Quantum theory of large amplitude collective motion: Natural fit between the Born-Oppenheimer and Kerman-Klein methods

Abraham Klein
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104

Niels R. Walet
Institüt für Theoretische Physik III, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany
(Received 29 September 1993)

Starting from the shell model, we develop the foundations for a quantum theory of large amplitude collective motion that generalizes and extends some of our earlier work and is otherwise distinct from other methods espoused in the literature. The technical basis of our approach is the amalgamation of the Born-Oppenheimer approximation into the framework of the Kerman-Klein method. The version of the latter that is utilized is one that is applicable to an arbitrary two-body interaction and in which the Pauli principle is satisfied at each level of approximation. In the approximation considered, the one-band or adiabatic approximation, the fit is smooth and seamless, so much so that it is suggested that a multiband approach will be necessary to uncover the Berry potentials. The physics is worked out to the first two orders in the reciprocal of the number of particles participating in the collective motion, comprising the mean-field approximation and the first quantum fluctuations thereto, respectively. It is emphasized that the quantization procedure is integral to the method: there is no *ad hoc* requantization of a classical limit.

PACS number(s): 21.60.Ev, 21.60.Jz, 03.65.Ca

I. INTRODUCTION

Over the past decade, during which the authors and their collaborators have been studying the subject of large amplitude collective motion of a many-particle system, attention has been focused on the quantum foundations only at the outset [1,2] and again recently [3,4]. Our original stimulus to reopen this chapter was the practical necessity to include, in an ongoing application [3], quantum corrections to the requantized mean-field approximation. The decision to proceed beyond the limits of this immediate necessity [4] was fueled by several more general considerations.

There was first of all a perception that the original work [1,2] should be refined and updated, especially in the light of the Berry phase developments [5] and the attendant increased interest in the properties and application of the Born-Oppenheimer approximation (BOA). It is surprising that this approximation, which provides the underpinning of much of molecular and condensed matter physics has barely penetrated the study of collective motion in nuclear physics. Indeed the only effort in this direction of which we are aware is that of Villars [6–8]. The reason for this long-term neglect is apparent. The BOA provides a natural means of separating slow motions from fast motions for situations where the Hamiltonian is already expressed in terms of coordinates that clearly belong to one or the other set. In nuclear physics there is the additional nontrivial problem of *discovering* the coordinates that affect this separation. It is remarkable that this process of discovery, with a history of two decades, has achieved notable successes without essential appeal to the BOA. (For a brief review and further references, consult Ref. [9].)

One of the two major aims of this work is to explain how this was possible, but at the same time to show how the incorporation of the BOA provides conceptual and other improvements in the foundations of the theory. We shall see that the incorporation of the BOA into the Kerman-Klein framework for the many-body problem [10,11] can be carried out in a way that is so smooth and seamless that there appears to be no change in the formalism other than a more explicit definition of the collective states whose properties are to be determined. Further analysis appears to uncover the Berry potentials, but our conclusion is that the direct study of these objects is not natural within the framework utilized in this paper, which can be characterized as the single-band or strictly adiabatic approximation. If one wishes to focus on these potentials, it is suggested that either the framework has to be broadened to that of a multiband approximation [12], as we intend to do in future work, or else it has to be modified, as in the paper that accompanies the present one [13]. Neither of these alternatives, however, should be interpreted as a rejection of the method described in the current work, which provides the basis for our ongoing program of application [3].

The work that follows has a second goal, however. There are at present several major collaborations [14,15] whose aim is the application of a quantum theory of collective motion to phenomena of current experimental interest, such as the properties of superdeformed bands. This work utilizes the method of generator coordinates as the basis for quantization because of the belief of its authors that the only alternative is the requantization of

a classical Bohr Hamiltonian. The latter method, naturally associated with the self-consistent theory of large amplitude collective motion [9], is criticized because of the ambiguity of requantization of a kinetic energy term with a coordinate-dependent mass tensor. The method developed in this paper, on the contrary, is quantum throughout and does not suffer from this ambiguity, at the same time that it incorporates the classical procedures that have previously been thought to predetermine the resulting theory to be classical.

Our work originally had a third aim, but one that is not satisfied in the present paper. In the first effort designed to reopen the study of quantum foundations [4], we combined the BOA with the self-consistent theory of large amplitude collective motion, in application to a quantum many-body Hamiltonian expressed in terms of a set of coordinates and momenta in a curved space. It was claimed that such a Hamiltonian was an appropriate starting point even for the nuclear problem, provided we could show that it could be derived from a general nuclear shell-model Hamiltonian. No such derivation is given in this paper, which provides, nevertheless, a satisfactory alternative basis for the theory, able to incorporate the algorithms developed previously in conjunction with the mean-field approach. A derivation that satisfies the requirement of justifying the work of Ref. [4] is given in an accompanying paper [13]. The reason for separating the two methods is that the latter is based on assumptions that are more difficult to justify than those imposed in the current work.

The order of exposition is as follows: In Sec. II, we give a general definition of the collective Hamiltonian starting from a shell-model Hamiltonian. This definition is not new [3] except insofar as it incorporates the BOA. In Sec. III we undertake the major task of this work, the formulation of a microscopic theory of the collective Hamiltonian, by deriving formulas for the so-called moments of the shell-model Hamiltonian in terms of moments of the generalized density matrix, the basic ingredient of the Kerman-Klein method. The equations of motion for the moments of this density matrix are derived in Sec. IV, in which we also review the restrictions imposed by the Pauli principle. Section V is devoted to a discussion of the relation between the microscopic theory just formulated and the existing classical theory of large amplitude collective motion, in order to show how the algorithms developed for this theory are naturally incorporated into the extended formalism. Quantum corrections to the preceding formalism are taken up in Sec. VI, where only a brief discussion is necessary, since a full discussion of this topic has already been published [3]. We conclude the body of the text with a summary of our procedure. Appendix A contains a brief review of the factorization assumption that leads to the form of the Kerman-Klein method used in this work. Appendix B is devoted to the completion of a proof, started in Sec. V, of the equivalence of the equations of motion for the moments of the density matrix with the classical decoupling conditions. In Appendix C we point out the equivalence of the Wigner transform to the moment expansion method and remark on a further use of this method.

II. DEFINITION OF THE EFFECTIVE HAMILTONIAN

We study the problem defined by the shell-model Hamiltonian

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

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 order to carry out the program we have in view, we assume that there exists a basis of localized states,

$$|Q^i, q^a\rangle \equiv |x^\mu\rangle \equiv |Q, q\rangle = |Q)|q], \qquad \langle Q, q|Q'q'\rangle = \delta(Q - Q')\delta(q - q'). \tag{2.2}$$

Here the indices i range over a finite, usually small, set of values, $i = 1, \ldots, k$, whereas the set $a = k + 1, \ldots, n$ can be large and, in limiting cases, even infinite. Notice the use of the notation x^μ, $\mu = 1, \ldots, n$, when it is unnecessary to distinguish between the two sets of variables. When that distinction is essential, it is reinforced by the introduction of round and square brackets to distinguish basis vectors in the two subspaces. In terms of this basis set, which remains to be characterized in more detail, we assume the existence of a Hilbert space of collective states, $|n\rangle$, that can be represented in the general Born-Oppenheimer form

$$|n\rangle = \sum_\nu \int dQdq|Q)|q](Q|n\nu)[q|\nu:Q]. \tag{2.3}$$

It is supposed that for each value of Q, the wave functions $[q|\nu:Q]$ represent a complete set of states in the space of the fast variables,

$$\sum_\nu [q|\nu:Q][\nu:Q|q'] = \delta(q - q'). \tag{2.4}$$

In contrast to the molecular case, or to specially chosen simple examples, it is generally not possible to specify ahead of time the Hamiltonian of which the $[q|\nu:Q]$ are the eigenfunctions. Ultimately, as a consequence of the further development of the theory, we shall be able to obtain an approximate characterization of the space of the fast variables, adequate for most of our needs. In the usual Born-Oppenheimer or adiabatic approximation (BOA), to which the considerations that follow pertain, we restrict the set ν to a single value 0. The generalization to multiple values, though formally straightforward, is far from trivial when we attempt to combine it with a Kerman-Klein approximation and is presently under development.

