q, the one-dimensional manifold that provides the domain of definition of the collective Hamiltonian. In any event this solution is to be *excluded* from the list of solutions that describe excited states. Henceforth, we use the symbols a, b to refer to the solutions of (3.39) exclusive of the lowest one(s).

There is, of course, a mathematical problem, the same one that we encounter when there is a Nambu-Goldstone mode, namely, that of mathematical completeness of the solutions of (3.39). The resolution of this problem, as we shall see in due course, is that the extra solution associated with the collective path enters the completeness relation in a manner completely analogous to that in which spurious modes do. We shall now study this mode using Eq. (2.18). Utilizing a matrix notation similar to that defined in (3.40), we calculate for the zeroth and first moments of the aforementioned equation,

$$\mathcal{M}_{\mathrm{php'h'}}\mathcal{Z}^{(0)}(\mathrm{p'h'}) = i(dV/dQ)\tau_3\mathcal{Z}^{(1)}(\mathrm{ph}) - \lambda Q, \quad (3.43)$$

$$\mathcal{M}_{\mathrm{php'h'}}\mathcal{Z}^{(1)}(\mathrm{p'h'}) = -i\bar{B}\tau_3\frac{d}{dQ}\mathcal{Z}^{(0)}(\mathrm{ph}) , \quad (3.44)$$

where

$$Q \equiv \begin{pmatrix} q^*_{\mathrm{ph}} \\ q_{\mathrm{ph}} \end{pmatrix} . \quad (3.45)$$

It is appropriate to refer to (3.43) and (3.44) as the equations of motion along the path.

The unambiguous solution of these equations is based on the recognition that (3.44) is one of the decoupling conditions in the theory of large amplitude collective motion, the so-called mass condition [1] in the classical theory of large amplitude adiabatic collective motion. The basis for this identification, described in Appendix B, includes the equations

$$\begin{aligned} d\mathcal{X}^{(0)}(\mathrm{ph})/dQ &= (d\rho/dQ)_{\mathrm{hp}} , \\ d\mathcal{Y}^{(0)}(\mathrm{ph})/dQ &= (d\rho/dQ)_{\mathrm{ph}} , \end{aligned} \quad (3.46)$$

that can be established directly from the definitions of these quantities, where ρ is the local density matrix, and also implies that

$$\begin{aligned} \mathcal{X}^{(1)}(\mathrm{ph}) &= -iq_{\mathrm{hp}} , \\ \mathcal{Y}^{(1)}(\mathrm{ph}) &= iq_{\mathrm{ph}} . \end{aligned} \quad (3.47)$$

From this last result we see that since $(dV/dQ) = \lambda$, a consistent solution of Eq. (3.43) is

$$\mathcal{Z}^{(0)}(\mathrm{ph}) = 0 . \quad (3.48)$$

This is a local equation, so that it is not inconsistent to have $d\mathcal{Z}^{(0)}(\mathrm{ph})/dQ \neq 0$. Starting from (3.48), which is also a consequence of the definition of the density matrix, we can unroll the same reasoning in the reverse direction.

We have not yet extracted all the information contained in Eqs. (3.43) and (3.44). If we differentiate the former with respect to Q (λ is *not* differentiated here), and use the results just established, we find the equation

$$\mathcal{M}_{\mathrm{php'h'}}\frac{d\mathcal{Z}^{(0)}(\mathrm{p'h'})}{dQ} = i\frac{d^2V}{dQ^2}\tau_3\mathcal{Z}^{(1)}(\mathrm{ph}) . \quad (3.49)$$

Together with (3.44), this provides the missing solution of the RPA, namely, the one that determines the collective path. We also see that $(d\mathcal{Z}^{(0)}/dQ)$ does not describe a spurious mode.

We are almost in possession of all the results necessary to carry out the calculation of $\int d\xi\langle Y|H|X\rangle$. One missing ingredient is the completeness relations for the solutions of the RPA to which we now turn.

