Quantum theory of large amplitude collective motion: Bosonization of all degrees of freedom

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In an accompanying paper we have described a method that provides a foundation for a quantum theory of large amplitude collective motion. In this method, only the collective degrees of freedom are initially bosonized, i.e., represented by canonical variables. By contrast, in this paper, we describe an alternative method in which all elementary (fermion) density operators defined in the shell model are bosonized. Once again it involves an amalgamation of the Born-Oppenheimer approximation with a version of the Kerman-Klein method. Compared to the alternative it has the advantages of bearing a closer resemblance to the corresponding molecular problem and bringing the role of the Berry potentials clearly into focus. On the other hand, the physical justification for bosonizing the noncollective degrees of freedom is not obvious, and the Pauli principle is only satisfied approximately at every stage of approximation. The method in this paper may also be considered to be an extension to the large amplitude domain of the quantum theory of anharmonic vibrations developed by Marshalek and Weneser. The boson formalism is applied to the problem of the coupling of the giant dipole mode to a quadrupole mode, studied recently for the effect of Berry potentials by LeTourneux and Vinet.

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I. INTRODUCTION

In an accompanying paper we have described a framework for a quantum theory of adiabatic large amplitude collective motion [1] that smoothly amalgamates the Born-Oppenheimer approximation (BOA) with the Kerman-Klein method. This is the version of the quantum theory that has been applied by us in our ongoing study of the spectrum of ^{28}Si [2,3]. In this method, the only states that enter the quantum theory initially are those in which the system may be in any of the collective states associated with the ground state of the noncollective variables. Excitations of the latter are studied subsequently as quantum fluctuations. This method permits us to treat a general shell-model interaction and to preserve the Pauli principle at every level of approximation. On the other hand, it fails to connect with the quantum theory of large amplitude collective motion that has previously been developed [4] starting from a general Hamiltonian in configuration space.

The purpose of this paper is to provide a foundation for this previous study, starting from a shell-model Hamiltonian. In order to succeed in this enterprise, we find that we must modify both the version of the Kerman-Klein formalism [5,6] to be applied and the manner in which we carry out approximations on that formalism. In the method utilized in the accompanying work, we never attempt to write down formally exact equations of motion, but restrict the approximation to one that we believe is valid for the collective subspace. In the version used in this paper, one can record equations of motion that are formally exact, but as soon as any necessary approximation is entered, the exact validity of the Pauli principle is surrendered. Furthermore, the approach can be justified on physical grounds only when the interaction is given explicitly as a sum of multipole and pairing terms. It does provide the natural means of justifying the previous treatment in configuration space [4]. It even simplifies the latter to some degree, by leading directly to a derivation of the starting point of that work. In this way, it seems to tie in with the corresponding treatment of molecular problems, certainly to a greater extent than the method developed in the accompanying paper.

There is another tie-in of the present work with the existing literature, one which did not become evident to us until we had to grapple seriously with the quantum fluctuations. We believe that the method in this paper can be viewed as an extension to the problem of large amplitude collective motion of the "reconstitution" method of Marshalek and Weneser [7–9]. This is, first of all, a general *quantum* method of dealing with anharmonic vibrations of both spherical and deformed nuclei, at the same time that the so-called Goldstone modes associated with the breaking of translational and rotational invariance and number conservation can be treated correctly. We have not discussed the latter problem in the current papers, but it can be dealt with, since the Kerman-Klein method was invented originally precisely for this purpose. The work of Marshalek and Weneser is based on the bosonization of all multipole and pair operators that can be formed within the given shell-model framework, uses Hartree rather than Hartree-Fock approximations, and has been formulated only for interactions written as

a sum of multipole and pairing parts. These are precisely the assumptions made in this paper. Thus we may consider the present work to represent an extension of the method of these authors, not presented here in full detail, to systems where some of the degrees of freedom may undergo large distortions.

In Secs. II–IV, we present the essential elements of our method in barest outline where there are only minor changes compared to the accompanying work, only dwelling at greater length on those aspects that differ, such as the treatment of quantum fluctuations. Section V presents an alternative and, we think, somewhat simplified study of the model of a giant dipole mode coupled to the low-energy quadrupole mode treated recently by LeTourneux and Vinet [10,11]. In an Appendix, we study Pauli principle constraints within the formalism used in this work.

II. DEFINITION OF AN EFFECTIVE HAMILTONIAN FOR THE COLLECTIVE DEGREES OF FREEDOM

In the accompanying paper we studied the problem of deriving a quantum theory of large amplitude collective motion starting with a shell-model Hamiltonian of the form

$$H = h_{\alpha\beta}a^\dagger_\alpha a_\beta + \frac{1}{4}V_{\alpha\beta\gamma\delta}a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma, \tag{2.1}$$

expressed in terms of the usual fermion creation (destruction) operators, $a^\dagger_\alpha(a_\alpha)$ describing the shell-model orbit α, and in terms of the Hermitian one- and two-particle Hermitian matrices h and V; the latter, as written, is also antisymmetric, separately, in the initial and in the final pair of indices. In the approach taken in several previous studies of the quantum foundations of a theory of large amplitude collective motion [12,4], we have not worked directly with the shell-model Hamiltonian of the form (2.1), but instead took the point of view that we had already transformed this Hamiltonian into a form expressed in terms of bosons, i.e., in terms of a Heisenberg-Weyl space of suitable dimensionality. The purpose of the present paper is to carry out this program of transformation in a practical form.