The goal of this section is to derive an effective Hamiltonian for the collective subspace, defined within the BOA by the equation

$$(n|H_{\text{eff}}(Q,P)|n') \equiv \langle n|H|n'\rangle = \int (n|Q)[0:Q|q]dQdq\langle Q,q|H|Q',q'\rangle \times dQ'dq'[q'|0:Q'](Q'|n'), \quad (2.5)$$

which has utilized the BOA in the form of Eq. (2.3) with the sum restricted to the single term $\nu = 0$.

We wish H_{eff} to depend only on the collective variables Q and their canonically conjugate momenta P. To reach this objective we must integrate over the fast variables q. If our aim is purely to derive the starting point of Ref. [4], which is a Hamiltonian of second order in all the momenta, collective and noncollective, then the method that suggests itself is to carry out a Wigner transform of the nonlocal Hamiltonian matrix that appears in Eq. (2.5), or what is the same thing, a moment expansion in all the variables. Aside from the fact that it would fulfill one of the aims of this work, such an approach has other points of interest and therefore is discussed in an accompanying paper [13]. It also has several weaknesses, such as the fact that the application of a semiclassical approximation to the fast variables is difficult to justify, and that it does not satisfy the Pauli principle at each stage of approximation. It is for these reasons that we have chosen to describe separately the alternative method in this paper, which is also related to ideas that we have favored in the past [3].

The point is that one can define an effective Hamiltonian for the slow variables without initially making an expansion of any kind in the fast variables. Toward this end, it is convenient to rewrite the definition of the effective Hamiltonian, Eq. (2.5), in the condensed form

$$(n|H_{\text{eff}}|n') = \int dQdQ'(n|Q)\langle Q|H|Q'\rangle(Q'|n'), \quad (2.6)$$

where

$$|Q\rangle = |0:Q]|Q). \quad (2.7)$$

The states (2.7) are normalized according to

$$\langle Q|Q'\rangle = \delta(Q-Q'). \quad (2.8)$$

The last observation encourages us to carry out a moment expansion for the entire structure $\langle Q|H|Q'\rangle$. We define

$$\langle Q|H|Q'\rangle \equiv K(\bar{Q},\tilde{Q}), \quad (2.9)$$

where

$$\bar{Q} = \frac{1}{2}(Q+Q'), \quad \tilde{Q} = Q-Q'. \quad (2.10)$$

With the assumption that the matrix elements (2.9) are peaked in the differences of collective coordinates, we can carry out an expansion in terms of the delta function and its derivatives with respect to such coordinates. This expansion has the form

$$K(\bar{Q},\tilde{Q}) = K^{(0)}(\bar{Q})\delta(\tilde{Q}) + K^{(1,i)}(\bar{Q})(-i\tilde{\partial}_i)\delta(\tilde{Q}) + \frac{1}{2}K^{(2,ij)}(\bar{Q})(-i\tilde{\partial}_i)(-i\tilde{\partial}_j)\delta(\tilde{Q}) + \cdots. \quad (2.11)$$

In this expression the various coefficient functions are examples of the set of moments

$$K^{(n,i_1,\ldots,i_n)}(\bar{Q}) = \int d\tilde{Q}(-i)^n\tilde{Q}^{i_1},\ldots,\tilde{Q}^{i_n}K(\bar{Q},\tilde{Q}). \quad (2.12)$$

As we have explained in Ref. [3] and many previous times, the moment expansion for the collective variables should generate a convergent series in powers of the reciprocal of the number of particles participating in the collective motion.

Inserting this expansion into Eq. (2.6) we easily succeed in identifying the operator $H_{\text{eff}}(Q,P)$, namely,

$$H_{\text{eff}} = V(Q) + \frac{1}{8}\{P_i,\{P_j,B^{ij}\}\}, \quad (2.13)$$

$$V(Q) = K^{(0)}(Q), \quad (2.14)$$

$$B^{ij}(Q) = K^{(2,ij)}(Q). \quad (2.15)$$

In reaching this result, we have assumed that the first moments vanish by time reversal invariance.

Two observations are in order concerning the result found at this stage. Note first the absence of any sign of the coupling of the fast variables to the slow ones. It will turn out that the way to bring this coupling back into the picture is in the form of quantum fluctuations according to the theory developed recently [3]. This matter will be taken up in Sec. VI. The second observation is to note the absence of any sign of the Berry potentials. In the present formulation their effect is buried in our definition of the moment expansion. We describe an attempt to unearth this effect.

The obvious way to attempt to locate the "missing" Berry potentials is to delve more deeply into the structure of the quantity

$$\langle Q|H|Q'\rangle = [0:Q|(Q|H|Q')|0:Q'] \quad (2.16)$$

by carrying out a moment expansion for the matrix element

$$(Q|H|Q') = H^{(0)}(\bar{Q})\delta(\tilde{Q}) + H^{(1,i)}(\bar{Q})(-i\tilde{\partial}_i)\delta(\tilde{Q}) + \frac{1}{2}H^{(2,ij)}(\bar{Q})(-i)^2\tilde{\partial}_i\tilde{\partial}_j\delta(\tilde{Q}) + \cdots. \quad (2.17)$$

Note that in this case the various moments are still operators in the Hilbert space of the fast variables, since we have taken matrix elements only with respect to states defined in the collective subspace.

The most straightforward way to proceed is to substitute this expansion into Eq. (2.6), integrating by parts as necessary to carry out the integration over the relative coordinates. This calculation differs from the standard calculation that brings the Berry potentials to the forefront, given in a form particularly convenient for our purposes in Ref. [4]. The difference arises from the operator character of the moments defined in Eq. (2.17). The resulting effective Hamiltonian will depend on the Berry potentials defined by the equations

$$i\partial_i[q|\nu:Q] = \sum_{\nu'}[q|\nu':Q][A_i(Q)]_{\nu'\nu}, \tag{2.18}$$

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

and on an additional set of moments,

$$L^{(n,i_1,\ldots,i_n)}_{\nu\nu'} \equiv [\nu:Q|H^{(n,i_1,\cdots,i_n)}|\nu':Q]. \tag{2.20}$$

With the help of these equations, we find that H_{eff} takes the form

$$H_{\text{eff}} = \bar{V}(Q) + \frac{1}{8}\{D_i,\{D_j,\bar{B}^{ij}\}\} + S(Q), \tag{2.21}$$

$$\bar{V}(Q) = L^{(0)}(Q), \tag{2.22}$$

$$\bar{B}^{ij} = L^{(2,ij)}(Q), \tag{2.23}$$

$$D_i = P_i - A_i, \tag{2.24}$$

$$S(Q) = \frac{1}{8}\sum_{\nu,\nu'\neq 0}[(A_i)_{0\nu}(A_j)_{\nu\nu'}L^{(2,ij)}_{\nu'0} + \cdots], \tag{2.25}$$

where in the last equation, in the sum over ν and ν', the term in which both of these indices have the value zero is excluded. Further, the continuation dots represent the additional terms that would arise from an original double anticommutator of the three operators, i.e., a complete symmetrization. As we now explain this is not a very useful form of H_{eff}.

