Formally exact quantum variational principles for collective motion based on the invariance principle of the Schrödinger equation

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The time-dependent variational principle of the Schrödinger equation is applied to a formally exact solution of the Schrödinger equation whose variational elements are operators which define a collective subspace of the many-body system under study. This generalizes the procedure employed to derive time-dependent Hartree-Fock theory. Four distinct formally exact time-independent variational principles, including several familiar forms, are derived. Application to a class of exactly soluble models, studied in the vibrational regime, illustrates the different modes of implementation of two of the principles. The general theory of large amplitude collective motion is derived. It is shown that the principles can be applied equally well, using either boson or fermion pair degrees of freedom. Some aspects of the relation to the semiclassical limit are discussed.

NUCLEAR STRUCTURE Time-dependent variational principle for collective motion. Invariance principle of Schrödinger equation. Generalized coherent state trial function. Exact time-independent variational principles. Variational principle for intrinsic state. Cranking variational principle. Large amplitude collective motion. Semiclassical limit.

I. INTRODUCTION

The purpose of this paper is to describe yet another formally complete quantum theory of nuclear collective motion.[1] Because of a superficial resemblance to a great deal of the previous literature, especially on large amplitude collective motion,[2–14] we want immediately to distinguish the basic idea of this work from that described in the references. (It should be remarked, however, that this distinction does not include the motivating ideas of Marumori *et al.*,[15] which are, for all intents and purposes, the same as those in this paper. It is in the implementation that the present method is to be distinguished from this previous work.)

States of the form (called generalized coherent states)

$$|\Phi(\underline{\beta},\underline{\beta}^*,t)\rangle=\exp[\underline{b}^\dagger\cdot\underline{\beta}(t)-\underline{\beta}^\dagger(t)\cdot\underline{b}]\,|\Phi\rangle \tag{1.1}$$

have been used widely as trial states for the variational principle of the time dependent Schrödinger equation. Here $\underline{\beta}^\dagger(t)$ is a row matrix

$$\underline{\beta}^\dagger(t)=\{\beta_\alpha^*(t)\}$$
$$=[\beta_1^*(t),\beta_2^*(t),\ldots,] \tag{1.2}$$

$\underline{b}^\dagger(t)$ is a corresponding operator-valued row matrix, and $\underline{\beta}(t)$ and $\underline{b}(t)$ are the associated column matrices. If, for example, $b_\alpha^\dagger$ is a particle-hole (*ph*) creation operator and the index α runs over a complete set associated with a fixed Slater determinant $|\Phi_0\rangle$, then (1.1) is itself, according to Thouless's theorem,[16] an arbitrary determinant, and the resulting theory is time dependent Hartree-Fock (TDHF). By further specialization we can derive the random phase approximation (RPA) or adiabatic TDHF (ATDHF), which provides a foundation for the study of large amplitude collective motion.

Another interpretation for (1.1) arises if we take b_α, $b_\alpha^\dagger$ as boson operators—which in practice may be very complicated functions of fermion pair operators—with $|\Phi_0\rangle$ the vacuum for these bosons

$$b_\alpha\,|\Phi_0\rangle=0\,, \tag{1.3}$$

or at least a subset of them and of any other boson degrees of freedom of the system not explicitly contained in the set $\underline{b}$. If the *vector space* constructed from the $b_\alpha^\dagger$ operating on $|\Phi_0\rangle$ is invariant under the action of the Hamiltonian, H, it follows that these states span a subspace, equally well spanned by a subset of eigenstates of H. The simple structure of this space impels us to name it the collective subspace. Since (1.1) is a state in that space with enviably simple properties, it is indeed reasonable that information about the collective subspace can be extracted from it with the help of a variational principle. In fact, it is well known[17,18] (and will emerge again in this work) that the collective Hamiltonian can be constructed completely in a semiclassical approximation from the associated theory.

It is our basic observation that we can go beyond the semiclassical limit to a formally complete quantum theory by applying the time-dependent variational principle to a

state which bears a superficial resemblance to (1.1), but which is a formally *exact* solution of the time dependent Schrödinger equation, namely (E_0 is the ground state energy)

$$|\Psi(\beta,\beta^*,t)\rangle = \exp[i(H-E_0)t] \times \exp[\underline{b}^\dagger\cdot\underline{\beta}-\underline{\beta}^\dagger\cdot\underline{b}]\,|\Phi\rangle\ . \tag{1.4}$$

In effect, (1.4) replaces time-dependent parameters by time-dependent Heisenberg operators $b(t)$ and $b^\dagger(t)$.

Though (1.4) is more difficult to work with than (1.1), it is, nevertheless, it turns out, quite tractable. For illustrative purposes, we have carried out all manipulations in the body of the paper with a single collective coordinate. The basic approach, which exploits the assumption that an operator pair $b,b^\dagger$ exists such that

$$\exp[i(H-E_0)t]\,|\Psi(\beta,\beta^*)\rangle \equiv |\Psi(\beta,\beta^*,t)\rangle$$

is in the same subspace as $|\Psi(\beta,\beta^*)\rangle$ itself, has been called the "invariance principle of the Schrödinger equation."[3,9]

The contents of this paper are presented in the following order: In Sec. II, conditions for the Hamiltonian of a degree of freedom $(b,b^\dagger)$ to decouple from the full Hamiltonian are specified and the generalized coherent state is defined. In Sec. III, the time-dependent variational principle is applied. It is shown that the time dependence can be integrated out, giving rise to two forms of time-independent variational principle, one, quite familiar, involving the so-called intrinsic Hamiltonian. In Sec. IV, the structure of the class of admissible variations is analyzed in detail, after which yet a third form (with two subforms) of time-independent variational principle is derived, again with a familiar structure. In Sec. V, the second and third variational principles are applied to a class of exactly soluble models, and the difference in their content is elucidated. In Sec. VI, a further analysis is given of the relationship between the collective Hamiltonian and the generalized intrinsic state (1.4). In Sec. VII, the analysis of the previous sections leads almost immediately to a fourth, cranking form of the variational principle. In Sec. VIII, the second and third variational principles are used to derive Villar's equations[5] characterizing large amplitude collective motion. In Sec. IX, it is shown that previous developments of this paper were based on the assumption that the shell model had been mapped onto a boson space. Here it is shown that the variational principles are equally applicable in a fermion setting. In Sec. X, the relation to the semiclassical approximation is discussed briefly. In Sec. XI, we present a summary and conclusions.

Concerning other fully quantum theories of collective motion, this is hardly the place for a review, but one observation is in order at least concerning methods which utilize coherent or generalized coherent states. In this case it has been widely believed that the road from TDHF or ATDHF to a full quantum theory is to utilize the coherent state as a generating state for a generator coordinate approach.[14,19–22] This is indeed a perfectly legitimate way to go. The observation on which we have acted is simply that it is not necessarily the only way to generalize to a completely quantum theory.

II. DECOUPLING OF COLLECTIVE SUBSPACE: INVARIANCE PRINCIPLE OF THE SCHRÖDINGER EQUATION

We contemplate a subset of eigenstates $|\Psi_n\rangle$, $n=0,1,\ldots,N$, of the Schrödinger equation for a many-body system described by the Hamiltonian H, where the possibility $N\to\infty$ is also admitted. Under the action of H, the subspace $|\Psi_n\rangle$ goes over into itself, i.e., it is invariant under the action of H. Because of the special structures we have in mind, we shall call the space in question an invariant collective subspace.

At least two classes of examples can be cited which will prove of ultimate practical importance: (i) H, as an operator function of canonical pairs x_α,p_α or of corresponding boson variables $b_\alpha,b_\alpha^\dagger$, can be written as a sum of at least two commuting parts,

$$H=H_1+H_2\ , \tag{2.1}$$

where H_1 depends on a subset of the x_α,p_α and H_2 on the complementary set. Then, the direct product of the eigenstates of H_1 with, for instance, the ground state of H_2, form a collective subspace. (ii) H is a polynomial in the generators of a Lie algebra. The space of the eigenstates decomposes into irreducible representations under the algebra, each of which is an invariant subspace.

In reality, we may aspire to achieve condition (i) or (ii) approximately at best. Even if the Hamiltonian confronting us bears little superficial resemblance to one of the preferred forms, experiment may suggest the relevance of bending all efforts to try to transform it to the form required. In this paper we shall be concerned with case (i). For illustrative purposes, we restrict attention to a single canonical or pseudocanonical (see below) degree of freedom. We assume that the states $|\Psi_n\rangle$ can be expanded in terms of a set of oscillatorlike states

$$|p\rangle=(b^\dagger)^p/\sqrt{p!}\,|0\rangle,\quad b\,|0\rangle=0\ , \tag{2.2}$$

where $b,b^\dagger$ satisfy the commutation relations

$$[b,b^\dagger]=\Gamma\ . \tag{2.3}$$

Here, if we are truly dealing with bosons, Γ is the unit operator. To include the situation of fundamental interest to us, the nuclear shell model, Γ, will, in general, be a projection operator onto a finite set of the states (2.2), and $b,b^\dagger$ may be defined as (generally rather complicated) functions of fermion pair or particle-hole operators.