C. Completeness relations

To evaluate quantum corrections to the potential energy, in addition to the results of the previous subsection, we also need the completeness relations associated with the quasiboson commutation relations. For example, we study the zeroth moment of the commutation relation

$$\int d\xi\langle Y|[A_{\mathrm{ph}}, A^*_{\mathrm{p'h'}}]|X\rangle = \delta_{\mathrm{pp'}}\delta_{\mathrm{hh'}} . \quad (3.50)$$

Utilizing a sum over intermediate states, the definitions (3.30)–(3.33), and a definition to be discussed below, we find straightforwardly at each point Q of the path

$$\sum_a[\mathcal{X}_a(\mathrm{ph})\mathcal{X}^*_a(\mathrm{p'h'}) - \mathcal{Y}_a(\mathrm{p'h'})\mathcal{Y}^*_a(\mathrm{ph})] + \frac{-i}{N}(q_{\mathrm{ph}}p_{\mathrm{p'h'}} + p_{\mathrm{ph}}q_{\mathrm{p'h'}}) = \delta_{\mathrm{pp'}}\delta_{\mathrm{hh'}} . \quad (3.51)$$

Here we have introduced the definition

$$(d/dQ)_{\mathrm{ph}} \equiv ip_{\mathrm{ph}}/N . \quad (3.52)$$

The point of this definition is that q and p can thus be identified as a set of (local) canonical coordinates. The consistency of this identification is justified in Appendix B. The contribution to the sum rule associated with these operators arises from transitions along the path, i.e., from

the quasispurious mode. The term involving the q and p's can be replaced by an expression involving the corresponding eigenvector of the RPA, in which case we find that Eq. (3.52) is equivalent to the usual RPA normalization condition.

From the vanishing commutator between two A operators, we obtain in a similar fashion

$$\sum_a [\mathcal{X}_a^*(\mathrm{p'h'})\mathcal{Y}_a(\mathrm{ph}) - \mathcal{X}_a^*(\mathrm{ph})\mathcal{Y}_a(\mathrm{p'h'})] = 0. \quad (3.53)$$

Notice that in this relation, there is no contribution from the quasispurious mode. These last two equations and their complex conjugates can be assembled into the usual completeness relation for the RPA in exactly the same fashion as when there is a spurious mode, implying all the textbook properties [26] such as normalization of solutions, that we shall require below.

IV. EVALUATION OF FIRST QUANTUM CORRECTIONS TO THE POTENTIAL ENERGY

For technical reasons, it is convenient to first evaluate the zeroth moment of Eq. (3.37), the effective Hamiltonian that yields the correct equations of motion in the quasiboson approximation. The method of evaluation is exactly the same as that used for the completeness relations including contributions from transitions along the collective path as well as from the RPA intermediate states "orthogonal" to the collective path. We find

$$H_{\mathrm{eff}}^{(0)}(Q) = \mathcal{A}_{\mathrm{php'h'}}[\mathcal{Y}_a^*(\mathrm{p'h'})\mathcal{Y}_a(\mathrm{ph}) - (i/N)(q_{\mathrm{p'h'}}p_{\mathrm{ph}} + p_{\mathrm{p'h'}}q_{\mathrm{ph}})] + \tfrac{1}{2}[\mathcal{B}_{\mathrm{php'h'}}\mathcal{X}_a^*(\mathrm{p'h'})\mathcal{Y}_a(\mathrm{ph}) + \mathrm{c.c.}], \quad (4.1)$$

where the term linear in the quasiboson operators does not contribute. This expression can be transformed with the help of the completeness relations (3.51) and (3.53). We thereby find

$$H_{\mathrm{eff}}^{(0)}(Q) = \tfrac{1}{2}\sum_a \mathcal{Z}_a^\dagger \mathcal{M}\mathcal{Z}_a - \tfrac{1}{2}\mathrm{tr}\mathcal{A} = \tfrac{1}{2}\sum_a \omega_a - \tfrac{1}{2}\mathrm{tr}\mathcal{A}\ . \quad (4.2)$$

This is the well-known result [26] for the zero-point energy associated with the standard bosonization procedure, except that it refers to the local solutions at a specific point of the path. As is well known (see, e.g., the discussion in Ref. [23]) this expression overcounts some contributions, due to the fact that we have not kept track of the Pauli principle.