In order to understand the connection between the two forms of H_{eff}, we need the relation between the two sets of functions, K and L. For this purpose we sandwich (2.17) between $[\chi(Q)|$ and $|\chi(Q')]$ and follow that by an expansion of the arguments in these states about the value $\bar{Q}$. Finally, by utilizing such properties of the delta function as

$$\begin{aligned} x_\lambda\partial_\mu\partial_\nu\delta(x) &= -(\delta_{\mu\lambda}\,\partial_\nu + \delta_{\nu\lambda}\partial_\mu)\delta(x), \\ x_\lambda x_\rho\partial_\mu\partial_\nu\delta(x) &= (\delta_{\mu\lambda}\delta_{\nu\rho} + \delta_{\mu\rho}\delta_{\nu\lambda})\delta(x), \end{aligned} \tag{2.26}$$

we find straightforwardly, keeping terms only up to second moments, and dropping the first moment terms,

$$K^{(0)}(Q) = [\chi(Q)|H^{(0)}(Q)|\chi(Q)] - \frac{1}{2}i[\chi|\{\partial_i,H^{(1,i)}\}|\chi] + \frac{1}{2}\left(\frac{1}{2}i\right)^2[\chi|\{\partial_i,\{\partial_j,H^{(2,ij)}\}\}|\chi], \tag{2.27}$$

$$K^{(2,ij)} = [\chi|H^{(2,ij)}|\chi]. \tag{2.28}$$

To apply these relations, we remark first that for time-reversal invariant systems, the vector potential A_i vanishes. Next, from Eq. (2.28), $\bar{B}^{ij} = B^{ij}$. Thus the kinetic energies can be identified. Finally, a study of Eq. (2.27) shows that it is equivalent to the equation,

$$V(Q) = \bar{V}(Q) + S(Q). \tag{2.29}$$

It will turn out, however, as we develop the theory further, that it is the total quantity $V(Q)$ that is convenient to study rather than the individual pieces, so that the analysis just attempted is not very useful and will therefore not be pursued.

There is another, more physical, way of approaching Berry phase effects, namely, within the framework of a coupled bands approach, currently under study. Meanwhile in the accompanying paper, we shall encounter no trouble in exposing the contribution of Berry potentials in quite a conventional manner. But there we shall encounter other limitations, including difficulties satisfying the Pauli principle.

III. CALCULATION OF THE EFFECTIVE HAMILTONIAN

The aim of this section is to express the moments of the Hamiltonian matrix, $\langle Q|H|Q'\rangle$, in terms of elements that can be determined dynamically. Toward this end we apply the Kerman-Klein factorization method [10,11] reviewed briefly in Appendix A. In terms of the generalized density matrix elements,

$$\rho(\alpha Q|\beta Q') \equiv \langle Q'|a^\dagger_\beta a_\alpha|Q\rangle, \tag{3.1}$$

we have

$$\langle Q'|H|Q\rangle = h_{\alpha\beta}\rho(\beta,Q|\alpha,Q') + \frac{1}{2}V_{\alpha\beta\gamma\delta}\rho(\delta,Q|\beta,Q'')\rho(\gamma,Q''|\alpha,Q'). \tag{3.2}$$

For the same reason that the Berry potentials did not appear in the previous section, they will also not appear in the current discussion.

The further study of this expression relies upon the use of a moment expansion for the density matrix elements,

$$\rho(\alpha Q|\beta Q') = \rho^{(0)}_{\alpha\beta}(\bar{Q})\delta(\tilde{Q}) + \rho^{(1,i)}_{\alpha\beta}(\bar{Q})(-i\tilde{\partial}_i)\delta(\tilde{Q}) \times\frac{1}{2}\rho^{(2,ij)}_{\alpha\beta}(\bar{Q})(-i\tilde{\partial}_i)(-i\tilde{\partial}_j)\delta(\tilde{Q}) + \cdots, \tag{3.3}$$

where

$$\rho^{(n,i_1,\ldots,i_n)}_{\alpha\beta}(\bar{Q}) = \int d\tilde{Q}(-i)^n\tilde{Q}^{i_1},\ldots,\tilde{Q}^{i_n}\rho(\alpha Q|\beta Q'). \tag{3.4}$$

By inserting Eq. (3.3) into Eq. (3.2) and carrying out the intermediate integrations in the interaction term, we can obtain the basic result that we are after here, namely, the expression of the moments of the Hamiltonian matrix in terms of those of the generalized density matrix.

For cataloging purposes, we shall say that an nth moment of the density matrix is of order n. In this spirit we record here only the contributions of order zero, one, and two to the corresponding moments of the Hamiltonian matrix; the technical basis for the following result is given below. We thus find, omitting the bar on Q,

$$K^{(0)}(Q) = h_{\alpha\beta}\rho^{(0)}_{\beta\alpha}(Q) + \frac{1}{2}V_{\alpha\beta\gamma\delta}\rho^{(0)}_{\gamma\alpha}(Q)\rho^{(0)}_{\delta\beta}(Q), \tag{3.5}$$

$$K^{(1,i)}(Q) = h_{\alpha\beta}\rho^{(1,i)}_{\beta\alpha}(Q) + \frac{1}{2}V_{\alpha\beta\gamma\delta}[\rho^{(0)}_{\gamma\alpha}(Q)\rho^{(1,i)}_{\delta\beta}(Q) + \rho^{(1,i)}_{\gamma\alpha}(Q)\rho^{(0)}_{\delta\beta}(Q)], \tag{3.6}$$

$$K^{(2,ij)}(Q) = h_{\alpha\beta}\rho^{(2,ij)}_{\beta\alpha}(Q) + \frac{1}{2}V_{\alpha\beta\gamma\delta} \times \left[\rho^{(1,i)}_{\alpha\gamma}(Q)\rho^{(1,j)}_{\delta\beta}(Q) + \frac{1}{2}\rho^{(0)}_{\gamma\alpha}(Q)\rho^{(2,ij)}_{\delta\beta}(Q) + \frac{1}{2}\rho^{(2,ij)}_{\gamma\alpha}(Q)\rho^{(0)}_{\delta\beta}(Q)\right]. \quad (3.7)$$

In addition to the terms recorded, there are higher-order contributions to each moment that arise naturally in the calculation. It is essential to emphasize that the moments that intervene in these formulas are those involving the full many-body states $|Q\rangle$. It is in terms of these states that the fit between the BOA and the Kerman-Klein method is "seamless." As we have argued in the previous section, it does not appear to be natural to analyze this formalism further for the presence of Berry potential effects, and therefore this subject will be encountered next in the exposition in the accompanying paper.

The expressions given above for the moments of the Hamiltonian in terms of the moments of the generalized density matrix depend for their derivation on the convolution theorem for moment expansions. Before continuing with the main development, we derive such a result to the order required for this and subsequent applications. We utilize a notation applicable to the entire space of states, which can then be applied to the collective subspace by a specialization of variables and indices.

