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Adiabatic time-dependent Hartree-Fock theory in the generalized valley approximation

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A classical theory of large amplitude, adiabatic collective motion, developed and applied previously to test examples, is transcribed into the language of time-dependent Hartree-Fock theory in order to initiate the application of the new method to problems in nuclear physics. The formulation which emerges can be characterized as a generalized cranking theory, in the sense that the cranking operator cannot be chosen arbitrarily, as in the conventional formulation of this method, but is instead fully constrained by the formalism. A procedure for obtaining approximate solutions to the new equations is described and illustrated with several simplified many-body models. It is inferred that traditional cranking calculations can serve as starting points for more realistic models. This paper also includes additional discussion concerning the calculation of collective masses and the problem of local stability of collective motion, not covered in our previous work.

I. INTRODUCTION

This paper is intended as the continuation of the development of a theory of large amplitude collective motion in the adiabatic limit.[1–6] During the past 20 years many important contributions have been made to the subject of large amplitude collective motion. References 7–28 contain a representative selection of these papers. Other work may be traced from these references.

In our version of the theory we seek within the framework of classical Hamiltonian dynamics the class of decoupled motions, i.e., motions confined to a submanifold of the total configuration space. This set of motions includes, but is more general than, those associated with integrable systems. For example, the Hamiltonian which governs the time development of the system on the decoupled manifold is not generally a constant of the motion, though it is independent of time on the decoupled manifold itself. (This follows trivially from the definitions given in Sec. II.)

The conditions for exact decoupling were formulated as differential equations that must be satisfied on the submanifold on which the motion occurs. Since for cases of practical interest exactly decoupled motion does not occur, the exact theory must be modified so as to provide for the actual construction of a submanifold that can be tested subsequently for how closely it approaches perfect decoupling. We have previously suggested a new construction with the following theoretical properties: It yields a valley for a one-dimensional submanifold and the exactly decoupled motions in any number of dimensions, if these exist. We shall refer to the multidimensional submanifolds on which these decoupled motions occur as generalized valleys. The formulation also includes a natural measure of the deviation from exact decoupling. In the work cited, we have applied the method just described and illustrated what can be achieved by subsequent quantization.[3,4,6] From the applications to date, it is apparent that our methods are suitable for the decoupling of one and two degrees of freedom from a parent system with a few more degrees of freedom and thus provide a useful approach to the approximate quantization of nonseparable systems.

The problem of major interest, however, is that of decoupling one or several degrees of freedom from a system with many degrees of freedom. We were led to study the problem within a classical framework from the well-known result[29,30] that the time-dependent Hartree-Fock (TDHF) equations are equivalent to Hamilton's equations. In this paper, we transcribe the results of our previous work back to the language of nuclear physics and begin the task of formulating and applying methods for solving the new equations. The latter are seen to assume the form of a sequence of cranking equations, of which the first alone defines the conventional cranking theory. The additional equations fully constrain the cranking operator, rather than leave its choice partly a matter of whim, as in existing theories. Indeed, the unambiguous determination of this operator is tantamount to fixing the approximately decoupled submanifold. An approximate method for solving the generalized cranking formulation is described that reduces the many-body problem to a few-body problem of the type treated in our previous work. The application of this method is illustrated for several simplified models.

Turning to the sequential contents of this paper, in Sec. II, we review some elements of the previously developed classical theory as required for the subsequent development. The transcription to TDHF is described in Sec. III, but is fully documented only for the case of one collective coordinate in the TDH approximation. The generalized cranking nature of the resulting equations is exhibited. A new method for the calculation of the collective mass tensor is described. In Sec. IV, we discuss

briefly the theory of local stability of an approximately decoupled manifold.

In Sec. V, we begin the discussion of applications with a new treatment of a simple many-body model for tunneling[31] that we have also studied recently.[4] We do a cranking calculation to obtain a two-dimensional submanifold, and show that this approach agrees within TDH accuracy with our previous work.

All the previous work was based on the theory of point canonical transformations. In Sec. VI we observe that the adiabatic approximation is consistent with an extended class of canonical transformations, and we derive the modifications of the formalism necessary to include these. In Sec. VII we study a model for a breathing mode for particles moving in one spatial dimension,[32–36] and again show that cranking yields the known result (see Appendix D) in the limit of a large number of particles, provided we utilize the formalism of the Sec. VI. The final section, VIII, contains a brief summary of the preceding developments and outlines the next steps to be taken in our program of applications. Three appendices provide some of the technical details for the preceding sections, whereas a fourth contains a derivation of the exact solution of the TDH equations for the model discussed in Sec. VII.

II. CLASSICAL THEORY OF DECOUPLED MOTION

A. Definition of decoupled motion

This section contains the only material that has been fully described in equivalent form in our work,[2,5] but it is so fundamental to all that follows that we consider its inclusion integral to the present discussion. We study a classical system with N canonical pairs ξ^α and π_α (the single-particle coordinates) described by the Hamiltonian,

$$H=\tfrac{1}{2}\pi_\alpha B^{\alpha\beta}(\xi)\pi_\beta+V(\xi)\ , \tag{2.1}$$

and consider the transformation to "collective" coordinates by means of a point canonical transformation,

$$\xi^\alpha=g^\alpha(q^1,\ldots,q^N)\ , \tag{2.2}$$

$$\pi_\alpha=f^\mu_{,\alpha}p_\mu\ , \tag{2.3}$$

with inverse

$$q^\mu=f^\mu(\xi)\ , \tag{2.4}$$

$$p_\mu=g^\alpha_{,\mu}\pi_\alpha\ , \tag{2.5}$$

where the comma indicates partial derivative.

We assume that in the new coordinate set we can identify a decoupled surface, defined as follows: We divide the set q into two subsets, q^i, $i=1,\ldots,K$, and $q^a, a=K+1,\ldots,N$, and suppose this division to be such that if at time $t=0$ both $q^a=0$ (by convention) and $\dot q^{\,a}=0$, then $q^a(t)\equiv 0$. Such motions evolve on a K-dimensional submanifold

$$\xi^\alpha=g^\alpha(q^1,\ldots,q^K)\equiv g^\alpha(q)\ , \tag{2.6}$$

designated as the surface Σ. In geometrical terms, if the system point is initially on Σ, and the initial velocity is on $T\Sigma$, the tangent plane to Σ at the given point, then provided the subsequent motion of the system is confined to this surface, Σ is said to be decoupled. It is as if the system had imposed on itself a set of holonomic constraints.

Before deriving the conditions which characterize such a motion, let us note that under the point transformation (2.2) and (2.3), the Hamiltonian becomes

$$H(\xi,\pi)=\overline{H}(q,p)=\tfrac{1}{2}p_\mu\overline{B}^{\,\mu\nu}(q)p_\nu+\overline{V}(q)\ , \tag{2.7}$$

where

$$\overline{B}^{\,\mu\nu}=f^\mu_{,\alpha}B^{\alpha\beta}f^\nu_{,\beta}\ . \tag{2.8}$$

Also, the chain rule relations

$$f^\mu_{,\alpha}g^\alpha_{,\nu}=\delta^\mu_\nu \tag{2.9}$$

permit us to reexpress (2.8) in the form

$$\overline{B}^{\,\mu\nu}g^\alpha_{,\nu}=B^{\alpha\beta}f^\mu_{,\beta}\ . \tag{2.10}$$

The conditions which characterize Σ are derived most readily from the equations of motion for the set q^a, p_a. These are

$$\dot q^{\,a}=\partial\overline{H}/\partial p_a=\overline{B}^{\,ai}p_i+\overline{B}^{\,ab}p_b\ , \tag{2.11}$$

$$-\dot p_a=\partial\overline{H}/\partial q^a=\overline{V}_{,a}+\tfrac{1}{2}\overline{B}^{\,ij}_{,a}p_ip_j+\overline{B}^{\,bi}_{,a}p_ip_b+\tfrac{1}{2}\overline{B}^{\,bc}_{,a}p_bp_c\ . \tag{2.12}$$

The requirements $\dot q^{\,a}=\dot p_a=0$ can be compatible with the requirements $q^a=p_a=0$ only if the equations

$$\overline{B}^{\,ai}p_i=0 \tag{2.13}$$

$$\overline{V}_{,a}+\tfrac{1}{2}p_ip_j\overline{B}^{\,ij}_{,a}=0\ , \tag{2.14}$$

are satisfied, as one sees from (2.11) and (2.12). Equations (2.13) and (2.14) are equivalent to three sets of conditions provided none of the p_i are constants of the motion, for in that case (2.14) yields two independent conditions, and altogether, we have

$$\overline{B}^{\,ai}=0\ , \tag{2.15}$$

$$\overline{V}_{,a}=0\ , \tag{2.16}$$

$$\overline{B}^{\,ij}_{,a}=0\ . \tag{2.17}$$

The modifications necessary when one or more of the p_i is a constant of the motion are described in Ref. 2, but are not germane to any of the examples studied in this paper.

The physical significance of these equations is apparent. The first tells us that we may choose the mass tensor block diagonal, i.e., it restricts the choice of noncollective coordinates at each point. The remaining two equations then demand the absence of both "real" and "geometrical" (centrifugal) forces orthogonal to the decoupled surface. Altogether (2.15)–(2.17) imply that an exactly decoupled surface is geodesic.[2]

It follows readily from the decoupling conditions that the Hamiltonian that governs the motion on Σ, the "collective" Hamiltonian, is the value of $\overline{H}$, Eq. (2.7), on the surface.

Equations (2.15)–(2.17) are the most transparent form

of the decoupling conditions, and in cases of exact decoupling (see Secs. V and VI) can be used to check assertions that exact solutions have been found. Though it appears feasible to develop an algorithm for obtaining approximate solutions directly from these conditions, the method that we shall follow in this paper involves the transformation of (2.15)–(2.17) into an equivalent set for which algorithms have already been developed.

The first, trivial, stage of transformation is to replace (2.15)–(2.17) by the equivalent set,

$$B^{\alpha\beta}f^{i}_{,\beta}=\bar{B}^{ij}g^{\alpha}_{,j}\ , \tag{2.18}$$

$$V_{,\alpha}=\bar{V}_{,i}f^{i}_{,\alpha}\ , \tag{2.19}$$

$$\bar{B}^{ij}_{,\alpha}=\bar{B}^{ij}_{,k}f^{k}_{,\alpha}\ . \tag{2.20}$$

Of these relations, (2.19) and (2.20) are chain rule relations which have been simplified by the imposition of (2.16) and (2.17), respectively, whereas Eq. (2.18) is a simplified version of Eq. (2.10) obtained by remembering (2.15). Geometrically, (2.18) states that the quantities $g^{\alpha}_{,i}$ and $f^{i}_{,\alpha}$ are equivalent sets of basis vectors on Σ, and (2.19), e.g., affirms that the gradient of V lies in $T\,\Sigma$.