As has been emphasized, to obtain the correct description of the ground state, we must be sure that we have not violated the Pauli principle to the required accuracy. It therefore behooves us to deal with the Hamiltonian before transformation by the number-operator method. We thus use the following approximate form of Eq. (3.9):

$$H = V_0(Q) + \bar{H}_{\mathrm{eff}}\ , \quad (4.3)$$

$$\bar{H}_{\mathrm{eff}} = H_{11} + H_{22} + (H_{40} + \mathrm{c.c.})\ . \quad (4.4)$$

Here the linear term has been omitted since it does not contribute to the final result.

If we now evaluate the zeroth moment of Eq. (4.4), as discussed in great detail in Ref. [23], we find that (4.2) overestimates the contributions of H_{11} and H_{40} by a factor of two. The right answer is therefore

$$V(Q) = V_0(Q) + \tfrac{1}{2}\left(\sum_a \omega_a(Q) - \mathrm{tr}\mathcal{A}\right) - [(H_{11})^{(0)} + (H_{04} + H_{40})^{(0)}]\ , \quad (4.5)$$

with

$$(H_{11})^{(0)} = \tfrac{1}{2}\sum_{\mathrm{php'h'}a} (\mathcal{H}_{\mathrm{pp'}}\delta_{\mathrm{hh'}} - \mathcal{H}_{\mathrm{hh'}}\delta_{\mathrm{pp'}}) \times \mathcal{Y}_a^*(\mathrm{ph})\mathcal{Y}_a(\mathrm{p'h'})\ , \quad (4.6)$$

$$(H_{04})^{(0)} = \tfrac{1}{4}\mathcal{B}_{\mathrm{php'h'}}\mathcal{X}_a^*(\mathrm{p'h'})\mathcal{Y}_a(\mathrm{ph})\ . \quad (4.7)$$

For $dV/dQ = 0$ this expression reduces to a value of the ground-state energy that agrees in the limit of weak residual interaction with the result of perturbation theory [22, 23] (of course after addition of term $\frac{1}{2}\omega_1$, associated with the collective coordinate Q). It also contains the zero-point energy calculated by Reinhard and Goeke [10] as a special case: If we discard the ω_a terms, and approximate the trace by the contribution along the collective path (discussed in more detail in the next section) we obtain the expression (4.4b) in Ref. [10].

V. APPLICATION OF THE RESULTS TO ^{28}Si

As an application of the result derived in the previous section consider the problem discussed in Ref. [8] (which we shall refer to as WDK in the following). Let us set the stage for the further discussion by giving a brief recapitulation of the relevant points of that paper. There we describe a calculation for ^{28}Si in the *sd* shell using Kuo's interaction. The most important features of this system for the present discussion are the fact that the HF equations have two stable solutions: a global minimum of oblate deformation and a local prolate minimum with slightly higher energy. In WDK we discuss in great detail the calculation of a path (where each point represents a triaxial Slater determinant) connecting the two minima. A projection of this path on the quadrupole-deformation β-γ plane is given in Fig. 1.

For the calculation of this path the algorithm consists of solving the local, constrained, Hartree-Fock equations (3.4), where the constraining operator (or rather the numbers q_{ph}) are obtained self-consistently from the iterated RPA equation

$$(\mathcal{A} + \mathcal{B})(\mathcal{A} - \mathcal{B})_{\mathrm{php'h'}}q_{\mathrm{p'h'}} = \omega_1^2 q_{\mathrm{ph}}\ . \quad (5.1)$$

Since it can easily be shown that there is a one-to-one correspondence between the left and right eigenvalues of the iterated RPA and the $\mathcal{X}_\mu$ and $\mathcal{Y}_\mu$ eigenvectors of the usual RPA, the complete set of solutions of Eq. (5.1) can be shown to provide all the information we will need to calculate the quantum corrections.