We wish then to determine the properties of the space $|\Psi_n\rangle$, supposing that $n=0$ corresponds to the exact ground state. Because of assumptions (2.2) and (2.3), regarding $|\Psi_n\rangle$, there exists a Hamiltonian, $H_c(b^\dagger;b)$, where the notation $(b^\dagger;b)$ implies normal ordering, which has the same excitation spectrum as H in the collective subspace (CS). By adjusting an additive constant, we may choose

$$H_c(b^\dagger;b)\,|\Psi_0\rangle=0\ . \tag{2.4}$$

We may thus write

$$H=H_c(b^\dagger;b)+H_{\text{in}} , \tag{2.5}$$

where H_{in}, the intrinsic Hamiltonian, must satisfy

$$H_{\text{in}}\,|\,\Psi_n\rangle=E_0\,|\,\Psi_n\rangle , \tag{2.6}$$

with E_0 the ground state energy, i.e., H_{in} is completely degenerate in the CS, or effectively a multiple of the unit operator in that space,

$$[b,H_{\text{in}}]=[b^\dagger,H_{\text{in}}]=0 . \tag{2.7}$$

Our goal is to develop means of decomposing H into the form (2.5). The techniques to accomplish this must also provide the means for transforming any other operator of interest. Thus, if H is some shell model Hamiltonian, a natural conclusion from (2.5) is that we shall be seeking a boson mapping that will express the fermion pairs in terms of the $b,b^\dagger$ and other less collective canonical pairs. We may expect this mapping or series of mappings to be determined both by the kinematical criterion (2.3) and the dynamical ones (2.4)—(2.7). We do not rule out the alternative reciprocal scheme of expressing the $b,b^\dagger$ in terms of fermion pairs, but delay discussion of this case until Sec. IX.

In any event, we may view the problem as the determination of the collective variables $b,b^\dagger$. As a dynamical criterion we shall apply, imminently, the variational principle of the time-dependent Schrödinger equation. We shall study the wave packet which evolves in time from a special initial state in the CS, of the form,

$$|\,\Psi(\beta,\beta^*)\rangle=U^{-1}(\beta,\beta^*)\,|\,\Psi_0\rangle , \tag{2.8}$$

where

$$U^{-1}=e^G,\quad G=\beta b^\dagger-\beta^* b , \tag{2.9}$$

which resembles a coherent state, except that $|\,\Psi_0\rangle$, as the exact ground state, *need not* be the vacuum for the operator b. We shall show that the application of (2.8) and (2.9) leads to a number of useful *time-independent* variational principles, several quite familiar. In the manipulations, the role of the operator U as a displacement operator,

$$Ub^\dagger U^{-1}=b^\dagger+\beta^*,\quad UbU^{-1}=b+\beta , \tag{2.10}$$

leads to great simplification. Other reasons for choosing this form will emerge.

III. TIME INDEPENDENT VARIATIONAL PRINCIPLES FROM THE TIME DEPENDENT VARIATIONAL PRINCIPLE

We study the state [different by a phase from (1.4)]

$$|\,\Psi(\beta,\beta^*,t)=\exp(iHt)U^{-1}(\beta,\beta^*)\,|\,\Psi_0\rangle , \tag{3.1}$$

which is a solution of the time-dependent Schrödinger equation (with the reversed sign of $\sqrt{-1}$) and, according to our assumptions, belongs to the invariant subspace, provided the operators $b,b^\dagger$ and the state $|\,\Psi_0\rangle$ have been properly chosen. By utilizing (2.3)—(2.7), (3.1) can be written

$$|\,\Psi(\beta,\beta^*,t)\rangle=\exp(iE_0t)U^{-1}(\beta,\beta^*,t)\,|\,\Psi_0\rangle , \tag{3.2}$$

where

$$U^{-1}(\beta,\beta^*,t)=e^{G(t)} , \tag{3.3}$$

$$G(t)=\beta b^\dagger(t)-\beta^* b(t) , \tag{3.4}$$

and

$$b^\dagger(t)=\exp(iH_ct)b\exp(-iH_ct) . \tag{3.5}$$

We characterize the state (3.2) by means of the time-dependent variational principle

$$\delta\int_{t_1}^{t_2}dt\,\langle\Psi(\beta,\beta^*,t)\,|\,[\tilde{H}+i\partial_t]\,|\,\Psi(\beta,\beta^*,t)\rangle=\delta\int_{t_1}^{t_2}dt\,\langle\Psi_0\,|\,U(\beta,\beta^*,t)[H+i\partial_t]U^{-1}(\beta,\beta^*,t)\,|\,\Psi_0\rangle=0 , \tag{3.6}$$

where

$$\tilde{H}=H+E_0 \tag{3.7}$$

is used to eliminate an irrelevant phase factor. The name *invariance principle of the Schrödinger equation* has been particularly applied to the special form (3.6) of the variational principle.[15]

We next manipulate the variational form so as to eliminate the time dependence. The main tool for this transformation is a well-known formula which permits us to calculate the time derivative of $U^{-1}(\beta,\beta^*,t)\equiv U^{-1}(t)$,

$$\frac{d}{dt}U^{-1}(t)=\frac{d}{dt}e^{G(t)}=\int_0^1 dv\,e^{G(t)v}[dG(t)/dt]e^{G(t)(1-v)}=\int_0^1 dv\,e^{G(t)v}[dG(t)/dt]e^{-G(t)v}U^{-1} . \tag{3.8}$$

With the aid of the multiple commutator expansion of $\exp(A)b\exp(-A)$, the equation of motion,

$$dG(t)/dt=-i[G(t),H_c(t)] , \tag{3.9}$$

and the formula

$$[b,H_c]=\partial H_c/\partial b^\dagger , \tag{3.10}$$

together with its Hermitian conjugate, we can readily derive the result

$$\int_0^1 dv\, e^{Gv}(dG/dt)e^{-Gv}=i\sum_{n=1}^{\infty}(-1)^{n+1}(1/n!)(\beta\partial/\partial b+\beta^*\partial/\partial b^\dagger)^n H_c \tag{3.11}$$

$$=i\{H_c(b^\dagger;b)-H_c(b^\dagger-\beta^*,b-\beta)\}\ . \tag{3.12}$$

In these equations we have suppressed the explicit time dependence, i.e., set $t=0$, since it is a trivial consequence that once the forms (3.11) or (3.12) have been reached the time dependence embodied in the time-development operators cancels out between operators and state vectors. Thus, the time integration yields (t_2-t_1), which is divided out.

From (3.11) and (3.12), we thus derive two forms of the variational principle. From (3.11) we obtain (as form I):

$$0=\delta\langle\Psi(\beta,\beta^*)|\left\{H-\sum_{n=1}^{\infty}(-1)^{n+1}(1/n!)(\beta\partial/\partial b+\beta^*\partial b^\dagger)^n H_c\right\}|\Psi(\beta,\beta^*)\rangle\ .$$

For the special case $H_c=\omega b^\dagger b$ this coincides with a result given previously in the literature.[3] To derive a second form, we make use of (2.10) followed by (2.4), in order to observe that

$$\langle\Psi(\beta,\beta^*)|H_c(b^\dagger-\beta^*;b-\beta)|\Psi(\beta,\beta^*)\rangle=\langle\Psi_0|H_c(b^\dagger;b)|\Psi_0\rangle=0\ . \tag{3.13}$$

The second term of (3.12) consequently disappears, and we are left with the variational principle (form II)

$$0=\delta\langle\Psi(\beta,\beta^*)|[H-H_c(b^\dagger;b)]|\Psi(\beta,\beta^*)\rangle$$
$$=\delta\langle\Psi(\beta,\beta^*)|H_{\rm in}|\Psi(\beta,\beta^*)\rangle\ .$$

To reach form II, we have certainly utilized the specific form of the trial state. This seems a little surprising since II is not only a familiar variational principle for a special intrinsic state, it also is a variational characterization of any intrinsic state. We shall find II extremely useful in application together with alternative forms which we can obtain by a study of the nature of admissible variations for II.