The form of the Hamiltonian given by Eq. (2.1) is, in fact, not suitable for the announced purpose. The theory in question requires for its physical (as opposed to its formal) justification that the general interaction in (2.1) be replaced by a sum of multipole and pairing interactions. Since we do not wish to carry along the extra details necessary to include the pairing effects, we shall omit them from this paper, with the understanding, however, that they can be reinstated when needed in future applications. We therefore replace the interaction term in (2.1) with the form

$$\frac{1}{2}\sum_\lambda F^{(\lambda)}_{\alpha\gamma}F^{(\lambda)*}_{\delta\beta}(a^\dagger_\alpha a_\gamma)(a^\dagger_\beta a_\delta) = \frac{1}{2}\sum_\lambda \mathbf{F}^{(\lambda)}\cdot\mathbf{F}^{(\lambda)\dagger}. \tag{2.2}$$

In carrying out this program, we do not wish to repeat those steps that are formally identical to those shown in the accompanying paper and works referred to there. In any event, we assume the existence of a localized basis of states $|x\rangle = |Q,q\rangle = |Q)|q]$ and the Born-Oppenheimer form for the collective band,

$$|n\rangle = \int dQdq|Q)|q](Q|n)[q|0:Q], \tag{2.3}$$

leading to the following expression for the effective Hamiltonian in the collective subspace

$$[n|H_{\rm eff}(Q,P)|n'] = \int (n|Q)[0:Q|q]dQdq\langle Q,q|H|Q',q'\rangle \times dQ'dq'[q'|0:Q'](Q'|n'). \tag{2.4}$$

In accordance with our announced intentions, the next step is to carry out a moment expansion to second order with respect to all variables. In terms of the sum and difference coordinates, $\bar{x}$ and $\tilde{x}$, respectively,

$$x = \bar{x} + \frac{1}{2}\tilde{x}, \qquad x' = \bar{x} - \frac{1}{2}\tilde{x}, \tag{2.5}$$

we expand

$$\langle x|H|x'\rangle = H^{(0)}(\bar{Q},\bar{q})\delta(\tilde{x}) + H^{(1,\mu)}(\bar{Q},\bar{q})(-i\tilde{\partial}_\mu)\delta(\tilde{x}) + \frac{1}{2}H^{(2,\mu\nu)}(-i\tilde{\partial}_\mu)(-i\tilde{\partial}_\nu)\delta(\tilde{x}) + \cdots. \tag{2.6}$$

Here

$$\tilde{\partial}_i = \frac{\partial}{\partial\tilde{Q}^i}, \quad \tilde{\partial}_a = \frac{\partial}{\partial\tilde{q}^a}, \tag{2.7}$$

and

$$H^{(n,\mu_1,\ldots,\mu_n)}(\bar{Q},\bar{q}) = \int d\tilde{x}(-i)^n\tilde{x}^{\mu_1},\ldots,\tilde{x}^{\mu_n}\langle x|H|x'\rangle. \tag{2.8}$$

In the following we shall assume that the odd moments vanish as a consequence of time-reversal invariance, and therefore we concentrate our attention on evaluating the contributions of the zeroth and second moments to the effective Hamiltonian for the slow variables.

The expansion (2.6) is based on the assumption that the matrix element of the Hamiltonian is strongly peaked in the difference coordinates. This is more likely to be the case for the collective than for the noncollective variables. The justification of the moment expansion on the basis of the strong-peaking argument is also the basis of the argument given many times and most recently in Ref. [3] that this expansion converges as a power of the reciprocal of the number of particles that participate in the collective motion. A corresponding argument for the noncollective coordinates is not apparent, though in Ref. [4] we have given an argument based on the geometrical structure of the configuration space that may have restricted validity.

Because of the lack of complete conviction on this point, we have avoided the moment expansion for the noncollective variables in our previous work. The use of this expansion for the fast variables, or some equivalent assumption, appears to be necessary, however, to make direct contact with the starting point of our previous work [4] as well as with all existing treatments of anharmonic vibrations.

The insertion of Eq. (2.6) into Eq. (2.4) allows us to carry out the integration over the relative coordinate $\tilde{q}$. The various moments that enter the resulting expressions are still unknown functions of $\bar{q}$. The only practical method of dealing with this problem is to assume that the functions involved are slowly varying functions of $\bar{q}$ and therefore can be expanded in a power series in these variables, which we limit, for purposes of illustration, to second-order terms only. We shall avoid the completely uninformative details of the resulting calculations, preferring to summarize the results instead.

Starting from the assumption that there is a special localized basis $|Q,q\rangle$, in which we can distinguish a set Q of collective or slow variables from another set q of noncollective or fast variables (using criteria that have been described many times [13]), we transform the general Hamiltonian matrix into a useful form first by making a moment expansion in the difference coordinates, keeping up to second-order terms, and second by expanding in powers of the average values of the fast variables, again only to second-order terms. The result can be summarized by a Hamiltonian $\bar{H}(Q,P,q,p)$ in the full space, arranged according to powers of the fast variables,

$$\bar{H} = \bar{H}_{(0)} + \bar{H}_{(1)} + \bar{H}_{(2)}, \tag{2.9}$$

$$\bar{H}_{(0)} = V(Q) + \tfrac{1}{8}\{P_i,\{P_j,B^{ij}(Q)\}\}, \tag{2.10}$$

$$\bar{H}_{(1)} = q^a[V_{,a} + \tfrac{1}{8}\{P_i,\{P_j,B^{ij}_{,a}(Q)\}\}] + p_a\tfrac{1}{2}\{P_i,B^{ai}(Q)\}, \tag{2.11}$$

$$\bar{H}_{(2)} = \tfrac{1}{2}q^aq^bV_{,ab}(Q) + \tfrac{1}{2}p_ap_bB^{ab}(Q). \tag{2.12}$$

Here

$$V(Q) \equiv H^{(0)}(Q,0), \tag{2.13}$$

$$B^{ij} \equiv H^{(2,ij)}(Q,0). \tag{2.14}$$

Furthermore, extending the original definition of H_{eff}, $\bar{H}$ is understood to define a matrix

$$(n,\nu|H_{\text{eff}}|n',\nu') = \int dQdq(n|Q)[\nu:Q|q]\,\bar{H}\,[\nu':Q'|q'] \times(Q'|n'), \tag{2.15}$$

of which the subset of elements for the values $\nu = \nu' = 0$ define the subspace comprehended by the original definition of H_{eff}.