B. Fundamental theorem of the generalized valley formulation

We turn then to the transformation of the foregoing conditions into the form we shall utilize. The basic idea which underlies the following considerations is that we should be able to construct the surface $\xi^{\alpha}=g^{\alpha}(q)$ provided we can specify the tangent plane at each point. We shall do this by constructing a complete set of basis vectors for the tangent plane from the "ingredients" of the given Hamiltonian.

To carry out this program, we define a sequence of single index point functions according to the definitions

$$X^{(0)}\equiv V(\xi)=\bar{V}(q)\ , \tag{2.21}$$

$$X^{(1)}\equiv V_{,\alpha}B^{\alpha\beta}V_{,\beta}=\bar{V}_{,\mu}\bar{B}^{\mu\nu}\bar{V}_{,\nu}\ , \tag{2.22}$$

$$X^{(\sigma+1)}\equiv X^{(\sigma)}_{,\alpha}B^{\alpha\beta}X^{(\sigma)}_{,\beta}=\bar{X}^{(\sigma)}_{,\mu}\bar{B}^{\mu\nu}\bar{X}^{(\sigma)}_{,\nu}\ . \tag{2.23}$$

Then for $\sigma\neq\tau$, we define a sequence of double index point functions,

$$X^{(\sigma\tau)}\equiv X^{(\sigma)}_{,\alpha}B^{\alpha\beta}X^{(\tau)}_{,\beta}=\bar{X}^{(\sigma)}_{,\mu}\bar{B}^{\mu\nu}\bar{X}^{(\tau)}_{,\nu}\ . \tag{2.24}$$

Thus the single index sequence is constructed with the help of the mass tensor, here in its role as metric tensor, by forming the gradient of the previous point function and then calculating the length of the new vector. The double index scalars are mixed scalar products of gradients. By finding the gradients of these we can form still additional sequences of point functions, all of which are subsumed under the considerations that follow.

The basic assertion is that for a decoupled surface, the gradient of every scalar, either defined previously or alluded to, is a vector field which lies in the tangent plane to Σ. The proof depends on induction. We first note that according to the fundamental decoupling condition (2.16), the gradient of $X^{(0)}$ lies in the tangent plane, i.e., $\bar{X}^{(0)}_{,a}=0$. Now let us assume that $\bar{X}^{(\sigma)}_{,a}=0$ and show that in consequence of this statement and all the remaining decoupling conditions, $\bar{X}^{(\sigma+1)}_{,a}=0$. We simply compute

$$\begin{aligned}\bar{X}^{(\sigma+1)}_{,a}&=2\bar{X}^{(\sigma)}_{,\mu a}\bar{X}^{(\sigma)}_{,\nu}\bar{B}^{\mu\nu}+\bar{X}^{(\sigma)}_{,\mu}\bar{X}^{(\sigma)}_{,\nu}\bar{B}^{\mu\nu}_{,a}\\&=2\bar{X}^{(\sigma)}_{,ba}\bar{X}^{(\sigma)}_{,i}\bar{B}^{bi}+2\bar{X}^{(\sigma)}_{,ia}\bar{X}^{(\sigma)}_{,j}\bar{B}^{ij}+\bar{X}^{(\sigma)}_{,i}\bar{X}^{(\sigma)}_{,j}\bar{B}^{ij}_{,a}\\&=0\ .\end{aligned} \tag{2.25}$$

In passing to the second line of (2.25), we have used only the statement $\bar{X}^{(\sigma)}_{,a}=0$; in order to obtain zero overall, we have then used (2.15) and (2.17) in the first and third terms, respectively, whereas the second term vanishes because $\bar{X}^{(\sigma)}_{,ai}=0$. The vanishing of the gradients of the multiply-indexed scalars follows from the same mode of proof.

The results obtained may be summarized in two equivalent forms. Let us suppose for the moment that all the point functions of interest have been arranged into a linear array designated $X^{(\sigma)}$, in the notation used previously only for the single index scalars. In the same way as (2.16) implied (2.19), we have more generally

$$X^{(\sigma)}_{,\alpha}=\bar{X}^{(\sigma)}_{i}f^{i}_{,\alpha}\ . \tag{2.26}$$

By using $B^{\alpha\beta}$ in the entire space and $\bar{B}^{ij}$ on Σ to raise indices, and remembering (2.18), (2.26) may be converted to the form

$$X^{(\sigma),\alpha}=\bar{X}^{(\sigma),i}g^{\alpha}_{,i}\ . \tag{2.27}$$

Equations (2.26) and (2.27) both state, one in covariant, the other in contravariant form, that the vector fields in question lie in the tangent plane to Σ.

In previous work,[3,4,6] we have begun the process of showing how these equations may be used in practice. In particular, we have emphasized a relation to a theory of generalized (more than one-dimensional) valley which provides an exact solution when such exists and in other cases provides what may be a good "approximate" solution. Here we wish to transcribe the formulas of this section back to the language of TDHF. The most complicated case that we shall consider in the near term is the case $K=2$. We utilize the simplest point functions $V=X^{(0)}$, $U=X^{(1)}$, and $T=X^{(01)}$ in the notation of Eq. (2.24). For example, (2.27) becomes, in this case,

$$V^{,\alpha}=\bar{V}^{,i}g^{\alpha}_{,i}\ , \tag{2.28}$$

$$U^{,\alpha}=\bar{U}^{,i}g^{\alpha}_{,i}\ , \tag{2.29}$$

$$T^{,\alpha}=\bar{T}^{,i}g^{\alpha}_{,i}\ . \tag{2.30}$$

We turn then to the problem of determining the form of these equations within the framework of nuclear physics. We shall give the details only for (2.28) and (2.29) because these are all that will be required for the applications to be studied in this paper. The general method should, however, be clear from the special case considered.

III. TRANSCRIPTION TO TDHF THEORY

A. Canonical variables and the adiabatic Hamiltonian

To utilize the theory described in the preceding section, we must recast the TDHF equations into the form

of Hamilton's equations. We therefore consider the former,

$$i\dot{\rho}_{ab}=[\mathcal{H},\rho]_{ab} , \tag{3.1}$$

where

$$\mathcal{H}_{ab}=h_{ab}+V_{acbd}\rho_{dc} , \tag{3.2}$$

and $h_{ab}=h^*_{ba}$, $V_{abcd}=-V_{bacd}=-V_{abdc}=V^*_{cdab}$ are the traditional elements of a nonrelativistic nuclear many-body Hamiltonian. The labels $a,b,\ldots$ refer to a complete orthonormal set of single-particle functions ϕ_a; this set will be further subdivided into a set h occupied in the reference Slater determinant and an unoccupied set p. We have

$$\rho=\sum_h \phi_h\phi^*_h, \quad (\rho^2)_{ab}=\rho_{ab} . \tag{3.3}$$

The most convenient choice of basis for exhibiting the canonical structure of (3.1) is the one in which ρ is instantaneously diagonal. In this basis (3.1) is equivalent to the pair of equations

$$\begin{aligned} i\dot{\rho}_{ph}&=\mathcal{H}_{ph}=(\delta H/\delta\rho_{hp}) ,\\ i\dot{\rho}_{hp}&=-\mathcal{H}_{hp}=-(\delta H/\delta\rho_{ph}) , \end{aligned} \tag{3.4}$$

where

$$H=W_{HF}[\rho]=h_{ab}\rho_{ba}+\tfrac{1}{2}V_{abcd}\rho_{ca}\rho_{db} , \tag{3.5}$$

the Hartree-Fock functional, serves as "Hamiltonian." Remarkably, Eqs. (3.4) are already in Hamiltonian form, where we identify ρ_{ph} and $\rho_{hp}=\rho^*_{ph}$ as complex canonical variables. We may introduce real canonical coordinates ξ and π,

$$\begin{aligned} \rho_{ph}&=\frac{1}{\sqrt{2}}(\xi^{ph}+i\pi_{ph}) ,\\ \rho_{hp}&=\frac{1}{\sqrt{2}}(\xi^{ph}-i\pi_{ph})=\frac{1}{\sqrt{2}}(\xi^{hp}+i\pi_{hp}) . \end{aligned} \tag{3.6}$$

The canonical coordinates (3.6) that provide such a concise proof of the canonicity of the TDHF equations are, however, not suitable for the study of the adiabatic limit. Note, in particular, that Eqs. (3.6) vanish at the particular instant of their utilization, though of course their derivatives do not. We describe briefly the alternative method to be utilized, based on a classical version of the Holstein-Primakoff boson mapping. (Further details are given in Appendix A.)

The formulas

$$\rho_{ph}=[\beta(1-\beta^\dagger\beta)^{1/2}]_{ph} , \tag{3.7}$$

$$\rho_{hp}=[(1-\beta^\dagger\beta)^{1/2}\beta^\dagger]_{hp} , \tag{3.8}$$

$$\rho_{pp'}=[\beta\beta^\dagger]_{pp'} , \tag{3.9}$$

$$\rho_{hh'}=[1-\beta^\dagger\beta]_{hh'} , \tag{3.10}$$

define a mapping from the elements of the density matrix in an arbitrary basis onto a set of complex numbers β_{ph}, which together with their complex conjugates are a set of complex canonical variables, convenient for the discussion of vibrational degrees of freedom. For the study of large amplitude motion, we introduce real canonical variables ξ and π, distinct from the variables in (3.6), according to the standard formulas

$$\beta=\frac{1}{\sqrt{2}}(\xi+i\pi), \quad \beta^\dagger=\frac{1}{\sqrt{2}}(\tilde{\xi}-i\tilde{\pi}) , \tag{3.11}$$

where tilde means transposed. We have

$$\xi^{ph}=\xi^{hp}, \quad \pi_{ph}=-\pi_{hp} . \tag{3.12}$$

In this transcription the classical Hamiltonian is given by the formula

$$H(\xi,\pi)=W_{HF}[\rho(\xi,\pi)] . \tag{3.13}$$

In the adiabatic limit by far the most convenient representation appears to be the one in which $\rho(\xi,\pi=0)\equiv\rho^{(0)}(\xi)$ *is diagonal.* This choice greatly simplifies the ensuing formulas.