Given an operator product

$$C = AB \quad (3.8)$$

in the space of the states $|x\rangle$, where each of the matrices, e.g.,

$$\langle x|A|x'\rangle \equiv A(x,x'), \quad (3.9)$$

can be approximated by a moment expansion

$$A(x,x') = A^{(0)}(\bar{x})\delta(\tilde{x}) + A^{(1,\mu)}(\bar{x})(-i\tilde{\partial}_\mu)\delta(\tilde{x}) \times \frac{1}{2}A^{(2,\mu\nu)}(\bar{x})(-i\tilde{\partial}_\mu)(-i\tilde{\partial}_\nu)\delta(\tilde{x}) + \cdots, \quad (3.10)$$

the problem is to find an expression for the moments of C in terms of those of A and B.

The elementary steps are as follows (i) Insert the expansions of A and B into (3.8) and do the integration over the intermediate variable; (ii) the result exhibits the product of A and B as a sum of delta functions and their derivatives, but there remains the task of expressing all the coefficients as functions of $\bar{x}$ rather than of x or of x'. This deficiency is rectified by expanding about the value $\bar{x}$ and using Eq. (2.26). Keeping only the lowest-order and next to lowest-order terms, we thus identify the results

$$C^{(0)}(x) = A^{(0)}B^{(0)} + \frac{1}{2}i[\partial_\mu A^{(0)}B^{(1,\mu)} - A^{(1,\mu)}\partial_\mu B^{(0)}], \quad (3.11)$$

$$C^{(1,\mu)}(x) = A^{(0)}B^{(1,\mu)} + A^{(1,\mu)}B^{(0)} + \frac{1}{2}i[\partial_\nu A^{(0)}B^{(2,\mu\nu)} - A^{(2,\mu\nu)}\partial_\nu B^{(0)}] + \frac{1}{2}i[\partial_\nu A^{(1,\mu)}B^{(1,\nu)} - A^{(1,\nu)}\partial_\nu B^{(1,\mu)}], \quad (3.12)$$

$$C^{(2,\mu\nu)}(x) = [A^{(0)}B^{(2,\mu\nu)} + A^{(2,\mu\nu)}B^{(0)} + A^{(1,\mu)}B^{(1,\nu)} + A^{(1,\nu)}B^{(1,\mu)}] + \frac{1}{2}i[\partial_\lambda A^{(2,\mu\nu)}B^{(1,\lambda)} - A^{(1,\lambda)}\partial_\lambda B^{(2,\mu\nu)} + \partial_\lambda A^{(1,\mu)}B^{(2,\nu\lambda)} - A^{(2,\nu\lambda)}\partial_\lambda B^{(1,\mu)} + \partial_\lambda A^{(1,\nu)}B^{(2,\mu\lambda)} - A^{(2,\mu\lambda)}\partial_\lambda B^{(1,\nu)}]. \quad (3.13)$$

In the last of these equations, there is, in principle, also a contribution involving products of the zeroth and third moments of the ingredients, but since we have excluded third moments from the considerations thus far, we continue this practice here. We now turn to the further application of these results.

IV. EQUATIONS OF MOTION AND PAULI PRINCIPLE RESTRICTIONS

A. Equations of motion

The collective Hamiltonian has been shown to be determined by the low-order moments of the Hamiltonian matrix. The latter have been shown to be determined by the low-order moments of the generalized density matrix. In this section we exhibit the equations of motion from which the latter may be computed. Our starting point here are the equations of motion for the generalized density matrix as given in Ref. [11]. A particularly useful form of these equations is one in which the single-particle indices are displayed explicitly, but the equation is in matrix form with respect to the collective coordinates Q, namely,

$$[\rho_{\alpha\beta}, H] = \frac{1}{2}\{\mathcal{H}_{\alpha\gamma}, \rho_{\gamma\beta}\} - \frac{1}{2}\{\mathcal{H}_{\gamma\beta}, \rho_{\alpha\gamma}\}. \quad (4.1)$$

Here H is the original shell-model Hamiltonian, and $\mathcal{H}_{\alpha\beta}$ is the generalized Hartree-Fock Hamiltonian whose matrix elements are given by the expression

$$\mathcal{H}(\alpha, Q|\beta, Q') = h_{\alpha\beta}\delta(Q - Q') + V_{\alpha\beta\gamma\delta}\rho(\delta, Q|\beta, Q'). \quad (4.2)$$

The equations upon which further developments are based are those which follow by taking the zeroth, first, and second moments of (4.1). This is a straightforward application of Eqs. (3.11)–(3.13). Remembering that the first moments $K^{(1,\mu)}$ are assumed to vanish, we shall also revert to the notation of Eqs. (2.14) and (2.15). The resulting equations may be written

$$i\rho^{(1,i)}_{\alpha\beta}(Q)\partial_i V(x) = [\rho^{(0)}, \mathcal{H}^{(0)}_{\alpha\beta}], \tag{4.3}$$

$$-i[(\partial_j\rho^{(0)})B^{ij} - \rho^{(2,ij)}\partial_j V] = [\rho^{(0)}, \mathcal{H}^{(1,i)}] + [\rho^{(1,i)}, \mathcal{H}^{(0)}], \tag{4.4}$$

$$i[\rho^{(1,k)}\partial_k B^{ij} - (\partial_k\rho^{(1,i)})B^{jk} - (\partial_k\rho^{(1,j)})B^{ik}] = [\rho^{(0)}, \mathcal{H}^{(2,ij)}] + [\rho^{(2,ij)}, \mathcal{H}^{(0)}] + [\rho^{(1,i)}, \mathcal{H}^{(1,j)}] + [\rho^{(1,j)}, \mathcal{H}^{(1,i)}]. \tag{4.5}$$

We remark that to this order the same equations would have been obtained if the right-hand side of (4.1) were replaced by $[\mathcal{H}, \rho]_{\alpha\beta}$, which is an older form of the Kerman-Klein equations [10].

B. Pauli principle restrictions

The zeroth moment equation (4.3) has the form of a constrained Hartree-Fock equation. We have not yet established, however, that solutions are to be sought in the space of Slater determinants. As reviewed in Appendix A, we can start from the Pauli principle restriction of the generalized density matrix formalism. Written as an operator in the many-body space, it takes the form

$$\rho_{\alpha\beta} = \frac{1}{2}\rho_{\alpha\gamma}\rho_{\gamma\beta} + \frac{1}{2}\rho_{\gamma\beta}\rho_{\alpha\gamma}. \tag{4.6}$$

When the zeroth, first, and second moments of this equation are computed in lowest-order approximation, these turn out to be indistinguishable from the well-known relations that follow from the equation $\rho^2 = \rho$, evaluated by an expansion, $\rho = \rho^{(0)} + \rho^{(1)} + \rho^{(2)} + \cdots$, except that, in the relations below, the superscripts refer to a moment of a distribution rather than to the order of smallness; in fact, we have already made this identification. We shall not provide any algebraic details of this standard procedure, but only quote the final results in their most useful form, namely,

$$(\rho^{(0)})^2 = \rho^{(0)}, \tag{4.7}$$

$$\sigma^{(0)}\rho^{(1,i)}\sigma^{(0)} = \rho^{(0)}\rho^{(1,i)}\rho^{(0)} = 0, \tag{4.8}$$

$$\rho^{(0)}\rho^{(2,ij)}\rho^{(0)} = -\rho^{(0)}(\rho^{(1,i)}\rho^{(1,j)} + \rho^{(1,j)}\rho^{(1,i)})\rho^{(0)}, \tag{4.9}$$

$$\sigma^{(0)}\rho^{(2,ij)}\sigma^{(0)} = \sigma^{(0)}(\rho^{(1,i)}\rho^{(1,j)} + \rho^{(1,j)}\rho^{(1,i)})\sigma^{(0)}, \tag{4.10}$$

$$\sigma^{(0)} = 1 - \rho^{(0)}. \tag{4.11}$$

We note that the Pauli principle puts no restrictions on the (ph) and (hp) elements of $\rho^{(2,ij)}$. If we assume that these values can be chosen to be zero, then it becomes easy to generalize the pattern established in lowest order by the equations above. 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. This pattern turns out to be correct for the representation of the density matrix that we use in practice.