Further remarks refer only to this submatrix. First we drop any further reference to the term $\bar{H}_{(1)}$, since strict satisfaction of the decoupling conditions requires that this term vanish; we shall in any event assume that this is a good approximation. For the remaining two terms we now perform the integration over q, and write the result in the form,

$$H_{\text{eff}} = H^{(0)}_{\text{eff}} + H^{(2)}_{\text{eff}}. \tag{2.16}$$

With the aid of the definitions

$$D_i = P_i - A_i, \tag{2.17}$$

$$(A_i)_{\nu\nu'} = \int dq[\nu:Q|q]\left(i\frac{\partial}{\partial Q^i}\right)[q|\nu':Q], \tag{2.18}$$

$$A_i = (A_i)_{00}, \tag{2.19}$$

$$S'_{ij}(Q) = \sum_{\nu\neq 0}(A_i)_{0\nu}(A_j)_{\nu 0}, \tag{2.20}$$

we find

$$H^{(0)}_{\text{eff}} = V(Q) + \frac{1}{8}\{D_i,\{D_j,B^{ij}(Q)\}\} + \frac{1}{2}S'_{ij}B^{ij}(Q). \tag{2.21}$$

This is the expected result for the leading term of the collective Hamiltonian [4]. The contribution of the second-order term is the leading contribution of the fast variables to the collective potential energy, the so-called quantum fluctuations. With the additional definition,

$$\langle\theta\rangle_Q = \int dq[0:Q|q]\theta(q,p)[q|0:Q], \tag{2.22}$$

the result is

$$H^{(2)}_{\text{eff}} = \frac{1}{2}\langle q^aq^b\rangle_QV_{,ab} + \frac{1}{2}\langle p_ap_b\rangle_QB^{ab}. \tag{2.23}$$

As we now explain and will demonstrate in Sec. IV, this last result is not quite correct. Briefly, the point is that $V(Q)$ is the collective potential energy associated with the Hartree approximation to the many-particle energy, i.e., that associated with an uncorrelated ground state. Since the quantum fluctuation energy is also a correlation energy, its value for the uncorrelated ground state should be zero. This will be true for the Hamiltonian, $\bar{H}^{(2)}$, provided the products q^aq^b and p_ap_b are replaced by normal-ordered products with respect to the uncorrelated vacuum. (The latter is the Hartree state associated with the value Q of the collective coordinate, i.e., the orbitals are determined by the solution of a constrained Hartree equation.) In order to achieve the normal ordering in a "natural" way, this means that both the moment expansion and the subsequent Taylor expansion with respect to the fast coordinates should be normal-ordered. This, in turn, may seem *ad hoc*, but can be justified by the bosonization procedure used in the Marshalek-Weneser reconstruction method [7–9] or by the analogous number-operator method that we have used recently [3].

In the next section, we shall summarize briefly the dynamical procedure by which the moments that appear in $H^{(0)}_{\text{eff}}$ are determined, since this procedure is essentially identical to the one described in the accompanying paper. In the succeeding section, we shall turn to the small vibrations problem represented by $H^{(2)}_{\text{eff}}$, associated with the correlation energy problem discussed above.

III. MICROSCOPIC CALCULATION OF THE EFFECTIVE HAMILTONIAN

A. Moments of the Hamiltonian

We start with the definition

$$(n|H_{\text{eff}}|n') = \int dxdx' \langle n|x\rangle\langle x|H|x'\rangle\langle x'|n'\rangle, \tag{3.1}$$

with

$$\langle x|n\rangle = (Q|n)[q|0:Q]. \tag{3.2}$$

The aim of this subsection is to express the Hamiltonian matrix in (3.1) in terms of elements that can be determined dynamically. Toward this end we apply the Kerman-Klein method in its most rudimentary form; namely, we evaluate the matrix element of a product of operators by the completeness relation. As the elementary operator we take the product $a^\dagger a$ of fermion operators. Applying this to the Hamiltonian Eq. (2.2), we find

$$\langle x'|H|x\rangle = h_{\alpha\beta}\rho[\beta x|\alpha x')] + \frac{1}{2}\sum_\lambda F^{(\lambda)}_{\alpha\gamma}F^{(\lambda)*}_{\delta\beta}\rho[\delta x|\beta x'')]\rho(\gamma x''|\alpha x'), \tag{3.3}$$

that involves the generalized density matrix

$$\rho(\alpha x|\beta x') = \langle x'|a^\dagger_\beta a_\alpha|x\rangle. \tag{3.4}$$

The evaluation of (3.4) again relies on a moment expansion

$$\rho(\alpha x|\beta x') = \rho^{(0)}_{\alpha\beta}(\bar{x})\delta(\tilde{x}) + \rho^{(1,\mu)}_{\alpha\beta}(\bar{x})(-i\tilde{\partial}_\mu)\delta(\tilde{x}) \times\frac{1}{2}\rho^{(2,\mu\nu)}_{\alpha\beta}(\bar{x})(-i\tilde{\partial}_\mu)(-i\tilde{\partial}_\nu)\delta(\tilde{x}) + \cdots, \tag{3.5}$$

where

$$\rho^{(n,\mu_1,\ldots,\mu_n)}_{\alpha\beta}(\bar{Q},\bar{q}) = \int d\tilde{x}(-i)^n\tilde{x}^{\mu_1},\ldots,\tilde{x}^{\mu_n}\rho(\alpha x|\beta x'). \tag{3.6}$$

By inserting Eq. (3.5) into Eq. (3.3) and applying the convolution theorem for moment expansions discussed in the accompanying paper, we obtain, to lowest order, the following formulas for the moments of the Hamiltonian:

$$H^{(0)}(x) = h_{\alpha\beta}\rho^{(0)}_{\beta\alpha}(x) + \sum_\lambda F^{(\lambda)}_{\alpha\gamma}F^{(\lambda)*}_{\delta\beta}\rho^{(0)}_{\gamma\alpha}(x)\rho^{(0)}_{\delta\beta}(x), \tag{3.7}$$

$$H^{(1,\mu)}(x) = h_{\alpha\beta}\rho^{(1,\mu)}_{\beta\alpha}(x) + \frac{1}{2}\sum_\lambda F^{(\lambda)}_{\alpha\gamma}F^{(\lambda)*}[\rho^{(0)}_{\gamma\alpha}(x)\rho^{(1,\mu)}_{\delta\beta}(x) + \rho^{(1,\mu)}_{\gamma\alpha}(x)\rho^{(0)}_{\delta\beta}(x)], \tag{3.8}$$

$$H^{(2,\mu\nu)}(x) = h_{\alpha\beta}\rho^{(2,\mu\nu)}_{\beta\alpha}(x) + \frac{1}{2}\sum_\lambda F^{(\lambda)}_{\alpha\gamma}F^{(\lambda)*}_{\delta\beta}\left[\rho^{(1,\mu)}_{\alpha\gamma}(x)\rho^{(1,\nu)}_{\delta\beta}(x) + \frac{1}{2}\rho^{(0)}_{\gamma\alpha}(x)\rho^{(2,\mu\nu)}_{\delta\beta}(x) + \frac{1}{2}\rho^{(2,\mu\nu)}_{\gamma\alpha}(x)\rho^{(0)}_{\delta\beta}(x)\right]. \tag{3.9}$$

In addition to the terms recorded, there are higher-order contributions to each moment that arise naturally in the calculation.