In order to expand $H(\xi,\pi)$ in powers of π to second-order terms, we first expand $\rho(\xi,\pi)$,

$$\begin{aligned} \rho(\xi,\pi)=&\rho^{(0)}(\xi)+\rho^{(1a)}(\xi)\pi_a\\ &+(\tfrac{1}{2})\rho^{(2ab)}(\xi)\xi\pi_a\pi_b+\cdots . \end{aligned} \tag{3.14}$$

From (3.14) and the condition that ρ is idempotent, we derive the well-known constraints

$$\rho^{(0)}=\rho^{(0)2} , \tag{3.15}$$

$$\rho^{(1a)}=\rho^{(0)}\rho^{(1a)}+\rho^{(1a)}\rho^{(0)} , \tag{3.16}$$

$$\rho^{(2ab)}=\rho^{(0)}\rho^{(2ab)}+\rho^{(2ab)}\rho^{(0)}+\rho^{(1a)}\rho^{(1b)}+\rho^{(1b)}\rho^{(1a)} . \tag{3.17}$$

Next, if we carry out a formal expansion of (3.7), after having substituted (3.11), we find to second order (indices temporarily suppressed)

$$\begin{aligned} \sqrt{2}\rho=&\xi(1-\tfrac{1}{2}\tilde{\xi}\xi)^{1/2}+i\pi(1-\tfrac{1}{2}\tilde{\xi}\xi)^{1/2}\\ &-\tfrac{1}{2}\xi\tilde{\pi}\pi(1-\tfrac{1}{2}\tilde{\xi}\xi)^{-1/2} . \end{aligned} \tag{3.18}$$

The consequences of (3.18) are, first, that in the representation in which $\rho^{(0)}$ is diagonal, we have

$$[\rho^{(0)}]_{ph}=[\xi(1-\tilde{\xi}\xi)^{1/2}]_{ph}=0 , \tag{3.19}$$

and therefore $\xi^{ph}=\xi^{hp}=0$. It follows that (3.18) reduces to

$$\sqrt{2}\rho^{(1)}_{ph}=i\pi_{ph}+O(\pi^3) . \tag{3.20}$$

Upon comparison with (3.14), we conclude that

$$\rho^{(1p'h')}_{ph}=-\rho^{(1p'h')}_{hp}=\frac{1}{\sqrt{2}}i\delta_{pp'}\delta_{hh'} , \tag{3.21}$$

$$\rho^{(2p'h'p''h'')}_{ph}=0 . \tag{3.22}$$

The adiabatic expansion of the Hamiltonian leading to the form (2.1) can be obtained by collecting the foregoing results, substituting into (3.13) and expanding to the required order. A more elegant derivation is to expand directly in powers of π_{ph} and then notice that for variation about the chosen representation, we have from (3.18) that

$$\sqrt{2}\delta\rho=\delta\xi+i\delta\pi \tag{3.23}$$

is also a consequence of (3.6). Following this latter procedure and remembering (3.23) we can write

$$\begin{aligned}H(\xi,\pi)&=W_{HF}[\rho(\xi,\pi)]\\&=W[\rho(\xi,0)]+\tfrac{1}{2}\pi_{ph}\pi_{p'h'}(\delta^2W/\delta\pi_{ph}\delta\pi_{p'h'})\\&\equiv V(\xi)+\tfrac{1}{2}\pi_\alpha B^{\alpha\beta}(\xi)\pi_\beta\ ,\end{aligned} \tag{3.24}$$

where the linear term vanishes,

$$\frac{\delta W}{\delta\pi_{ph}}=\frac{i}{\sqrt{2}}\left[\frac{\delta W}{\delta\rho_{ph}}-\frac{\delta W}{\delta\rho_{hp}}\right]=\frac{i}{\sqrt{2}}(\mathcal{H}_{hp}-\mathcal{H}_{ph})=0\ , \tag{3.25}$$

since the matrix elements of $\mathcal{H}$ can be chosen real if the system under study is time-reversal invariant. Furthermore

$$\begin{aligned}\frac{\delta^2W}{\delta\pi_{ph}\delta\pi_{p'h'}}&=B^{php'h'}\\&=-\frac{1}{2}\left[\frac{\delta^2W}{\delta\rho_{ph}\delta\rho_{p'h'}}-\frac{\delta^2W}{\delta\rho_{ph}\delta\rho_{h'p'}}\right.\\&\quad\left.-\frac{\delta^2W}{\delta\rho_{hp}\delta\rho_{p'h'}}+\frac{\delta^2W}{\delta\rho_{hp}\delta\rho_{h'p'}}\right].\end{aligned} \tag{3.26}$$

The techniques necessary to evaluate (3.26) are reviewed in Appendix B. The result is

$$\begin{aligned}B^{php'h'}&=\tfrac{1}{2}\delta_{hh'}(\mathcal{H}_{pp'}+\mathcal{H}_{p'p})-\tfrac{1}{2}\delta_{pp'}(\mathcal{H}_{hh'}+\mathcal{H}_{h'h})\\&\quad+\tfrac{1}{2}(V_{ph'hp'}+V_{hp'ph'}-V_{pp'hh'}-V_{hh'pp'})\ .\end{aligned} \tag{3.27}$$

The preceding formula simplifies if we consider either separable interactions in the Hartree approximation or Skyrme interactions in conjunction with spin and isospin saturated systems, for in those cases the last set of terms depending explicitly on the two-body matrix elements cancel. Since our initial applications all conform to one or the other of these approximations, the remaining formulas of the transcription will apply only to these cases. It is straightforward to elaborate formulas corresponding to the general case.

Though in the classical discussion we have given formulas applicable to the case of two collective coordinates, in the further transcription we shall restrict attention to the case of a single collective coordinate. Again when these will be needed, there will be no essential difficulty in adding the formulas applicable in more general instances. Thus the point function U, defined prior to Eq. (2.28), takes the form

$$U=\mathcal{H}_{ph}B^{php'h'}\mathcal{H}_{p'h'}\ . \tag{3.28}$$

With the help of Eq. (3.27), simplified according to the remarks following it, a more explicit form of (3.28), expressed as a trace, is

$$U=\mathrm{Tr}[\rho\mathcal{H}(1-\rho)\mathcal{H}(1-\rho)\mathcal{H}-(1-\rho)\mathcal{H}\rho\mathcal{H}\rho\mathcal{H}]\ , \tag{3.29}$$

where in all such formulas we henceforth mean the density matrix in the limit of vanishing momenta, i.e., the first term of (3.14).

B. Equations for the collective path

In Eqs. (2.28)–(2.30) we have given in contravariant form the equations to determine a two-dimensional decoupled surface. The main purpose of the present discussion is to transcribe the first two of these equations, that are the ones appropriate for the study of a collective path. In a practice it is convenient in the nuclear case to utilize the covariant form of the equations, since (2.28) will then be thoroughly familiar as the equations of the standard cranking method. It is also natural to make a change in the notation, this change being partly defined by writing the point transformation equations (2.2) and (2.4) in the form

$$\xi^{ph}=\xi^{ph}(Q^i)\ , \tag{3.30}$$

$$Q^i=Q^i(\xi)\ . \tag{3.31}$$

For a collective path the superscript i becomes superfluous. We also set

$$\delta V/\delta\rho_{hp}=\mathcal{H}_{ph}\ , \tag{3.32}$$

$$\delta U/\delta\rho_{hp}\equiv\mathcal{H}^{(1)}_{ph}\ , \tag{3.33}$$

$$\delta Q/\delta\rho_{hp}\equiv f_{ph}\ . \tag{3.34}$$

With this nomenclature Eqs. (2.28) and (2.29) take the concise forms

$$\mathcal{H}_{ph}=\lambda f_{ph}\ , \tag{3.35}$$

$$\mathcal{H}^{(1)}_{ph}=\mu f_{ph}\ , \tag{3.36}$$

where $\lambda=d\bar{V}/dQ$ and $\mu=d\bar{U}/dQ$. Each of these equations is of the cranking form, differing in the structure of the cranking Hamiltonians and in the definition of the cranking parameters, but both driven by the same cranking operator f. The cranking operator which accomplishes this heavy burden is no longer freely at our disposal, but must be a self-consistent solution of the two sets of conditions. We shall see this idea in practice starting with Sec. V.

The specification of the contents of Eq. (3.36) is not yet complete, since we must evaluate the additional cranking Hamiltonian, $\mathcal{H}^{(1)}$. We shall do so for the choice

$$V_{abcd}=\sum_\sigma\kappa_\sigma(q_\sigma)_{ac}(q_\sigma)_{bd}\ , \tag{3.37}$$

where q_σ is a single-particle operator and κ_σ an associated interaction strength. A straightforward application of the formulas from Appendix B then yields the result

$$\mathcal{H}^{(1)}=\mathcal{H}(1-\rho)\mathcal{H}(1-\rho)\mathcal{H}-2\mathcal{H}\rho\mathcal{H}(1-\rho)\mathcal{H}-2\mathcal{H}(1-\rho)\mathcal{H}\rho\mathcal{H}+\mathcal{H}\rho\mathcal{H}\rho\mathcal{H}$$
$$+\sum_\sigma \kappa_\sigma q_\sigma \mathrm{Tr}[\rho q_\sigma(1-\rho)\mathcal{H}(1-\rho)\mathcal{H}+\rho\mathcal{H}(1-\rho)q_\sigma(1-\rho)\mathcal{H}+\rho\mathcal{H}(1-\rho)\mathcal{H}(1-\rho)q_\sigma$$
$$-(1-\rho)q_\sigma\rho\mathcal{H}\rho\mathcal{H}-(1-\rho)\mathcal{H}\rho q_\sigma\rho\mathcal{H}-(1-\rho)\mathcal{H}\rho\mathcal{H}\rho q_\sigma]$$
$$=\mathcal{H}^{(1)NL}+\mathcal{H}^{(1)L}\ . \tag{3.38}$$

Here the terms proportional to one of the q_σ have been designated by the superscript L, for local, and the remaining terms recognized as nonlocal.

C. Calculation of the collective mass

The solution of the generalized cranking equations, of which the equations for the collective path previously given represent only a special case, yields a density matrix, $\rho(Q^i)$, which depends parametrically on the collective coordinates Q^i. This density matrix specifies the collective surface and is thus equivalent to the determination of the form of Eq. (3.30). On the other hand, the collective mass tensor, which we require equally, is determined by the tangent vectors to the collective surface. It seems most natural to apply Eq. (2.8), adapted to the collective subspace. In the language of nuclear physics, this formula utilizes the components of the cranking operators. As noted in Eq. (2.18), when there is exact decoupling these quantities span a basis for the tangent plane. In practice, however, this is usually no longer the case. At each point of the collective surface there is now a distinct plane determined by the dynamical vector fields that intervene in the fundamental theorem of Sec. II B. The solution of the generalized cranking equations expresses the fact that the components of the cranking operators span a basis in this plane, which differs generally from the tangent plane. On the other hand the covariant form of (2.8), namely

$$\bar{B}_{ij}=\frac{\partial\xi^{ph}}{\partial Q^i}B_{php'h'}\frac{\partial\xi^{p'h'}}{\partial Q^j}\ , \tag{3.39}$$

clearly entails use of the true tangent vectors. It can be shown that it is this form that is related directly to the usual cranking formula for the mass parameters. Thus the proposed construction carries with it two candidates for the collective mass tensor. To distinguish them, we shall designate the one determined by the cranking operators as $\tilde{B}$. This suggests that an invariant measure of their relative difference at each point will, on average, measure the exactness of decoupling, since such a measure must vanish for exact coupling. We shall henceforth adopt the measure

$$D\equiv K^{-1}\mathrm{Tr}[(\bar{B}^{-1}-\tilde{B}^{-1})\bar{B}]\ , \tag{3.40}$$

where K is the dimensionality of the collective space. Equation (3.40) differs slightly from a measure suggested in Ref. 2, but has the advantage of being completely intuitive. Thus for the case $K=1$ it reduces to the fractional difference of the masses.