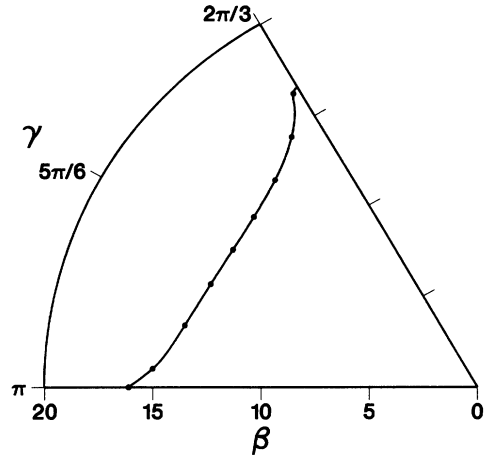

FIG. 1. The one-dimensional collective path projected onto the quadrupole deformation β-γ plane. ($\beta^2 = \langle Q_{20}\rangle^2 + 2\langle Q_{22}\rangle^2$.) The oblate minimum is attained for $\gamma = \pi$, corresponding to symmetry around the z axis. The dots indicate the points $Q = i/4$, starting from the oblate minimum where $i = 0$.

In WDK we make the additional approximation of only considering the space of shapes of even multipolarity, i.e., of ellipsoidal symmetry. This reduces the dimension of the RPA matrix considered by a factor of 4. (This means that the space of excitations, or equivalently the RPA matrix, is divided in four equal parts. One part gives the ellipsoidal excitations, the other three parts each contain an excitation corresponding to a rigid rotation of the system as well as some other modes that are disregarded.) The rotational modes are used to calculate the position-dependent moments of inertia, so that the collective dynamics is described by the Hamiltonian

$$H = \sum_i \frac{J_i^2}{2\mathcal{I}_i} + \frac{P^2}{2} + V_0(Q) \ . \tag{5.2}$$

For future reference the potential $V_0(Q)$ is given in Fig. 2. We have quantized the Hamiltonian (5.2) and found that

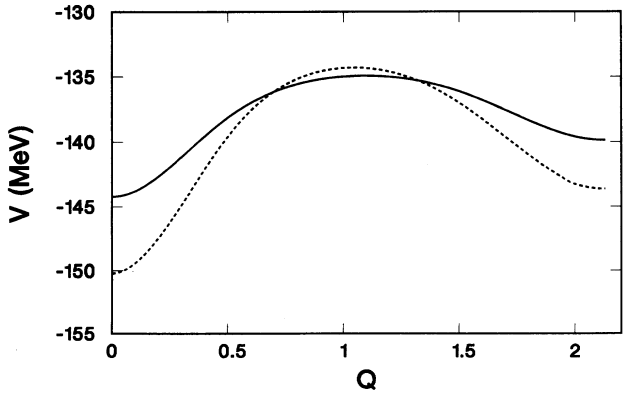

FIG. 2. The potential energy $V_0(Q)$ along the collective path (solid line) as well as the quantum corrected potential energy $V(Q)$ (dashed line). $Q = 0$ corresponds to the oblate minimum, whereas $Q = 2.15$ for the prolate minimum.

the description of the spectrum as compared to the exact shell-model spectrum is quite good for the ground-state band, but of limited quality for the first excited band, which is the band built on the prolate minimum. Let us now study how quantum corrections to the potential change this picture.

We write

$$V(Q) = V_0(Q) + \tfrac{1}{2}\left(\sum_a \omega_a - \mathrm{tr}(A)\right) - [(H_{11})^{(0)} + (H_{04} + H_{40})^{(0)}] - \sum_i \frac{\langle J_i^2\rangle}{2\mathcal{I}_i} \ . \tag{5.3}$$

The first two corrections terms are the ones described in the previous section and do not need further explanation apart from the statement that we use only the ellipsoidal excitations to calculate these two terms; the last term, which is a subtraction of the expectation value of the rotational energy in the local Hartree-Fock state, is just a part of the total expression for the quantum corrections obtained from the remaining three quarters of the space (see, e.g., Ref. [26], Eq. (8.111)).