V. RELATION TO CLASSICAL MECHANICS

A. Canonicity conditions

The purpose of this section is to show that the first three moments of the equations of motion for the density matrix, as embodied in Eqs. (4.3)–(4.5), are equivalent to the so-called decoupling conditions of large amplitude adiabatic collective motion. These conditions, together with the canonicity condition, to be reviewed below, provide the basis for the algorithms that have been applied in practice. The importance of this proof is that the algorithms in question determine the ingredients of the collective Hamiltonian, called H_{eff} in this paper, namely, the potential energy and the mass tensor. Since the algorithms are formulated on the basis of a purely classical theory of collective motion, this shows that by following the reasoning of this paper, we have derived a quantum theory of collective motion without *ad hoc* requantization of the kinetic energy. The symmetric or Weyl form of the kinetic energy is prescribed.

The classical conditions in question arise as follows: As described in Ref. [4] and many antecedent works, we assume that the Hamiltonian has been given in terms of an arbitrary set of coordinates and momenta, ξ^α and π_α, $\alpha = 1, \ldots, n$ that do not separate naturally into a fast and a slow set. A preferred set, the coordinates that we have labeled x^μ, is one for which the transformed Hamiltonian has no terms linear in the fast coordinates or momenta. (The indices α and μ have the same range, but are chosen from different ends of the Greek alphabet in order to distinguish starting and transformed variables.) The two sets are assumed to be related to one another by a (locally invertible) point transformation,

$$\xi^\alpha = g^\alpha(x), \tag{5.1}$$

$$x^\mu = f^\mu(\xi). \tag{5.2}$$

In reality, the existing theory [9] does not determine a transformation such as (5.1) but only a projection of such a transformation onto the submanifold $(x) = (Q, q = 0)$, or (at best) an additional small neighborhood of this submanifold.

There is one important change of viewpoint compared to Ref. [4], a change already implied by some of our remarks above. In Ref. [4] we started with a quantum Hamiltonian in the "old" coordinates and transformed it to get the quantum Hamiltonian in the new coordinates. In this paper, we construct the quantum collective Hamiltonian directly in the favored coordinates. In the approximation under discussion, we require only the *classical* Hamiltonian in the old variables in order to construct the elements of the collective Hamiltonian, which are, after all, a set of point functions. Thus we start with H in the classical form

$$H = \tilde{H}(\xi, \pi) = \frac{1}{2}\pi_\alpha \tilde{B}^{\alpha\beta}\pi_\beta + \tilde{V}(\xi), \tag{5.3}$$

written down to define the elements $\tilde{V}$ and $\tilde{B}^{\alpha\beta}$ that occur, together with their derivatives, in the considerations below. For nuclear physics it is highly relevant that

the source of this classical Hamiltonian is the Hartree-Fock energy associated with a solution of time-dependent Hartree-Fock theory.

As we have already stated, the theory (in the guise of the decoupling conditions discussed below) determines the point transformation only in the subspace $q = 0$. In the classical limit, the quantum commutators among the collective variables, Q^i, P_j, become the Poisson bracket relations among the corresponding classical variables. For purposes of normalization, we shall use instead the chain-rule relations

$$\begin{aligned}\delta^i_j &= (\partial Q^i/\partial Q^j) \\ &= \frac{\partial Q^i}{\partial \xi^\alpha}\frac{\partial \xi^\alpha}{\partial Q^j} + \frac{\partial Q^i}{\partial \pi_\alpha}\frac{\partial \pi_\alpha}{\partial Q^j}.\end{aligned} \tag{5.4}$$

The equivalence of these equations and of the other partial derivatives involving the canonical coordinates to the Poisson bracket relations implies the validity of equations such as (5.7) below, that are well known to be sufficient conditions for a canonical transformation [16].

In order to utilize this connection as well as to carry out the comparison that is the major goal of this section, we must relate the arbitrary initial coordinates and momenta to the matrix elements of the density matrix in a corresponding arbitrary single-particle basis. As we have shown [17], there are two aspects to this identification. The first is the correspondence of indices, $\alpha \to (ph)$. The second is a one-to-one but nonlinear mapping between the elements $\rho^{(0)}_{ph}, \rho^{(0)}_{hp} = \rho^{(0)*}_{ph}$ and the canonical coordinates and momenta. To the order of accuracy of our theory this relationship can be taken as linear,

$$\begin{aligned}\rho^{(0)}_{ph} &= \frac{1}{\sqrt{2}}(\xi^{ph} + i\pi_{ph}), \\ \rho^{(0)*}_{ph} &= \frac{1}{\sqrt{2}}(\xi^{ph} - i\pi_{ph}).\end{aligned} \tag{5.5}$$

These equations show that we can treat the density matrix elements as complex canonical coordinates. It follows that (5.4) can be rewritten (suppressing the superscript zero)

$$\delta^i_j = \frac{\partial Q^i}{\partial \rho_{ph}}\frac{\partial \rho_{ph}}{\partial Q^j} + \frac{\partial Q^i}{\partial \rho_{hp}}\frac{\partial \rho_{hp}}{\partial Q^j}. \tag{5.6}$$

To obtain the final form of these equations, we use a well-known canonicity condition alluded to above, that follows from the comparison of Poisson bracket relations with the chain-rule equation that we are studying. In terms of the complex variables, it has the form

$$\begin{aligned}\frac{\partial Q^i}{\partial \rho_{ph}} &= i\frac{\partial \rho^*_{ph}}{\partial P_i} \\ &= i\rho^{(1,i)*}_{ph} = i\rho^{(1,i)}_{hp}.\end{aligned} \tag{5.7}$$

That we have correctly identified the first moment of the density matrix is most evident if one calculates the Wigner transform of the density matrix, $\rho(x', x'') \to \rho(x, p)$. The moments are then the coefficients of the expansion of $\rho(x, p)$ in a power series in p, as we verify in Appendix C.

B. Equivalence of equations of motion to decoupling conditions

The form of the decoupling conditions that we shall study corresponds to the case that the system has no constants of the motion in addition to the energy. These equations, which have been given in Ref. [9] and in numerous others of our previous works, take the form

$$V_{,a}(Q) = 0, \tag{5.8}$$

$$B^{ai}(Q) = 0, \tag{5.9}$$

$$B^{ij}_{,a} = 0. \tag{5.10}$$

We remind the reader that indices $i, j, \ldots$ refer to collective variables whereas indices $a, b, \ldots$ stand for noncollective coordinates. The case where there are additional constants of the motion [9] can be dealt with most conveniently by means of the Wigner transform, but will not be considered explicitly.