We conclude this section with an alternative (but numerically equivalent) method of calculating the tilde mass tensor. For brevity we use the notation of Sec. II. The general case will already be clear from the case $K=2$. Consider the point function

$$U=V_{,\alpha}B^{\alpha\beta}V_{,\beta}=\bar{V}_{,i}\tilde{B}^{ij}\bar{V}_{,j}\ . \tag{3.41}$$

To the preceding, we adjoin the two next simplest point functions

$$T=\bar{U}_{,i}\tilde{B}^{ij}\bar{V}_{,j}\ , \tag{3.42}$$

$$W=\bar{U}_{,i}\tilde{B}^{ij}\bar{U}_{,j}\ . \tag{3.43}$$

The transformation between the two forms of (3.41) and the completely analogous calculations for (3.42) and (3.43) identify the collective mass tensor which enters as the tilde form. Since the mass tensor is symmetric, Eqs. (3.41)–(3.43) constitute three linear inhomogeneous equations for its three independent components, the other ingredients being known. In the one-dimensional case, (3.41) by itself suffices and we obtain the simple formula

$$\tilde{B}=U/(dV/dQ)^2\ . \tag{3.44}$$

IV. CONDITIONS FOR LOCAL STABILITY

A problem of supreme importance, which we have considered previously only within the context of special models,[3,4] is that of local stability. Given even an exactly decoupled surface, suppose that there is a small perturbation in the initial conditions which pushes the system off the collective surface. Will the system then remain in the neighborhood of the surface?

To study this question, we consider a point ξ^α in the neighborhood of the decoupled surface,

$$\xi^\alpha=\xi_0^\alpha+\delta\xi^\alpha\ , \tag{4.1}$$

where ξ_0^α is a point on the surface, and the variation is a vector orthogonal to the surface at every point. It thus has the form

$$\delta\xi^\alpha=\xi^\alpha_{,a}\delta Q^a\ . \tag{4.2}$$

When we now expand the potential energy about the point ξ_0^α, the first-order term vanishes because grad$V$ is assumed to lie in the collective surface (though in practice this is an approximation). We thus obtain

$$V(\xi)=V(\xi_0)+\tfrac{1}{2}\bar{V}_{,ab}\delta Q^a\delta Q^b\equiv V_C+V_{NC}\ , \tag{4.3}$$

i.e., the sum of the collective contribution and of a noncollective part which is quadratic in the deviations of the coordinates away from the starting surface. For a prescribed deviation we have

$$\bar{V}_{,ab}=V_{,\alpha\beta}\xi^\alpha_{,a}\xi^\beta_{,b}\ . \tag{4.4}$$

We shall return to the determination of this quantity.

Because of the decoupling condition on the mass ma-

trix, the kinetic energy, T, also decomposes in the immediate neighborhood of the decoupled surface into the sum of a collective and of a noncollective part,

$$T=T_C+T_{NC}\equiv\tfrac{1}{2}P_i\bar{B}^{ij}P_j+\tfrac{1}{2}P_a\bar{B}^{ab}P_b\ , \tag{4.5}$$

where

$$\bar{B}^{ab}=Q^a_{,\alpha}B^{\alpha\beta}Q^b_{,\beta}\ . \tag{4.6}$$

We wish to study the noncollective energy,

$$H_{NC}=V_{NC}+T_{NC}\ , \tag{4.7}$$

since wherever it is positive, we have local stability. We see from Eqs. (4.4) and (4.6) that this requires the specification at each point of the surface of a coordinate system spanning the space orthogonal to the collective space. This is, in principle, an elementary problem which can be solved in such a way that at the same time the mass matrix in the noncollective space can be chosen to be the unit matrix at every point. With such a choice, we then have only to diagonalize the matrix $\bar{V}_{,ab}$ to check whether the resulting eigenvalues are positive. These numbers are also of great interest after quantization if we are interested in absolute energies of our system rather than just excitation energies.

In the transcription to nuclear physics, it remains only to specify the formula for $V_{,\alpha\beta}$, which is needed for (4.4), namely,

$$\begin{aligned}V_{,\alpha\beta}=&\frac{1}{2}\left[\frac{\delta^2V}{\delta\rho_{ph}\delta\rho_{p'h'}}+\frac{\delta^2V}{\delta\rho_{ph}\delta\rho_{h'p'}}\right.\\&\left.+\frac{\delta^2V}{\delta\rho_{hp}\delta\rho_{p'h'}}+\frac{\delta^2V}{\delta\rho_{hp}\delta\rho_{h'p'}}\right]\\=&\tfrac{1}{2}\delta_{hh'}(\mathcal{H}_{pp'}+\mathcal{H}_{p'p}-\tfrac{1}{2}\delta_{pp'}(\mathcal{H}_{hh'}+\mathcal{H}_{h'h})\\&+\tfrac{1}{2}(V_{ph'hp'}+V_{hp'ph'}+V_{pp'hh'}+V_{hh'pp'})\ .\end{aligned} \tag{4.8}$$

All elements necessary to carry out the test of stability have now been specified. The remainder of this paper will be devoted to the study of a pair of simple many-body problems; the main purpose of this study is to introduce methods that may be utilized for the study of the nuclear many-body problem.

V. MODEL OF A MANY-BODY SYSTEM WITH TUNNELING

A. Description of model

The model Hamiltonian to be analyzed in this section was introduced by Arve *et al.*[31] in order to illustrate the applicability of the (imaginary) time-dependent Hartree(-Fock) [(I)TDH(F)] method to the tunneling in a many-body system. This model has two degenerate ground states, separated by a large barrier. Since the Hamiltonian is exactly soluble (numerically), it is excellent testing ground for different many-body techniques aimed at describing large amplitude collective motion. In a previous paper[4] we also analyzed this model, observing that the problem can be reduced to a Hamiltonian with only two active degrees of freedom. Subsequently, by applying the techniques developed for systems with only a few degrees of freedom, we determined the collective path, the collective Hamiltonian, and the measure of the goodness of the decoupling; we also demonstrated the quantum stability of the collective mode. The eigenvalues of the collective Hamiltonian were in excellent agreement with the corresponding exact eigenvalues.

In this section we shall attack this same problem, but in a truly many-body manner, in order to demonstrate that we are in possession of a method that can be applied to cases with initially a large number of degrees of freedom. Though the model to be studied is one of bosons (with spin), the method of study and the formulas to be applied are readily adapted from those described in Secs. III and IV.

In the second quantized form the Hamiltonian describing this model system reads

$$\begin{aligned}\hat{H}=&\int dx\ \psi^\dagger_\alpha(x)\tfrac{1}{2}(p^2+x^2)\psi_\alpha(x)\\&+\kappa\int dx\ \psi^\dagger_\alpha(x)\psi_\alpha(x)x\int dy\ \psi^\dagger_\beta(y)\psi_\gamma(y)(\sigma_z)_{\beta\gamma}\\&-\lambda\left[\int dx\ \psi^\dagger_\alpha(x)\psi_\beta(y)(\sigma_x)_{\alpha\beta}\right]^2\ ,\end{aligned} \tag{5.1}$$

where the summation over repeated spin indices is implied. As in the original paper[31] we shall treat this Hamiltonian in the Hartree approximation. The only quantity needed for our study is the density matrix,

$$\begin{aligned}\tilde{\rho}_{\alpha\beta}(x,y)=&\langle\Phi|\psi^\dagger_\beta(y)\psi_\alpha(x)|\Phi\rangle\\=&N\phi_\alpha(x)\phi^*_\beta(y)\equiv N\rho_{\alpha\beta}(x,y)\ ,\end{aligned} \tag{5.2a}$$

where N stands for the total number of particles, and $|\Phi\rangle$ is the coherent state,

$$|\Phi\rangle=\frac{(a^\dagger_0)^N}{\sqrt{N!}}|0\rangle\ , \tag{5.2b}$$

$$a^\dagger_0=\int dx\ \psi^\dagger_\alpha(x)\phi_\alpha(x)\ . \tag{5.2c}$$

Since we are dealing with a many-boson system, only one single-particle wave function (SPWF) is needed.

The total energy in this approximation is

$$\begin{aligned}W_H=&\langle\Phi|\hat{H}|\Phi\rangle\\=&N\left\{\int dx\ \phi^*_\alpha(x)\tfrac{1}{2}[p^2+x^2]\phi_\alpha(x)\right.\\&+\kappa_0\int dx\ \phi^*_\alpha(x)\phi_\alpha(x)x\int dy\ \phi^*_\alpha(y)\phi_\beta(y)(\sigma_z)_{\alpha\beta}\\&\left.-\lambda_0\left[\int dx\ \phi^*_\alpha(y)\phi_\beta(y)(\sigma_x)_{\alpha\beta}\right]^2\right\}\ ,\end{aligned} \tag{5.3}$$

where the rescaled coupling constants are

$$\kappa_0=\kappa N=0.256\,12\ , \tag{5.4a}$$

$$\lambda_0=\lambda N=0.02\ . \tag{5.4b}$$

In a standard fashion one can derive the TDH equation ($\hbar=1$)

$$i\partial_t\rho=[\mathcal{H},\rho] \tag{5.5}$$

where

$$\mathcal{H}=\tfrac{1}{2}(p^2+x^2)+\kappa_0 x\,\mathrm{Tr}(\rho\sigma_z)+\kappa_0\sigma_z\mathrm{Tr}(\rho x)-2\lambda_0\sigma_x\mathrm{Tr}(\rho\sigma_x)\ . \tag{5.6}$$