The quantum corrected potential energy is given in Fig. 2 as the dashed line. Clearly we have deeper minima and a higher barrier, so that the wave functions will become more strongly localized on the minima. In Fig. 3 we give each of the corrections to the potential energy separately. The solid line represents the quasiboson result $\frac{1}{2}[\sum_a \omega_a - \mathrm{tr}(\mathcal{A})]$, the dashed line represents the rotational energy $-\sum_i \langle J_i^2\rangle/2\mathcal{I}_i$, and the dotted line represents the overcounting correction $-[(H_{11})^{(0)} + (H_{04} + H_{40})^{(0)}]$. We find that to good approximation the contribution $(H_{40}+H_{04})$ equals -2 times H_{11}, a result that can be shown to become exact in the perturbation limit. We do not understand why this relation holds so well for our calculation, but it may be due to a weak residual interaction. In any event, in the following we shall disregard this

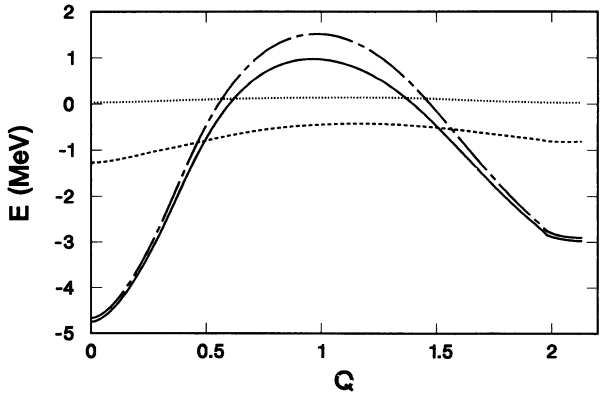

FIG. 3. The quantum correction to the potential energy, decomposed in the quasiboson result $[\sum_a \omega_a - \mathrm{tr}(\mathcal{A})]$, given by the solid line, the rotational zero-point energy $[\sum_\mu \langle J_\mu^2\rangle/2\mathcal{I}_\mu]$, given by the dashed line, and the overcounting correction $(-[(H_{11})^{(0)} + (H_{40})^{(0)} + (H_{04})^{(0)}])$, given by the dotted line. The dash-dotted line represents the approximation (5.4) to the quasiboson result.

term, and concentrate on the two remaining terms. We have also calculated the quantum correction corresponding to Eq. (4.4b) in Ref. [10]. Recasting this expression, which is given in terms of the Gaussian overlap approximation, into a form using our standard notation, we find the following approximate result for the quasiboson part of the correction:

$$E_{\rm corr} = -\tfrac{1}{4}(|f|^{-2}\bar{B}^{11} + |f|^2\bar{V}_{11}) = -\tfrac{1}{4}(|f|^{-2} + |f|^2\omega_1^2)\ . \tag{5.4}$$

Here $|f|^2 = \sum_{\rm ph}(f^{(1)}_{\rm ph})^2$, and we have used our choice of normalization of f (i.e., $\bar{B}^{11} = 1$, see WDK) in the second half of the equation. Clearly we find that this approximate quantum correction is always smaller than $-\frac{1}{2}\omega_1$. As can be seen from the dash-dotted line in Fig. 3, that represents this result, this is in general a good approximation to the quasiboson result, except near the top of the barrier.

In Table I we give the numerical values we have calculated for some low-lying 0^+ states. We give both absolute and excitation energies to show the effects of various approximation schemes in the best possible way. The first column gives the exact shell-model result, as a benchmark to measure the quality of various approximations. The second and the third column give the results of a requantization of the one-dimensional Hamiltonian without (second column) and with (third column) the inclusion of quantum corrections. Not surprisingly the absolute value for the energies becomes closer to the true value if we include quantum corrections, even though we apparently still need more to attain the correct result. It is gratifying to see that the excitation energy of the first excited 0^+ state, the bandhead of the first excited band, is much closer to the true value.