IV. ADMISSIBLE VARIATIONS

In our view, the variational principles appropriate to the study of collective motion have a special character distinct from those used to characterize a single state such as the ground state. We are after a variational characterization of a space of states built on a predetermined ground state, even if in practice that predetermination may not be divorced from the rest of the calculation and may end up being a codetermination. Thus, we take the theoretical view that

$$\delta|\Psi(\beta,\beta^*)\rangle=\delta U^{-1}(\beta,\beta^*)|\Psi_0\rangle\ , \tag{4.1}$$

i.e., we are seeking to optimize the choice of the collective operators $b,b^\dagger$; we write

$$\delta U^{-1}=e^{G+\delta G}-e^G\ . \tag{4.2}$$

We must then distinguish two cases: (i) δG commutes with G, i.e., with b and $b^\dagger$. Such variations correspond to δG in the space of operators kinematically independent of b and $b^\dagger$. Remarkably, such variations may be obtained equivalently from a variation of the ground state vector $|\Psi_0\rangle$ with fixed U^{-1}, namely,

$$\delta|\Psi_0\rangle=\delta G|\Psi_0\rangle\ . \tag{4.3}$$

(δG is, of course, skew-Hermitian.) This can be seen easily, since with $[\delta G,G]=0$, (4.2) may be written

$$\delta U^{-1}=\delta G U^{-1}=U^{-1}\delta G\ , \tag{4.4}$$

and, in consequence, for (4.1),

$$\delta|\Psi(\beta,\beta^*)\rangle=U^{-1}\delta G|\Psi_0\rangle$$
$$=U^{-1}\delta|\Psi_0\rangle\ . \tag{4.5}$$

Secondly, since we have, together with (4.4),

$$\delta U=-U\delta G=-\delta G U\ , \tag{4.6}$$

we may write from variational principle II,

$$0=\langle\Psi_0|[\delta G,(UHU^{-1}-UH_cU^{-1})]|\Psi_0\rangle$$
$$=\langle\Psi_0|[\delta G,UHU^{-1}]|\Psi_0\rangle\ , \tag{4.7}$$

since δG commutes with UH_cU^{-1}. (ii) $[\delta G,G]\neq 0$. We may still write

$$\delta U^{-1}=\delta G_L U^{-1}=U^{-1}\delta G_R\ , \tag{4.8a}$$

$$\delta U=-U\delta G_L=-\delta G_R U\ , \tag{4.8b}$$

where $\delta G\neq\delta G_L\neq\delta G_R$, in general. Nevertheless, as we vary δG over a complete set of noncommuting variations, we expect δG_L and δG_R to form a complete set. Using the form involving δG_R, this implies first that Eq. (4.5) holds for all variations, and thus our care in distinguishing what is to be varied turns out in practice to be unnecessary. (We have learned, however, that we may vary U^{-1} or $|\Psi_0\rangle$ and that varying both is redundant.) Finally, the first form of (4.7) holds for all G.

We may summarize the results of this section by stating a third form of the variational principle, which can be given in two forms, namely,

$$0=\langle\Psi_0|[\delta G,(UHU^{-1}-UH_cU^{-1})]|\Psi_0\rangle$$
$$=\langle\Psi(\beta,\beta^*)|[\delta G,(H-H_c)]|\Psi(\beta,\beta^*)\rangle\ .$$

The second form of III may also be considered to be a trivial consequence of II.

V. ELEMENTARY APPLICATIONS

A. The generalized Lipkin model

Before continuing with the theoretical development, it may be useful to illustrate the ideas presented so far with elementary examples based on the two-level LMG (Lipkin) model[23] and the various n-level generalizations of it.[24,25] In the latter, we consider n single particle levels, each with the same degeneracy, N. The operator $\alpha_{ir}^{\dagger}$ creates a "nucleon" in level r ($r=1\cdots n$), sublevel i ($i=1\cdots N$); α_{ir} is the corresponding destruction operator. The number-conserving bilinear sums

$$A_r^s=(A_s^r)^{\dagger}=\sum_{i=1}^{N}\alpha_{ir}^{\dagger}\alpha_{is} \tag{5.1}$$

are well-known generators of the Lie algebra $U(n)$, whereas the operators

$$J_0^{(k)}=\tfrac{1}{2}[A_{k+1}^{k+1}-A_1^1]\ , \tag{5.2}$$

$$J_+^{(k)}=(J_-^k)^{\dagger}=A_{k+1}^1,\quad k=1\cdots n-1\ , \tag{5.3}$$

together with the remaining A_{r+1}^{s+1}, $r\neq s$, generate SU(n).

We study a very special Hamiltonian within the algebra of SU(n),

$$H=\epsilon\sum_{k=1}^{n-1}\{\eta_k J_0^{(k)}+(f/2N)[(J_+^{(k)})^2+(J_-^{(k)})^2]\}\ , \tag{5.4}$$

$$\sum\eta_k=1,\quad \eta_{k+1}\geq\eta_k\ , \tag{5.5}$$

which is a sum of a single particle term and a "monopole-monopole" interaction. This class of models has the virtue that it can be studied profitably using either the Lie algebra, or, as is our current interest, a mapping to bosons.

We confine attention to the standard problem in which the number of nucleons is N, the degeneracy of each level. The ground state then belongs to the symmetric representation $(N,0\cdots 0)\equiv(N)$ of SU(n). For this representation, we can map to a space of $n-1$ bosons by means of a generalized Holstein-Primakoff transformation,[26,27]

$$(J_-^{(k)})^{\dagger}=J_+^{(k)}=a_k^{\dagger}\sqrt{N-\hat{n}}\ , \tag{5.6}$$

$$J_0(k)=-\tfrac{1}{2}(N-\hat{n})+\tfrac{1}{2}a_k^{\dagger}a_k\ , \tag{5.7}$$

$$A_{k+1}^{l+1}=a_k^{\dagger}a_l\quad (k,l=1,\ldots,n-1)\ , \tag{5.8}$$

$$A_1^1=N-\hat{n}\ , \tag{5.9}$$

$$n=\sum_{k=1}^{n-1}a_k^{\dagger}a_k\ , \tag{5.10}$$

where

$$[a_k,a_l^{\dagger}]=\delta_{kl}\ . \tag{5.11}$$

With the help of (5.6)–(5.10), (5.4) becomes

$$H=H_0+H_1'\ , \tag{5.12}$$

$$H_0=-\tfrac{1}{2}\epsilon(N-\hat{n})+\tfrac{1}{2}\sum_k\eta_k a_k^{\dagger}a_k\ , \tag{5.13}$$

$$H_1'=\tfrac{1}{2}f\epsilon\sum_k\{a_k^{\dagger}a_k^{\dagger}[1-(\hat{n}+1)/N]^{1/2}[1-(\hat{n}/N)^{1/2}]+\text{H.c.}\}\ . \tag{5.14}$$

To the first two terms in powers of N^{-1}, the interaction H_1' may be replaced by the simple polynomial H_1,

$$H_1=\tfrac{1}{2}f\epsilon\left[1-\frac{1}{2N}\right]\sum_k(a_k^{\dagger}a_k^{\dagger}+a_k a_k)-\frac{f\epsilon}{2N}[a_k^{\dagger}a_k^{\dagger}\hat{n}+\hat{n}a_k a_k]\ . \tag{5.15}$$

We shall work with the sum of (5.13) and (5.15). In any event, our aim in this section is only to illustrate methodology rather than to engage in curve fitting. The discussion which follows is applicable only to the vibrational regime (see below).

B. The two-level model

Let us first consider the case $n=2$. Then the effective Hamiltonian takes the form (one boson)

$$H=-\tfrac{1}{2}\epsilon N+\epsilon a^{\dagger}a+\tfrac{1}{2}f\epsilon\left[1-\frac{1}{2N}\right](a^{\dagger}a^{\dagger}+aa)-(f\epsilon/2N)[a^{\dagger}a^{\dagger}a^{\dagger}a+a^{\dagger}aaa]\ . \tag{5.16}$$

Of course, from the dynamical point of view, this model is trivial. There is no subspace to decouple. Up to an additive constant required to ensure the condition (2.4), (5.16) is already the collective Hamiltonian H_c. It seems that the only reasonable procedure at this point is to diagonalize it numerically. Nevertheless, something can be learned from this model by proceeding along the lines suggested by the theory developed in the preceding sections. For example, how is the boson, a, related to the boson, b, of those sections? The point is that this question does not have a unique interesting answer. There are instead several possibly interesting answers: (i) $a=b$ as already stated. (ii) As we shall see below there is some simplification in the theoretical structure if we define b to have the property

$$b\,|\,\Psi_0\rangle=0\ . \tag{5.17}$$

Combined with (2.4) this further requires that

$$[b,H_c]\,|\,\Psi_0\rangle=0\ . \tag{5.18}$$

Equations (5.17) and (5.18) imply that as a function of $b,b^{\dagger}$, H_c has no "dangerous diagrams," i.e., no terms of the form $b^p+(b^{\dagger})^p$ for any (integer) value of p. Thus, H_c will have the form

$$H_c=h_{11}b^{\dagger}b+h_{31}[(b^{\dagger})^3b+\text{H.c.}]+h_{22}(b^{\dagger})^2(b)^2+h_{51}[(b^{\dagger})^5b+\text{H.c.}]+\cdots\ . \tag{5.19}$$