Note that

$$\rho^2=\rho,\quad \tilde{\rho}^2=N\tilde{\rho}\ . \tag{5.7}$$

B. Modification of fermion formalism for bosons

The theory that follows is now developed in quite close analogy with the fermion case, as we have already observed. All the formulas of Sec. III can readily be adapted to the present case or derived anew easily enough. Except for factors of N, which depend on the choice of scale, the structure of all formulas is the same, with the replacement of all indices $h,h',\ldots$ by the single index 0. We shall study Eq. (5.5) in the representation in which ρ is instantaneously diagonal. Then

$$\rho_{00}=1,\quad \rho_{0p}=\rho_{p0}=\rho_{pp'}=0\ , \tag{5.8}$$

where the index 0 is for the hole (occupied) state while p (p') stand for particle (unoccupied) states. Then just as in Eq. (3.4), Eq. (5.5) can be shown to imply the following set of equations for the matrix elements of the density matrix:

$$i\partial_t\rho_{0p}=-\mathcal{H}_{0p}=-\frac{1}{N}\frac{\partial W_H}{\partial\rho_{p0}}\ , \tag{5.9a}$$

$$i\partial_t\rho_{p0}=\mathcal{H}_{p0}=\frac{1}{N}\frac{\partial W_H}{\partial\rho_{0p}}\ . \tag{5.9b}$$

Consequently, the set of matrix elements $\sqrt{N}\rho_{0p}$ and $\sqrt{N}\rho_{p0}$ form an infinite set of complex canonical variables. Though we can introduce real canonical coordinates and momenta by the standard transformation,

$$\rho_{0p}=\rho^*_{p0}=\frac{1}{\sqrt{2N}}(\xi^p+i\pi_p)\ , \tag{5.10}$$

in the adiabatic limit we turn again to the Holstein-Primakoff alternative and the representation in which $\rho(\xi,\pi=0)$ is diagonal. One can then define the corresponding kinetic- and potential-energy terms

$$W_H(\xi,\pi)=\tfrac{1}{2}\pi_p B^{pp'}\pi_{p'}+V(\xi)\ . \tag{5.11}$$

In analogy with (3.26) and (3.27), we can also derive the following formula for the inverse mass matrix, applicable to separable interactions,

$$B^{pp'}=\frac{\partial^2 W}{\partial\pi_p\partial\pi_{p'}}=\tfrac{1}{2}(\mathcal{H}_{pp'}+\mathcal{H}_{p'p}-2\delta_{pp'}\mathcal{H}_{00})\ , \tag{5.12}$$

where $\mathcal{H}_{00}$ and $\mathcal{H}_{pp'}$ are the hole-hole and particle-particle matrix elements, respectively, of the single-particle Hamiltonian (5.6). One can also construct the so-called U functional, that in the present case is given by the following expression,

$$U=\frac{1}{2}\frac{\partial V}{\partial\xi^p}B^{pp'}\frac{\partial V}{\partial\xi^{p'}}=\frac{N}{2}\mathrm{Tr}[\rho\mathcal{H}(1-\rho)\mathcal{H}(1-\rho)\mathcal{H}-(1-\rho)\mathcal{H}\rho\mathcal{H}\rho\mathcal{H}]\ . \tag{5.13}$$

Returning to the specific model under study, we introduce the following definitions,

$$q=\mathrm{Tr}(\rho x)\ , \tag{5.14}$$

$$\cos\zeta=\mathrm{Tr}(\rho\sigma_z)\ , \tag{5.15a}$$

$$\sin\zeta=\mathrm{Tr}(\rho\sigma_x)\ . \tag{5.15b}$$

Equation (5.6) now reads

$$\mathcal{H}=\tfrac{1}{2}[p^2+x^2]+\kappa_0 x\cos\zeta+\kappa_0 q\sigma_z-2\lambda_0\sin\zeta\sigma_x\ , \tag{5.16}$$

which can be interpreted as describing a spin one-half particle in a displaced harmonic oscillator well interacting with an effective magnetic field

$$\mathbf{B}_0=(4\lambda_0\sin\zeta,0,-2\kappa_0 q)\ . \tag{5.17}$$

The generalized valley equations are [cf. (3.35) and (3.36)]

$$\mathcal{H}_{p0}=\mu\frac{\delta Q}{\delta\rho_{0p}}\ , \tag{5.18a}$$

$$\mathcal{H}^{(1)}_{p0}=\omega\frac{\delta Q}{\delta\rho_{0p}}\ . \tag{5.18b}$$

For the cases treated in this paper, Q has a particularly simple form, namely

$$Q=\mathrm{Tr}\{\rho f\}\ , \tag{5.19}$$

with f a density-independent single-particle operator; μ and ω are the appropriate Lagrange multipliers. For more realistic models to be considered in the future, we shall have to consider a more general relation than (5.19); this point will be taken into account in some of the reasoning to be carried out next.

C. Method of solution

To see how to construct an approximate solution of (5.18), we remark first that we are dealing with an infinite-dimensional vector space labeled by the unoccupied levels, p (and by the spin). The quantities $\mathcal{H}_{p0}$ and $\mathcal{H}^{(1)}_{p0}$ are the components of two vectors in this space. We are looking for a basis, or rather a continuous, differentiable one-dimensional manifold of bases, such that the two vectors are everywhere parallel to each other, and in so far as possible, also parallel to the tangent to the manifold (collective path).

Of the two operators $\mathcal{H}$ and $\mathcal{H}^{(1)}$, the first, the Hartree Hamiltonian, has a simple, almost transparent form for the models under study in this paper. For all intents and purposes it resides in a finite-dimensional vector space.

On the other hand, if we study the structure of $\mathcal{H}^{(1)}$ with the aid of Eq. (3.38), we can easily convince ourselves that in general the latter spans a larger vector space than does the Hartree Hamiltonian. This is true for all realistic models and implies furthermore that for such models we cannot expect exact decoupling, because if we attempt to enlarge the vector space for $\mathcal{H}$, this will still further enlarge the space for $\mathcal{H}^{(1)}$, and so on, without apparent convergence.

It turns out, however, that for the simple models considered in this section and the next, $\mathcal{H}^{(1)}$ spans the same vector space as $\mathcal{H}$, and thus we have exact decoupling. Proofs of this assertion within the present context will be provided in this section and the next, whereas the algebraic basis for these results will be pointed out in Sec. VIII and illustrated in Appendix D.

We now describe a method which yields the exact solution when the latter exists and should serve as a reasonable approximation otherwise. In this method, we consider a set of one-body observables, Q^i, $(i=1\ldots L)$,

$$Q^i=\mathrm{Tr}(\rho f^i)\ , \tag{5.20}$$

and assume that the "true" collective coordinate, Q, is a function of the L Q^i,

$$Q=Q(Q^i)\ . \tag{5.21}$$

Then the cranking operator, f, is given by the expression

$$f=(\delta Q/\delta\rho)=\sum_{i=1}^{L} a_i f^i\ , \tag{5.22a}$$

$$a_i=(\delta Q/\delta Q^i),\quad f^i=(\delta Q^i/\delta\rho)\ . \tag{5.22b}$$

By a suitable rescaling at every point on the collective path, we may choose $a_1=1$.

With these assumptions, Eq. (5.18a) takes the form

$$\overline{\mathcal{H}}_{p0}=\left[\mathcal{H}-\mu\sum_i a_i f^i\right]_{p0}=0\ , \tag{5.23}$$

which is recognized as a constrained Hartree problem determining (by variation of the L independent parameters μ, $a_2,\ldots a_L$) an L-dimensional submanifold. Given the density matrix on this submanifold, we can evaluate the potential energy and the mass tensor, as well as any other physical quantity of interest in the collective subspace. In this way the problem is reduced precisely to the type studied in our previous work[3,4,6] namely that of finding a valley on a submanifold with L degrees of freedom, where L is some "manageable" number from the computational point of view.

Let us apply this method to the model under study. As a special case of (5.21), we choose

$$Q=Q(q,\cos\zeta)\ , \tag{5.24}$$

where the quantities q and ζ were defined in (5.14) and (5.15). Some details of the calculation following from the assumption (5.24) are given in Appendix C. In broad outline, the cranking Hamiltonian takes the form

$$\overline{\mathcal{H}}=\tfrac{1}{2}(p^2+x^2)+qx-B(\sin\zeta\sigma_x+\cos\zeta\sigma_z)\ , \tag{5.25}$$

which again describes a displaced harmonic oscillator with the spin coupled to an external magnetic field. The SPWF,

$$\phi(x,\sigma)=\phi_0(x-q)\begin{bmatrix}\cos\frac{1}{2}\zeta\\ \sin\frac{1}{2}\zeta\end{bmatrix}\ , \tag{5.26}$$

where $\phi_0(x)$ is the wave function for the ground state of an harmonic oscillator, determines the dynamics of the solution and shows clearly that only two independent parameters intervene.

The result proved in Appendix C is that the cranking solution based on Eq. (5.24) reproduces to the leading order in N^{-1} the exact formulation given in Ref. 4. This is perhaps not too surprising in view of the result that the ostensible many-body problem is in reality only a problem in two dimensions. From the point of view of the exact decoupling conditions, Eqs. (2.15)–(2.17), the solution of the cranking equations may always be carried out so as to satisfy (2.15) and (2.16). The crucial conditions become (2.17). The essential observation here is that the evaluation of $\overline{B}^{ij}$, $(i,j=1,2)$ is completely general and yields a tensor that depends only on the collective coordinates introduced for the cranking. Thus they are independent of any noncollective coordinates that we may choose to introduce; consequently (2.17) is also satisfied.

On the basis of the results given in Appendix C, we can calculate the expressions for the V and U functionals, respectively,

$$V=\tfrac{1}{2}N+N[\tfrac{1}{2}(q+\kappa_0\cos\zeta)^2-\tfrac{1}{2}\kappa_0^2\cos^2\zeta-\lambda_0\sin^2\zeta]\ , \tag{5.27}$$

$$\begin{aligned}U=N[&\tfrac{1}{2}(q+\kappa_0\cos\zeta)^2-2\kappa_0^3q^3\sin^2\zeta\cos\zeta\\&+4\kappa_0^2\lambda q^2(3\cos^4\zeta-4\cos^2\zeta+1)\\&+8\kappa_0\lambda_0^2 q\cos\zeta(3\cos^4\zeta-5\cos^2\zeta+2)\\&+16\lambda_0^3\sin^4\zeta\cos^2\zeta]\ .\end{aligned} \tag{5.28}$$

It is noteworthy that in both of these expressions the leading terms have the same structure, namely $(q+\kappa_0\cos\zeta)^2$. The remaining terms, which contain different powers of the coupling constants κ_0,λ_0 are much smaller. [In comparing (5.27) with the corresponding Eq. (11) in Ref. 4, one has to be aware of some changes in notation, namely $\kappa_0\to N\kappa$, $\lambda_0\to N\lambda$, $q\to qN^{-1/2}$, $\zeta\to\xi$.] The combination $q+\kappa_0\cos\zeta$ has to be interpreted as an approximate expression for the noncollective coordinate, characterized by the largest frequency of the system, and correspondingly the approximate solution for the collective path will be $q+\kappa_0\cos\zeta=0$, which, in our previous analyses, corresponds exactly to what we termed the Born-Oppenheimer approximation. The collective Hamiltonian in this limit, Eq. (30) of Ref. 4, is

$$H_{\mathrm{coll}}=-2N\kappa^2S_z^2-4\lambda S_x^2\ , \tag{5.29}$$

where S_x,S_z are the operators for the total spin of the system, proved to be an almost perfect approximation for the "exact" collective Hamiltonian we constructed using our procedure.