For sake of comparison we give the RPA value for the oblate and prolate minima, which are $V(Q) + \frac{1}{2}\omega_1$, as well as the excitations obtained by adding ω_1 (or ω_2) to this value. As can be seen ω_1 and ω_2 are quite close. This has to do with the fact that we should really use a two-dimensional coordinate surface. Stopping short of that approach we have done a poor man's calculation along the collective path. We realize that our path can be imbedded in the (Q_1, Q_2) plane, and that due to the poor decoupling it does not follow the line $Q_2 = 0$. Actually, in WDK we have calculated the change ΔQ_2 from point to point. If we evaluate the sum of these numbers we have an estimate for $Q_2 = q_2(Q_1)$ along the path. Since we are at the bottom of a valley, we know that to lowest order the potential as a function of Q_2 is harmonic about the points of the valley, with frequency ω_2. Using all this information we requantize the approximate Hamiltonian (valid for 0^+ states alone),

$$H = \tfrac{1}{2}(P_1^2 + P_2^2) + E_{\rm HF}(Q^1) + \tfrac{1}{2}\omega_2^2[Q_2 - q_2(Q_1)]^2 + \tfrac{1}{2}\sum_{a>2}\omega_a - \tfrac{1}{2}{\rm tr}[\mathcal{A}(Q_1)] - \tfrac{1}{2}\sum_j \langle J_j^2\rangle/\mathcal{I}_j(Q_1)\ . \tag{5.5}$$

The results of this calculation are given in the column labelled "2D" and can be seen to give a much better overall result for the excitation spectrum.

VI. CONCLUDING REMARKS

We have shown that it is possible to calculate the leading quantum corrections to the theory of large amplitude collective motion without undue effort. The theory is closely linked to that of the ground-state correlation energy for the RPA, and requires only knowledge about the RPA matrix and its eigenvalues that we have to evaluate anyway to solve for the collective surface in the theory of large amplitude collective motion.

Since our discussion starts directly from the Hartree-Fock equations, and not just from the Hartree equations, we have to be careful about possible overcounting of higher-order terms that have already been accounted for in lower terms through the exchange mechanism. This leads to the appearance of the "overcounting corrections," which fortunately appear to be small for the present calculation.

Inclusion of the quantum corrections in our calcula-

TABLE I. A comparison of various approximate calculations of the 0^+ energies. E_μ gives absolute energies, whereas E^x_μ represents the excitation energies. The first column gives the exact shell-model results. The next two columns represent the results of quantization of the one-dimensional collective Hamiltonian; the first without quantum corrections, and the second with inclusion of these corrections. The column labelled "2D" gives the results of the approximate two-dimensional calculation discussed in the text. The last column gives the results obtained from the RPA on either minimum.

	Shell model	1D		2D	RPA	
		no zero pt.	zero pt.			
$E_{0_1^+}$	-149.638	-140.535	-146.941	-146.904	-147.556	
$E_{0_2^+}$	-145.121	-137.580	-141.987	-142.163	-142.381	
$E_{0_3^+}$	-140.409	-132.822	-134.929	-138.134	-138.256	(-138.058)
$E_{0_4^+}$	-139.634	-127.841	-130.858	-137.347	-136.618	(-136.187)
$E^x_{0_2^+}$	4.517	2.954	4.953	4.741	5.175	
$E^x_{0_3^+}$	9.229	7.712	12.012	8.670	9.300	(9.498)
$E^x_{0_4^+}$	10.004	12.693	16.091	9.557	10.937	(11.369)

tion for ^{28}Si improves the calculation of both binding and excitation energies. We have shown that a quasi-two-dimensional calculation improves the results even more. This makes it even more compelling to perform a real two-dimensional calculation, which is currently in progress.