B. Equations of motion

The moments of the Hamiltonian have thus been given in terms of the moments of the generalized density matrix. The latter are to be determined by solving the equations of motion. We take the equation of motion for the density matrix to be of the form

$$\rho(\alpha x|\beta x'')H(x'',x') - H(x,x'')\rho(\alpha x''|\beta x') = \mathcal{H}(\alpha x|\gamma x'')\rho(\gamma x''|\beta x') - \rho(\alpha x|\gamma x'')\mathcal{H}(\gamma x''|\beta x'), \tag{3.10}$$

where

$$\mathcal{H}(\alpha x|\beta x') = h_{\alpha\beta}\delta(x-x') + \sum_\lambda F^{(\lambda)}_{\alpha\beta}F^{(\lambda)}_{\gamma\delta}\rho(\delta x|\gamma x') \tag{3.11}$$

is the generalized single-particle Hamiltonian corresponding to the choice (2.2) for the many-body Hamiltonian. As opposed to the equation of motion used in the alternative method, these equations are formally exact.

The equations upon which further developments are based are those which follow by taking the zeroth, first, and second moments of (3.10), using the convolution theorem. Remembering that the first moments $H^{(1,\mu)}$ are assumed to vanish, we shall also revert to the notation

$$V(x) \equiv H^{(0)}(x), \tag{3.12}$$

$$B^{\mu\nu}(x) \equiv H^{(2,\mu\nu)}(x). \tag{3.13}$$

The resulting equations may be written

$$i\rho^{(1,\mu)}_{\alpha\beta}(x)\partial_\mu V(x) = [\rho^{(0)},\mathcal{H}^{(0)}_{\alpha\beta}], \tag{3.14}$$

$$-i[(\partial_\nu\rho^{(0)})B^{\mu\nu} - \rho^{(2,\mu\nu)}\partial_\nu V] = [\rho^{(0)},\mathcal{H}^{(1,\mu)}] + [\rho^{(1,\mu)},\mathcal{H}^{(0)}], \tag{3.15}$$

$$i[\rho^{(1,\lambda)}\partial_\lambda B^{\mu\nu} - (\partial_\lambda \rho^{(1,\mu)})B^{\nu\lambda} - (\partial_\lambda \rho^{(1,\nu)})B^{\mu\lambda}]$$

$$= [\rho^{(0)}, \mathcal{H}^{(2,\mu\nu)}] + [\rho^{(2,\mu\nu)}, \mathcal{H}^{(0)}]$$

$$+[\rho^{(1,\mu)}, \mathcal{H}^{(1,\nu)}] + [\rho^{(1,\nu)}, \mathcal{H}^{(1,\mu)}]. \tag{3.16}$$

To construct the collective submanifold, we have solved these equations only for the values $q = 0$ and for the indices $\mu, \nu, \ldots$ taking on the values $i, j, \ldots$. In this case these equations have the same geometrical structure as the corresponding Hartree-Fock equations studied in the accompanying paper, and therefore the entire discussion of their equivalence to decoupling conditions derived from classical Hamiltonian mechanics can be taken over unchanged.

C. Pauli principle restrictions

We can dispose summarily of the Pauli principle constraints by considering the Hartree approximation as a subapproximation of the Hartree-Fock approximation. We can then utilize the same constraints as for the latter

$$(\rho^{(0)})^2 = \rho^{(0)}, \tag{3.17}$$

$$\sigma^{(0)}\rho^{(1,i)}\sigma^{(0)} = \rho^{(0)}\rho^{(1,i)}\rho^{(0)} = 0, \tag{3.18}$$

$$\rho^{(0)}\rho^{(2,ij)}\rho^{(0)} = -\rho^{(0)}(\rho^{(1,i)}\rho^{(1,j)} + \rho^{(1,j)}\rho^{(1,i)})\rho^{(0)}, \tag{3.19}$$

$$\sigma^{(0)}\rho^{(2,ij)}\sigma^{(0)} = \sigma^{(0)}(\rho^{(1,i)}\rho^{(1,j)} + \rho^{(1,j)}\rho^{(1,i)})\sigma^{(0)}, \tag{3.20}$$

$$\sigma^{(0)} = 1 - \rho^{(0)}. \tag{3.21}$$

Since these equations have been justified by reference to the alternative approach, the various moments depend on the collective coordinates Q and only the collective indices $\mu = i$ occur. As was done previously, we also assume that the odd moments have only nonvanishing (ph) and (hp) elements (and are to be determined dynamically), whereas the even moments have no such elements and their (pp) and (hh) elements are determined by the nonvanishing elements of lower order.

The remarks above do not dispose of all questions associated with the Pauli principle. Let us consider the equations of motion, for instance. Whereas the equations that underlie the method described in the accompanying paper strictly preserve the Pauli principle at every level of approximation, in the equations of motion in this paper the Pauli principle lies buried in the folds of the completeness relation used in the derivation of these equations. As soon as an approximation occurs here as a necessary dynamical compromise, that compromise propagates to the kinematics and the Pauli principle is also violated to some degree. This violation also obtains for the quantum fluctuations to which we turn below.

An attempt at a more formal treatment of the kinematical aspects of the Pauli principle can be found in the Appendix.

IV. COUPLING TO FAST COORDINATES: QUANTUM FLUCTUATIONS

The effect of the motion of the fast variables on the collective motion occurs both through the Berry potentials and the zero-point motion of the fast modes. The former has been discussed to some degree in Ref. [4], where the contributions were worked out in detail for some examples. The general formalism will not be repeated here, but a short discussion will be given at the end of this subsection. First we devote our attention to the fast modes that follow from the Hamiltonian $H^{(2)}_{\text{eff}}$, Eq. (2.23), as modified by the discussion subsequent to this equation. If we introduce creation and annihilation operators in the standard way,

$$q^a = \frac{1}{\sqrt{2}}(a_a + a_a^\dagger), \tag{4.1}$$

$$p_a = \frac{-i}{\sqrt{2}}(a_a - a_a^\dagger), \tag{4.2}$$

the normal form of $H^{(2)}_{\text{eff}}$ then becomes

$$H^{(2)}_{\text{eff}} = \frac{1}{2}(a_b a_c^\dagger + a_b^\dagger a_c)\mathcal{A}_{bc} + \frac{1}{2}(a_b a_c + a_b^\dagger a_c^\dagger)\mathcal{B}_{bc} - \frac{1}{2}\text{tr}\mathcal{A}, \tag{4.3}$$

$$\mathcal{A}_{ab} = \frac{1}{2}(V_{,ab} + B^{ab}), \tag{4.4}$$

$$\mathcal{B}_{ab} = \frac{1}{2}(V_{,ab} - B^{ab}). \tag{4.5}$$

The subtracted quantity in Eq. (4.3) is the zero-point energy associated with the Tamm-Dancoff approximation (TDA) (see below).

