Quantum theory of large amplitude collective motion and the Born-Oppenheimer method

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(Received 19 March 1993)

We study the quantum foundations of a theory of large amplitude collective motion for a Hamiltonian expressed in terms of canonical variables. In previous work the separation into slow and fast (collective and noncollective) variables was carried out without the explicit intervention of the Born-Oppenheimer approach. The addition of the Born-Oppenheimer assumption not only provides support for the results found previously in leading approximation, but also facilitates an extension of the theory to include an approximate description of the fast variables and their interaction with the slow ones. Among other corrections, one encounters the Berry vector and scalar potential. The formalism is illustrated with the aid of some simple examples, where the potentials in question are actually evaluated and where the accuracy of the Born-Oppenheimer approximation is tested. Variational formulations of both Hamiltonian and Lagrangian type are described for the equations of motion for the slow variables.

PACS number(s): 21.60.−n, 21.60.Ev, 0.3.65.Ca, 03.65.Sq

I. INTRODUCTION

For the past decade, the authors and their collaborators have been involved in the development of a theory of large amplitude collective motion. This enterprise began with a pair of papers [1,2] on possible quantum foundations for such a program. Soon thereafter [3] it was realized that the leading approximation, to which most previous studies had been confined, was classical in nature, (with subsequent requantization) and, as a consequence, almost all later systematic theoretical development, reviewed in Ref. [4], was based on the study of this limit.

Quantum corrections can be important in selected circumstances, however. Consequently, the elements of a systematic method for including quantum corrections by expansion about the classical limit has recently been developed [5], distinct from the approaches found in our initial papers. We consider it worthwhile, nevertheless, in the light of subsequent developments, especially within the context of the Berry phase idea [6,7], to update, augment, and improve the work described in those initial efforts and to tie them, where possible, to more recent work. In a paper currently in preparation, we shall contrast the nuclear-physics foundations of the method described in this paper with that found in Ref. [5], both approaches requiring elaboration compared to what has already been published.

In Sec. II we give a condensed but at the same time more precise account of the essential theoretical content of Ref. [1], namely, a method for separating and identifying a collective subspace for a specified class of Hamiltonians. This is done in an approximation that suppresses

any coupling to noncollective degrees of freedom. As opposed to the corresponding problem in molecular physics, the Hamiltonian is generally given in a form where the coordinates are not appropriate to make the separation of the Hamiltonian into a collective and a noncollective part. The discovery of new coordinates that will effect the separation is an essential part of the problem. In the regime of large amplitude collective motion, a reasonably complete theory that can be implemented [4,5] has been developed so far only for the case that the transformations to new coordinates and momenta are restricted to point transformations.

In Sec. III, we describe how the previous theory may be extended to include the interaction between the fast and slow variables. This is done by means of a standard Born-Oppenheimer (BO) representation of the states of the slow variables. Though some of the ensuing details are similar to those encountered in the molecular problem, leading, for example, to the occurrence of Berry potentials [6,7], others are characteristic of the problem of large amplitude collective motion. In order to evaluate the corrections found to the potential energy of the collective variables, it is necessary to obtain wave functions for the fast variables. This is done by an extension of the analysis carried out in Sec. II. At the same time this development provides a justification for some of the assumptions of the previous analysis.

In Sec. IV, we present material that has no direct counterpart in any previous work in this field, outside our own. One of the results of Sec. III was to establish a complete effective quantum mechanics in the collective subspace, i.e., we not only computed an effective Hamiltonian operator in the collective subspace, but also proved that it was expressed in terms of canonical variables. In Sec. IV we study variational principles for the associated Heisenberg matrix mechanics. If we put aside, momentarily, special difficulties associated with

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the curved spaces that we allow in our general formulation, we find quantum analogues of variational principles both for Hamilton's and for Lagrange's equations. The connection between the two forms is the standard one, even when Berry phase terms are included, in contrast to a result based on the use of path integrals [7]. For the general case of a curved space the situation is more involved, and only a variational principle for Hamilton's equations is presented and analyzed.

The corrections to the potential energy of collective motion found in Sec. III are of three types. There is first a "quantum" potential arising from the curved space (position-dependent mass tensor). This term cannot be evaluated fully with the tools developed in our previous work [4]. In practical applications to systems with N degrees of freedom, this term is of order N^{-2}, and therefore should be small for a many-body system. A second term consists of the eigenvalue for the state of the fast variables for a fixed value of the slow variables. In our approximation this state is that of a set of independent harmonic oscillators, with frequencies dependent on the instantaneous value of the collective coordinates. We are mainly (though not exclusively) interested in the zero-point motion associated with the ground state. This contribution, which is only of order N^{-1} compared to the leading term, has been studied previously in simple examples [8]. A third correction, referred to as the Berry scalar potential, occurs together with the Berry vector potential, both appearing in the collective Hamiltonian as a consequence of the BO approximation.

Examples in the literature relevant to the approach described in this paper are not numerous. The examples studied by Bulgac [9,10] have been stimulating, but a bit too simple for our purposes. On the other hand, the work by Girard, LeTourneux, and Vinet [11] on the dipole-quadrupole problem in spherical nuclei is too complex to satisfy our initial needs. Section V is devoted to the study of several "in-between" models sufficiently simple that the BO approximation can be carried out, including the calculation of the Berry potentials, and compared with more exact results. Some technical details associated with the material of Secs. II and III, respectively, are provided in two appendices.

II. SUMMARY OF PREVIOUS RESULTS

In this paper we base our study on a Hamiltonian that with the help of the summation convention takes the form

$$H = \tilde{H}(\xi^\alpha, \pi_\alpha) = \frac{1}{8}\{\pi_\alpha, \{\pi_\beta, \tilde{B}^{\alpha\beta}(\xi)\}\} + V(\xi), \quad (2.1)$$

that describes N coordinate and momentum pairs, ξ^α and π_α, $\alpha = 1 \cdots N$, that satisfy canonical commutation relations ($\hbar = 1$),

$$[\xi^\alpha, \pi_\beta] = i\delta^\alpha_\beta. \quad (2.2)$$

We thus allow for a curved space described by a (reciprocal) mass tensor $\tilde{B}^{\alpha\beta}$. Not only is this formulation of interest for a range of applications outside of nuclear

physics [4,8], but it is also possible [12] to transform the large amplitude problem of nuclear collective motion into this form as the basis for further development. Associated with this Hamiltonian is a form for the scalar product in Hilbert space that is discussed in Appendix A.

The problem of immediate interest is to find a decomposition of the operator $\tilde{H}$ into two parts, exactly in rare cases, approximately under most circumstances, that describe slow and fast (or collective and noncollective) degrees of freedom. A basic difficulty of the class of problems that interest us is that we cannot assume that this separation occurs for the initial choice of coordinates. Instead, we assume that it is possible to effect such a decomposition, at least approximately, by means of a point transformation of the form

$$\begin{aligned} \xi^\alpha &= g^\alpha(x), \\ x &= \{Q^i, q^a\}, \\ \\ i &= 1 \cdots K, \\ a &= K + 1 \cdots N, \end{aligned} \quad (2.3)$$

that is locally invertible,

$$x^\mu = f^\mu(\xi). \quad (2.4)$$

Though we have discussed, in the past [3,4], the possible interest of going beyond point transformations in the study of large amplitude collective motion, it is only for this simpler class of transformations that a substantial theoretical underpinning can be claimed to exist, a foundation that we wish to widen in the present work. (Of course, there is a substantial literature based on transformations that are polynomial in coordinates and momenta that are applicable to anharmonic vibrations (see, for instance [13,14]), but this is not the subject of the current paper.)

A first step is to carry out a formal transformation of the Hamiltonian, H, to the new variables. For the potential energy, we have, trivially enough,

$$\tilde{V}(\xi) = \tilde{V}[g^\alpha(Q,q)] \equiv V(Q,q). \quad (2.5)$$

Turning then to the consideration of the kinetic energy, $\tilde{T}$,

$$\tilde{T} = \frac{1}{8}\{\pi_\alpha, \{\pi_\beta, \tilde{B}^{\alpha\beta}(\xi)\}\}, \quad (2.6)$$

this expression can be transformed to the new variables with the aid of the relations [1]

$$\pi_\alpha = \tfrac{1}{2}\{f^\mu_{,\alpha}, p_\mu\}, \quad (2.7)$$

$$B^{\mu\nu} = f^\mu_{,\alpha}\tilde{B}^{\alpha\beta}f^\nu_{,\beta}. \quad (2.8)$$

The derivation of (2.7) is given in Appendix A, whereas (2.8) confirms the tensorial character of the mass tensor. In terms of the new variables, the kinetic energy consequently takes the form

$$T = \frac{1}{8}\{p_\mu, \{p_\nu, B^{\mu\nu}(Q,q)\}\} + U(Q,q), \quad (2.9)$$

where the second term, which is specifically a quantum potential arising from the noncommutativity of coordinates and momenta, has the form

$$8U(Q,q) = [f^\mu_{,\alpha\gamma}g^\gamma_{,\nu}g^\alpha_{,\lambda}B^{\nu\lambda}]_{,\mu} - [f^\mu_{,\alpha\gamma}g^\gamma_{,\mu}]_{,\nu}g^\alpha_{,\lambda}B^{\nu\lambda}. \quad (2.10)$$

For further work, the momenta are also divided into collective and noncollective subsets,

$$p_\mu = \{P_i, p_a\}. \quad (2.11)$$

We now remind ourselves that the initial, even primary, goal of the present considerations is to identify a piece of the transformed Hamiltonian as collective. This collective Hamiltonian, H_C, should depend only on the variables Q^i, P_i, that we suppose to be canonical pairs. The simplest possible choice would appear to be the restriction of the full Hamiltonian to the values $q^a = 0$, $p_a = 0$, and thus (see below)

$$H_C \cong \frac{1}{8}\{P_i, \{P_j, B^{ij}(Q,0)\}\} + V(Q,0). \quad (2.12)$$

This choice is purely formal until we specify a procedure for determining the unknown functions $V(Q,0) \equiv V(Q)$ and $B^{ij}(Q,0) \equiv B^{ij}(Q)$ in terms of the elements of the original Hamiltonian and of the point transformation (2.3) and (2.4). The criteria for such a determination must be chosen so as to somehow minimize the coupling between the collective and noncollective variables.