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APPENDIX A: EQUATIONS OF MOTION ALONG THE PATH

Let us extend the concise discussion given in Sec. II A, by giving some more details. We study the equations of motion for an arbitrary operator, θ, within the collective subspace,

$$\begin{aligned}\langle X|[\theta,H]|X'\rangle &= \langle X|[\theta,\mathcal{H}_{\rm col}]|X'\rangle \\ &\cong [V(X')-V(X)]\langle X|\theta|X'\rangle \\ &\cong (dV/dQ)(X'-X)\langle X|\theta|X'\rangle \ , \end{aligned} \tag{A1}$$

where we have made the adiabatic assumption that the collective Hamiltonian, $\mathcal{H}_{\rm col}$, is dominated by the potential energy V.

Using the operator $\hat{Q}$, for which the states $|X\rangle$ are its eigenvectors with eigenvalues X, we can rewrite (A1) as

$$\langle X|[\theta, H-(dV/dQ)\hat{Q}]|X'\rangle = 0 \ . \tag{A2}$$

It turns out, however, that neither (A2) nor its predecessor (A1) is sufficiently accurate for the needs of Sec. III. For these latter purposes, by utilizing the moment expansion, the right-hand side of (A1) can be rewritten in terms of the first moment of $\langle X|\theta|X'\rangle$,

$$\begin{aligned}(X-X')\langle X|\theta|X'\rangle &= \xi\theta^{(1)}(Q)(-i\partial/\partial\xi)\delta(\xi) \\ &= i\delta(\xi)\theta^{(1)}(Q) \ , \end{aligned} \tag{A3}$$

and will thus contribute to the zeroth moment of the corresponding equations of motion. But we shall also need the leading contribution to the first moment. A lengthier, but elementary calculation shows that the collective kinetic energy contributes an additional amount

$$\delta'(\xi)\bar{B}(Q)(d/dQ)\theta^{(0)}(Q) \ , \tag{A4}$$

where

$$\bar{B} \equiv M^{-1} \equiv H^{(2)} \tag{A5}$$

is the inverse collective mass. Thus we have derived Eq. (2.20).

APPENDIX B: RPA IDENTITIES

We consider the solution of Eqs. (3.43) and (3.44). We first note that if we use Eqs. (3.46) and (3.47) [the latter already expressing the solution of (3.43)] in (3.44), then, for example, the first row of the latter becomes

$$(\mathcal{A}-\mathcal{B})_{\rm php'h'}q_{\rm p'h'} = (1/M)(d\rho_{\rm ph}/dQ) \ . \tag{B1}$$

In fact, the difference matrix that appears on the left-hand side of (B1) coincides with the quantity that is defined as the reciprocal mass matrix, B, in the theory of large amplitude collective motion based on time-dependent Hartree-Fock theory [6, 7]. According to the definitions (3.35) and (3.36) we have (the use of superscripts is borrowed from previous work)

$$B^{\rm php'h'} = (\mathcal{H}_{\rm pp'}\delta_{\rm hh'} - \mathcal{H}_{\rm hh'}\delta_{\rm pp'}) + V_{\rm p'hh'p} - V_{\rm hh'pp'} \ , \tag{B2}$$

and the further identification

$$q_{\rm ph} = (\partial Q/\partial\rho_{\rm hp}) \ . \tag{B3}$$

Thus Eq. (B1) becomes

$$B^{\rm php'h'}\frac{\partial Q}{\partial\rho_{\rm p'h'}} = \frac{1}{M}\frac{d\rho_{\rm ph}}{dQ} \ . \tag{B4}$$

This is the standard mass condition in the theory of large amplitude collective motion and also one of the RPA equations determining the matrix elements $q_{\rm ph}$.