The normal modes of the Hamiltonian under discussion are determined by the equations of motion

$$\Omega\psi_a = \mathcal{A}_{ab}\psi_b + \mathcal{B}_{ab}\chi_b, \tag{4.6}$$

$$-\Omega\chi_a = \mathcal{A}_{ab}\chi_b + \mathcal{B}_{ab}\psi_b, \tag{4.7}$$

where, in a more detailed notation,

$$\psi_a^{(b)} = [0{:}Q|a_a|\Psi^{(b)}], \tag{4.8}$$

$$\chi_a^{(b)} = [0{:}Q|a_a^\dagger|\Psi^{(b)}], \tag{4.9}$$

$$|\Psi^{(a)}] = b_a^\dagger|0{:}Q], \tag{4.10}$$

$$b_a|0{:}Q] = 0, \tag{4.11}$$

$$b_a^\dagger = \psi_b^{(a)}a_b^\dagger - \chi_b^{(a)}a_b, \tag{4.12}$$

$$a_b^\dagger = \psi_b^{(a)*}b_a^\dagger + \chi_b^{(a)}b_a. \tag{4.13}$$

If we neglect the matrix $\mathcal{B}$, Eqs. (4.6) and (4.7) reduce to the TDA with eigenvalues ω. We thus have

$$\text{tr}\mathcal{A} = \sum_a \omega_a. \tag{4.14}$$

Introducing the normal mode operators b and $b^\dagger$, we thus obtain by a standard calculation [14]

$$H^{(2)}_{\text{eff}} = \sum_a \Omega_a b_a^\dagger b_a + \frac{1}{2}\sum_a(\Omega_a - \omega_a). \tag{4.15}$$

It remains for us to reassure ourselves that we can compute the matrices $\mathcal{A}$ and $\mathcal{B}$, that occur in the equations of motion or rather the pieces of which they are made, namely,

$$B^{ab} = f^a_{,\alpha}\tilde{B}^{\alpha\beta}f^b_{,\beta}, \tag{4.16}$$

$$V_{,ab} = g^\alpha_{,a}\tilde{V}_{,\alpha\beta}g^\beta_{,b}. \tag{4.17}$$

This matter has been discussed in Refs. [12,13]. First of all, the tilde matrices are determined by the Hartree energy; this point has been discussed exhaustively in previous works. Furthermore, without entering into all the subtleties, we may say that the decoupling conditions that determine the leading part of the collective Hamiltonian do so by determining a basis of tangent vectors, $g^\alpha_{,i}$, to the decoupled manifold and, at the same time, another basis of tangent vectors, $f^i_{,\alpha}$, where the two can be considered as the covariant and contravariant components of the same basis at the point in question. Given the k-dimensional basis ($i = 1,\ldots,k$) thus assembled, it is straightforward to define a complementary basis in the total space, with basis vectors, $f^a_{,\alpha}$ and $g^\alpha_{,a}$. Together with the known input matrices, these suffice to determine the matrices (4.16) and (4.17). The equations of motion are of the standard RPA form and hardly require further discussion except to note that they define an $(n-k)$-dimensional manifold of solutions.

The last observation leads us to pursue the current discussion just a bit further. In the course of constructing the decoupled manifold one already encounters a random-phase approximation (RPA) formalism, the one that produces the k basis vectors $f^i_{,\alpha}$ as solutions. But the equation in question lives in the entire configuration space. It is not surprising to find that the $n-k$ solutions discarded in the decoupling algorithm are precisely the solutions of Eqs. (4.6) and (4.7). To show this, it is convenient to consider the "real" form of these equations of motion,

$$\Omega\mathcal{Q}^a = iB^{ab}\mathcal{P}_b, \tag{4.18}$$

$$\Omega\mathcal{P}_a = -iV_{ab}\mathcal{Q}^b, \tag{4.19}$$

$$\mathcal{Q}^a = [0{:}Q|q^a|\Psi], \tag{4.20}$$

$$\mathcal{P}_a = [0{:}Q|p_a|\Psi]. \tag{4.21}$$

From (4.18) and (4.19), we obtain the two equations

$$\Omega^2\mathcal{P}_a = V_{ac}B^{cb}\mathcal{P}_b, \tag{4.22}$$

$$\Omega^2\mathcal{Q}^a = B^{ac}V_{cb}\mathcal{Q}^a. \tag{4.23}$$

Utilizing the definitions (4.16) and (4.17), and the decoupling condition

$$B^{ia} = f^i_\gamma\tilde{B}^{\gamma\delta}f^a_\delta = 0, \tag{4.24}$$

we can write, for example,

$$V_{ac}B^{cb} = g^\alpha_{,a}\tilde{V}_{,\alpha\gamma}\tilde{B}^{\gamma\beta}f^b_{,\beta}. \tag{4.25}$$

With the definition

$$\delta\pi_\alpha = f^a_{,\alpha}\mathcal{P}_a, \tag{4.26}$$

Eq. (4.22) takes the form

$$\Omega^2\delta\pi_\alpha = (f^a_{,\alpha}g^\beta_{,a})V_{\alpha\gamma}B^{\gamma\beta}\delta\pi_\beta. \tag{4.27}$$

The quantity in parentheses on the right-hand side of this equation is a projection operator onto the configuration space orthogonal to the (decoupled) collective manifold. It follows that

$$g^\alpha_{,i}\delta\pi_\alpha = 0, \tag{4.28}$$

i.e., solutions are to be sought in the space orthogonal to the collective manifold. It is, however, permissible to drop this projection operator, since we have previously identified the excluded solutions. What remains is precisely one form of the local RPA equation, of which a suitably chosen subset of solutions defines a basis associated with the collective submanifold, that is automatically orthogonal to the vectors that now interest us, the two sets together forming a complete set of solutions.