The simplest approach to this problem is to consider H_C, (2.12), as the first term of a Taylor expansion in powers of the noncollective variables, q^a, remembering at the same time that we have a polynomial of degree two in the noncollective momentum operators, p_a. Assuming that higher-order terms are successively of lesser importance, basically the same assumption that governs the treatment of all variables in the small vibrations domain, we adopt the same assumption that defines optimum decoupling in the classical limit [4], namely that the terms linear in the noncollective variables vanish. This yields the two sets of conditions

$$V_{,a}(Q) + \frac{1}{8}\{P_i, \{P_j, B^{ij}_{,a}(Q)\}\} = 0, \quad (2.13)$$

$$B^{ai}(Q) = 0, \quad (2.14)$$

recognizable as the coefficients of q^a and p_a, respectively. The operator character of these conditions is apparent only from the second term of (2.13). However, if we introduce the Wigner transform of these equations, because of the special symmetrization that we have adopted for the kinetic energy, they reduce exactly to the classical conditions studied extensively in our previous work [4]. There, starting from these classical conditions, we have described and illustrated suitable algorithms for the determination of the elements of the collective Hamiltonian.

With the determination of the elements of the Hamiltonian, (2.12), the theory is completed by the assumption that the eigenstates of this operator are defined on a K-dimensional Hilbert space of (round-bracketed) states $|n)$,

$$|n) = \int dQ|Q)(Q|n), \quad (2.15)$$

and that these states accurately model a corresponding subspace, $|n\rangle$, of states of the full Hilbert space. The theory described above is very close to the theory that has been applied in a number of early applications, such as [15,16]. A major aim of the present work is to critique and generalize this procedure.

We emphasize that in this program, the elements of the collective Hamiltonian are determined from a K-dimensional manifold in configuration space, parametrized by the coordinates $\{Q\}$, whereas the quantum mechanics is determined in a Hilbert space defined by the same coordinates. Upon further reflection, it may strike the reader that this is a strange result, or, at least, a very limited one. The reason is that the true collective states, $|n\rangle$, though they define a subspace of the full Hilbert space, are nevertheless states in this space and therefore depend also on the noncollective coordinates, at the very least through the zero-point motion of the latter. Though we have been able to neglect this dependence in the approximation considered so far, this will no longer be true if we seek to include the effect of the coupling to the fast variables on the properties of the collective states, or in directly describing the motion of the fast variables.

III. GENERALIZATION OF THE FORMALISM TO INCLUDE THE EFFECTS OF THE FAST VARIABLES

In this section, we set ourselves two tasks. We shall first find the forms of the leading corrections to the collective Hamiltonian given above, arising from the coupling of the fast to the slow variables. This will be done with the help of the standard Born-Oppenheimer (BO) approximation. In order to evaluate these corrections explicitly, however, we shall then commit ourselves to further approximations for the dependence of the full Hamiltonian on the fast variables, that yield a normal mode description of the latter.

To generalize the restricted ideas of the previous section, we thus introduce the BO picture into the theory of large amplitude collective motion. As stated above this amounts to an extension of the complexity of structure allowed for the states of the collective subspace so as to take into account the influence of the fast variables, We first assume, more generally, that the collective states $|n\rangle$ have coordinate space representatives

$$\langle Q^i q^a | n \rangle \equiv \langle Q, q | n \rangle$$
$$= \sum_\nu (Q|n\nu)[q|\nu : Q], \quad (3.1)$$

where the index ν is not to be confused with its previous use as a coordinate index. Here and for the remainder of this paper, we adopt a notation where angular brackets indicate states in the full Hilbert space, square brackets states in the space of fast variables (though dependent

parametrically on the slow variables, as denoted by : Q in the state vector), and parentheses states in the collective space. We suppose that for fixed Q, the states $[q|\nu:Q]$ are a complete set of functions for the fast coordinates,

$$\sum_{\nu}[q|\nu:Q][\nu:Q|q'] = \delta(q - q'). \qquad (3.2)$$

Though for the moment we have not specified the equation of which they are the solutions, we shall be able to do so, at least approximately, as a consequence of the developments to be carried out in this section.

For the remainder of the current discussion, we shall consider the simplest case in which the fast variables occupy, for any given value of the slow variables, their state of lowest energy, which is assumed to be nondegenerate. For the case to be studied here, ν takes a single value denoted by zero. The coefficient function, usually denoted in this case by $(Q|n)$, that appears in (3.1), can then be identified as the wave function for the collective motion, and this identification will agree with the one that has been made in the previous section, where the description of large amplitude collective motion was not tied to the BO approximation. There we emphasized a connection between the decoupled Hilbert space of the collective coordinates and the crucial existence of a K-dimensional decoupled coordinate manifold described by the functions $g^{\alpha}(Q, q = 0)$. The approximate separability of the associated Hilbert space is based on the assumption that the functions $[q|\nu:Q]$ describing the fast variables are confined to a narrow region in q space in the neighborhood of the collective surface. If this picture holds, we may expect the mathematical details to work out reasonably.

Adopting the BO approximation, we set ourselves the task of finding an effective Hamiltonian to describe the motion of the collective variables. This operator is defined, though not yet operationally, by means of the equation

$$(n'|H_{\text{eff}}(Q, P)|n) = \langle n'|\tilde{H}(\xi, \pi)|n\rangle. \qquad (3.3)$$

This relation will assume the status of a definition of the collective Hamiltonian within the space of slow variables and H_{eff} recognized as a generalization of H_C only after we specify how to eliminate the fast variables from the right-hand side. The procedure that we shall follow is closely akin to the traditional BO approach, with characteristic differences arising from the facts that at the beginning we cannot specify which are the slow and which the fast variables, and that the treatment of the fast variables comes as a kind of afterthought, dependent in detail on the prior treatment of the collective variables.

Let us start with the potential energy,

$$\tilde{V}(\xi) = \tilde{V}[g^{\alpha}(Q, q)] \equiv V(Q, q), \qquad (3.4)$$

and evaluate the associated piece of (3.3)

$$\langle n'|\tilde{V}(\xi)|n\rangle \equiv (n'|V_{\text{eff}}|n)$$
$$\cong \int dQ\, dq (n'|Q)[0:Q|q]\tilde{V}[g^{\alpha}(Q, q)]$$
$$\times [q|0:Q](Q|n), \qquad (3.5)$$

within the BO approximation. The only feasible way, in general, of integrating out the fast variables is to expand $\tilde{V}$ in powers of q^a,

$$V(Q, q) = V(Q) + V_{,a}q^a + \tfrac{1}{2}V_{,ab}q^aq^b + \cdots, \qquad (3.6)$$

leading to

$$V_{\text{eff}}(Q) = V(Q) + V^{(1)}(Q) + V^{(2)}(Q) + \cdots, \qquad (3.7)$$

where assuming that the function $[q|0:Q]$ is normalized,

$$V(Q) = V(Q, 0), \qquad (3.8)$$
$$V^{(1)}(Q) = V_{,a}\int |[q|0:Q]|^2 q^a$$
$$\equiv V_{,a}(Q)\langle q^a\rangle_Q, \qquad (3.9)$$
$$V^{(2)}(Q) = \tfrac{1}{2}V_{,ab}(Q)\langle q^aq^b\rangle_Q. \qquad (3.10)$$

We thus see that the leading term is independent of the wave function for the fast variables, coinciding with the standard result for the potential energy of large amplitude collective motion [1,4] presented in the previous section. The computation only requires the form of the collective submanifold, $\xi^{\alpha} = g^{\alpha}(Q, 0)$, which can be determined by well-defined procedures [4]. To go beyond this lowest order, we need, besides the wave function of the fast variables, to rearrange the expansion of V, as explained in Appendix B. There it is shown that if we wish to interpret the small quantities q^a as components of a vector, we must replace the ordinary second derivative by a covariant second derivative, $V_{;ab}$, that can be computed from known or calculable quantities according to the equations

$$V_{,a}(Q) = \tilde{V}_{,\alpha}g^{\alpha}_{,a}, \qquad (3.11)$$
$$V_{;ab}(Q) = \tilde{V}_{;\alpha\beta}g^{\alpha}_{,a}g^{\beta}_{,b}. \qquad (3.12)$$

These equations are simplified by introducing one of the decoupling conditions that follow from Eq. (2.13), namely that (3.11) should be zero. (Here we are assuming that the two terms of (2.13) vanish separately. Conditions for this to be true and modifications necessary when it is not have been discussed in Ref. [4].) The third term $V^{(2)}(Q)$, is the first, $\Delta^{(1)}V(Q)$, of a sequence of contributions that we shall identify as the leading corrections to the potential energy. Further discussion of the evaluation of this term and of the additional correction terms, to be identified below, will be continued later in this section, following the identification of all the pieces.