The equations above have a simple geometrical significance, characterizing a K-dimensional decoupled (collective) coordinate manifold parametrized by the preferred coordinate set $\{Q\}$. The first and third demand that the dynamical and geometrical forces, respectively, orthogonal to the decoupled manifold, vanish. The second condition states that a local coordinate system can be chosen at each point of the collective manifold such that the noncollective axes are orthogonal to the collective ones. We shall show that Eqs. (4.3)–(4.5) are equivalent to a different version of Eqs. (5.8)–(5.10), expressed in terms of relationships between the potential energy in the two sets of coordinates and other such relationships involving the mass tensor. Thus as a consequence of Eqs. (5.8)–(5.10), the chain rule for differentiation, and the tensor character of the mass tensor, the potential energy and the mass tensor expressed in terms of the old (tilde quantities) are related to the corresponding quantities in the preferred coordinate system by means of the equations

$$\tilde{V}_{,\alpha} = V_{,i} f^i_{,\alpha}, \tag{5.11}$$

$$\tilde{B}^{\alpha\beta} f^i_{,\beta} = B^{ij} g^\alpha_{,j}, \tag{5.12}$$

$$B^{ij}_{,\alpha} = B^{ij}_{,k} f^k_{,\alpha}. \tag{5.13}$$

In order to carry out a demonstration of the equivalence of Eqs. (4.3)–(4.5) to Eqs. (5.11)–(5.13), it is convenient to consider the latter in the form appropriate for complex canonical coordinates.

We revert then to the derivation promised, first considering Eq. (4.3). In view of the structure of this equation, only the ph or hp matrix elements are nonvanishing. We have, for example,

$$\mathcal{H}^{(0)}_{ph} = -i\rho^{(1,i)}_{ph}\partial_i V. \tag{5.14}$$

Since

$$\mathcal{H}^{(0)}_{ph} = \frac{\partial W_{\mathrm{HF}}[\rho_{ph}]}{\partial \rho^{(0)}_{hp}} = \frac{\partial V}{\partial \rho^*_{hp}}, \tag{5.15}$$

where W_{HF} is the Hartree-Fock functional, we can identify (5.14) with (5.11) provided

$$-i\rho_{ph}^{(1,i)} = \frac{\partial Q^i}{\partial \rho_{ph}^{(0)*}} \equiv f_{ph}^i, \tag{5.16}$$

which is the complex conjugate of (5.7). With this last identification, we have proved the equivalence to Eq. (5.11), albeit in terms of complex canonical coordinates.

Consider next Eq. (4.4). This equation has nonvanishing pp' and hh' elements that will be considered first. Recalling the fact that $\partial_i \rho^{(0)}$ has only ph and hp nonvanishing elements and using Eqs. (4.9) and (4.10) relating the hh' and pp' matrix elements of the second moment of the density matrix to the nonvanishing elements of the first moment, it is a straightforward exercise to see that the pp' and hh' elements of (4.4) are a consequence of the preceding equation (4.3). To study the ph and hp parts of (4.4) we need to know the quantities $\rho_{ph}^{(2,ij)}$ and $\rho_{hp}^{(2,ij)}$. We shall drop these quantities as a consequence of the argument given previously: There are no kinematical constraints on these quantities requiring them to be nonvanishing, and it also appears to be consistent with the dynamics to the order that we are working to do so. In any event, omitting these terms, we are left, for example, with the equation

$$-B^{php'h'}(i\rho_{p'h'}^{(1,j)}) = (\partial_j \rho_{ph}^{(0)}) B^{ij}, \tag{5.17}$$

$$B^{php'h'} = \frac{1}{2}(\mathcal{H}_{pp'}^{(0)} + \mathcal{H}_{p'p}^{(0)})\delta_{hh'} - \frac{1}{2}(\mathcal{H}_{h'h}^{(0)} + \mathcal{H}_{hh'}^{(0)})\delta_{pp'} + \frac{1}{2}(V_{ph'hp'} + V_{hp'ph'} - V_{pp'hh'} - V_{hh'pp'}). \tag{5.18}$$

This result can be identified with the complex conjugate of (5.12).

We turn finally to the analysis of the structure of Eq. (4.5). The details are somewhat more tedious, and are relegated to Appendix B. There we show that the ph elements can be identified with Eq. (5.13). Altogether we have shown that we can utilize the classical theory developed previously and apply this theory to the nuclear case by means of the "dictionary" developed in Ref. [17]. This dictionary is justified by the considerations of this section.

VI. COUPLING TO FAST COORDINATES: QUANTUM FLUCTUATIONS

Up to now we have almost completely suppressed any reference to the fast or noncollective variables. The next order of accuracy in the development of a collective Hamiltonian requires us to study this coupling, that in the current method is described as the inclusion of quantum fluctuations. By this we mean that we must include the possibility of excited states for the fast variables and of transitions between the ground-state collective band and these excited states. A study of this subject within the framework of ideas found in this paper has, in fact, already been carried out and applied to our study of ^{28}Si [3]. Since we consider this work to be the best we can muster in this respect, and indeed quite satisfactory except for the fact that we did not recognize the BOA explicitly, here we shall repeat and elaborate only one relatively small part of this development. Because it dovetails so well with some of the material found in the present work, we believe that this partial repetition will help clarify the ideas in question.

The object of the investigation is to compute an improved value for the collective potential energy, identified as the zeroth moment of $\langle Q|H|Q'\rangle$. This is done in terms of additional matrix elements of the generalized one-particle density operator connecting states already included in the collective space with excited states previously excluded from this space. Within the framework of the BOA, these additional states are of the form

$$|Q,\mu\rangle = |\mu{:}Q]|Q), \tag{6.1}$$

where here the symbol μ refers to other than the ground state of the fast system. These states are taken to satisfy the following conditions:

$$\langle Q,\mu|Q'\mu'\rangle = \delta_{\mu\mu'}\delta(Q-Q'), \tag{6.2}$$

$$\langle Q,\mu|Q'\rangle = 0, \tag{6.3}$$

$$\hat{Q}|Q,\mu\rangle = Q|Q,\mu\rangle, \tag{6.4}$$

where the last equation is a partial definition of the operator $\hat{Q}$.

To calculate matrix elements of the density operator connecting the collective space $|Q\rangle$ to these new states, we solve equations of motion for the single-particle operators of interest, namely, density operators or linear combinations thereof. Let θ be any one of these operators. Since the matrix elements within the collective subspace also occur in the formalism we shall first consider the equation of motion

$$\langle Q|[\theta,H]|Q'\rangle = -i\theta^{(1,i)}(\bar{Q})[\partial_i V(\bar{Q})]\delta(\tilde{Q}) + i[B^{ij}\partial_i\theta^{(0)} - \partial_i V\theta^{(2,ij)}][-i\tilde{\partial}_j\delta(\tilde{Q})]. \tag{6.5}$$

Here the evaluation of the matrix element of the commutator, that has been carried through to first-order moments, may be compared with the left-hand sides of Eqs. (4.3) and (4.4). We have already assumed that the first moment of the Hamiltonian vanishes. In the following we shall also drop the second moment of θ, as we have argued previously in this work, if it is to be identified with a particle-hole matrix element of the density operator. Furthermore, from the elementary properties of the operator Q, the first term on the right-hand side of (6.5) can be written as $\langle Q|[\theta,\hat{Q}\partial_i V(\bar{Q})]|Q'\rangle$. With all these specifications, Eq. (6.5) takes the final form useful for our purposes,

$$\langle Q|[\theta,[H-\hat{Q}\partial_i V(\bar{Q})]]|Q'\rangle = B^{ij}(\bar{Q})\partial_i\theta^{(0)}(\bar{Q})[\tilde{\partial}_j\delta(\tilde{Q})]. \tag{6.6}$$