With a corresponding set of arguments for Eq. (4.23) we can show that it can be replaced by the alternative form of (4.27), namely,

$$\Omega^2\delta\xi^\alpha = \tilde{B}^{\alpha\gamma}\tilde{V}_{,\gamma\beta}\delta\xi^\beta, \tag{4.29}$$

where

$$\delta\xi^\alpha = g^\alpha_{,a}\mathcal{Q}^a, \tag{4.30}$$

and the solutions of current interest satisfy

$$f^i_{,\alpha}\delta\xi^\alpha = 0. \tag{4.31}$$

We now turn to the problem of calculating the Berry potentials. In fact, the appropriate general formulas have already been given in Ref. [4] and will only be quoted as needed. There they were applied to special models that violated time-reversal invariance. Here we suppose that our model does not violate this symmetry. As a consequence, we know that we can choose a single-particle basis in which all the shell-model matrix elements of the interaction are real. It follows that the ground-state correlation amplitudes can be chosen real, in further consequence of which the diagonal element of the Berry vector potential vanishes,

$$A_i = i[0{:}Q|\partial_i|0{:}Q] = 0. \tag{4.32}$$

However, the off-diagonal elements, as given by the equation,

$$(A_i)_{ab} = i[ab{:}Q|\partial_i|0{:}Q] = i[\psi^{(b)}_c\partial_i\chi^{(a)}_c - \chi^{(b)}_c\partial_i\psi^{(a)}_c], \tag{4.33}$$

where $|ab{:}Q]$ are "two-phonon" excitations in the non-collective space, do not vanish, in general. Therefore, the Berry scalar potential will contribute to the collective potential energy.

V. BERRY POTENTIALS IN THE MODEL OF LeTOURNEUX AND VINET

The purpose of this section is to provide another application of the formalism developed in Ref. [4], the basis for

which has just been derived. We shall redo, within the framework established, the recent work of LeTourneux and Vinet [10,11] that includes the effect of Berry potentials in a model with two interacting modes, the low-energy quadrupole mode and the higher-energy giant dipole mode.

Before defining the model, it is convenient to define the variables that will occur because several different choices are introduced that are each convenient for different purposes. For the description of the quadrupole mode, for instance, we utilize in turn a symmetric traceless tensor, $\mathcal{Q}_{ij}$, with i and j three-dimensional Cartesian indices, five real coordinates Q_m, and the usual spherical-tensor coordinates, $\alpha_{2\mu} = (-1)^\mu \alpha^\dagger_{2-\mu}$. These different objects are connected by the relations

$$Q_1 = \frac{\sqrt{3}}{2}\mathcal{Q}_{33} = -\frac{\sqrt{3}}{2}(\mathcal{Q}_{11} + \mathcal{Q}_{22}) = \alpha_{20}, \tag{5.1}$$

$$Q_2 = \mathcal{Q}_{13} = \frac{1}{\sqrt{2}}(\alpha_{21} - \alpha_{2-1}), \tag{5.2}$$

$$Q_3 = \mathcal{Q}_{23} = -\frac{i}{\sqrt{2}}(\alpha_{21} + \alpha_{2-1}), \tag{5.3}$$

$$Q_4 = \frac{1}{2}(\mathcal{Q}_{11} - \mathcal{Q}_{22}) = \frac{1}{\sqrt{2}}(\alpha_{22} + \alpha_{2-2}), \tag{5.4}$$

$$Q_5 = \mathcal{Q}_{12} = -\frac{i}{\sqrt{2}}(\alpha_{22} - \alpha_{2-2}). \tag{5.5}$$

In terms of these tensors, the quadratic invariant takes the forms (summation convention)

$$\frac{1}{2}\mathcal{Q}_{ij}\mathcal{Q}_{ij} = Q_m Q_m = \alpha^\dagger_{2\mu}\alpha_{2\mu}. \tag{5.6}$$

To describe the dipole mode we use Cartesian variables q_i.

For illustrative purposes, we choose to study essentially the same Hamiltonian as in previous work,

$$H = H_S + H_F, \tag{5.7}$$

$$H_S = \frac{1}{2}(P_m P_m + \omega_2^2 Q_m Q_m), \tag{5.8}$$

$$H_F = H_1 + H_{12}, \tag{5.9}$$

$$H_1 = \frac{1}{2}(p_i p_i + \omega_1^2 q_i q_i), \tag{5.10}$$

$$H_{12} = \omega_1^2 \kappa \mathcal{Q}_{ij} q_i q_j. \tag{5.11}$$

Here S and F refer to slow and fast parts of the Hamiltonian, respectively. The former is taken as a harmonic oscillator in the quadrupole variables and the latter as the sum of a harmonic oscillator in the dipole variables plus a trilinear coupling term dependent on the coordinates only.

We can put H_F into normal form by means of a real orthogonal transformation O that brings the matrix $\mathcal{Q}$ to diagonal form,

$$q_i = O_{ij}\bar{q}_j, \tag{5.12}$$

$$\tilde{O}O = I(\text{unit matrix}), \tag{5.13}$$

$$\tilde{O}\mathcal{Q}O = \Lambda(\text{diagonal matrix}). \tag{5.14}$$

Since the matrix Λ is traceless, we can represent its eigenvalues, Λ_i, in the form,

$$\Lambda_i = \beta\cos\left(\gamma - \frac{2\pi i}{3}\right), \tag{5.15}$$

involving the conventional quadrupole shape parameters. If we define

$$\Omega_i^2 = \omega_1^2 K_i(\beta,\gamma), \tag{5.16}$$

$$K_i = 1 + 2\kappa\beta\cos\left(\gamma - \frac{2\pi i}{3}\right), \tag{5.17}$$

the fast Hamiltonian takes the simple form

$$H_F = \frac{1}{2}\sum_i(\bar{p}_i\bar{p}_i + \Omega_i^2\bar{q}_i\bar{q}_i). \tag{5.18}$$

It is apparent that the barred variables refer to the intrinsic frame.