The remaining terms will arise from the study of the kinetic energy, given after transformation of coordinates by Eqs. (2.9) and (2.10). In order to integrate out the fast variables in the contribution that these terms make to H_{eff}, consider the first term of the kinetic energy. We expand the mass tensor in powers of q, and keep initially only the leading term $B^{\mu\nu}(Q, 0) \equiv B^{\mu\nu}(Q)$. In this approximation, we first restrict the study to the contribution of those terms where the indices μ, ν take on values i, j in the collective subset.

As a preliminary to this calculation, we study the simpler object

$$
\begin{aligned}
(n'|(P_i)_{\text{eff}}|n) &= \langle n'|P_i|n\rangle \\
&= (n'|(P_i - A_i)|n) \\
&\equiv (n'|D_i|n).
\end{aligned}
\tag{3.13}
$$

Here P_i is the collective momentum operator identified in the previous section, and

$$
A_i \equiv i \int dq[0\!:\!Q|q]\partial_i[q|0\!:\!Q],
\tag{3.14}
$$

where ∂_i means partial derivative with respect to Q^i. Notice, however, that if we calculate straightforwardly,

$$
\begin{aligned}
(n'|(P_iP_j)_{\text{eff}}|n) &= \langle n'|P_iP_j|n\rangle \\
&= (n'|(P_iP_j - A_iP_j - A_jP_i + S_{ij})|n),
\end{aligned}
\tag{3.15}
$$

where

$$
S_{ij} = -\int dq[0\!:\!Q|q](\partial^2/\partial Q^i\partial Q^j)[q|0\!:\!Q].
\tag{3.16}
$$

As a consequence of this result, we are reassured that the effective value of zero is zero, i.e.,

$$
0 = \langle n'|[P_i, P_j]|n\rangle = (n'|[P_i, P_j]|n).
\tag{3.17}
$$

It is easy to see that the remaining canonical commutators also project without change.

It is useful to rewrite (3.15) in a form that makes contact with standard results. We have

$$
(i\partial_j)[q|\nu\!:\!Q] = \sum_{\nu'}[q|\nu'\!:\!Q]A_j(Q)_{\nu'\nu},
\tag{3.18}
$$

$$
(A_j)_{\nu'\nu} = i \int dq[\nu'\!:\!Q|q]\partial_j[q|\nu\!:\!Q].
\tag{3.19}
$$

Because of the Q dependence of the matrix element, it now follows that

$$
\begin{aligned}
S_{ij} &= \sum_\nu (A_i)_{0\nu}(A_j)_{\nu 0} + (i\partial_i)A_j \\
&= (i\partial_i)A_j + A_iA_j + S'_{ij},
\end{aligned}
\tag{3.20}
$$

where

$$
(A_j)_{00} = A_j,
\tag{3.21}
$$

$$
S'_{ij} = \sum_{\nu\neq 0}(A_i)_{0\nu}(A_j)_{\nu 0}.
\tag{3.22}
$$

Consequently, we may also rewrite Eq. (3.15) as

$$
(n'|(P_iP_j)_{\text{eff}}|n) = (n'|(D_iD_j + S'_{ij})|n).
\tag{3.23}
$$

In the simplest case, where $[0\!:\!Q|q]$ is a real wave function, and it follows that A_i vanishes, the contribution S'_{ij} remains to be taken into account.

We are now in a position to apply to the computation of the collective kinetic energy the same reasoning as just carried out for a product of momentum operators. Making use of the analogue of (3.23), the result is

$$
\tfrac{1}{8}\{D_i, \{D_j, B^{ij}(Q)\}\} + \tfrac{1}{2}S'_{ij}B^{ij},
\tag{3.24}
$$

where the second term can be incorporated into the collective potential energy as a second such contribution, $\Delta^{(2)}V(Q)$.

An additional contribution of this type is obtained by setting $q^a = 0$ in Eq. (2.10),

$$
\Delta^{(3)}V(Q) = U(Q, 0),
\tag{3.25}
$$

where $U(Q, q)$ is the quantum potential defined in Eqs. (2.9) and (2.10).

It remains for us to discuss the contributions from T that depend on $B^{ai}(Q)$ that "mix" the collective and noncollective indices and those that depend on the noncollective mass tensor $B^{ab}(Q)$. The former can be neglected because of one of the decoupling conditions, Eq. (2.14). The leading contribution of the latter is seen to be another contribution to the potential energy,

$$
\Delta^{(4)}V = \tfrac{1}{2}B^{ab}(Q)\langle p_a p_b\rangle_Q.
\tag{3.26}
$$

To summarize our findings, we have derived the following effective Hamiltonian:

$$
H_{\text{eff}} = \frac{1}{8}\{D_i, \{D_j, B^{ij}(Q)\}\} + V(Q) + \Delta V(Q),
\tag{3.27}
$$

where $\Delta V(Q)$ is the sum of four terms that summarize the leading quantum corrections including the coupling to the fast variables,

$$
\Delta V = \sum_{i=1}^{4}\Delta^{(i)}V,
\tag{3.28}
$$

given respectively in or in relation to Eqs. (3.10), (3.24), (3.25), and (3.26). Let us contrast this result with the corresponding form appropriate to the more familiar molecular case. The introduction of a curved metric aside, the main difference is that in the molecular case, the ground state wave function of the fast variables, for a fixed value of Q, may be assumed known, and its eigenvalue, $\epsilon_0(Q)$, together with $\Delta^{(2)}V$, contained in Eq. (3.24) constitutes the collective potential energy [6,7].

In the present instance we cannot assume that we know the Hamiltonian of the fast variables, except in an approximate sense that we now discuss. We need to extend the considerations of the previous section that led to the definition of the quantum collective Hamiltonian operator H_C. Instead of specializing the transformed Hamiltonian operator to the values $q^a = p_a = 0$, we now retain terms up to second order in these variables. In this treatment, we may replace $U(Q, q)$ by $U(Q, 0)$, since this term is already a small correction, and the remaining terms linear in the fast variables may be dropped because of the decoupling conditions. To the specified accuracy, we obtain the following quantum Hamiltonian:

$$
H = H_C + U(Q) + H_{NC},
\tag{3.29}
$$

$$
H_{NC} = \tfrac{1}{2}p_a p_b B^{ab}(Q) + \tfrac{1}{2}q^a q^b V_{ab}(Q).
\tag{3.30}
$$

In Appendix B, we point out that once the elements of H_C have been determined, one can choose a set of

fast variables and calculate the matrices that appear in (3.30). For each value of Q, the Hamiltonian H_{NC} represents a standard normal mode problem. Let $c_\alpha, c_\alpha^\dagger$ be normal mode destruction and creation operators, Ω_α the corresponding frequencies, and $\hat{n}_\alpha = c_\alpha^\dagger c_\alpha$. Assuming local stability, i.e., Ω_α real and positive, we have

$$H_{NC}(Q) = \sum_\alpha (\hat{n}_\alpha + \tfrac{1}{2})\Omega_\alpha(Q). \qquad (3.31)$$

The practical importance of the contribution of (3.31) has been noted in several applications carried out in the past [8,15].

The quantum Hamiltonian, expressed in terms of the optimum choice of variables, but in a restricted approximation, has thus been found. Except for the term $U(Q)$, it has been expressed in terms of elements that can be calculated. Evaluation of $U(Q)$ appears to require some properties of the point transformation that have not so far been studied. Comparison of approximate calculations (with this term omitted) with exact calculations indicates that it is probably a small correction. As previously remarked, it is of order N^{-2} compared to the main term in the potential energy, where N is the number of degrees of freedom. We shall make no further allusion to this term in the present paper.

Let us now return to a discussion of the correction terms, ΔV by which H_{eff}, Eq. (3.27), differs from H_C. We have just discarded $\Delta^{(3)}V$. The sum $\Delta^{(1)}V + \Delta^{(4)}V$ has been seen in (3.31) to be a sum of oscillator terms in the approximation considered, its contribution then depending, naturally, on the state of motion of the fast variables. As stated above, in this section we shall consider only the lowest-energy state for these variables, so that the contribution of this term is just the zero-point energy.

It remains for us to discuss the contribution of the term $\Delta^{(2)}V$, the Berry scalar potential, associated with the projection of the kinetic energy onto the collective subspace. This contribution goes together with that from the "vector potential," A_i. In Sec. V, we shall study examples where these terms contribute. In fact, the manner in which both the vector and scalar potentials contribute is best studied within the context of these illustrations.