We also consider the justification of Eq. (3.52) by computing

$$\begin{aligned}1 = \frac{dQ}{dQ} &= \frac{dQ}{d\rho_{\rm ph}}\frac{d\rho_{\rm ph}}{dQ} + \frac{dQ}{d\rho_{\rm hp}}\frac{d\rho_{\rm hp}}{dQ} \\ &= (-i/N)(q_{\rm hp}p_{\rm ph} - p_{\rm hp}q_{\rm ph}) \\ &= (-i/N)[q,p]_{\rm hh} = 1 \ . \end{aligned} \tag{B5}$$

APPENDIX C: COVARIANT FORM OF THE RPA

In this appendix we discuss the derivation of the covariant RPA in the context discussed in this paper. As we have shown in Sec. II B, the Hamiltonian relevant for the study of local RPA excitations is $H-\lambda\hat{Q}$. We now allow $\hat{Q}$ to be a sum of one- and two-body operators,

$$Q[\rho] = {\rm tr}(\rho q^{(1)}) + \tfrac{1}{2}{\rm tr}(\rho q^{(2)}\rho) \ . \tag{C1}$$

Arranging $\hat{Q}$ into normal form as we did with H, we find to the accuracy to which we are working,

$$\hat{Q} = Q[\rho] + \hat{Q}_1 + \Delta H_{11} + \Delta H_{22} + (\Delta H_{40} + {\rm H.c.}) \ . \tag{C2}$$

Of course, the role of the first term is that it furnishes the constraint in the derivation of the constrained Hartree-Fock equation (3.4) from the variational expression

$$\delta(W[\rho] - \lambda Q[\rho]) = 0 \ . \tag{C3}$$

The term $-\lambda\hat{Q}_1$ combines with a contribution to H, as we have already shown in the study of the RPA in the main text. The remaining terms that have not been treated in the text have the values

$$\Delta H_{11} = -\lambda(q_{\rm pp'}\psi^\dagger_{\rm p}\psi_{\rm p'} - q_{\rm hh'}\psi_{\rm h}\psi^\dagger_{\rm h'}) \ , \tag{C4}$$

$$\Delta H_{22} = -\lambda q^{(2)}_{\mathrm{ph'hp'}}(\psi^\dagger_{\mathrm{p}}\psi_{\mathrm{h}})(\psi^\dagger_{\mathrm{h'}}\psi_{\mathrm{p'}}), \tag{C5}$$

$$\Delta H_{40} = -\lambda \tfrac{1}{4} q^{(2)}_{\mathrm{pp'hh'}}\psi^\dagger_{\mathrm{p}}\psi^\dagger_{\mathrm{p'}}\psi_{\mathrm{h'}}\psi_{\mathrm{h}} \ . \tag{C6}$$

Thus the RPA matrices $\mathcal{A}$ and $\mathcal{B}$ have the additional contributions

$$\Delta\mathcal{A}_{\mathrm{php'h'}} = -\lambda(q_{\mathrm{pp'}}\delta_{\mathrm{hh'}} - q_{\mathrm{hh'}}\delta_{\mathrm{pp'}} + q^{(2)}_{\mathrm{p'hh'p}}) \ , \tag{C7}$$

$$\Delta\mathcal{B}_{\mathrm{php'h'}} = -\lambda q^{(2)}_{\mathrm{hh'pp'}} \ . \tag{C8}$$

These are special cases of the more general formulas

$$\Delta\mathcal{A}_{\mathrm{php'h'}} = -\lambda\left(\frac{\delta^2 Q[\rho]}{\delta\rho_{\mathrm{ph}}\delta\rho_{\mathrm{h'p'}}}\right) \ , \tag{C9}$$

$$\Delta\mathcal{B}_{\mathrm{php'h'}} = -\lambda\frac{1}{2}\left(\frac{\delta^2 Q[\rho]}{\delta\rho_{\mathrm{ph}}\delta\rho_{\mathrm{p'h'}}} + \mathrm{c.c.}\right) \ , \tag{C10}$$

that are equivalent to general formulas developed in our previous work and reviewed in Ref. [1] in the context of the *iterated* RPA. (The extra contributions displayed here correspond to what we have called the "symplectic RPA.") Our tentative conclusion based on calculations carried out for ^{28}Si is that these extra terms are not numerically significant in this case. This is fortunate, since their inclusion does complicate the algorithm. We should be alert, however, that we may not always be so fortunate in future applications.

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