We shall find it convenient in the sequel to replace the coordinates and momenta by creation and annihilation operators by means of the standard formulas

$$q_i = \frac{1}{\sqrt{2\omega_1}}(a_i + a_i^\dagger), \tag{5.19}$$

$$p_i = -i\sqrt{\frac{\omega_1}{2}}(a_i - a_i^\dagger), \tag{5.20}$$

$$\bar{q}_i = \frac{1}{\sqrt{2\Omega_i}}(b_i + b_i^\dagger), \tag{5.21}$$

$$\bar{p}_i = -i\sqrt{\frac{\Omega_i}{2}}(b_i - b_i^\dagger). \tag{5.22}$$

By means of these definitions and Eq.(5.12), we have the following relations between the two sets of annihilation operators,

$$b_i = \frac{1}{2}[K_i^{\frac{1}{4}}O_{ji}(a_j + a_j^\dagger) + K_i^{-\frac{1}{4}}O_{ji}(a_j - a_j^\dagger)], \tag{5.23}$$

$$a_i = \frac{1}{2}O_{ij}[K_j^{-\frac{1}{4}}(b_j + b_j^\dagger) + K_j^{\frac{1}{4}}(b_j + b_j^\dagger)]. \tag{5.24}$$

In terms of these variables, the Hamiltonian now takes its simplest form

$$H = \frac{1}{2}\sum_m(P_m^2 + \omega_2^2 Q_m^2) + \sum_i\left(b_i^\dagger b_i + \frac{1}{2}\right)\Omega_i. \tag{5.25}$$

The two parts are coupled, of course, through the dependence of the frequencies Ω_i on the quadrupole degrees of freedom.

Since the Berry vector potential vanishes for this system when the dipole mode is unexcited, as we have previously explained, we shall look at the case where a single phonon is excited. Since the three possible states for which this can occur are almost degenerate, we must include all three in a Born-Oppenheimer description. With the standard definition of the one-phonon correlated state,

$$|i] = b_i^\dagger|0], \tag{5.26}$$

we look for approximate eigenstates of the form

$$|n\rangle = \sum_{i=1}^{3} \int dQ|Q)(Q|ni)|i]. \tag{5.27}$$

Applying the Hamiltonian (5.25) and taking a scalar product with a phonon basis state, we can derive an effective Schrödinger equation for the quadrupole motion in the form

$$H_{ij}(Q|nj) = E_n(Q|ni), \tag{5.28}$$

$$H_{ij} = \frac{1}{2}[P_m\delta_{ik} - (A_m)_{ik}][P_m\delta_{kj} - (A_m)_{kj}] + \frac{1}{2}\omega_2^2 Q_m Q_m + \delta_{ij}\left(\Omega_i + \frac{1}{2}\mathrm{tr}\Omega\right). \tag{5.29}$$

The derivation of the last equation follows the same path used in Ref. [4]. Here the vector potentials,

$$(A_m)_{ij} = \left[i\left|i\frac{\partial}{\partial Q_m}\right|j\right], \tag{5.30}$$

are both quadrupole tensors and SO(3) matrices.

The vector potential can be evaluated in terms of the elements defined by the equation

$$b_i^\dagger = \psi_j^{(i)} a_j^\dagger - \chi_j^{(i)} a_j, \tag{5.31}$$

that, in fact, can be read off from Eqs.(5.23) (all coefficients are real),

$$\psi_j^{(i)} = \frac{1}{2}O_{ji}(K_i^{\frac{1}{4}} - K_i^{\frac{-1}{4}}), \tag{5.32}$$

$$\chi_j^{(i)} = -\frac{1}{2}O_{ji}(K_i^{\frac{1}{4}} + K_i^{\frac{-1}{4}}). \tag{5.33}$$

Following techniques described and illustrated in Ref. [4], we then find

$$(A_m)_{ij} = (i\partial_m\psi_k^{(j)})\psi_k^{(i)} - (i\partial_m\chi_k^{(j)})\chi_k^{(i)}. \tag{5.34}$$

This completes the calculation of the effective Hamiltonian in the laboratory system, a result not given by the previous authors. If we chose to carry out numerical calculations in a basis of vibrational states, we could, in fact, stop here.

To make contact with previous work, however, we shall carry out one last task; namely, the transformation of the Hamiltonian matrix H_{ij} to the intrinsic system of the quadrupole tensor. Though we wish to be as brief as possible, it is necessary to recall a few standard formulas. In these considerations, we utilize the irreducible spherical tensor components, $\alpha_{2\mu}$ and their canonically conjugate variables, $\pi_{2\mu}$. The intrinsic components, indicated by bars, are related to a general choice by the formulas,

$$\bar{\alpha}_{2\mu} = \sum_\nu \alpha_{2\nu} D^{(2)*}_{\nu\mu}, \tag{5.35}$$

$$\bar{\alpha}_{20} = \beta\cos\gamma = a_0, \tag{5.36}$$

$$\bar{\alpha}_{22} = \bar{\alpha}_{2-2} = \frac{\beta}{\sqrt{2}}\sin\gamma = \frac{a_2}{\sqrt{2}}, \tag{5.37}$$

$$\bar{\alpha}_{21} = \bar{\alpha}_{2-1} = 0. \tag{5.38}$$

In terms of spherical tensor components, the two essential formulas needed to transform the kinetic energy, including vector-potential terms, are

$$\pi_{2\mu} = \frac{-i}{\sqrt{2}}\frac{(D^{(2)*}_{\mu 1} + D^{(2)*}_{\mu -1})}{2\beta\sin(\gamma - \frac{2\pi}{3})}L_1 + \frac{1}{\sqrt{2}}\frac{(D^{(2)*}_{\mu 1} - D^{(2)*}_{\mu -1})}{2\beta\sin(\gamma - \frac{4\pi}{3})}L_2 + \frac{i}{\sqrt{2}}\frac{(D^{(2)*}_{\mu 2} - D^{(2)*}_{\mu -2})}{2\beta\sin\gamma}L_3$$
$$-i\left(D^{(2)*}_{\mu 0}\cos\gamma + \frac{1}{\sqrt{2}}(D^{(2)*}_{\mu 2} + D^{(2)*}_{\mu -2})\right)\sin\gamma\frac{\partial}{\partial\beta} + i\left(D^{(2)*}_{\mu 0} - \frac{1}{\sqrt{2}}(D^{(2)*}_{\mu 2} + D^{(2)*}_{\mu -2})\cos\gamma\right)\frac{\partial}{\beta\partial\gamma}, \tag{5.39}$$

$$(A_{2\mu})_{ij} = i[(K_i/K_j)^{\frac{1}{4}} + (K_j/K_i)^{\frac{1}{4}}]\frac{1}{4\sqrt{2}}\left(-i\epsilon_{1ij}\frac{(D^{(2)*}_{\mu 1} + D^{(2)*}_{\mu -1})}{\beta\sin(\gamma - \frac{2\pi}{3})} + \epsilon_{2ij}\frac{(D^{(2)*}_{\mu 1} - D^{(2)*}_{\mu -1})}{\beta\sin(\gamma - \frac{4\pi}{3})} + i\epsilon_{3ij}\frac{(D^{(2)*}_{\mu 2} - D^{(2)*}_{\mu -2})}{\beta\sin\gamma}\right). \tag{5.40}$$