To find the relationship between a and b, it suffices to assume that it can be written in the form

$$a^\dagger = \sum_{r=0,1,\ldots,} [x_{2r+1}(b^\dagger)^{2r+1} + y_{2r+1}(b)^{2r+1}] , \tag{5.20}$$

and $a=(a^\dagger)^\dagger$. We may choose the x_{2r+1} and y_{2r+1} real. In detail, consider the approximation which includes $r=0,1$ only. We then have four coefficients to determine. From the commutation relation

$$[a,a^\dagger]=1 , \tag{5.21}$$

we can conclude, consistently, by substituting (5.20),

$$1=x_1^2-y_1^2+6(x_3^2-y_3^2) , \tag{5.22a}$$

$$0=x_1x_3-y_1y_3 . \tag{5.22b}$$

For the remaining conditions substitute (5.20) and its Hermitian conjugate into (5.16), and reorder into normal form. The result is of the form

$$H=\sum_{r,s} g_{rs}(b^\dagger)^r(b)^s \equiv E_0+H_c . \tag{5.23}$$

By comparison of (5.23) with (5.19) (which has little, at first sight, to do with the variational theory in Secs. III and IV, but see below), we conclude that insofar as the terms in H and H_c are sufficiently well approximated,

$$g_{rs}=h_{rs}, \quad (r\neq 0, s\neq 0) . \tag{5.24}$$

We also have

$$g_{00}=E_0\equiv H_{\text{in}} . \tag{5.25}$$

The remaining conditions which determine x_{2r+1} and y_{2r+1} come from the values of r and s, in (5.24) for which h_{rs} in (5.19) vanishes, namely,

$$g_{20}=g_{40}=0 , \tag{5.26}$$

which are the conditions for the vanishing of the "dangerous diagrams." On the other hand, if $h_{rs}\neq 0$, we have a definition (of h_{rs}), rather than a condition.

This procedure, as stated above, is clearly of interest only in the vibrational or weak coupling regime. In this regime, as may easily be checked for the particular case under study,

$$(x_{2r+1}/x_{2r-1})\sim(y_{2r+1}/y_{2r-1})=0(N^{-1}) \tag{5.27}$$

and

$$h_{rs}=0(N^{1-(1/2)(r+s)}) , \tag{5.28}$$

i.e., the expansion in powes of $b,b^\dagger$ converges because the operators are 0 (1) and the successive coefficients decrease in the stated way. The case of large amplitude collective motion, where other criteria obtain, will be dealt with later in this paper.

Now how do the variational principles of Secs. III and IV enter, if at all? In place of the inclusive reasoning, following (5.23), let us apply the variational principle (VP) II [following Eq. (3.13)]. We calculate

$$E_0=\langle\Psi(\beta,\beta^\dagger)|[H-H_c]|\Psi(\beta,\beta^*)\rangle \equiv\sum(g_{rs}-h_{rs})(\beta^*)^r(\beta)^s , \tag{5.29}$$

and first require

$$\partial E_0/\partial\beta^*=\partial E_0/\partial\beta=0 . \tag{5.30}$$

The resulting double power series can only vanish if (5.24) is satisfied. The special condition (5.25) is not included. However, (5.30) now reduces (5.29) to (5.25).

Since all conditions necessary to determine the transformation (5.22) have been found, there should be no further variational requirements. Nevertheless, we cannot help wondering whether the expansion coefficients x_r and y_r can be treated as variational parameters so that we would have, e.g.,

$$0=\partial E_0/\partial x_r=\sum(\partial g_{ts}/\partial x_r)(\beta^*)^t(\beta)^s , \tag{5.31}$$

and similarly for variations with respect to y_r. Here we have checked in detail the simplest possible example, $x_3=y_3=0$, and have verified that the conditions $\delta E_0=\delta g_{00}=0$ (ground state variational principle) and $\delta(x_1^2-y_1^2)=0$ [cf. (5.22a)] together imply $g_{20}=0$. This result should generalize, as will be evident from the further considerations.

The same results as follow from (5.30) can be derived from variational principle III at the end of Sec. IV. Choosing $G=(b-\beta)$ or its Hermitian conjugate, the calculation equivalent to (5.30) is

$$\langle\Psi(\beta,\beta^*)|[b,(H-H_c)]|\Psi(\beta,\beta^*)\rangle=0 , \tag{5.32}$$

leading to the same consequences.

This is about all we can learn from the two level model, unless we want to define b as the boson in the representation in which H is diagonal,

$$H=E_0+h_1b^\dagger b+h_2(b^\dagger)^2b^2+\cdots . \tag{5.33}$$

We still have (5.17), and (5.20) has to be replaced by a more general expansion. The same principles apply, however, to the determination of the expansion coefficients.

C. Three-level model

To augment our knowledge, we turn next to the three-level model and two bosons a_k. In order to reach the understanding sought in the simplest possible terms, we restrict our study of the decoupling problem to quadratic terms. We introduce two bosons b_1 and b_2, each satisfying (5.17), related to a_1 and a_2 by the equations ($k=1,2$; $\lambda=1,2$)

$$a_k^\dagger=x_{k\lambda}b_\lambda^\dagger+y_{k\lambda}b_\lambda , \tag{5.34a}$$

$$a_k=x_{k\lambda}b_\lambda+y_{k\lambda}b_\lambda^\dagger , \tag{5.34b}$$

$$b_\lambda=x_{k\lambda}a_k-y_{k\lambda}a_k^\dagger , \tag{5.34c}$$

$$b_\lambda^\dagger=x_{k\lambda}a_k^\dagger-y_{k\lambda}a_k . \tag{5.34d}$$

The eight coefficients $x_{k\lambda}$ and $y_{k\lambda}$ satisfy four kinematical constraints following from the canonical commutation relations (summation convention),

$$\delta_{kk'}=x_{k\lambda}x_{k'\lambda}-y_{k\lambda}y_{k'\lambda} , \tag{5.35}$$

$$0=x_{1\lambda}y_{2\lambda}-y_{1\lambda}x_{2\lambda} , \tag{5.36}$$

where (5.35) provides three conditions and (5.36) the fourth. Substituting (5.34) into H, Eq. (5.15), yields the form

$$H=\sum g_{r_1r_2,s_1s_2}(b_1^\dagger)^{r_1}(b_2^\dagger)^{r_2}(b_1)^{s_1}(b_2)^{s_2}$$
$$\equiv E_0+H_c\ . \tag{5.37}$$

Proceeding as in the sequel to (5.23), the conditions which determine the remaining transformation coefficients are the vanishing of the terms proportional to $(b_1^\dagger)^2$, $(b_2^\dagger)^2$, $b_1^\dagger b_2^\dagger$, and $b_1^\dagger b_2$ (plus H.c. in every case). These are the four conditions

$$g_{20,00}=g_{02,00}=g_{11,00}=g_{10,01}=0\ . \tag{5.38}$$

If $g_{10,10}<g_{01,01}$, as we suppose, after Eqs. (5.35), (5.36), and (5.38) are solved, we set further terms depending on $b_2,b_2^\dagger$ in H, such as $b_2^\dagger b_2$, to zero, in order to be able to satisfy (5.37), since H_c depends only on $b_1,b_1^\dagger$. Though this last step appears a bit *ad hoc,* it is equivalent (as we shall now see) to what the variational principles do automatically.

Consider VP II. As in (5.29), we now find

$$E_0=\sum(g_{r0,s0}-h_{rs})(\beta^*)^r(\beta)^s\ . \tag{5.39}$$

Here Eq. (5.30) yields, in a consistent order, only *one* dynamical condition, namely,

$$g_{20,00}=g_{00,20}=0\ , \tag{5.40}$$

and we are missing three conditions. This tells us that we were correct to pay attention to the arguments associated with (5.31). The appropriate form appears to be

$$0=\delta E_0-\sum_{\alpha=1}\Lambda_\alpha\delta\mathcal{N}_\alpha=\delta g_{00,00}-\sum\Lambda_\alpha\delta\mathcal{N}_\alpha\ . \tag{5.41}$$

Here $\mathcal{N}_\alpha=0$ are the four kinematical constraints (5.35) and (5.36) and Λ_α are associated Lagrange multipliers. Since there are eight variables, when the Λ_α are eliminated we obtain four conditions which must be equivalent to (5.38). In this case (5.40) is redundant. It thus appears that for VP II, the procedures based on (5.31) or (5.41) are the natural ones, when we *first* evaluate the expectation value of $(H-H_c)$ and *then* consider c-number variations.

Though the ground state variational principle (5.41) suffices, as we know from experience, to fix the harmonic approximation, it is almost certain that when we go beyond this approximation, the optimum determination of the transformation coefficients must involve the "β dependence," i.e., must bring in excited eigenstates. How to make this determination within the present framework is a question worthy of further study, though it can be avoided in practice by utilizing the method described below.

If we turn to VP III, where we utilize q-number variations, it is the direct derivation of (5.38) which is the natural outcome. To be specific we have, in a consistent approximation,

$$H=g_{00,00}+g_{10,10}b_1^\dagger b_1+g_{01,01}b_2^\dagger b_2$$
$$+g_{20,00}[(b_1^\dagger)^2+(b_1)^2]+g_{02,00}[(b_2^\dagger)^2+(b_2)^2]$$
$$+g_{11,00}[b_1^\dagger b_2^\dagger+b_2b_1]+g_{10,01}[b_1^\dagger b_2+b_2^\dagger b_1]\ , \tag{5.42}$$

$$H_c=h_{11}b_1^\dagger b_1\ . \tag{5.43}$$

We apply VP III with the variations $\delta G=(b_1-\beta)$, b_2, and $(b_2)^2$ and find easily that these yield the four conditions (5.38). For instance,

$$0=\langle\Psi(\beta,\beta^*)\,|\,[b_2,(H-H_c)]\,|\,\Psi(\beta,\beta^*)\rangle$$
$$=g_{11,00}\beta^*+g_{10,01}\beta\ , \tag{5.44}$$

which yields two of the conditions.