In this section we have thus gone as far as we shall in defining a quantum theory of the slow variables, having derived an effective Hamiltonian and shown that it is expressed in terms of canonical variables. Thus we are also free to study this problem with the help of the Heisenberg equations of motion. In the next section we shall consider variational formulations of these equations.

IV. VARIATIONAL PRINCIPLES: LAGRANGIAN FORMULATION

Having defined an effective quantum theory within the collective subspace, we can imagine that we study this theory by means of Heisenberg's equations of motion,

$$-i[Q^i, H_{\text{eff}}] = \frac{\partial}{\partial P_i} H_{\text{eff}}, \qquad (4.1)$$

$$i[P_i, H_{\text{eff}}] = \frac{\partial}{\partial Q^i} H_{\text{eff}}. \qquad (4.2)$$

The purpose of this section is to show that these equations can be derived from a variational principle, the so-called trace variational principle, involving H_{eff}, or an operator closely related to it; it is to show, further, that a reworking of this principle leads to a second version of the variational principle, involving an effective Lagrangian, L_{eff}, that is defined in the natural way as the Legendre transform of H_{eff}. According to Moody, Schapere, and Wilzek [7], when L_{eff} is defined by means of a path integral, it is not exactly the Legendre transform of H_{eff}. We shall not encounter any such difficulty as long as the mass tensor is independent of coordinates, the only case studied by previous authors. When the mass tensor enters in full generality, the formulation of a variational principle of the type we have in mind is not quite as straightforward as in previous instances that we have studied [17,18].

In order not to have to deal with all subtleties at once, let us first consider the case that the mass tensor does not depend on coordinates. In that case we may utilize the standard version

$$\delta \text{Tr}\{H_{\text{eff}} - i\Lambda[Q^i, P_i]\} = 0. \qquad (4.3)$$

Here the trace is taken over a *finite* subspace of the collective Hilbert space. This assumption allows us to utilize the invariance of the trace under cyclic permutation, a property that plays an essential role in the manipulation of the second term of (4.3). In this term, Λ is a Lagrange multiplier operator associated with a set of constraints that are the nonvanishing canonical commutation relations. These, at least, must be imposed because, to start with, the variational quantities are arbitrary matrix elements within the space included in the trace, and these variations must be subject to the kinematical constraints. The fact that we can limit the constraints to the commutators for canonical pairs is, at the moment, an observation.

In order to come out with the Heisenberg equations of motion upon variation, it is necessary, as well, to choose variations of the coordinates that depend only on the coordinates themselves, so as to validate the formula

$$\delta V(Q) = [\partial V(Q)/\partial Q^k]\delta Q^k. \qquad (4.4)$$

The equations of motion that follow from these assumptions are

$$-i[Q^i, \Lambda] = \frac{\partial H_{\text{eff}}}{\partial P_i}, \qquad (4.5)$$

$$i[P_i, \Lambda] = \frac{\partial H_{\text{eff}}}{\partial Q^i}. \qquad (4.6)$$

To make these agree with Heisenberg's equations, the choice $\Lambda = H_{\text{eff}}$ is indicated.

We apply this formalism to the case with nonvanishing Berry potentials but constant mass matrix, described by

the Hamiltonian operator,

$$H_{\text{eff}} = \tfrac{1}{2} D_i D_j B^{ij} + V, \tag{4.7}$$

where it is understood that V may include the correction terms discussed in the previous section. The operator equations of motion that follow from (4.5), (4.6), and (4.7), after some standard manipulations, are

$$\dot{Q}^i = D_j B^{ji}, \tag{4.8}$$

$$\dot{D}_i = -V_{,i} + \tfrac{1}{2}\{\dot{Q}^j, \mathcal{F}_{ij}\}, \tag{4.9}$$

where

$$A_i = \tfrac{1}{2}\{(\partial A_i/\partial Q^j), \dot{Q}^j\}, \tag{4.10}$$

$$\mathcal{F}_{ij} = (\partial A_i/\partial Q^j) - (\partial A_j/\partial Q^i), \tag{4.11}$$

and

$$D_i = \dot{Q}^j B_{ji}, \tag{4.12}$$

with B_{ji} the matrix inverse to B^{ji}, is the solution of Eq. (4.8) for the gauge-covariant momentum.

From the combination of (4.9) and (4.12), we can derive the familiar Lagrangian equations of motion

$$\ddot{Q}^j B_{ji} + V_{,i} - \tfrac{1}{2}\{\mathcal{F}_{ji}, \dot{Q}^j\} = 0. \tag{4.13}$$

Of some interest is that the associated variational principle from which these equations can be derived, namely

$$\begin{aligned} 0 &= \delta \operatorname{Tr}(-L_{\text{eff}}) \\ &= \delta \operatorname{Tr}(-\tfrac{1}{2}\dot{Q}^i \dot{Q}^j B_{ji} - \dot{Q}^i A_i + V), \end{aligned} \tag{4.14}$$

can be obtained directly from the starting trace variational principle, (4.3), simply by eliminating the momenta in favor of the velocities by means of the relations given above. Instead of independent variations of coordinates and momenta, only the coordinates are to be varied. In this variation, the velocity $\dot{Q}^i$ is to be replaced by $-i[Q^i, H_{\text{eff}}]$ and H_{eff} is not to be varied. One obtains the correct equations of motion because algebraic manipulation of the resulting trace expressions, containing commutators with H_{eff}, that is aimed at isolating the coordinate variations, produces the same results as integration by parts of the time derivatives in the corresponding classical variational principle, proper attention being paid to the order of noncommuting factors. For the case just concluded, the outcome is thus completely satisfactory.

When we reinstate the Q dependence of the mass tensor, an additional problem is encountered. If we insist on the cyclic invariance of the trace, which has played an essential role in the previous applications of the trace variational principle, then we have

$$\operatorname{Tr}\{P_i, \{P_j, B^{ij}\}\} = 2 \operatorname{Tr}\{P_i P_j, B^{ij}\}. \tag{4.15}$$

However, direct transformation, using the commutation relations, yields

$$\{P_i, \{P_j, B^{ij}\}\} = 2\{P_i P_j, B^{ij}\} + B^{ij}_{,ij}, \tag{4.16}$$

leading to an apparent contradiction upon formation of the trace. Of course, in deriving (4.16), we have used the commutation relations appropriate to an infinite Hilbert

space. The point is the same as that $\operatorname{Tr}QP \neq \operatorname{Tr}PQ$ for a truly canonical pair. In order to derive the equations of motion from a trace variational principle, we deal with this problem by adopting (4.15), but including the last term in (4.16) as part of the potential energy. This implies the assumption that the trace is taken, to start with, only over a finite-dimensional vector space and that therefore the invariance of the trace under cyclic permutation is a correct operation. As a consequence, the equations of motion are given in matrix form. The operator form of the equations of motion is recognized as a limit of these equations. In this limit, the application of (4.16) *after variation*, can be seen to yield the equations of motion in the desired symmetrical (Weyl) structure. Thus the final variational principle takes the form

$$\delta \operatorname{Tr}\{H_{\text{mod}} - iH_{\text{eff}}[Q^i, P_i]\}, \tag{4.17}$$

where

$$H_{\text{mod}} = H_{\text{eff}} + \frac{1}{8} B^{ij}_{,ij}. \tag{4.18}$$

In the discussion above, we have noted a problem only in connection with the part of the kinetic energy quadratic in the momenta. It may be verified that a similar difficulty does not occur for the terms that are bilinear in the momenta and the "vector potential."

Unfortunately, in the transition from Hamilton's equations to Lagrange's equations for this case additional complications are encountered; because of the noncommutativity of the mass tensor with the momentum, the Lagrange equations do not follow from the expression obtained by eliminating the momenta in favor of the velocities in the starting variational principle. The equations of motion that follow from this conjectured Lagrangian variational expression differ from the correct equations of motion by additional "quantum" potentials. This line of inquiry does not appear to be illuminating and therefore will not be pursued.

V. ILLUSTRATIVE MODELS

It is simplest to illustrate the main points by choosing models in which the collective coordinates have already been identified, so that we need not enter into the intricacies of the theory of large amplitude collective motion *per se*. For instance, in the first model studied below, there are no terms in the Hamiltonian linear in the fast variables. Thus the model satisfies the decoupling conditions exactly. In both of the models to be studied, we break time-reversal invariance, and in that sense they are somewhat artificial.