VI. EXTENDED ADIABATIC APPROXIMATION

In order to accomplish all our aims in the study of a second soluble model, it is necessary to generalize the considerations of Secs. II and III, because of the following observation: A point transformation is not the most general transformation that preserves the structure of (2.1)! To see this rather simple point, we generalize (2.2) and (2.3) to[32]

$$\xi^{\alpha}=g^{(0)\alpha}(q)+\tfrac{1}{2}g^{(1)\alpha\mu\nu}(q)p_{\mu}p_{\nu}+\mathcal{O}(p^4)\ , \tag{6.1}$$

$$\pi_{\alpha}=f^{(0)\mu}_{,\alpha}p_{\mu}+\mathcal{O}(p^3)\ . \tag{6.2}$$

From the standard Poisson bracket relations, we find once more the chain rule relations

$$\begin{aligned} &g^{(0)\alpha}_{,\mu}f^{(0)\nu}_{,\alpha}=\delta^{\mu}_{\nu}\ ,\\ &g^{(0)\alpha}_{,\mu}f^{(0)\mu}_{,\beta}=\delta^{\alpha}_{\beta}\ , \end{aligned} \tag{6.3}$$

and one new condition, namely, that the quantity

$$\tau^{\alpha\beta\gamma}=g^{(1)\gamma\mu\nu}g^{(0)\beta}_{,\mu}g^{(0)\alpha}_{,\nu} \tag{6.4}$$

is symmetric in all three indices (supposed that $g^{(1)}$ is symmetric in its last two indices).

Inserting the transformation (6.1) and (6.2) into (2.1) and neglecting terms of higher than second order in the momenta in the Hamiltonian, the transformed Hamiltonian takes the form

$$\begin{aligned} \overline{H}(q,p)&=\tfrac{1}{2}p_{\mu}\{f^{(0)\mu}_{,\alpha}B^{\alpha\beta}[g(q)]f^{(0)\nu}_{,\beta}\\ &\quad+V_{,\gamma}[g(q)]g^{(1)\gamma\mu\nu}\}p_{\nu}+V[g(q)]\\ &\equiv\tfrac{1}{2}p_{\mu}\overline{B}^{\mu\nu}p_{\nu}+\overline{V}(q)\ . \end{aligned} \tag{6.5}$$

This establishes the immediate point, but raises a new problem. How is one to determine the added set of functions $g^{(1)}$? We shall not give a general solution of this problem, but rather one that suffices for the immediate needs of this work. (A general solution has been worked out and will be described in our future work.)

The solution consists of prescribing the structure of the transformation inverse to (6.1) and (6.2), in terms of a set of density-independent single-particle operators f^{μ}, according to the equations

$$\begin{aligned} Q^{\mu}&=\mathrm{Tr}(f^{\mu}\rho)\\ &=Q^{\mu}(\xi,\pi)\\ &=f^{(0)\mu}(\xi)+\tfrac{1}{2}f^{(1)\mu\alpha\beta}(\xi)\pi_{\alpha}\pi_{\beta}+\mathcal{O}(\pi^4)\ . \end{aligned} \tag{6.6}$$

The transformation of the momenta is

$$p_{\mu}=g^{(0)\alpha}_{,\mu}\pi_{\alpha}+\mathcal{O}(\pi^3)\ . \tag{6.7}$$

If the structure of the f^{μ} is known or can be obtained by independent means, as we now assume (we shall see in practice how this can be done), then the last form of (6.6) can be evaluated by the substitution of (3.14), and the quantities $f^{(1)}$ thus obtained. Next we substitute (6.6) and (6.7) into (6.5) and thus find

$$\begin{aligned} H(\xi,\pi)=\tfrac{1}{2}\pi_{\alpha}B^{\alpha\beta}(\xi)\pi_{\beta}+\tfrac{1}{2}V_{,\gamma}(g^{(1)\gamma\mu\nu}g^{(0)\alpha}_{,\mu}g^{(0)\beta}_{,\nu}\\ +g^{(0)\gamma}_{,\mu}f^{(1)\mu\alpha\beta})\pi_{\alpha}\pi_{\beta}+V(\xi)\ , \end{aligned} \tag{6.8}$$

and requiring this to coincide with (2.1) shows that

$$g^{(1)\gamma\mu\nu}=-f^{(0)\mu}_{,\alpha}f^{(0)\nu}_{,\beta}g^{(0)\gamma}_{,\lambda}f^{(1)\lambda\alpha\beta}\ . \tag{6.9}$$

The upshot of these calculations is that the augmented transformed mass tensor defined in (6.5) is now calculable. The decoupling conditions and fundamental theorem go through as before in terms of this new quantity. It is evident, however, that the formulas of Sec. III are modified in detail, as we now demonstrate.

Let us concentrate once more on the case of decoupling one collective coordinate, so that we only need the two point functions

$$X^{(1)}=\overline{V}=V[g^{(0)}(q)]\ , \tag{6.10}$$

$$\begin{aligned} X^{(2)}&=\overline{U}=\overline{V}_{,\mu}\overline{B}^{\mu\nu}\overline{V}_{,\nu}\\ &=V_{,\alpha}B^{\alpha\beta}V_{,\beta}+\tau^{\alpha\beta\gamma}V_{,\alpha}V_{,\beta}V_{,\gamma}\ . \end{aligned} \tag{6.11}$$

Translating these conditions to TDH(F) again, we have

$$V=W(\rho)\ , \tag{6.12}$$

$$V_{,ph}=\mathcal{H}_{ph}=\lambda f_{ph}\ , \tag{6.13}$$

$$\begin{aligned} U&=\mathcal{H}_{hp}\mathcal{H}_{pp'}\mathcal{H}_{p'h}-\mathcal{H}_{ph}\mathcal{H}_{hh'}\mathcal{H}_{h'p}\\ &\quad+d\overline{V}/dQ(\mathcal{H}_{ph}f_{hh'}\mathcal{H}_{h'p}-\mathcal{H}_{hp}f_{pp'}\mathcal{H}_{p'h})\\ &=\mathcal{H}_{hp}\overline{\mathcal{H}}_{pp'}\mathcal{H}_{p'h}-\mathcal{H}_{ph}\overline{\mathcal{H}}_{hh'}\mathcal{H}_{h'p}\ , \end{aligned} \tag{6.14}$$

$$U_{,ph}=\mathcal{H}^{(1)NL}_{ph}+\mathcal{H}^{(1)L}_{ph}=\mu f_{ph}\ . \tag{6.15}$$

In the evaluation of U we have used Eq. (6.13) as well as the explicit form of $f^{(1)}$ obtained from (6.6). The two terms of (6.15) given in detail in the following were calculated directly from (6.14), whereas rigorously the calculation of the gradient should have been made before the substitution of (6.13). Because the terms that are thereby omitted play no role in the present paper, we shall not enter into a more detailed discussion of this point, but will return to it in our future work, where it will be germane. The two operators in (6.15) are found to have the form

$$\begin{aligned} \mathcal{H}^{(1)NL}&=-\overline{\mathcal{H}}\rho\mathcal{H}(1-\rho)\mathcal{H}-\mathcal{H}(1-\rho)\mathcal{H}\rho\overline{\mathcal{H}}+\mathcal{H}\rho\overline{\mathcal{H}}\rho\mathcal{H}-\overline{\mathcal{H}}(1-\rho)\mathcal{H}\rho\mathcal{H}-\mathcal{H}\rho\mathcal{H}(1-\rho)\overline{\mathcal{H}}+\mathcal{H}(1-\rho)\overline{\mathcal{H}}(1-\rho)\mathcal{H}\ ,\\ \mathcal{H}^{(1)L}&=\sum_{\sigma}\kappa_{\sigma}q_{\sigma}\mathrm{Tr}[\rho q_{\sigma}(1-\rho)\overline{\mathcal{H}}(1-\rho)\mathcal{H}+\rho\mathcal{H}(1-\rho)q_{\sigma}(1-\rho)\mathcal{H} \end{aligned} \tag{6.16}$$

$$+\rho\mathcal{H}(1-\rho)\overline{\mathcal{H}}(1-\rho)q_{\sigma}-(1-\rho)q_{\sigma}\rho\overline{\mathcal{H}}\rho\mathcal{H}-(1-\rho)\mathcal{H}\rho q_{\sigma}\rho\mathcal{H}-(1-\rho)\mathcal{H}\rho\overline{\mathcal{H}}\rho q_{\sigma}]\ . \tag{6.17}$$

These formulas should be compared with (3.38). Because the local coordinate system is the one in which $\overline{\mathcal{H}}$ is diagonal, (6.16) and (6.17) are actually simpler to use than the former. Finally, the formula for the collective mass can be read off from (6.14), namely,

$$\tfrac{1}{2}\overline{B}=f_{hp}\overline{\mathcal{H}}_{pp'}f_{p'h}-f_{ph}\overline{\mathcal{H}}_{hh'}f_{h'p}\ . \tag{6.18}$$

This formalism will now be applied to an exactly soluble model.

VII. MONOPOLE MODEL IN ONE SPATIAL DIMENSION (SUZUKI MODEL)

In this section we study a system of spinless fermions in one spatial dimension, described by a Hamiltonian that in second quantized form is written

$$\hat{H}=\int dx\ \psi^{\dagger}(x)\tfrac{1}{2}(p^2+x^2)\psi(x)+\tfrac{1}{2}\kappa\hat{Q}^2\ , \tag{7.1}$$

where

$$\hat{Q}=\int dx\ \psi^{\dagger}(x)x^2\psi(x) \tag{7.2}$$

is a monopole operator. This model has been studied previously by several authors.[33–37]

If we consider a system of N particles and neglect the Fermi statistics, it then becomes possible to exactly decouple a degree of freedom corresponding to the operator $\hat{Q}$, which can be interpreted as the square of the radius in a space of N dimensions. Decoupling will then occur upon the introduction of hyperspherical coordinates. In Appendix D, we derive an exact solution of the TDH equation which indicates that also for the problem with Fermi statistics, we have exact decoupling as a consequence of the simple algebraic structure of the model. In this section we show that the same solution can be obtained by applying the method of Sec. V in conjunction with the formulas of Sec. VI.