The considerations of this section apply only to the vibrational regime. The theory of large amplitude collective motion developed in Secs. VIII and IX can also be applied to these models, but these applications will be presented in a separate publication.

VI. RECONSTRUCTION OF THE COLLECTIVE HAMILTONIAN FROM THE INTRINSIC STATE

We wish to formalize the procedures of the previous section, to draw a few lessons therefrom, and finally to consider one necessary generalization. Consider the latter first, in reference to the three-level model, in order to be concrete. We have written H in the form

$$H=H(b_1^\dagger,b_2^\dagger;b_1,b_2) \tag{6.1}$$

and imposed the condition

$$b_i\,|\,\Psi_0\rangle=0\ . \tag{6.2}$$

In the regime of large amplitude collective motion to be discussed, it remains convenient to impose condition (6.2) for the *noncollective modes,* but this condition becomes less than convenient for the collective mode. Under these more general circumstances, with $b_1=b$, we have, assuming

$$H_c=\sum h_{rs}(b^\dagger)^r(b)^s \tag{6.3}$$

and using (2.10),

$$\langle\Psi(\beta,\beta^*)\,|\,H_c\,|\,\Psi(\beta,\beta^*)\rangle=\langle\Psi_0\,|\,H_c(b^\dagger+\beta^*;b+\beta)\,|\,\Psi_0\rangle=\sum\tilde{h}_{rs}(\beta^*)^r\beta^s\ , \tag{6.4}$$

where by straightforward expansion, we find

$$\tilde{h}_{rs}=\sum_{n_1,n_2}h_{r+n_1,s+n_2}\frac{(r+n_1)!(s+n_2)!}{r!n_1!s!n_2!}\langle\Psi_0\,|\,(b^\dagger)^{n_1}b^{n_2}\,|\,\Psi_0\rangle\ . \tag{6.5}$$

In the vibrational domain, the series (6.5) should be rapidly convergent in consequence of condition (5.28). Therefore, given $\tilde{h}_{rs}$, Eq. (6.5) can be solved by iteration for the h_{rs}, starting from the approximation $h_{rs}\cong\tilde{h}_{rs}$.

Of course the determination of the $\tilde{h}_{rs}$ must trace back to the properties of the given Hamiltonian. In fact, we have

$$H_c(\beta^\dagger;\beta)\equiv\langle\Psi(\beta,\beta^*)\,|\,H\,|\,\Psi(\beta,\beta^*)\rangle-\langle\Psi_0\,|\,H\,|\,\Psi_0\rangle\ . \tag{6.6}$$

As we have seen in the preceding section, once the "b bosons" are introduced, H will take the general form

$$H=\sum g_{rs}(b^\dagger)^r b^s+H'\equiv E_0+H_c+H'\ , \tag{6.7}$$

where H' contains all dependence on the noncollective bosons, and therefore includes coupling between the collective and noncollective spaces. As long as we retain (6.2) for the *noncollective bosons,* we must have the equations

$$\begin{aligned}0&=\langle\Psi(\beta,\beta^*)\,|\,H'\,|\,\Psi(\beta,\beta^*)\rangle\\&\equiv\langle\Psi(\beta,\beta^*)\,|\,[\delta G,H']\,|\,\Psi(\beta,\beta^*)\rangle\ ,\end{aligned} \tag{6.8}$$

where the second condition holds for any δG completely *within* the collective subspace. Both conditions (6.8) follow from (6.2) and the dual condition $\langle\Psi_0\,|\,b_i^\dagger=0$ for the noncollective degrees of freedom.

Another important conclusion to be drawn from the preceding section, as well as from the remarks just made, is that all that can be learned from variations within the collective subspace using VP III can be learned from linear variations

$$\delta G=\epsilon b^\dagger-\epsilon^* b\ . \tag{6.9}$$

This could be gleaned from our examples, but follows in general from VP II, since it is equivalent to Eq. (5.30). Thus, we can conclude that the most general set of variations consists of the direct sum of (6.9) and variations which commute with the collective operators. From VP III with $\delta G=$(6.9), we learn that

$$\tilde{g}_{rs}=\tilde{h}_{rs}\ , \tag{6.10}$$

whereas $\tilde{g}_{rs}$ is related to g_{rs} by a series of form (6.9). It follows that

$$g_{rs}=h_{rs}\ . \tag{6.11}$$

As pointed out previously, these conditions fall into two sets. Where $h_{rs}\neq0$, they are determinations of h_{rs} in terms of the known (or to be computed) quantities g_{rs}. If $h_{rs}=0$, $g_{rs}=0$ is a condition for the determination of the b_i bosons. Further conditions are obtained by choosing δG outside the collective subspace, or as (5.41), by applying energy minimization conditions.

VII. CRANKING VARIATIONAL PRINCIPLE

We are finally in a position to derive yet another form of variational principle. We shall deal directly with the case

$$b\,|\,\Psi_0\rangle\neq0\ . \tag{7.1}$$

Details simplify when the right-hand side (rhs) of (7.1) vanishes, but the same general forms will hold. We write

$$\begin{aligned}\langle\Psi(\beta,\beta^*)\,|\,H_c(b^\dagger;b)\,|\,\Psi(\beta,\beta^*)\rangle&=\tilde{H}_c(\beta^*,\beta)\\&\equiv\sum\tilde{h}_{rs}(\beta^*)^r\beta^s\ .\end{aligned} \tag{7.2}$$

We have from VP II

$$0=\delta\langle\Psi(\beta,\beta^*)\,|\,H\,|\,\Psi(\beta,\beta^*)\rangle-\delta\tilde{H}_c(\beta^*,\beta)\ . \tag{7.3}$$

Since the $\tilde{h}_{rs}$ are not variational quantities, the second term on the right may be rewritten

$$\begin{aligned}\delta\tilde{H}_c(\beta^*,\beta)&=(\partial\tilde{H}_c/\partial\beta^*)\delta\beta^*+(\partial H_c/\partial\beta)\delta\beta\\&\equiv\lambda\delta\beta^*+\lambda^*\delta\beta\\&=\delta\langle\Psi(\beta,\beta^*)\,|\,[\lambda b^\dagger+\lambda^* b]\,|\,\Psi(\beta,\beta^*)\rangle\ .\end{aligned} \tag{7.4}$$

In the last form of (7.4) we recognize that λ and λ^* are to remain fixed and thus play the role of Lagrange multipliers. We thus have transformed the variational principle into form IV:

$$\begin{aligned}0&=\delta\langle\Psi(\beta,\beta^*)\,|\,[H-\lambda b^\dagger-\lambda^* b]\,|\,\Psi(\beta,\beta^*)\rangle\\&=\delta\langle\Phi(\lambda,\lambda^*)\,|\,[H-\lambda b^\dagger-\lambda^* b]\,|\,\Phi(\lambda,\lambda^*)\rangle\\&\equiv\delta[\langle H\rangle_{\lambda,\lambda^*}-\lambda\langle b^\dagger\rangle_{\lambda,\lambda^*}-\lambda^*\langle b\rangle_{\lambda,\lambda^*}]\ ,\end{aligned}$$

where we have written

$$\Phi(\lambda,\lambda^*)\equiv\Psi(\beta,\beta^*)\ . \tag{7.5}$$

Applications of IV (as of I) will not be considered in this paper (see Ref. 18, however).

VIII. LARGE AMPLITUDE COLLECTIVE MOTION

We have been concerned until now with general principles and with practice applicable to anharmonic vibrations. We now show how the same general methods can be applied to the case of large amplitude collective motion, where the adiabatic approximation—expansion in powers of the momentum—is applicable. One of us recently gave an exhaustive account of this subject based on the equations of motion approach.[28,29] Here, it is our aim to show how the same basic equations, Villars's equations, can be derived from the present standpoint. These equations are valid under semiclassical conditions; one feature of the present formulation is that it provides a clear method for including quantum corrections.