Next, we evaluate the matrix element $\langle Q,\mu|[\theta,H]|Q'\rangle$. For this evaluation we do a sum over intermediate states, utilizing the two sets $|Q\rangle$ and $|Q,\mu\rangle$. The evaluation of the individual terms makes use of the equations

$$\langle Q,\mu|H|Q'\rangle = 0, \tag{6.7}$$

$$\langle Q,\mu|H|Q',\mu'\rangle = \langle Q|H|Q'\rangle\delta_{\mu\mu'} + \Omega_\mu\delta(Q-Q')\delta_{\mu\mu'}, \tag{6.8}$$

where the latter equation defines the excitation energy, Ω_μ. With the aid of these relations the remainder of the calculation parallels that done to derive (6.6). The result is

$$\langle Q,\mu|[\theta,H-\hat{Q}^i\partial_i V(\bar{Q})]|Q'\rangle = -\Omega_\mu\langle Q,\mu|\theta|Q'\rangle. \tag{6.9}$$

The manner in which the equations of motion derived above are used is to calculate the commutator $[\theta,H-\hat{Q}^i\partial_i V]$ from the shell-model Hamiltonian, and then to study the lowest moments of both sides, the zeroth and first moments for (6.6) and the zeroth moment for (6.9). The full analysis has been given in Ref. [3], to which we refer for all algebraic details and further discussion. The ultimate aim of the previous study was to find the quantum corrections to the potential energy that contains, in addition to the zero-point energy of the modes Ω_μ, correction terms associated with the correct treatment of the Pauli principle.

VII. SUMMARY

In this paper we have described a quantum theory of large amplitude collective motion based on an expansion in moments of the matrix of the shell-model Hamiltonian with respect to a basis of localized states. These localized states are assumed to be a direct product of a collective and of a noncollective subspace. The moment expansion is carried out with respect to the states of the collective subspace that are represented by means of a Born-Oppenheimer approximation. Our goal is a microscopic theory that is achieved by the following sequence of steps.

(i) Definition of a collective Hamiltonian whose elements are determined by zeroth and second moments of the shell-model Hamiltonian. These moments determine the potential and kinetic energies, respectively.

(ii) Expression of the moments of the Hamiltonian in terms of the moments of the generalized density matrix of the Kerman-Klein method.

(iii) Derivation of the equations of motion for the moments of the generalized density matrix.

(iv) Proof that the preceding equations are equivalent to the decoupling conditions previously established within the framework of classical Hamiltonian mechanics and for which several successful algorithms have been established.

(v) Generalization of the previous considerations to include the leading effect of quantum fluctuations that bring the noncollective degrees of freedom back into the picture.

The preceding theory is, except for the problem of band crossing, sufficient to deal with the topics of current interest in large amplitude collective motion. The problem of band crossing within the framework of the Kerman-Klein method is currently under investigation.

This work was supported in part by the U.S. Department of Energy under Grant No. 40264-5-25351.

APPENDIX A: GENERALIZED DENSITY MATRIX FORMALISM

We review briefly those aspects of the equation of motion method [11], designed to preserve the Pauli principle when approximations are made. The computation of matrix elements of the Hamiltonian of the type $\langle Q|H|Q'\rangle$ is predicated on the factorization of the two-body density matrix

$$\begin{aligned}\langle Q|a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma|Q'\rangle \cong \frac{1}{2}[&\langle Q|a^\dagger_\beta a_\delta|Q''\rangle\langle Q''|a^\dagger_\alpha a_\gamma|Q'\rangle \\ &-(\beta\leftrightarrow\alpha)-(\delta\leftrightarrow\gamma) \\ &+(\beta\leftrightarrow\alpha,\delta\leftrightarrow\gamma)],\end{aligned} \tag{A1}$$

which is assumed to be valid when pairing correlations are absent. The simplest qualitative arguments in favor of this approximate factorization are as follows: (i) it satisfies the Pauli principle; (ii) by suitable choice of the states $|Q\rangle$, it leads to equations that preserve the symmetries broken by standard Hartree-Fock theory, namely, translation and rotation invariance; (iii) it reduces to Hartree-Fock theory in the appropriate limit. It should be remarked, however, that there is a certain danger in taking the factorization too literally, since there are certainly important neglected two-particle correlations. Furthermore, the intermediate states must be restricted, since carrying the sum over too large a space must lead eventually to overcounting. At the present stage of development of the applications, this does not represent an imminent danger.

The validity of the ensuing theory only requires the accuracy of two special averages of this factorization to be valid, the one carried out with the matrix elements of the two-body potential that determines the equations of motion and the one that leads to Pauli principle restrictions on the single-particle density matrix. The results of this factorization are exhibited as Eqs. (4.1) and (4.6) of the text. The derivation of these equations has been discussed thoroughly in Ref. [11] and will not be repeated here.

APPENDIX B: EQUIVALENCE OF THE EQUATIONS OF MOTION WITH THE DECOUPLING CONDITIONS

In Sec. V we have studied the equivalence of the various moments of the equations of motion with the decoupling conditions, succeeding in establishing the result through the first-order moments. Here we study the second-order moment equation (4.5). Basically, we wish to prove that the ph elements of this equation have the form

$$B^{ij}_{,ph} = B^{ij}_{,k}\frac{\partial Q^k}{\partial\rho_{ph}} = B^{ij}_{,k}(-i\rho^{(1,k)}_{hp}). \tag{B1}$$

Remembering that the second moment of ρ has no ph elements, and also reordering the terms of (4.5), we have

$$(-i\rho^{(1,k)}_{hp})B^{ij}_{,k} = -i\left(\frac{\partial\rho^{(1,i)}_{ph}}{\partial Q^k}B^{jk} + \frac{\partial\rho^{(1,j)}_{ph}}{\partial Q^k}B^{ik}\right) - \mathcal{H}^{(2,ij)}_{ph} + \rho^{(2,ij)}_{pp'}\mathcal{H}^{(0)}_{p'h} - \mathcal{H}^{(0)}_{ph'}\rho^{(2,ij)}_{h'h}$$
$$+\rho^{(1,i)}_{ph'}\mathcal{H}^{(1,j)}_{h'h} - \mathcal{H}^{(1,j)}_{pp'}\rho^{(1,i)}_{p'h} + \rho^{(1,j)}_{ph'}\mathcal{H}^{(1,i)}_{h'h} - \mathcal{H}^{(1,i)}_{pp'}\rho^{(1,j)}_{p'h}. \tag{B2}$$