A. The first model: Berry phase in excited states

We study the Hamiltonian

$$\begin{aligned} H &= H_{\text{core}} + H_{\text{sp}} + H_{\text{int}} \\ &= H_{\text{core}} + H_{NC}, \end{aligned} \tag{5.1}$$

$$H_{\text{core}} = \frac{\mathbf{P}^2}{2M} + V(Q), \tag{5.2}$$

$$H_{\text{sp}} = \omega(Q)(a_1^\dagger a_1 + a_2^\dagger a_2 + 1), \tag{5.3}$$

$$H_{\text{int}} = -G(Q_- a_1^\dagger a_2 + Q_+ a_2^\dagger a_1). \tag{5.4}$$

Here the coordinates $\mathbf{Q}$ and the canonical momenta $\mathbf{P}$ are both two-dimensional vectors. We use the notation $\mathbf{Q} = (Q_1, Q_2)$, $Q_\pm = Q_1 \pm iQ_2$, and $Q = (Q_1^2 + Q_2^2)^{1/2}$. (In this section, we are not maintaining the distinction between upper and lower indices.) Furthermore, the $a_i, a_i^\dagger, i = 1, 2$ are boson destruction and creation operators, G is a coupling strength, and the frequency, $\omega(Q)$, of the uncoupled boson modes has been given a so far unspecified dependence on Q that will be chosen for analytic and numerical convenience. Note that the Hamiltonian, (5.1) conserves the boson number,

$$N = a_1^\dagger a_1 + a_2^\dagger a_2 = \text{const.} \qquad (5.5)$$

Since the $N = 0$ problem is completely trivial, the first interesting case for the present model is $N = 1$. Here, the state vectors may be written exactly as a superposition

$$|n\rangle = \int d\mathbf{Q}\{(\mathbf{Q}|n1)a_1^\dagger|0] + (\mathbf{Q}|n2)a_2^\dagger|0]\}, \qquad (5.6)$$

where $|0]$ is the vacuum state. The use of square brackets for the vacuum state of the fast variables is consistent with the notation introduced in Sec. III. The resulting eigenvalue equation in the space of the collective variables, $\mathbf{Q}$, is determined by the 2×2 effective Hamiltonian, H_{eff}, with matrix elements

$$(H_{\text{eff}})_{11} = H_{\text{core}} + 2\omega(Q) = (H_{\text{eff}})_{22},$$
$$(5.7)$$
$$(H_{\text{eff}})_{12} = -GQ_- = (H_{\text{eff}})_{21}^*.$$

Below we shall describe our solutions of the associated Schrödinger equation.

These exact solutions are to be compared with the adiabatic approximation, with and without the Berry potential terms. For this approximation, we require the normal modes of H_{NC}, which we calculate in a standard way from the equations of motion,

$$[a_1, H_{NC}] = \omega a_1 - GQ_- a_2,$$
$$(5.8)$$
$$[a_2, H_{NC}] = \omega a_2 - GQ_+ a_1,$$

by forming the matrix elements,

$$\psi_i = [0|a_i|\Psi]. \qquad (5.9)$$

With Ω representing the energy of the state $|\Psi]$, we obtain the equations

$$\Omega\psi_1 = \omega\psi_1 - GQ_-\psi_2,$$
$$(5.10)$$
$$\Omega\psi_2 = -GQ_+\psi_1 + \omega\psi_2,$$

that yield the eigenvalues

$$\Omega^{(1)}(Q) = \omega(Q) - GQ,$$
$$(5.11)$$
$$\Omega^{(2)}(Q) = \omega(Q) + GQ,$$

that are degenerate when $Q = 0$. The associated normal-

ized solutions of (5.10) are represented most conveniently by introducing the normal-mode creation operators

$$b_i^\dagger = \psi_j^{(i)} a_j^\dagger. \qquad (5.12)$$

In detail we have as a possible choice

$$b_1^\dagger = \frac{1}{\sqrt{2}}a_1^\dagger + \frac{1}{\sqrt{2}}\exp i\phi(\mathbf{Q})a_2^\dagger, \qquad (5.13)$$

$$b_2^\dagger = \frac{1}{\sqrt{2}}\exp i\phi(\mathbf{Q})a_1^\dagger - \frac{1}{\sqrt{2}}a_2^\dagger, \qquad (5.14)$$

where

$$\tan\phi(\mathbf{Q}) = Q_2/Q_1. \qquad (5.15)$$

We now apply these elementary results to the adiabatic approximation. In this case we represent a suitable subset of the eigenfunctions (5.6) in the form

$$|n\rangle = \int d\mathbf{Q}(\mathbf{Q}|n)b_1^\dagger|0\!:\!Q], \qquad (5.16)$$

where the notation $0 : Q$ refers to the vacuum for the normal modes. (For the current model, it coincides with the uncoupled vacuum.) The considerations of Sec. III now apply to this class of state vectors and, in particular, we apply Eq. (3.23). As a special case of this equation, we have

$$\sum_i (P_i)^2 \rightarrow \sum_i (P_i - A_i)^2 + \sum_i |(A_i)_{21}|^2, \qquad (5.17)$$

where

$$A_i = i[0\!:\!Q|b_1\partial_i b_1^\dagger|0\!:\!Q], \qquad (5.18)$$
$$(A_i)_{21} = i[0\!:\!Q|b_2\partial_i b_1^\dagger|0\!:\!Q], \qquad (5.19)$$

where ∂_i means the partial derivative with respect to Q_i. With the help of Eqs. (5.13) and (5.14), the quantities of interest are found to take the values

$$\mathbf{A} = \frac{1}{2Q^2}(Q_2, -Q_1), \qquad (5.20)$$

$$\sum_i |(A_i)_{21}|^2 = (1/4Q^2). \qquad (5.21)$$

The singular character of these results was to be expected.

The collective or adiabatic Hamiltonian, H_C, that thus emerges from the assumption that the state vectors of interest can be written in the form (5.16), has the structure

$$H_C = (1/2M)[(\mathbf{P} - \mathbf{A})^2 + (\mathbf{A}_{21})^2]$$
$$+ V(Q) + (3/2)\Omega^{(1)}(Q) + (1/2)\Omega^{(2)}(Q). \qquad (5.22)$$

We turn to the problem of solving the associated eigenvalue problem. We wish to compare the results of exact (numerical) calculations with the eigenvalues of the collective Hamiltonian. It is useful to choose $\omega(Q)$ such that the latter is exactly solvable. One such choice is

$$\omega(Q) = \frac{1}{2}GQ. \qquad (5.23)$$

In this case the additional contribution to the potential is zero,

$$\frac{3}{2}\Omega^{(1)}(Q) + \frac{1}{2}\Omega^{(2)}(Q) = 0. \tag{5.24}$$

We further take $M = 1$ and $V(Q) = \frac{1}{2}Q^2$.

We use the definition of the two-dimensional angular momentum,

$$L = -i\frac{\partial}{\partial \phi}$$
$$= -i(Q_1P_2 - Q_2P_1), \tag{5.25}$$

to simplify the $\mathbf{P} \cdot \mathbf{A}$ term. We can further simplify the equation $H_C\psi(\vec{Q}) = E\psi(\vec{Q})$ by substituting

$$\psi(\vec{Q}) = Q^{-1/2}\chi(Q)e^{im\phi} \tag{5.26}$$

and find

$$\left\{-\frac{1}{2}\frac{d^2}{dQ^2} + \frac{1}{2Q^2}\left[m^2 + m + \frac{1}{4}\right] + \frac{1}{2}Q^2\right\}\chi(Q) = E\chi(Q). \tag{5.27}$$

Even though the centrifugal term has changed, this is still very similar to the radial equation for the two-dimensional harmonic oscillator. It can be solved by the substitution

$$\chi(q) = q^{\alpha+1/2}e^{-q^2/2}L_n^{(\alpha)}(q^2). \tag{5.28}$$

As is well known the right-hand side of this equation satisfies the condition

$$-\frac{d^2}{dq^2}\chi + \left(q^2 + \frac{1-4\alpha^2}{4q^2}\right)\chi = (4n + 2\alpha + 2)\chi. \tag{5.29}$$

We thus find that

$$\alpha(m) = \sqrt{1/4 + (m+1/2)^2} \tag{5.30}$$

and

$$E_{nm} = [2n + \alpha(m) + 1]. \tag{5.31}$$

Without the Berry's phase terms we would have found

$$E_{nm} = (2n + |m| + 1). \tag{5.32}$$

When $G = 0$ the solution (5.32) is exact. Thus Eq. (5.31), which is independent of G, cannot be valid for all G. It should be valid in the adiabatic limit, which means that the two frequencies Ω must be very different. This occurs when G is very large.

The exact solution of the problem can be calculated using a spherical harmonic oscillator basis for the Q co-ordinates. This is coupled to a state containing either one $a_1^\dagger$ or one $a_2^\dagger$ boson,

$$|n, m, n_1, n_2\rangle = |n, m\rangle(a_1^\dagger)^{(n_1)}(a_2^\dagger)^{(n_2)}|0]. \tag{5.33}$$

The interaction Hamiltonian only couples states with $n_1 = 1, m = m_1$ to states with $n_2 = 1, m = m_1 + 1$. If we thus choose the value m_1 we have only a relatively small matrix to diagonalize. Since we wish to obtain accurate results for large G, we allow the number of Q harmonic oscillator quanta to be fairly large. We have used up to 200 harmonic oscillator states in each block (which leads to a 400 × 400 matrix eigenvalue problem).

In Table I we give a selected set of results for $m_1 = 0$ and a number of values of G. Similar results for $m_1=1$ are listed in Table II. We clearly see the convergence to the the collective model results including the Berry phase for large G.

B. The second model: Ground state

We next study a model that is also exactly decoupled, differing from the one just investigated only in the form of the interaction. In this model Eqs. (5.1)–(5.3) stand as given, but Eq. (5.4) is modified to

$$H_{\rm int} = -G_0Q(a_1^\dagger a_2 + a_2^\dagger a_1) - G_1(Q_+a_1a_2 + Q_-a_1^\dagger a_2^\dagger). \tag{5.34}$$

TABLE I. The lowest 10 eigenvalues of the coupled problem for $m_1 = 0$ as a function of G. The column labeled Berry lists the eigenenergies of the collective Hamiltonian (5.22).