Confining attention to a single collective degree of freedom described by a boson, b, we introduce canonical coordinates $\hat{x}$, and $\hat{p}$ by the usual transformation

$$b^\dagger=\frac{1}{\sqrt{2}}(\hat{x}-i\hat{p})\ , \tag{8.1a}$$

$$b=\frac{1}{\sqrt{2}}(\hat{x}+i\hat{p})\ . \tag{8.1b}$$

In the following, we take the coherent state in the form

$$|\,q,p\,\rangle=|\,\Psi(q,p)\rangle=\exp(i\hat{x}p)\exp(-i\hat{p}q)\,|\,\Psi_0\rangle\ , \tag{8.2}$$

which differs only by a phase from the form utilized previously. We shall also write

$$|\,q,p\,\rangle = \exp(i\hat{x}p)\,|\,q\,\rangle\ . \tag{8.3}$$

The collective Hamiltonian will be taken in the form

$$H_c = \tfrac{1}{2}\hat{p}K(\hat{x}\,)\hat{p} + V(\hat{x}\,)\ . \tag{8.4}$$

In this expression, $V(\hat{x})$ is of 0 (1) (because the ground state energy has been subtracted), $K(x)$ is 0 (1), but because we assume $\hat{x}\simeq\Omega^{1/2}$, where Ω is some large parameter of the order of the number of particles in the system, $\hat{p}\sim\Omega^{-1/2}$ and the kinetic energy is small compared to the potential energy. It will become evident that this implies that in the evaluation of $\langle q,p\,|\,H_c\,|\,q,p\,\rangle$, an expansion in powers of p is permissible. To second order,

$$\langle q,p\,|\,H_c\,|\,q,p\,\rangle \cong \langle q\,|\,\{H_c - ip[\hat{x},H_c] - \tfrac{1}{2}p^2[\hat{x},[\hat{x},H_c]]\}\,|\,q\,\rangle\ . \tag{8.5}$$

With the corresponding expression for the expectation value of H, we apply VP II. To zero and first order in p, we find

$$\delta\langle q\,|\,(H - H_c)\,|\,q\,\rangle = 0\ , \tag{8.6}$$

$$\delta\langle q\,|\,[\hat{x},(H - H_c)]\,|\,q\,\rangle = 0\ . \tag{8.7}$$

We shall return below to consider second (and higher) order variational conditions. Also among the possible variations is differentiation with respect to the parameter p. It is a simple exercise to show that the consequences of such variations are included in (8.6) and (8.7).

To see how to implement the variational conditions (8.6) and (8.7), we suppose in this section that the Hamiltonian has the form

$$H = \tfrac{1}{2}\pi_\alpha\kappa^{\alpha\beta}\pi_\beta + v(\underline{\xi})\ , \tag{8.8}$$

where

$$\underline{\xi} = (\xi^1 \cdots \xi^n)\ . \tag{8.9}$$

For example, for the SU(n) model, the form (8.8) can be reached by the substitution

$$a^\dagger_\alpha = \frac{1}{\sqrt{2}}(\xi^\alpha - ip_\alpha)\ , \tag{8.10a}$$

$$a_\alpha = \frac{1}{\sqrt{2}}(\xi^\alpha + ip_\alpha)\ . \tag{8.10b}$$

The substitution of (8.10) into (5.13) and (5.15) leads to the form (8.8) provided we drop terms in π_α higher than the second (up to fourth order terms occur).

As has been discussed at great length in our recent previous work,[28] we can define the collective coordinate x by first considering an invertible point transformation

$$\xi^\alpha = \phi^\alpha(x^1 \cdots x^n)\ , \tag{8.11a}$$

$$x^\alpha = f^\alpha(\xi^1 \cdots \xi^n)\ , \tag{8.11b}$$

then suppose the collective subspace to be defined by the conditions

$$x^2 = \cdots = x^n = 0\ , \tag{8.12}$$

and by choosing

$$x = x^1 = \xi^1 + \text{constant}\ , \tag{8.13}$$

where the constant may be used to shift to the position of a "deformed" minimum as origin.

[If H described a set of uncoupled oscillators and ξ^1 corresponded to the lowest frequency, the collective subspace would be defined by setting $\xi^2 = \cdots = \xi^n = 0$. Equation (8.12) generalizes this condition when coupling is present.]

Turning now to a study of the variational conditions, for (8.6) we consider first the class of variations

$$\delta\,|\,q\,\rangle = -i\pi_\alpha\,|\,q\,\rangle\ . \tag{8.14}$$

(Together with the variations

$$\delta\,|\,q\,\rangle = i(\xi^\alpha - \langle\xi^\alpha\rangle)\,|\,q\,\rangle\ , \tag{8.15}$$

these should constitute a complete set of variations.) We calculate

$$i[\pi_\alpha,H] = \tfrac{1}{2}\pi_\beta\kappa^{\beta\gamma}{}_{,\alpha}\pi_\delta + v_{,\alpha}\ , \tag{8.16}$$

where the notation $O_{,\alpha}$ means differentiation with respect to ξ^α. To calculate $[\pi_\alpha,H_c]$, we use a Hermitian representation in the collective subspace, namely,

$$\pi_\alpha \to \frac{1}{2i}\left\{\frac{\partial x}{\partial\xi^\alpha},\frac{\partial}{\partial x}\right\} \equiv \tfrac{1}{2}\{f_{,\alpha},p\}\ . \tag{8.17}$$

We then calculate

$$i[\pi_\alpha,H_c] = f_{,\alpha}V_{,x} + \tfrac{1}{4}\{f_{,\alpha},pK_{,x}p\} - \tfrac{1}{4}\{p,\{p,Kf_{,\alpha,x}\}\}\ . \tag{8.18}$$

Furthermore, with (8.17) and the displacement operator property

$$e^{i\hat{p}q}O(\hat{x}\,)e^{-i\hat{p}q} = O(\hat{x}+q)\ , \tag{8.19}$$

the variational condition "reduces" to the form

$$\tfrac{1}{8}\langle\{f_{,\beta}(q+\hat{x}\,),p\}\kappa^{\beta\gamma}{}_{,\alpha}(q+\hat{x}\,)\{f_\gamma(q+\hat{x}\,),p\}\rangle + \langle v_{,\alpha}(q+\hat{x}\,)\rangle = \langle f_{,\alpha}(q+\hat{x}\,)V_{,x}(q+\hat{x}\,)\rangle + \tfrac{1}{4}\langle\{f_{,\alpha}(q+\hat{x}\,),pK_{,x}(q+\hat{x}\,)p\}\rangle - \tfrac{1}{4}\langle\{p,\{p,K(q+\hat{x}\,)f_{,\alpha,x}(q+\hat{x}\,)\}\}\rangle\ , \tag{8.20}$$

where

$$\langle\Theta(q+\hat{x},p)\rangle = \langle\Psi_0\,|\,\Theta(q+\hat{x},p)\,|\,\Psi_0\rangle\ . \tag{8.21}$$

Equation (8.20) can be simplified if we take advantage of various orders of magnitude. We already know that $\hat{p}\sim\Omega^{-1/2}$. In the case of the variable $\hat{x}$ we shall assume that we have made a displacement, if necessary, so that $\hat{x}\sim 1$. Thus, if we have an expression such as

$$\langle \Theta(q+\hat{x}) \cong \Theta(q)+\tfrac{1}{2}\Theta''(q)\langle \hat{x}^2\rangle + \cdots \tag{8.22}$$

(we assume $\langle x\rangle=\langle p\rangle=0$), since $\Theta''(q)/\Theta(q)\sim\Omega^{-1}$ and $\langle \hat{x}^2\rangle\sim 1$, we have a convergent expansion. With these assumptions, we find that the largest terms in (8.20) yield the condition

$$v_{,\alpha}(q)=f_{,\alpha}(q)V_{,q}(q)\ . \tag{8.23}$$

The leading correction terms, which will not be recorded, depend on $\langle \hat{x}^2\rangle$, $\langle p^2\rangle$, and the functions in (8.23) and their derivatives. Before we can understand how to calculate these we must understand the structure of the remaining equations which follow from (8.6) and (8.7). For this purpose we shall use (8.11), (8.12), and (8.17) below.

Equation (8.23) plus corrections are, in fact, all we can deduce from (8.6). Thus, the variation (8.15) does not contribute here because we assume $\langle \hat{p}\rangle=0$. Turning then to (8.7), we use (8.15) *here* and compute easily (and exactly)

$$-[\xi^{\alpha},[x,H]]=\kappa^{\alpha\beta}f_{,\beta}(x)\ , \tag{8.24}$$

$$[\xi^{\alpha},[xH_c]]=\phi^{\alpha}{}_{,x}K(x)\ . \tag{8.25}$$

The equality of the expectation values of these operators in the states $|q\rangle$ implies the equality of the expressions themselves. In conformity with (8.23), we replace x by q and write

$$\kappa^{\alpha\beta}f_{,\beta}(q)=\phi^{\alpha}{}_{,q}K(q)\ . \tag{8.26}$$

In fact (8.23) and (8.26) are Villars's dynamical conditions, and as we have discussed,[28] have only to be appended by the kinematical condition

$$\langle q\,|\,[\hat{x},\hat{p}]\,|\,q\rangle=i \tag{8.27}$$

to provide a complete or deterministic theory. From (8.27) we deduce

$$f_{,\alpha}\phi^{\alpha}{}_{,x}=1\ , \tag{8.28}$$

if we evaluate by means of the Hermitian substitution

$$\hat{p}=\tfrac{1}{2}\{\phi^{\alpha}{}_{,x},\pi_{\alpha}\}\ . \tag{8.29}$$

Equation (8.28) is the condition that accompanies (8.23) and (8.26). Thus, from (8.26) and (8.28) we can conclude

$$K(q)=f_{,\alpha}\kappa^{\alpha\beta}f_{,\beta}\ , \tag{8.30}$$

and from (8.23), to an additive constant,

$$V(q)=v[\xi^1(q)\cdots\xi^n(q)]\ . \tag{8.31}$$

These equations define the collective parameters in terms of the parameters of the given Hamiltonian and of the equations of the collective subspace. The same equations follow in the same approximation from the definition

$$H_c(q,p)=\langle q,p\,|\,H\,|\,q,p\rangle-\langle H\rangle_0\ . \tag{8.32}$$

We leave this last calculation as an exercise.