We would like to show that the right-hand side of this equation equals $(\partial B^{ij}/\partial\rho_{ph})$. Since

$$B^{ij} = \rho^{(1,i)}_{ph}B^{php'h'}\rho^{(1,j)}_{p'h'} + (i \leftrightarrow j), \tag{B3}$$

differentiation with respect to ρ_{ph} leads to two sorts of terms. Those arising from the differentiation of the explicit factors of the first moments of ρ are precisely the first two terms on the right-hand side of (B2). Therefore, we need only consider the remaining terms which should be identified with the derivative of $B^{php'h'}$. We exhibit these terms in the form obtained by inserting the definitions of $\mathcal{H}^{(1,i)}$ and $\mathcal{H}^{(2,ij)}$ as well as the expressions for the pp' elements of the second moments of ρ in terms of the nonvanishing elements of the first moments. We thus find the array of terms

$$\rho^{(1,i)}_{ph'}\rho^{(1,j)}_{h'p'}\mathcal{H}^{(0)}_{p'h} + (i \leftrightarrow j) + \mathcal{H}^{(0)}_{ph'}\rho^{(1,i)}_{h'p'}\rho^{(1,j)}_{p'h} + (i \leftrightarrow j) - \rho^{(1,i)}_{p'h'}V_{pp''hp'}\rho^{(1,j)}_{h'p''} - (i \leftrightarrow j) + \rho^{(1,i)}_{h'p'}V_{p'h''hh'}\rho^{(1,j)}_{p'h''} + (i \leftrightarrow j)$$

$$+\rho^{(1,i)}_{ph'}V_{h'p'hh''}\rho^{(1,j)}_{h''p'} + (i \leftrightarrow j) + \rho^{(1,i)}_{ph'}V_{h'h''hp'}\rho^{(1,j)}_{p'h''} + (i \leftrightarrow j) - \rho^{(1,i)}_{p'h}V_{ph'p'p''}\rho^{(1,j)}_{p''h'}$$

$$-(i \leftrightarrow j) - \rho^{(1,i)}_{p'h}V_{pp''p'h'}\rho^{(1,j)}_{h'p''} - (i \leftrightarrow j). \tag{B4}$$

To show that this is the required set of terms, we must differentiate $B^{p'h'p''h''}$, Eq. (5.18), with respect to ρ_{ph}. For this purpose, we apply the differentiation formulas for one-particle operators Θ_{ab},

$$\frac{\partial\Theta_{ab}}{\partial\rho_{ph}} = -\delta_{ap}\Theta_{hb} + \delta_{bh}\Theta_{ap}, \tag{B5}$$

$$\frac{\partial\Theta_{ab}}{\partial\rho_{hp}} = -\delta_{bp}\Theta_{ah} + \delta_{ah}\Theta_{pb}, \tag{B6}$$

as well as the corresponding one for two-particle operators V_{abcd},

$$\frac{\partial V_{abcd}}{\partial\rho_{ph}} = -\delta_{ap}V_{hbcd} - \delta_{pb}V_{ahcd} + \delta_{ch}V_{abpd} + \delta_{dh}V_{abcp}, \tag{B7}$$

$$\frac{\partial V_{abcd}}{\partial\rho_{hp}} = -\delta_{pc}V_{achd} - \delta_{pd}V_{abch} + \delta_{ah}V_{pbcd} + \delta_{bh}V_{apcd}. \tag{B8}$$

The formulas given above have been derived several times in our previous work, for instance, in [17]. The simplest means of derivation is to note the formulas

$$\delta|h) = \sum_p |p)\delta\rho_{ph},$$
$$\delta|p) = -\sum_h |h)\delta\rho_{hp}. \tag{B9}$$

The application of these formulas to the terms of $B^{php'h'}$, together with the recognition of the properties of the resulting terms under exchange of indices soon reveals the identity sought.

APPENDIX C: EQUIVALENCE OF THE MOMENT EXPANSION TO THE WIGNER TRANSFORM

We define the Wigner transform of a matrix

$$\langle Q|A|Q'\rangle \equiv A(Q,Q') \tag{C1}$$

as the Fourier transform with respect to the difference coordinate $\tilde{Q} = Q - Q'$,

$$\tilde{A}(\bar{Q},\bar{P}) = \int d\tilde{Q}\exp(-i\bar{P}\tilde{Q})A(Q,Q') = \sum_{n=0}\frac{1}{n!}A^{(n,i_1,\ldots,i_n)}\bar{P}_{i_1},\ldots,\bar{P}_{i_n}. \tag{C2}$$

This transform is of particular value when the original function A is sharply peaked in the variables $\tilde{Q}$. It is then a slowly varying function of the variables $\bar{P}$, thus justifying the multiple Taylor series in these variables. The coefficients in this expansion are seen to be the moments utilized in the body of the text. Dropping the bars, we thus have

$$A^{(n,i_1,\ldots,i_n)}(Q) = \frac{\partial}{\partial P_{i_1}}\cdots\frac{\partial}{\partial P_{i_n}}\tilde{A}(Q,P)|_{P=0}. \tag{C3}$$

We consider next the convolution theorem for the Wigner transform. Confining our attention to the leading terms only, we have

$$\tilde{C}(Q,P) = \tilde{A}(Q,P)\tilde{B}(Q,P) + \frac{1}{2}i\sum_i\left(\frac{\partial\tilde{A}}{\partial Q^i}\frac{\partial\tilde{B}}{\partial P_i} - \frac{\partial\tilde{A}}{\partial P_i}\frac{\partial\tilde{B}}{\partial Q^i}\right). \tag{C4}$$

The convolution equations for moment functions utilized in the text are trivial consequences of (C3) and (C4). Finally, if we interpret the P_i as classical canonical mo-

menta and if some subset of them are constants of the motion instead of continuously variable, we are led most naturally in the present framework to modify the conclusions that can be drawn from convolution theorems. This would allow us to make contact with the version of the classical theory where there are indeed additional constants of the motion, but we shall not pursue these matters in detail here.

[1] A. Klein, Nucl. Phys. **A410**, 70 (1983).
[2] A. Klein, Nucl. Phys. **A431**, 90 (1984).
[3] N. R. Walet, A. Klein, and G. do Dang, Phys. Rev. C **45**, 249 (1992).
[4] A. Klein and N. R. Walet, Phys. Rev. C **48**, 178 (1993).
[5] M. V. Berry, in *Geometric Phases in Physics*, edited by A. Schapere and F. Wilczek (World Scientific, Singapore, 1989), p. 7.
[6] F. M. H. Villars, Nucl. Phys. **A420**, 61 (1984).
[7] F. M. H. Villars, Nucl. Phys. **A473**, 539 (1987).
[8] N. Zettili and F. M. H. Villars, Nucl. Phys. **A469**, 77 (1987); **A469**, 93 (1987).
[9] A. Klein, N. R. Walet, and G. do Dang, Ann. Phys. (N.Y.) **208**, 90 (1991).
[10] A. Klein, in *Progress in Particle and Nuclear Physics*, edited by D. Wilkinson (Pergamon, London, 1983), Vol. 10, p. 39.
[11] A. Klein, Phys. Rev. C **30**, 1680 (1984).
[12] D. Brink and G. Schütte, Z. Phys. A **310**, 307 (1983).
[13] A. Klein and N. R. Walet, Phys. Rev. C **49**, 1439 (1994), the following paper.
[14] P.-H. Heenen, P. Bonche, J. Dobaczewski, H. Flocard, S. J. Krieger, J. Meyer, J. Skalski, N. Tajima, and M. S. Weiss, in *International Workshop on Nuclear Structure Models*, edited by R. Bengsston, J. Draayer, and W. Nazarewicz (World Scientific, Singapore, 1992), p. 3.
[15] J.-F. Berger, J. Decharge, and D. Gogny, in *International Workshop on Nuclear Structure Models*, edited by R. Bengsston, J. Draayer, and W. Nazarewicz (World Scientific, Singapore, 1992), p. 26.
[16] H. Goldstein, *Classical Mechanics* (Addison-Wesley, Reading, MA, 1980), p. 391.
[17] A. Bulgac, A. Klein, N. R. Walet, and G. do Dang, Phys. Rev. C **40**, 945 (1989).