G	0.01	0.1	1	10	100	1000	Berry
E_1	1.00875	1.07849	1.36229	1.58463	1.66532	1.69302	1.7071
E_2	2.01328	2.13134	2.92007	3.48844	3.63505	3.68298	3.7071
E_3	3.01540	3.14492	4.09426	5.39473	5.60870	5.67438	5.7071
E_4	4.01827	4.18125	5.30157	7.29413	7.58443	7.66658	7.7071
E_5	5.01997	5.19061	6.57000	9.17666	9.56145	9.65932	9.7071
E_6	6.02221	6.22068	7.66964	11.0262	11.5393	11.6525	11.7071
E_7	7.02367	7.22768	8.90918	12.8133	13.5177	13.6459	13.7071
E_8	8.02558	8.25425	10.0230	14.4981	15.4965	15.6396	15.7071
E_9	9.02687	9.25972	11.1883	16.0926	17.4754	17.6335	17.7071
E_{10}	10.0286	10.2840	12.3410	17.7119	19.4544	19.6276	19.7071

TABLE II. The lowest 10 eigenvalues of the coupled problem for $m_1 = 1$ as a function of G. The column labeled Berry lists the eigenenergies of the collective Hamiltonian (5.22).

G	0.01	0.1	1	10	100	1000	Berry
E_1	2.01308	2.11333	2.41566	2.54921	2.57601	2.58042	2.58114
E_2	3.01670	3.17369	4.20360	4.51926	4.57057	4.57959	4.58114
E_3	4.01807	4.16340	5.44213	6.48766	6.56479	6.57866	6.58114
E_4	5.02086	5.21512	6.43129	8.45380	8.55880	8.57766	8.58114
E_5	6.02202	6.20307	7.86356	10.4165	10.5527	10.5766	10.58114
E_6	7.02436	7.25000	8.79958	12.3739	12.5464	12.5755	12.58114
E_7	8.02538	8.23691	10.1070	14.3218	14.5400	14.5744	14.58114
E_8	9.02745	9.28063	11.1975	16.2512	16.5336	16.5733	16.58114
E_9	10.0284	10.2669	12.3141	18.1346	18.5270	18.5721	18.58114
E_{10}	11.0302	11.3082	13.5364	19.8627	20.5204	20.5709	20.58114

The second term of this interaction spoils the conservation of boson number used to simplify the solution of the previous problem. For the present problem, it is already interesting to study the spectrum when the fast variables are in their ground levels, since there are now nontrivial ground state correlations and associated nontrivial Berry potentials, that we shall calculate.

We first turn to the study of the BO approximation. As before we need the normal modes of the fast variables, as determined from the equations of motion

$$[a_1, H_{NC}] = \omega a_1 - G_0 Q a_2 - G_1 Q_- a_2^\dagger,$$

$$[a_2, H_{NC}] = \omega a_2 - G_0 Q a_1 - G_1 Q_- a_1^\dagger,$$

$$(5.35)$$

and their Hermitian conjugates. In terms of the definitions

$$b_i^\dagger = \psi_j^{(i)} a_j^\dagger - \chi_j^{(i)} a_j, \qquad (5.36)$$

$$\psi_j^{(i)} = [0\!:\!Q|a_j|\Psi^{(i)}], \qquad (5.37)$$

$$\chi_j^{(i)} = [0\!:\!Q|a_j^\dagger|\Psi^{(i)}], \qquad (5.38)$$

$$|\Psi^{(i)}] = b_i^\dagger |0\!:\!Q], \qquad (5.39)$$

we obtain the eigenvalue equations

$$\Omega \psi_1 = \omega \psi_1 - G_0 Q \psi_2 - G_1 Q_- \chi_2,$$

$$\Omega \psi_2 = \omega \psi_2 - G_0 Q \psi_1 - G_1 Q_- \chi_1,$$

$$\qquad (5.40)$$

$$-\Omega \chi_1 = \omega \chi_1 - G_0 Q \chi_2 - G_1 Q_+ \psi_1,$$

$$-\Omega \chi_2 = \omega \chi_2 - G_0 Q \chi_1 - G_1 Q_+ \psi_1.$$

The physical eigenvalues are the positive roots of

$$\Omega^2(Q) = (\omega \mp G_0 Q)^2 - G_1^2 Q^2, \qquad (5.41)$$

which are again degenerate at $Q = 0$. As for the first model studied, we label these solutions $\Omega^{(i)}, i = 1, 2$. The corresponding amplitudes are determined from the equations of motion and the normalization conditions

$$|\psi_1|^2 + |\psi_2|^2 - |\chi_1|^2 - |\chi_2|^2 = 1. \qquad (5.42)$$

The simplest forms for the amplitudes are achieved by repeated use of the eigenvalue equation (5.41). We thus find

$$\psi_2^{(j)} = (-1)^{j+1} \psi_1^{(j)} = \text{real}, \qquad (5.43)$$

$$\chi_i^{(j)} = \exp(i\phi) \tilde{\chi}_i^{(j)}, \qquad (5.44)$$

$$\tilde{\chi}_2^{(j)} = (-1)^{j+1} \tilde{\chi}_1^{(j)} = \text{real}, \qquad (5.45)$$

$$\psi_1^{(j)} = \frac{(\Omega^{(j)} + \omega) + (-1)^j G_0 Q}{\sqrt{2}\{(\omega + \Omega^{(j)})[(\omega + \Omega^{(j)}) + (-1)^j 2 G_0 Q] + (G_0^2 - G_1^2)Q^2\}^{1/2}}, \qquad (5.46)$$

$$\chi_1^{(j)} = (-1)^{j+1} f^{(j)}(Q) \psi_1^{(j)}, \qquad (5.47)$$

$$f^{(j)} = \frac{G_1 Q}{(\Omega^{(j)} + \omega) + (-1)^j G_0 Q}. \qquad (5.48)$$

Here ϕ is the polar angle for $\mathbf{Q}$, $\phi = \arctan(Q_2/Q_1)$.

These results are thus available for application to the BO approximation studied by means of the assumption

$$|n\rangle = \int d\mathbf{Q}|\mathbf{Q}\rangle\langle\mathbf{Q}|n\rangle|0\!:\!Q]. \qquad (5.49)$$

It follows that the Berry vector potential is given by the

formula

$$A_i = i[0\!:\!Q|\partial_i|0\!:\!Q]. \qquad (5.50)$$

To carry out this calculation, we need the form of the correlated vacuum state, as given by the equation [19]

$$|0\!:\!Q] = \mathcal{N} \exp[\tfrac{1}{2} Z_{ij} a_i^\dagger a_j^\dagger]|0], \qquad (5.51)$$

where $\mathcal{N}$ is a real normalization factor, whose value we shall not need, $a_i|0] = 0$, and Z_{ij} is a generally complex array whose values will be considered below. Using the constancy of the norm of the correlated ground state as a function of the values of $\mathbf{Q}$, we can rewrite (5.50) as

$$A_i = \tfrac{1}{2}i\{[0:Q|\partial_i|0:Q] - [\partial_i 0:Q|0:Q]\}, \qquad (5.52)$$

which shows that the (real) normalization factor $\mathcal{N}$ does not contribute. This leaves the result

$$A_i = \frac{1}{4}i[\langle a_k^\dagger a_l^\dagger\rangle \partial_i Z_{kl} - \langle a_k a_l\rangle \partial_i Z_{kl}^*], \qquad (5.53)$$

where the averages, indicated by angular brackets, are with respect to the correlated vacuum.

We next indicate how (5.53) can be evaluated in terms of the solutions we have found above for the equations of motion. The quantities Z_{kl} are solutions of the equations

$$\psi_j^{(i)} Z_{jk}^* = \chi_k^{(i)} \qquad (5.54)$$

that follow from the definition $b_i|0:Q] = 0$. The expectation values can also be evaluated with the help of the formulas

$$a_i = \psi_i^{(j)} b_j + \chi_i^{(j)*} b_j^\dagger, \qquad (5.55)$$

and their Hermitian conjugates that are the inverse to Eq. (5.36). An elementary calculation now yields

$$\langle a_k^\dagger a_l^\dagger\rangle = \langle a_k a_l\rangle^* = \chi_k^{(j)}\psi_l^{(j)*}. \qquad (5.56)$$

Thus for the vacuum Berry potential, we obtain the formula

$$A_i = \frac{1}{4}i[\chi_k^{(m)}\psi_l^{(m)*}\partial_i Z_{kl} - \chi_k^{(m)*}\psi_l^{(m)}\partial_i Z_{kl}^*]. \qquad (5.57)$$