The Hartree approximation corresponding to the Hamiltonian (7.1) is

$$\mathcal{H}=\tfrac{1}{2}(p^2+x^2)+\kappa Q x^2\ , \tag{7.3}$$

with

$$Q=\mathrm{Tr}(\rho x^2) \tag{7.4}$$

the "natural" first choice of collective coordinate in a cranking treatment. From the discussion in Sec. V it follows that if there is to be an exactly decoupled coordinate then it must be Q, i.e., the cranking operator must be x^2, and the associated cranking Hamiltonian, also of oscillator form, is

$$\overline{\mathcal{H}}=\tfrac{1}{2}(p^2+\omega^2x^2)\ , \tag{7.5}$$

$$\omega^2=1+2(\kappa Q-\lambda)\ . \tag{7.6}$$

The N lowest-energy eigenfunctions of $\overline{\mathcal{H}}$, ϕ_h, (energy ϵ_h), will provide a density matrix $\rho(Q)$ which specifies a submanifold of dimension one.

We outline the calculation of the collective potential energy and the collective mass from the solutions ϕ_h. We have first

$$\begin{aligned}\overline{V}(Q)&=\mathrm{Tr}[\tfrac{1}{2}(p^2+x^2)\rho]+\tfrac{1}{2}\kappa Q^2\\&=\sum_h\epsilon_h(Q)-\tfrac{1}{2}\kappa Q^2+Q\frac{d\overline{V}}{dQ}\ ,\end{aligned} \tag{7.7}$$

where we have remembered the definition $\lambda=(d\overline{V}/dQ)$. The sum over single-particle energies is transformed by means of virial theorem,

$$\sum\epsilon_h=\omega^2\mathrm{Tr}(x^2\rho)=\omega^2Q\ . \tag{7.8}$$

We thus arrive at the first-order differential equation

$$\overline{V}=Q\left[\omega^2+\frac{d\overline{V}}{dQ}\right]-\frac{1}{2}\kappa Q^2\ , \tag{7.9}$$

of which the solution, by inspection, is

$$\overline{V}(Q)=\tfrac{1}{2}Q+\tfrac{1}{2}\kappa Q^2+\frac{\beta}{Q}\ , \tag{7.10}$$

where the value of the constant β has yet to be determined.

To calculate β, we proceed as follows. Let Q_0 be the equilibrium value of Q, as fixed in part from the equation

$$0=\frac{d\overline{V}}{dQ}=\frac{1}{2}+\kappa Q_0-\frac{\beta}{Q_0^2}\ . \tag{7.11}$$

From the virial theorem applied once more, we find

$$Q_0=\frac{N^2}{2\omega_0}\ , \tag{7.12}$$

where ω_0 is determined from the equilibrium value of (7.6)

$$\omega_0^2=1+2\kappa Q_0\ . \tag{7.13}$$

Combining the various results, we find that $\beta=(1/8)N^4$. Equation (7.10) now agrees with the exact result (D12).

It is easy to see that the relation (7.12) between Q and ω holds for any point on the collective path. Combining this observation with Eq. (7.6) leads to another derivation of the value of β.

We remark parenthetically that the second term of (7.10) is associated in an obvious way with the interaction term of the original many-body Hamiltonian, and that if in the latter we were to make the replacement,

$$\tfrac{1}{2}\kappa\hat{Q}^2\rightarrow\mathcal{V}(\hat{Q})\ , \tag{7.14}$$

then the corresponding replacement would take place in (7.10). The value of Q_0 would change, but assuming the system to be stable, the value of β would be unaffected.

We consider next the calculation of the collective mass, utilizing Eq. (6.18), which for the present example takes the form

$$\tfrac{1}{2}\overline{B}=\mathrm{Tr}[\rho x^2(1-\rho)\overline{\mathcal{H}}(1-\rho)x^2-(1-\rho)x^2\rho\overline{\mathcal{H}}\rho x^2]\ . \tag{7.15}$$

This formula can be transformed following a standard ar-

gument into the simpler structure (only because $\overline{\mathcal{H}}$ is diagonal)

$$\overline{B}=\mathrm{Tr}[x^2,(\overline{\mathcal{H}},x^2)]=4Q \ . \tag{7.16}$$

We thus see that to obtain the correct collective mass and thus the exact value for the collective Hamiltonian requires the modified theory of Sec. VI. Since the collective mass depends only on Q, it follows within the present context that the motion is decoupled, since this implies that (2.17) is satisfied, (2.16) has previously been solved, and (2.15) can always be satisfied by the proper choice of coordinate system.

One may finally wish to verify the conditions of the fundamental theorem. As an example one may check (6.15). We shall not pause here to perform this exercise, which requires taking into account restrictions on the contributions to the various gradient vectors implied by the simplified algebraic structure of the model. These restrictions are important for our work in progress and will be described when the latter is reported.

VIII. ADDITIONAL REMARKS AND FUTURE PROSPECTS

In this paper we have described how the generalized valley method, applied previously to rather simple problems of decoupling collective modes from a few-particle, or in special cases, from a many-particle system in the classical limit, might be applied to problems in nuclear physics. We have also indicated the possible need for an extension of the usual adiabatic approach. In Secs. V and VII we studied two simple examples. These were simple enough so that they could be shown to represent exactly decoupled motions in two and one dimension, respectively. This was done by direct application of the original decoupling conditions and by analytic rather than numerical treatment. We now remark that these results can also be understood from the algebraic structure of the models.

Consider first the model of Sec. V. The Hamiltonian (5.1) belongs to the enveloping algebra of SU(2) $\times$[W(1)$\oplus$SU(1,1)], i.e., the direct product of the SU(2) of the spin with the semidirect sum of the Heisenberg-Weyl canonical algebra W(1) and the associated SU(1,1) formed from x^2, p^2, and $(xp+px)$. It can be shown that if at time $t=0$, the system is described by a coherent state defined by a wave function of the form (5.26), a displaced harmonic oscillator with the spin pointing in a certain direction, then the exact solution of the TDH equation will also be a coherent state with generally a different displacement and a different spin orientation. The result described in Sec. V is simply the adiabatic limit of the same result.

For the "monopole" model of Sec. VII, the exact solution of the TDH equation has been given explicitly[37] as a generalized coherent state (Slater determinant) of harmonic-oscillator functions with a time-dependent frequency. The persistence in time of the harmonic-oscillator character is in this instance based on the underlying algebra SU(1,1) of the model. In Appendix D, the reader will find a brief self-contained study of this problem. We were able to verify in Sec. VII that the modified theory of Sec. VI was capable of yielding the exact solution found in this appendix.

The algebra SU(1,1) is isomorphic to SP(2,R). Exact solutions of the TDH equation can be obtained for a family of models based on the algebra Sp(2n,R), including a generalized version of the Nilsson model for $n=3$. Of more physical interest is the study of models which are not exactly soluble by algebraic methods, but go over to these models in a suitable limit. Such models, requiring the full power of the method described in Sec. V, will form the subject matter of the next paper of the current development.

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APPENDIX A: TDHF AS A FORM OF HAMILTON'S EQUATIONS

There are a number of ways of transforming the TDHF equations into the form of Hamilton's equations. We describe briefly a method based on a classical version of the Holstein-Primakoff transformation.[29,30,38] The most general Slater determinant not orthogonal to a given determinant, $|0\rangle$, where

$$|0\rangle=\prod_h a_h^\dagger|\mathrm{vac}\rangle \tag{A1}$$

has the (unnormalized) form

$$|z\rangle=\exp(z_{ph}a_p^\dagger a_h)|0\rangle \ , \tag{A2}$$

where h signifies the orbitals occupied in $|0\rangle$ and p those unoccupied. The density matrix associated with $|z\rangle$ is

$$\rho_{ab}=\langle z|a_b^\dagger a_a|z\rangle/\langle z|z\rangle\equiv\langle a_b^\dagger a_a\rangle \ , \tag{A3}$$

where now a and b are general single-particle labels. One evaluates

$$\rho_{ph}=\langle a_h^\dagger a_p\rangle=[Z(1+Z^\dagger Z)^{-1}]_{ph} \ , \tag{A4}$$

$$\rho_{hp}=\langle a_p^\dagger a_h\rangle=[(1+Z^\dagger Z)^{-1}Z^\dagger]_{hp} \ , \tag{A5}$$

$$\rho_{pp'}=\langle a_{p'}^\dagger a_p\rangle=[Z(1+Z^\dagger Z)^{-1}Z^\dagger]_{pp'} \ , \tag{A6}$$

$$\rho_{hh'}=\langle a_{h'}^\dagger a_h\rangle=[(1+Z^\dagger Z)^{-1}]_{hh'} \ . \tag{A7}$$

In place of the matrix Z, we shall employ another set of complex variables which will be identified as a set of complex canonical variables, namely

$$\beta=Z(1+Z^\dagger Z)^{-1/2}=(1+ZZ^\dagger)^{-1/2}Z \ , \tag{A8}$$

$$\beta^\dagger=(1+Z^\dagger Z)^{-1/2}Z^\dagger=Z^\dagger(1+ZZ^\dagger)^{-1/2} \ . \tag{A9}$$

In terms of these new variables Eqs. (A4)–(A7) are replaced by the formulas

$$\rho_{ph}=[\beta(1-\beta^\dagger\beta)^{1/2}]_{ph} \ , \tag{A10}$$

$$\rho_{hp}=[(1-\beta^\dagger\beta)^{1/2}\beta]_{ph} \ , \tag{A11}$$

$$\rho_{pp'}=[\beta\beta^\dagger]_{pp'} \ , \tag{A12}$$

$$\rho_{hh'}=[1-\beta^\dagger\beta]_{hh'} \ , \tag{A13}$$

which constitute the classical Holstein-Primakoff transformation.

It may now be shown that when the $\beta^\dagger$ and β are taken as the variational parameters in the time-dependent variational principle applied to the Slater determinant (A,2), then the resulting equations are of the form

$$i\dot{\beta}=\partial H/\partial\beta^\dagger \tag{A14}$$

and complex conjugate equation, where H is the Hartree-Fock energy functional associated with the same Slater determinant.