The derivation of these formulas is almost a textbook exercise [15,16] starting from (5.35)–(5.38) and the equations

$$\pi_{2\mu} = -i\frac{\partial}{\partial\alpha_{2\mu}} = \sum_i \frac{\partial\theta_i}{\partial\alpha_{2\mu}}L_i + \sum_{\alpha=0,2}\frac{\partial a_\alpha}{\partial\alpha_{2\mu}}(-i)\frac{\partial}{\partial a_\alpha}, \tag{5.41}$$

$$(L_l O_{kj})O_{ki} = \tilde{O}_{ik}L_l O_{kj} \tag{5.42}$$
$$= (i|L_l|j) \tag{5.43}$$
$$= i\epsilon_{lij}. \tag{5.44}$$

Here θ_i measures a rotation about the ith intrinsic axis and L_i is the corresponding intrinsic component of the angular momentum.

Putting these ingredients together, we can arrive at the final formula for the Hamiltonian matrix:

$$H_{ij} = \sum_{l,k} \frac{1}{8\beta^2 \sin^2(\gamma - \frac{2\pi l}{3})} \left\{ L_l \delta_{ik} + \frac{i}{2} \left[\left(\frac{K_i}{K_k} \right)^{\frac{1}{4} i} + \left(\frac{K_k}{K_i} \right)^{\frac{1}{4}} \right] \epsilon_{lik} \right\} \left\{ L_l \delta_{kj} + \frac{i}{2} \left[\left(\frac{K_k}{K_j} \right)^{\frac{1}{4}} + \left(\frac{K_j}{K_k} \right)^{\frac{1}{4}} \right] \epsilon_{lkj} \right\}$$
$$- \frac{1}{2\beta^4} \frac{\partial}{\partial \beta} \beta^4 \frac{\partial}{\partial \beta} - \frac{1}{2\beta^2 \sin 3\gamma} \frac{\partial}{\partial \gamma} \sin 3\gamma \frac{\partial}{\partial \gamma} + \frac{1}{2} \omega_2^2 \beta^2 + \delta_{ij} \left(\Omega_i + \frac{1}{2} \mathrm{tr} \Omega \right). \quad (5.45)$$

The interpretation of the extra terms in the kinetic energy compared to the well-known form for the quadrupole oscillator viewed in the intrinsic system has the obvious interpretation as the contribution of the dipole mode to the intrinsic angular momentum.

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APPENDIX: PAULI PRINCIPLE FOR METHOD I

We have pointed out in Sec. III that there is a conceptual difficulty in applying the Pauli principle to the method in this paper, which evaluates matrix elements of products of operators by means of a straight sum over intermediate states. Any approximation to this sum necessarily introduces some violation of the Pauli principle. In practice, we opted to impose the same conditions as in the alternative method, where the standard conditions that define a Slater determinant can be derived from the fundamental equations of the method. This is because, in practice, we use the same intermediate states as in the antisymmetric factorization. We can then argue that we have a Hartree approximation to a Hartree-Fock theory, and though we may have thus made a dynamical approximation, there is no reason not to retain the correct kinematics.

In this appendix, we investigate to what degree we can actually derive the Pauli principle restrictions from the equations of the method. Let $|x\rangle$ be the basis states for a system with N particles. We start with the identity

$$\langle x | a_\beta^\dagger a_\gamma^\dagger a_\gamma a_\alpha | x' \rangle = (N-1) \rho(\alpha, x | \beta, x'), \quad (A1)$$

where

$$\rho(\alpha, x | \beta, x') = \langle x | a_\beta^\dagger a_\alpha | x' \rangle,$$
$$\tau(\alpha, x | \beta, x') = \langle x | a_\alpha a_\beta^\dagger | x' \rangle, \quad (A2)$$
$$\rho + \tau = 1.$$

By commuting the fermion operators on the left-hand side of (A1) and summing over intermediate states, this equation may be rewritten as

$$\rho^2(\alpha, x | \beta, x') = \delta_{\alpha\beta} \delta(x - x') N - (N-1) \rho(\alpha, x | \beta, x')$$
$$= \rho(\alpha, x | \beta, x') + N \tau(\alpha, x | \beta, x'). \quad (A3)$$

Another pair of equations that can be derived from (A2) and (A3) by multiplying by the appropriate powers of ρ are

$$\rho^3 = \rho^2 - \rho^2 \tau, \quad (A4)$$

$$\rho^3 = \rho^2 + N \rho \tau. \quad (A5)$$

We study the zeroth moments of Eqs. (A2)–(A5). We need hardly record all of them. As a single example, (A3) becomes

$$(\rho^{(0)})^2_{\alpha\beta} = \rho^{(0)}_{\alpha\beta} + N \tau^{(0)}_{\alpha\beta}. \quad (A6)$$

From the zeroth moment of (A2), we conclude that $\rho^{(0)}$ and $\tau^{(0)}$ commute and can be diagonalized simultaneously. By combining the zeroth moments of (A4) and (A5), we obtain the equation

$$(\rho^{(0)} + N) \rho^{(0)} \tau^{(0)} = 0. \quad (A7)$$

In the representation in which the two matrices involved are diagonal, this equation requires that, for each eigenstate, one of the eigenvalues be zero. It follows from the remaining equations that the eigenvalue of the other is unity. Together with the condition

$$\mathrm{tr} \rho = N, \quad (A8)$$

this appears to be a satisfactory derivation of the condition that $\rho^{(0)}$ describe a Slater determinant. It also appears to be possible to derive the remaining ones of Eqs. (3.17)–(3.20), but we leave this as an exercise.

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