Any other matrix element, $(A_i)_{\nu 0}$ of the Berry potential can be calculated by similar techniques. In fact, the only nonvanishing elements of this type are $(A_i)_{11,0}$, $(A_i)_{20,0}$, and $(A_i)_{02,0}$, where, for example, $\nu = 20$ means a state with two correlated bosons of type 1 and none of type 2. We quote formulas for these matrix elements that follow from the same elementary techniques that furnished Eq. (5.57). We thus have

$$\begin{aligned}(A_i)_{11,0} &= i[11:Q|\partial_i|0:Q]\\ &= -i[\partial_i\,11:Q|0:Q]\\ &= -i[0:Q|b_1\partial_i(b_2)|0:Q]\}\\ &= -i\left(\sum_j \psi_j^{(1)*}\partial_i\chi_j^{(2)*} - \chi_j^{(1)*}\partial_i\psi_j^{(2)*}\right). \end{aligned} \qquad (5.58)$$

Similarly, remembering the normalization of the states, we find

$$(A_i)_{20,0} = \frac{1}{i\sqrt{2}}\left(\sum_j \psi_j^{(1)*}\partial_i\chi_j^{(1)*} - \chi_j^{(1)*}\partial_i\psi_j^{(1)*}\right). \qquad (5.59)$$

Finally, the matrix element $(A_i)_{02,0}$ is obtained from (5.59) simply by replacing all superscripts 1 by 2. In order to implement fully the BO approximation, it is necessary to evaluate these matrix elements in terms of the explicit solutions of the model displayed in Eqs. (5.43)–(5.46). It is also appropriate to remark here that in consequence of these relations and Eq. (5.54) we can write

$$Z_{jk} = \exp(-i\phi)\tilde{Z}_{jk}, \quad \tilde{Z}_{jk} = \text{real}. \qquad (5.60)$$

The calculation of the Berry potentials as defined above is now straightforward. In terms of purely real quantities, we find, for example,

$$A_i = (\partial_i\phi)[(\tilde{\chi}_1^{(1)}\psi_1^{(1)} + \tilde{\chi}_1^{(2)}\psi_1^{(2)})\tilde{Z}_{11} + (\tilde{\chi}_1^{(1)}\psi_1^{(1)} - \tilde{\chi}_1^{(2)}\psi_1^{(2)})\tilde{Z}_{12}]. \qquad (5.61)$$

Using the real form of Eq. (5.54), this expression can be simplified to

$$\begin{aligned}A_i &= \partial_i\phi[(\tilde{\chi}_1^{(1)})^2 + (\tilde{\chi}_1^{(2)})^2]\\ &= \frac{G_1^2}{2}\left[\frac{1}{(\omega+\Omega^{(1)})(\omega+\Omega^{(1)}-2G_0Q)+(G_0^2-G_1^2)Q^2} + \frac{1}{(\omega+\Omega^{(2)})(\omega+\Omega^{(2)}+2G_0Q)+(G_0^2-G_1^2)Q^2}\right](-Q_2,Q_1)_i.\end{aligned} \qquad (5.62)$$

In contrast to the previous model the vector potential is not singular at the origin, but take the finite value

$$\mathbf{A}(0) = \frac{G_1^2}{4\omega(0)^2}(-Q_2,Q_1). \qquad (5.63)$$

Turning to the off-diagonal matrix elements, we find by similar calculations

$$(A_i)_{11,0} = 0, \qquad (5.64)$$

$$\begin{aligned}(A_i)_{20,0} &= \sqrt{2}\exp(-i\phi)[(\partial_i\phi)\psi_1^{(1)}\tilde{\chi}_1^{(1)} + i(\psi_1^{(1)}\partial_i\tilde{\chi}_1^{(1)} - \tilde{\chi}_1^{(1)}\partial_i\psi_1^{(1)}]\\ &= -\sqrt{2}\exp(-i\phi)\left(\psi_1^{(1)}\right)^2 f^{(1)}\left[\partial_i\phi + i(\partial_i Q)\partial_Q\ln f^{(1)}\right]\\ &= \sqrt{2}\exp(-i\phi)\frac{G_1[(\Omega^{(1)}+\omega)-G_0Q]}{2[(\omega+\Omega^{(1)})(\omega+\Omega^{(1)}-2G_0Q)+(G_0^2-G_1^2)Q^2]}\left[\frac{1}{Q}(-Q_2,Q_1) + i\frac{1}{Q}(Q_1,Q_2)Q\partial_Q\ln f^{(1)}\right],\end{aligned} \qquad (5.65)$$

$$(A_i)_{02,0} = -\sqrt{2}\exp(-i\phi)\frac{G_1[G_0Q + (\Omega^{(2)} + \omega)]}{2[(\omega + \Omega^{(2)})(\omega + \Omega^{(2)} - 2G_0Q) + (G_0^2 - G_1^2)Q^2]}\left[\frac{1}{Q}(-Q_2, Q_1) + i\frac{1}{Q}(Q_1, Q_2)Q\partial_Q\ln f^{(2)}\right].$$

$$(5.66)$$

These off-diagonal potentials are also regular as Q goes to zero, for reasonably well behaved $\omega(Q)$.

We now study the numerical solution of the adiabatic Hamiltonian,

$$H_C = \frac{1}{2}[(\mathbf{P} - \mathbf{A})^2 + |\mathbf{A}_{20,0}|^2 + |\mathbf{A}_{02,0}|^2]$$
$$+ \frac{1}{2}Q^2 + \frac{1}{2}[\Omega^{(1)}(Q) + \Omega^{(2)}(Q)], \qquad (5.67)$$

where we have once again made the choice $M = 1, V(Q) = \frac{1}{2}Q^2$. For simplicity we take $G_0 = 0$, and write $G_1 = G$. For this special choice $\Omega^{(1)} = \Omega^{(2)} = \Omega$ and $(A_i)_{02,0} = -(A_i)_{20,0}$. A simple form for $\omega(Q)$, chosen such that Ω is positive definite, is

$$\omega(Q) = \omega_0 + GQ. \qquad (5.68)$$

In Fig. 1 we show some of the relevant quantities in the collective Hamiltonian for the choice $G = 1$, $\omega_0 = 2$.

We diagonalize the collective Hamiltonian by first going to spherical coordinates, and use the fact that m is conserved to write down a radial equation. We then map the Q values from the interval $[0, \infty)$ to the interval $[0, 1]$. Finally we make a finite difference approximation to the radial equation, and solve the approximate equation by matrix diagonalization.

Solving the complete problem without making the adiabatic approximation is somewhat involved. Since the
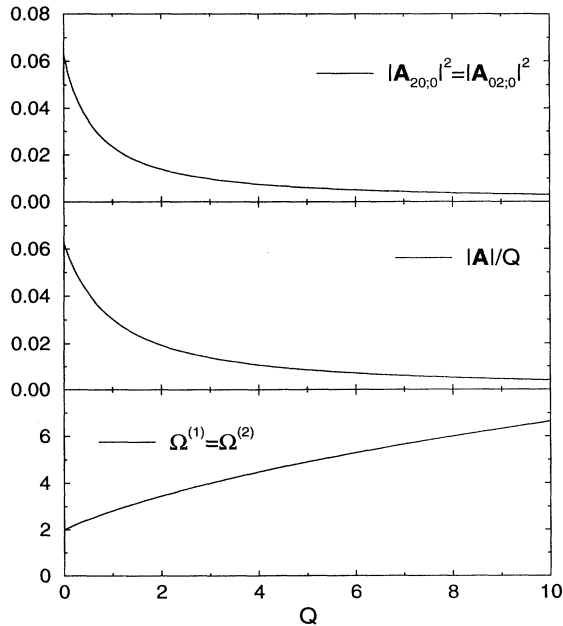

FIG. 1. Parameters in the collective Hamiltonian for $G = 1$, $\omega_0 = 2$. The lower panel shows the frequencies $\Omega^{(j)}$, the middle panel shows the size of the diagonal Berry potential, and the upper panel shows the square of the off-diagonal Berry potentials.

Hamiltonian is invariant under the interchange $a_1^\dagger \leftrightarrow a_2^\dagger$, we introduce new operators that are invariant under this parity transformation,

$$a_\pm^\dagger = \frac{1}{\sqrt{2}}(a_1^\dagger \pm a_2^\dagger). \qquad (5.69)$$

The interaction Hamiltonian takes the simple form

$$H_{\text{int}} = -G_0(a_+^\dagger a_+ - a_-^\dagger a_-)$$
$$- \frac{G_1}{2}(Q_+[a_+^2 - a_-^2] + Q_-[a_+^{\dagger 2} - a_-^{\dagger 2}]). \qquad (5.70)$$

We now make the expansion

$$\Psi = \sum_{K,\kappa} \psi_{K,\kappa}(Q)\frac{\left(a_+^\dagger\right)^{2K-2\kappa}\left(a_-^\dagger\right)^{2\kappa}}{\sqrt{(2K - 2\kappa)!(2\kappa)!}}|0]. \qquad (5.71)$$

(The even powers in this equation constitute the only combination that includes the vacuum for the fast degrees of freedom.)