Two problems remain in this section. First there is the problem of quantum corrections to (8.23). These can be obtained perturbatively or iteratively by using the solution in their absence to calculate the appropriate derivatives of $f(\xi)$, $V(\hat{x})$, and $K(\hat{x})$, and a suitable candidate for the ground state $|\Psi_0\rangle$ to calculate $\langle x^2\rangle$and $\langle p^2\rangle$. We shall not enter into details.

The second problem is the one we promised to discuss earlier, that of higher order variational conditions. For the Hamiltonian (8.8) there are no nontrivial higher order conditions. For example, the next order variation condition is

$$\delta\langle q\,|\,[\hat{x},[\hat{x},(H-H_c)]]\,|\,q\rangle=0\ . \tag{8.33}$$

However, for the Hamiltonian (8.8), the double commutator in (8.33) vanishes identically in consequence of Eq. (8.30). A fortiori still higher order variational conditions are identically satisfied.

Summarizing the results of this section, we have found that except for quantum corrections to the collective potential energy, for Hamiltonians of the form (8.8), Villars's equations are the full consequences of VP II. The content of these equations has been fully explored in recent work.[28–33]

IX. CALCULATIONS WITH FERMION DEGREES OF FREEDOM

The theory developed until now has been based on the assumption that the shell model problem has been mapped onto a subspace of a boson space as an intermediate step before any major attempt at decoupling the collective subspace is made. Another approach, the prevailing one thus far with realistic shell models, is to attempt to relate the collective variables directly to shell model variables. This is the approach found in the earlier and concomitant work of two of us (Marumori and Une). In this section, we shall indicate in outline form how both the large and small amplitude collective motion may be studied from this standpoint, using the methods of this paper.

We apply VP III, assuming that $|q,p\rangle$ is a Slater determinant. That this is the appropriate starting point for a correct, semiclassical approximation has been justified repeatedly in the literature cited, and recently again by one of us, utilizing the Wigner transform.[29] We choose the usual form of shell-model Hamiltonian

$$H=\tfrac{1}{2}h_{\alpha\beta}a^{\dagger}_{\alpha}a_{\beta}+\tfrac{1}{4}V_{\alpha\beta\gamma\delta}a^{\dagger}_{\alpha}a^{\dagger}_{\beta}a_{\delta}a_{\gamma}\ , \tag{9.1}$$

where

$$h_{\alpha\beta}=h^{*}_{\beta\alpha}\ , \tag{9.2}$$

$$V_{\alpha\beta\gamma\delta}=-V_{\beta\alpha\gamma\delta}=-V_{\alpha\beta\delta\gamma}=V^{*}_{\gamma\delta\alpha\beta}\ . \tag{9.3}$$

As variations for VP III, we take

$$\delta G\propto\hat{\rho}_{\alpha\beta}\ , \tag{9.4}$$

$$\hat{\rho}_{\alpha\beta}=a^{\dagger}_{\beta}a_{\alpha}\ . \tag{9.5}$$

Thus, we are to explore the dynamical consequences of the equation

$$\langle q,p\,|\,[\hat{\rho}_{\alpha\beta},(H-H_c)]q,p\rangle=0\ . \tag{9.6}$$

[Even here, as is well known, there is a certain redundancy, since the particle-hole (ph) and hole-particle (hp) operators ρ_{ph} and ρ_{hp} are a complete set of operators to

specify the system under study, since $\rho_{pp'}$ and $\rho_{hh'}$ can be expressed in terms of them.[34]]

To evaluate (9.6), we have first, because $|q,p\rangle$ is a Slater determinant,

$$\langle q,p\,|\,[\hat{\rho}_{\alpha\beta},H]\,|\,q,p\rangle=[\mathscr{H}(\rho(q,p)),\rho(q,p)]_{\alpha\beta}\,, \tag{9.7}$$

where

$$\rho_{\alpha\beta}(q,p)=\langle q,p\,|\,\hat{\rho}_{\alpha\beta}\,|\,q,p\rangle \tag{9.8}$$

and $\mathscr{H}$ is the Hartree-Fock Hamiltonian

$$\mathscr{H}_{\alpha\beta}[\rho]=h_{\alpha\beta}+V_{\alpha\gamma\beta\delta}\rho_{\delta\gamma}(q,p) \tag{9.9}$$

for the Slater determinant $|q,p\rangle$. Below we shall expand the rhs of (9.7) in powers of p by means of the expression

$$\rho_{\alpha\beta}(q,p)=\rho^{(0)}_{\alpha\beta}(q)+p\rho^{(1)}_{\alpha\beta}(q)+\cdots\,. \tag{9.10}$$

(In a more careful treatment, one can keep terms up to second order in p and show that they are determined in the semiclassical limit by the terms of order zero and one.) In order to evaluate $[\hat{\rho}_{\alpha\beta},H_c]$, we require an operator form of (9.10). Let us assume that

$$\hat{\rho}_{\alpha\beta}=\rho^{(0)}_{\alpha\beta}(\hat{x})+\tfrac{1}{2}\{\hat{p},\rho^{(1)}_{\alpha\beta}(\hat{x})\}+\cdots\,. \tag{9.11}$$

We then have, using the displacement operator properties,

$$\begin{aligned}\langle q,p\,|\,\hat{\rho}_{\alpha\beta}\,|\,q,p\rangle&=\langle\rho^{(0)}(q+\hat{x})\rangle\\&\quad+\tfrac{1}{2}\langle\{(\hat{p}+p),\rho^{(1)}(q+\hat{x})\}\rangle\\&\cong\rho^{(0)}(q)+p\rho^{(1)}(q)\,,\end{aligned} \tag{9.12}$$

according to the arguments presented in the previous section in conjunction with Eqs. (8.20)–(8.22). Similarly, we compute to leading order, using (8.4) and (9.11),

$$\begin{aligned}\langle q,p\,|\,[\hat{\rho}_{\alpha\beta},H_c]\,|\,q,p\rangle&=\langle q,p\,|\,[\tfrac{1}{2}i\{\rho^{(0)}_{\alpha\beta,x}K,\hat{p}\}-i\rho^{(1)}_{\alpha\beta}(x)V_{,x}]\,|\,q,p\rangle+O(p^2)\\&\cong i\rho^{(0)}_{\alpha\beta}(q)_{,q}Kp-i\rho^{(1)}_{\alpha\beta}(q)V_{,q}\,.\end{aligned} \tag{9.13}$$

With the help of (9.7), (9.12), and (9.13), we obtain zero and first order conditions,

$$[\mathscr{H}^{(0)},\rho^{(0)}]=-i\rho^{(1)}(dV(q)/dq)\,, \tag{9.14}$$

$$[\mathscr{H}^{(0)},\rho^{(1)}]+[\mathscr{H}^{(1)},\rho^{(0)}]=i(d\rho^{(0)}/dq)K(q)\,. \tag{9.15}$$

We have shown[29] that (9.14) and (9.15) are equivalent to (8.23) and (8.26), respectively, provided we identify the quantities as follows:

$$(d\phi^{\alpha}/dq)\rightarrow\{d\rho^{(0)}_{ph}/dq,d\rho^{(0)}_{hp}/dq\}\,, \tag{9.16}$$

$$f_{,\alpha}\rightarrow\{-i\rho^{(1)}_{ph},i\rho^{(1)}_{hp}\}\,, \tag{9.17}$$

i.e., the index α which runs over all the coordinates here runs over the sets (ph) and (hp).