APPENDIX B: VARIATION WITH RESPECT TO THE DENSITY MATRIX

If Θ_{ab} is a matrix element of an arbitrary single-particle operator in a basis in which the density matrix ρ is diagonal, we need formulas for how these matrix elements vary when we vary the density matrix. One derivation of such formulas has already been given in Ref. 38. Here we describe an alternative derivation. The trick is to write

$$\Theta_{ab}=(a|\Theta|b)=(a|\rho\Theta\rho|b)+(a|\rho\Theta(1-\rho)|b) +(a|(1-\rho)\Theta\rho|b)+(a|(1-\rho)\Theta(1-\rho)|b) , \tag{B1}$$

where ρ is the density matrix corresponding to the set $|a),|b)$. From (B1) one then verifies that

$$\partial\Theta_{ab}/\partial\rho_{ph}=\Theta_{hb}(-\delta_{ap})+\Theta_{ap}\delta_{bh} , \tag{B2}$$

$$\partial\Theta_{ab}/\partial\rho_{hp}=\Theta_{pb}\delta_{ah}-\Theta_{ah}\delta_{pb} . \tag{B3}$$

By the same technique we derive, for example,

$$\partial V_{abcd}/\partial\rho_{ph}=-\delta_{ap}V_{hbcd}+\delta_{ch}V_{abpd} -\delta_{bp}V_{ahcd}+\delta_{dh}V_{abcp} . \tag{B4}$$

Finally by combining (B2)–(B4), we can derive the formulas

$$\partial\mathcal{H}_{ab}/\partial\rho_{ph}=-\mathcal{H}_{hb}\delta_{ap}+\mathcal{H}_{ap}\delta_{bh}+V_{ahbp} , \tag{B5}$$

$$\partial\mathcal{H}_{ab}/\partial\rho_{hp}=\mathcal{H}_{pb}\delta_{ah}-\mathcal{H}_{ah}\delta_{bp}+V_{apbh} . \tag{B6}$$

APPENDIX C: CRANKING SOLUTION FOR THE TUNNELING MODEL

We supply the details of the cranking calculation which yields the leading term in powers of N^{-1} of the exact solution, as found in our previous work.[4] We choose the collective operator to be of the form

$$Q=q+a\cos\xi , \tag{C1}$$

corresponding to a cranking operator

$$f=x+a\sigma_x . \tag{C2}$$

The cranking Hamiltonian is thus of the form

$$(\mathcal{H}-\mu f)\equiv\overline{\mathcal{H}}=\tfrac{1}{2}[p^2+x^2]+x_0x -B(\cos\xi\sigma_z+\sin\xi\sigma_x) , \tag{C3}$$

where

$$x_0=(\kappa_0\cos\zeta-\mu) , \tag{C4a}$$

$$B\cos\zeta=-(\kappa_0q-\mu a),\quad B\sin\xi=2\mu\sin\zeta , \tag{C4b}$$

and the various symbols are defined in Eqs. (5.14), (5.15), and (5.18) of the text. The lowest eigenstate of $\overline{\mathcal{H}}$, the one that specifies the reduced density matrix ρ, is of the form given in (5.25) and (5.26) with $q=-x_0$ and $\zeta=\xi$; the eigenvalue is $\frac{1}{2}-B_0$. The collective potential energy is obtained by inserting the solution (5.26) into (5.3), reexpressing the first term as $\overline{\mathcal{H}}$ plus "corrections." The result is the expression

$$(V/N)=\tfrac{1}{2}q^2+\kappa_0q\cos\zeta-\lambda_0\sin^2\zeta . \tag{C5}$$

When account is taken of a difference in scale, this result agrees with Eq. (11) of Ref. 4, except for terms of relative order N^{-1}.

It remains to establish a similar concordance with the mass tensor. Here we emphasize that we are studying the properties of a two-dimensional submanifold parametrized by the collective coordinates $Q^1=q$ and $Q^2=\xi$. For the associated mass tensor, we have the formula

$$\bar{B}^{ij}=\frac{\partial Q^i}{\partial\xi^p}B^{pp'}\frac{\partial Q^j}{\partial\xi^{p'}},\quad i=1,2 . \tag{C6}$$

Remembering Eq. (5.10), we have, for example,

$$B^{11}=\frac{2}{N}\mathrm{Tr}[\rho x(1-\rho)\mathcal{H}(1-\rho)x-(1-\rho)x\rho\mathcal{H}\rho x] . \tag{C7}$$

This becomes the standard sum-rule evaluation if we replace $\mathcal{H}$ by $\overline{\mathcal{H}}$, the difference not contributing in this case, and we thereby find

$$B^{11}=N^{-1} . \tag{C8}$$

Next, to obtain the formula for B^{22} we replace x by σ_z in (C7). The only wave functions needed in the direct evaluation of the resulting formula are given by Eq. (5.26) and the corresponding state with the spin flipped. Also converting from $\cos\xi$ to ξ as collective coordinate, we find the result

$$\bar{B}^{\xi\xi}N=8\lambda_0\sin^2\xi-4\kappa_0q\cos\xi . \tag{C9}$$

It is easy to show that the off-diagonal mass vanishes. Again comparison of (C8) and (C9) with Eqs. (13) and (14) of Ref. 4 registers agreement when the scale is adjusted.

APPENDIX D: EXACT SOLUTION OF THE TDH EQUATIONS FOR THE SUZUKI MODEL

In the following we lean heavily on the properties of the symmetry algebra, SU(1,1) of the model. We utilize the generators

$$4\hat{T}_1=\int\psi^\dagger(x^2-p^2)\psi\equiv\hat{Q}-2\hat{K} , \tag{D1}$$

$$4\hat{T}_2=\int\psi^\dagger(xp+px)\psi , \tag{D2}$$

$$4\hat{T}_3=\int\psi^\dagger(x^2+p^2)\psi\equiv\hat{Q}+2\hat{K} , \tag{D3}$$

that satisfy the commutation relations (dropping the hats)

$$[T_1,T_2]=iT_3 \ , \tag{D4}$$

$$[T_2,T_3]=-iT_1 \ , \tag{D5}$$

$$[T_3,T_1]=-iT_2 \ . \tag{D6}$$

The Casimir invariant, I_2, is

$$I_2=T_3^2-T_1^2-T_2^2 \ . \tag{D7}$$

Let us study (D7) for a system of N fermions and for the irreducible representation (irrep) that contains the lowest-energy Slater determinant formed from the one-particle eigenstates of T_3. First we evaluate (D7) for any state in the irrep for which the Hartree approximation is valid, allowing us to replace the average of the square by the square of the average. We thus obtain the formula

$$I_2=\tfrac{1}{2}QK-\langle T_2\rangle^2 \ , \tag{D8}$$

where

$$Q=\langle \hat{Q}\rangle, \quad K=\langle \hat{K}\rangle \ , \tag{D9}$$

We can obtain the numerical value of I_2 for this same irrep by evaluating the rhs of (D8) for the Slater determinant constructed from the eigenstates of T_3. We thus find the value $N^4/16$. Furthermore, from the equation of motion for $\hat{Q}$, we learn that $\dot{Q}=4\langle T_2\rangle$. Combining the last two results, we thereby obtain a formula for K, namely

$$K=\frac{N^4}{8Q}+\frac{\dot{Q}^2}{8Q} \ . \tag{D10}$$

In turn this formula determines a time-dependent collective Hamiltonian, H_C, defined as

$$H_C\equiv\langle H\rangle=\frac{\dot{Q}^2}{8Q}+V(Q) \ , \tag{D11}$$

where

$$V(Q)=\tfrac{1}{2}Q+\tfrac{1}{2}\kappa_2Q^2+\frac{N^4}{8Q} \ . \tag{D12}$$

Henceforth the state utilized in the average will be understood to be the solution we are seeking of the TDH equation. By relating (D11) in the standard way to a Lagrangian, we may introduce a canonical momentum,

$$\dot{Q}=4QP \ , \tag{D13}$$

and thus rewrite H_C as

$$H_C=2QP^2+V(Q) \ . \tag{D14}$$

We next show how we can infer important information about the structure of the density matrix from the formulas already at hand. We write

$$\bar{\rho}(x,x'|Q,P)=\sum_h \psi_h(x|Q,P)\psi_h^*(x'|Q,P) \ . \tag{D15}$$

We are assuming that the density matrix will depend on time only through the time dependence of the canonical pair Q and P. It is important to notice, however, that the individual modes may each be multiplied by a time- and mode-dependent phase factor without modifying (D15).

It is informative to display the principal definitions and results found above in the ordered form

$$\langle \hat{Q}\rangle=Q \ , \tag{D16}$$

$$\langle T_2\rangle=QP \ , \tag{D17}$$

$$\langle \hat{K}\rangle=\frac{N^4}{8Q}+2QP^2 \ . \tag{D18}$$

These equations can be interpreted as a (classical) mapping from the SU(1,1) algebra onto a pair of canonical variables. The averages (D16) and (D17) suggest that the modes appearing in (D15) can be written in the form

$$\psi_h(x|Q,P)=\exp[iS(x|Q,P)]\phi_h(x,|Q) \ , \tag{D19}$$

i.e., in terms of real phase and amplitude functions, S and ϕ_h, respectively, with only the former depending on P. A straightforward investigation of (D17) yields the solution

$$S=Px^2 \ . \tag{D20}$$

To complete our considerations we must finally turn to the equations for the modes themselves in order to determine the form of ϕ_h. We thus look for solutions of the equation

$$i\frac{d\tilde{\psi}}{dt}=\mathcal{H}\tilde{\psi} \ , \tag{D21}$$

where $\mathcal{H}$ is the Hartree Hamiltonian (7.3) and $\tilde{\psi}$ is related to ψ (the mode index h having been temporarily suppressed) by the formula

$$\tilde{\psi}=\exp\left[-i\int^t\epsilon[Q(t')]dt'\right]\psi \ . \tag{D22}$$

Thus, for a given mode, writing out the various contributions to the time derivative, we are lead to the equation

$$\epsilon_h\psi_h+i\dot{P}(\partial\psi_h/\partial P)+i\dot{Q}(\partial\psi_h/\partial Q)=\mathcal{H}\psi_h \ . \tag{D23}$$

When the form (D19) and the solution (D20) are introduced into (D23), and the time derivatives of Q and P are replaced by the appropriate partial derivatives of H_C, we find that only terms of zero and first order in P survive, yielding the equations

$$\epsilon_h\phi_h=\overline{\mathcal{H}}\phi_h \ , \tag{D24}$$

$$4Q(\partial\phi_h/\partial Q)=-\phi_h-2x(d\phi/dx) \ , \tag{D25}$$

where

$$\overline{\mathcal{H}}=\mathcal{H}-(dV/dQ)x^2 \tag{D26}$$

is the expected cranking Hamiltonian. The solution of (D24) that also satisfies (D25) is

$$\phi_h(x|Q)=\tilde{\omega}^{1/4}\phi_h^{(h0)}(\tilde{\omega}^{1/2}x) \ , \tag{D27}$$

where the superscript $(h0)$ indicates harmonic oscillator and the frequency is determined by the equation

$$\tilde{\omega}^2=1+2\kappa_2Q-2(d\bar{V}/dQ)=N^4/4Q^2 \ . \tag{D28}$$

The use of a properly normalized solution is essential for (D25), which then turns out to be satisfied provided the product $Q\tilde{\omega}$=constant, a relation that is evident from (D28).

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