An approximate solution is obtained by limiting the sum over K, while summing over all allowed κ. At the same time we expand $\psi_{K,\kappa}(Q)$ in a finite number of spherical harmonic oscillator eigenfunctions $\langle Q|nm\rangle$. We denote the m value used in the expansion of $\psi_{K,\kappa}(Q)$ by $m_{K,\kappa}$. The interaction does not couple states of different κ for fixed K. We thus find that $m_{K,\kappa} = m_K = m_{K-1} - 1$. Thus the value m_0 is a constant of the motion, and can be used to specify different solutions. This quantity corresponds directly to the value of m in the collective Hamiltonian. We have performed matrix diagonalizations for $\omega_0 = 2, 10$ and $G = 1$. We have used harmonic oscillator states up to principal quantum number 70, and K values up to 20. (This corresponds to a 61 401 × 61 401 matrix.) The resulting matrix, which is very sparse, was diagonalized using a Lanczos algorithm. The eigenvalues were checked for convergence by comparing a calculation with smaller cutoffs on n and K against one with larger cutoffs. In Tables III and IV we compare a few selected ground state energies of the complete collective Hamiltonian with the exact solution. The splitting between states with opposite values of m is completely due to the vector potential. For the case $\omega_0 = 2$, where the adiabatic approximation we see that the size of the

TABLE III. A comparison between the exact numerical ground state energies and those for the collective Hamiltonian. $\omega_0 = 2, G = 1$, and the values of m are listed in the table.

	$m = -5$	$m = 5$	$m = -1$	$m = 1$
Exact	9.54715	9.73101	4.97309	5.03405
Collective	9.56722	9.74656	4.98669	5.04375

	$m = -5$	$m = 5$
Exact	18.0745	18.0918
Collective	18.0750	18.0922

splitting is very close to the exact value. The difference is probably due to nonadiabatic effects that cannot be completely neglected for $\omega_0 = 2$. For the case $\omega_0 = 10$ the correspondence is much closer, but the size of the Berry vector potential is much smaller as well.

APPENDIX A: SCALAR PRODUCT AND TRANSFORMATION OF MOMENTUM OPERATORS

In this appendix we provide the proof of Eq. (2.7), which specifies how the momentum operator transforms under a general point transformation. It will be essential to recognize that this result is tied to a choice of scalar product. We suppose that the Hamiltonian (2.1) is to be used in conjunction with the metric

$$\langle \Psi_a | \Psi_b \rangle \equiv \int d\xi^1 \cdots d\xi^N \Psi_a^*(\xi) \Psi_b(\xi). \tag{A1}$$

Thus

$$\pi_\alpha \rightarrow -i(\partial/\partial\xi^\alpha). \tag{A2}$$

Now carry out the point transformation (2.3) with Jacobian J,

$$J = |\partial\xi^\alpha/\partial x^\beta|. \tag{A3}$$

If we introduce a new wave function

$$\psi_a = J^{\frac{1}{2}} \Psi_a, \tag{A4}$$

the metric is preserved in the sense

$$(\Psi_a, \Psi_b) = (\psi_a, \psi_b) = \int dx^1 \cdots dx^N \psi_a^*(x)\psi_b(x). \tag{A5}$$

This is the metric that is associated with Eq. (2.7), as we proceed to show.

With $d\xi^1 \cdots d\xi^N \equiv [d\xi]$, we study

$$\int [d\xi] \Psi_a^* \pi_\alpha \Psi_b = \int [dx] \psi_a^* J^{\frac{1}{2}} \pi_\alpha J^{-\frac{1}{2}} \psi_b. \tag{A6}$$

Thus we must show that

$$J^{\frac{1}{2}} \pi_\alpha J^{-\frac{1}{2}} = \frac{1}{2}\{f_\alpha^i, (-i\partial/\partial x^i)\}. \tag{A7}$$

We have first

$$J^{\frac{1}{2}} \pi_\alpha J^{-\frac{1}{2}} = J^{-\frac{1}{2}} J \frac{\partial x^i}{\partial\xi^\alpha} \frac{1}{i} \frac{\partial}{\partial x^i} J^{-\frac{1}{2}}. \tag{A8}$$

For ease of notation, consider below a three-dimensional space, since this will exhibit the general features. By utilizing the equation, equivalent to the definition of J as a determinant,

$$J \frac{\partial x^i}{\partial\xi^\alpha} = \frac{1}{2}\epsilon_{ijk}\epsilon_{\alpha\beta\gamma}\frac{\partial\xi^\beta}{\partial x^j}\frac{\partial\xi^\gamma}{\partial x^k}, \tag{A9}$$

with ϵ_{ijk} the alternating symbol, we display the algebraic manipulation leading to the desired result,

$$\begin{aligned}
J^{\frac{1}{2}}\pi_\alpha J^{-\frac{1}{2}} &= \frac{1}{i}J^{-\frac{1}{2}}\frac{1}{2}\epsilon_{ijk}\epsilon_{\alpha\beta\gamma}\frac{\partial\xi^\beta}{\partial x^j}\frac{\partial\xi^\gamma}{\partial x^k}\frac{\partial}{\partial x^i}J^{-\frac{1}{2}} \\
&= \frac{1}{2i}J^{-\frac{1}{2}}\left\{\frac{\partial}{\partial x^i}, \frac{1}{2}\epsilon_{ijk}\epsilon_{\alpha\beta\gamma}\frac{\partial\xi^\beta}{\partial x^j}\frac{\partial\xi^\gamma}{\partial x^k}\right\}J^{-\frac{1}{2}} \\
&= \frac{1}{2i}J^{-\frac{1}{2}}\left(\frac{\partial}{\partial x^i}\frac{1}{2}\epsilon_{ijk}\epsilon_{\alpha\beta\gamma}\frac{\partial\xi^\beta}{\partial x^j}\frac{\partial\xi^\gamma}{\partial x^k}J^{-\frac{1}{2}}\right) \\
&\quad + \frac{1}{2i}\left(J^{-\frac{1}{2}}\frac{1}{2}\epsilon_{ijk}\epsilon_{\alpha\beta\gamma}\frac{\partial\xi^\beta}{\partial x^j}\frac{\partial\xi^\gamma}{\partial x^k}\frac{\partial}{\partial x^i}\right)J^{-\frac{1}{2}}.
\end{aligned} \tag{A10}$$

By an application of (A9), this becomes

$$\frac{1}{2i}J^{-\frac{1}{2}}\frac{\partial}{\partial x^i}\left(J^{\frac{1}{2}}\frac{\partial x^i}{\partial\xi^\alpha}\right) + \frac{1}{2i}\left(J^{\frac{1}{2}}\frac{\partial x^i}{\partial\xi^\alpha}\right)\frac{\partial}{\partial x^i}J^{-\frac{1}{2}}$$

$$= \frac{1}{2i}\left\{\frac{\partial x^i}{\partial\xi^\alpha}, \frac{\partial}{\partial x^i}\right\}, \tag{A11}$$

the result sought.

APPENDIX B: POTENTIAL ENERGY FOR THE FAST VARIABLES

In terms of the original coordinates, let us consider the change in the potential energy between two neighboring points, ξ and $\xi + \delta\xi$. To second order in $\delta\xi$ we have the usual terms of a Taylor expansion,

$$\begin{aligned}
\Delta V &= V(\xi + \delta\xi) - V(\xi) \\
&= V_{,\alpha}\delta\xi^\alpha + \frac{1}{2}V_{\alpha\beta}\delta\xi^\alpha\delta\xi^\beta,
\end{aligned} \tag{B1}$$

that now appears most unsatisfactory, since ΔV is a scalar, but the second term of (B1) contains the ordinary rather than the covariant second derivative. This defect is removed by replacing the quantity $\delta\xi^\alpha$ by substitution from the relation

$$d\xi^\alpha = \delta\xi^\alpha + \frac{1}{2}\Gamma_{\beta\gamma}^\alpha\delta\xi^\beta\delta\xi^\gamma, \tag{B2}$$

that contains the Christoffel symbol,

$$\Gamma_{\beta\gamma}^\alpha = \frac{1}{2}\tilde{B}^{\alpha\delta}(\tilde{B}_{\delta\beta,\gamma} + \tilde{B}_{\delta\gamma,\beta} - \tilde{B}_{\beta\gamma,\delta}). \tag{B3}$$

We thus obtain the form

$$\Delta V = V_{,\alpha}d\xi^\alpha + \tfrac{1}{2}V_{;\alpha\beta}d\xi^\alpha d\xi^\beta, \qquad \text{(B4)}$$

where the second term contains the covariant derivative

$$V_{;\alpha\beta} = V_{,\alpha\beta} - \Gamma^\delta_{\alpha\beta}V_\delta. \qquad \text{(B5)}$$

It is now apparent from (B4) that $d\xi^\alpha$ are the components of a vector, and therefore transformation to any alternative set of coordinates such as the q^μ is standard.

This allows us to calculate the quantity $V^{(2)}$ of Eq. (2.10) from given dynamical quantities, provided we can define a complete set of coordinate axes at each point of the decoupled manifold. This is done in two stages. In the first stage, the basis vectors at each point of the tangent space to the collective submanifold, for example, the set f^i_α, are determined by the algorithm that discovers the collective submanifold. A set of basis vectors f^a_α, orthogonal to the tangent space is then determined (non-uniquely) by the requirement that these be orthogonal to the f^i_α and to each other with respect to the metric $\tilde{B}^{\alpha\beta}$. The basis vectors orthogonal to the tangent space are precisely the elements needed to compute the Hamiltonian of the fast variables.

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