This identification is fortified by showing that the canonical commutation relation

$$\langle qp\,|\,[x,p]\,|\,\hat{q},\hat{p}\rangle=i \tag{9.18}$$

can be transformed into the relation

$$(-i\rho^{(1)}_{ph})^*\frac{d}{dx}\rho^{(0)}_{ph}+(i\rho^{(0)}_{hp})^*\frac{d}{dx}\rho^{(0)}_{hp}=1\,, \tag{9.19}$$

which is to be understood as a complex form of (8.28), namely,

$$f^*_{,\alpha}(d\phi^{\alpha}/dx)=1\,. \tag{9.20}$$

To carry out the demonstration, (9.10) or (9.11) and the remarks associated with (9.16) and (9.17) imply that we may write

$$\hat{x}=f(\rho^{(0)}_{ph},\rho^{(0)}_{hp})\,. \tag{9.21}$$

Thus, (9.18) is evaluated as

$$\frac{\partial f}{\partial\rho^{(0)}_{ph}(q)}\frac{d\rho^{(0)}_{ph}}{dq}+\frac{\partial f}{\partial\rho^{(0)}_{hp}(q)}\frac{d\rho^{(0)}_{hp}}{dq}=1\,. \tag{9.22}$$

The transformation of this into (9.19) requires the use of a classical condition for a set of variables to be canonical. Now the (ph) and (hp) elements of $\rho^{(0)}$ are not canonical, but the complex numbers β_{ph} and $i\beta^*_{ph}$ related to $\rho_{ph}\equiv(\underline{r})_{ph}$ and $\rho_{hp}=(\underline{r})_{hp}$ by the matrix equations

$$\underline{r}=\underline{\beta}(1-\underline{\beta}^{\dagger}\underline{\beta})^{1/2}\,, \tag{9.23a}$$

$$\underline{r}^{\dagger}=(1-\underline{\beta}^{\dagger}\underline{\beta})^{1/2}\underline{\beta}^{\dagger}\,, \tag{9.23b}$$

are canonical.[34] Introducing the real combinations

$$Q_{ph}=\frac{1}{\sqrt{2}}(\beta_{ph}+\beta_{hp})=\frac{1}{\sqrt{2}}(\beta_{ph}+\beta^*_{ph})\,, \tag{9.24a}$$

$$P_{ph}=-\frac{i}{\sqrt{2}}(\beta_{ph}-\beta^*_{ph})\,, \tag{9.24b}$$

if q,p are considered as a pair of classical canonical variables (remaining pairs unspecified) (we shall see in the next section that they satisfy Hamilton's equations in the limit under study), then it follows[35] that

$$\frac{\partial x}{\partial Q_{ph}}=\frac{\partial P_{ph}}{\partial p},\quad\frac{\partial x}{\partial P_{ph}}=-\frac{\partial Q_{ph}}{\partial p}\,. \tag{9.25}$$

One more simplification: If (ph) and (hp) refer to the representation in which $\rho^{(0)}$ is diagonal, then we may replace[29] (for purposes of differentiation only) $\underline{\beta}$ in (9.24) by $\underline{\rho}^{(0)}$. Applying (9.25), we then find

$$\frac{\partial f}{\partial\rho^{(0)}_{ph}(q)}=i\rho^{(1)}_{hp}\,, \tag{9.26}$$

which together with its complex conjugate provides the missing elements of our proof.

The results obtained in this section so far are completely equivalent to the theory of the preceding section. However, the harmonic limit of small amplitude collective motion is also contained, provided we augment the size of

the collective subspace to the number of independent (*ph*) excitations we care to describe and we replace the general potential energy function hitherto assumed by a harmonic approximation.

In a true vibrational regime, however, where anharmonic terms are of importance, we must treat p and q on an equal footing, and since this requires going to higher order than quadratic terms in p, the present formalism becomes cumbersome. It is more convenient to return to the $b,b^\dagger$ operators. From this standpoint by utilizing VP III, we may derive the RPA and higher RPA. Such a formalism has been explored recently by two of us (Marumori and Une) and will not be repeated here.[36]

X. CLASSICAL EQUATIONS OF MOTION

In contrast to our completely quantum starting point in the trial state (3.2), one encounters most frequently in the literature a trial state in which $G(t)$, Eqs. (3.4) and (3.5), has been replaced by

$$G_{\rm cl}(t)=\beta(t)b^\dagger-\beta^*(t)b \ . \tag{10.1}$$

Under these conditions, if we imagine that H has been put into the form of Eq. (6.7), then Eq. (3.6) is evaluated as

$$0=(t_2-t_1)\delta E_0 + \delta\int_{t_1}^{t_2}dt[\tilde{H}_c(\beta^*;\beta)-i\dot{\beta}^*(t)\beta(t)+i\dot{\beta}(t)\beta^*(t)] \ , \tag{10.2}$$

where $\tilde{H}_c$ is discussed below, but is temporarily understood to be Eq. (6.4). Thus, in this instance, as has been remarked very frequently in the literature,[37] varying with respect to $\beta(t)$ and $\beta^*(t)$ yields Hamilton's classical equations of motion (note the unconventional sign of i)

$$i\dot{\beta}^*=\frac{\partial H_c}{\partial\beta} \ , \tag{10.3a}$$

$$-i\dot{\beta}=\frac{\partial H_c}{\partial\beta^\dagger} \ . \tag{10.3b}$$

To make further progress, let us suppose that H_c has the form appropriate to vibrations,

$$H_c=H_c(b^\dagger;b)=h_1b^\dagger b+h_2(b^\dagger)^2b^2+\cdots \ . \tag{10.4}$$

If Eq. (6.2) is satisfied for all degrees of freedom including b, then

$$\tilde{H}_c(\beta^*;\beta)=H_c(\beta^*,\beta) \ , \tag{10.5}$$

and from (10.3) we find easily, e.g.,

$$-i\dot{\beta}(t)=[h_1+2h_2n+\cdots]\beta(t) \equiv\omega(n)\beta(t) \ , \tag{10.6}$$

where

$$n(t)=n(0)=\beta^*(t)\beta(t) \tag{10.7}$$

is a classical constant of the motion, corresponding to the quantum operator $\hat{n}=b^\dagger b$. Equation (10.6) has the solution

$$\beta(t)=e^{i\omega(n)t}\beta(0) \ . \tag{10.8}$$

Classically n is a function of the energy, E, so that we may write

$$\omega(n)=h_1+2h_2n+\cdots \equiv\bar{\omega}(E) =\omega_0+\omega_1E+\cdots \ . \tag{10.9}$$

Furthermore, from (10.4)

$$E(n)=h_1n+h_2n(n-1)+\cdots \ . \tag{10.10}$$

From (10.9) and (10.10) together we conclude:

$$\omega_0=h_1, \ \ \omega_1h_1=2h_2, \ldots, \ . \tag{10.11}$$

Since in practice a classical calculation would give us $\bar{\omega}(E)$ (see below), the calculation outlined above shows that if indeed we could obtain H_c in the form (10.4), with the associated conditions on $|\Psi_0\rangle$, a classical calculation would allow us to determine the parameters of the collective Hamiltonian. In practice, however, we cannot know the Hamiltonian in the form (10.4) without having diagonalized H, in which event we hardly need the aftermath of classical mechanics. It is nevertheless an amusing observation that in a suitable representation, we can obtain exact quantum results from a classical Hamiltonian. Another way of saying the same thing is that in this case the quantum theory reduces to a classical theory. This can be seen by studying the matrix element

$$\beta(t)=\langle\beta,\beta^*\,|\,b(t)\,|\,\beta,\beta^*\rangle =\langle\beta,\beta^*\,|\,e^{+i\omega(\hat{n})t}b\,|\,\beta,\beta^*\rangle \ , \tag{10.12}$$

since the quantum analog of (10.8) holds. Furthermore, (10.12) now yields (10.8). In practice we would be studying the classical equations of motion in a representation in which H_c is not diagonal in form and furthermore the condition $b\,|\,\Psi_0\rangle=0$ is not truly satisfied: Nevertheless the considerations of Sec. VI lead us to the conclusion that solution of the classical equations of motion by a Fourier series will yield $\bar{\omega}(E)$ from which a set of quantities $h_1,h_2,\ldots,$ can be constructed from (10.9) and (10.10), which can be associated with the corresponding quantities discussed in Sec. VI and thus identified with the true quantities up to corrections of order Ω^{-1}, in general.

Though we have confined our remarks to vibrational motion, a corresponding development can be carried out for large amplitude collective motion.

Furthermore, if we are not in the representation in which H is diagonal, then the exact equation of motion for $\beta(t)$ no longer coincides with the classical equation. Solutions of the latter yield essential information on the collective Hamiltonian. Higher order corrections to the classical equation undoubtedly contain important dynamical information. However, the exact connection with the fully quantum methods of the preceding sections of this paper remain to be investigated, perhaps through VP I.

XI. SUMMARY AND CONCLUSIONS

We have shown that starting from the time-dependent variational principle and a trial state of generalized

coherent form, we can derive a number of formally exact time independent variational principles, VP's I—IV, each of which should contain a complete theory of nuclear collective motion. We have illustrated how this program can be implemented for VP's II and III. VP IV is of cranking form and the means of exploiting it are well known. Only VP I is unfamiliar, though it appears useful at least for obtaining higher order corrections to classical equations of motion. We have shown how theories of both small and large amplitude collective motion can be treated starting from either boson or from fermion variables. Finally, we have indicated a connection with classical mechanics.

Note added in proof. It has recently been shown by K. Tanabe and one of the authors that variational principles II and III are true for any intrinsic state in the collective subspace, but principles I and IV require the coherent state. See A. Klein and K. Tanabe, University of Pennsylvania report UPR-0235T, 1983, to be published in Phys. Lett.

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