

Classical mappings of the symplectic model and their application to the theory of large-amplitude collective motion

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We study the algebra $\text{Sp}(n, R)$ of the symplectic model, in particular for the cases $n=1,2,3$, in a new way. Starting from the Poisson-bracket realization we derive a set of partial differential equations for the generators as functions of classical canonical variables. We obtain a solution to these equations that represents the classical limit of a boson mapping of the algebra. We show further that this mapping plays a fundamental role in the collective description of many-fermion systems whose Hamiltonian may be approximated by polynomials in the associated algebra, as is done in the simplest versions of the symplectic model. The relationship to the collective dynamics is formulated as a theorem that associates the mapping with an exact solution of the time-dependent Hartree approximation. This solution determines a decoupled classical symplectic manifold, thus satisfying the criteria that define an exactly solvable model in the theory of large amplitude collective motion. The models thus obtained also provide a test of methods for constructing an approximately decoupled manifold in fully realistic cases. We show that an algorithm developed in one of our earlier works reproduces the main results of the theorem.

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I. INTRODUCTION

We have been engaged for a decade in an effort to formulate a theory of large amplitude collective motion with the special aim of applying it to nuclear physics. The theory has both a classical and a quantum dimension. The classical aspect has been most fully developed and described in a review [1]. The quantum aspect is presently in a stage of vigorous development [2,3], supplanting the early work on this part of the theory [4,5]. At the same time a program of applications to problems of nuclear structure has been undertaken [6-9].

Early in the latter work, we became aware of a paucity of solvable models with some physical content. The usefulness of such models is that they provide a testing ground for the algorithms that would later be applied to more realistic models. For our initial investigation we selected a well-known model of monopole vibrations [10], exactly solvable because the Hamiltonian is a polynomial in the generators of the algebra $\text{Sp}(1, R)$ [or $\text{SU}(1,1)$]. We studied this model in two ways. First, by utilizing the classical limit of the algebra, we were able to produce an exact solution of the time-dependent Hartree equations (derived previously by rather less transparent techniques [11]) and by means of this solution a decoupled collective Hamiltonian for the monopole vibration. Second, and more important, we could check if the same Hamiltonian emerged from the application of the theory of large am-

plitude collective motion. The monopole model provided us with an apparently ideal test of the soundness of our algorithms. This test failed initially, forcing us eventually to recognize and correct an incompleteness in our previous theory.

The first goal of this paper is to show that the method developed for the algebra of $\text{Sp}(1, R)$ can be extended to the algebra of $\text{Sp}(n, R)$. In particular, we work out fully the cases $n=2$ and $n=3$. The former leads to a Hamiltonian with three collective coordinates, describing the interaction of a monopole degree of freedom with a quadrupole tensor in two spatial coordinates and is thus only of interest as a toy model. On the other hand $n=3$ leads to a Hamiltonian with 6 degrees of freedom describing both a monopole and a three-dimensional quadrupole. This defines the model as not only one of physical interest *per se*, but also because of its connection with the symplectic [12] and pseudosymplectic [13] models. The latter, in particular, provides a possibly useful truncation scheme for shell-model calculations for other than the lightest deformed nuclei.

Although not one of the aims of the present paper, this identification will allow us on a future occasion to compare the quantum consequences of the collective Hamiltonian to be derived in this paper with the results of an exact diagonalization carried out for the original many body Hamiltonian. In fact such a comparison has broader implications than the accuracy achieved for the special Hamiltonian considered, since it has been demonstrated that Hamiltonians consisting of suitably chosen polynomials in the generators can give a rather precise fit to the low-energy spectra and other properties of even deformed nuclei [13].

The second aim of this paper is to demonstrate that the extended algorithm formulated in connection with the monopole model also provides correct results for the

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generalized models.

The presentation is organized as follows: In Sec. II we give a brief summary of the properties of the algebra of $\text{Sp}(n, \mathcal{R})$ needed in the ensuing development as well as a discussion of the model Hamiltonians to be studied. In the following three sections we then study separately cases $n=1,2,3$. We describe in each instance the mapping of the algebra onto a classical symplectic manifold, which is tied to the existence of a manifold of solutions of the time-dependent Hartree equation and an associated decoupled collective Hamiltonian. We then show how the same collective Hamiltonian can be derived from our theory of large-amplitude collective motion. The material for the monopole case is a rearrangement with different emphasis of results presented previously [6]. All other results are new. In Sec. VI, we make suggestions for further work, involving both applications and extensions of the results of this paper, as well as the study of possible connections with previous research. Two appendixes, A and C, contain important details of the calculations that would impede the flow of the argument in the main text. In Appendix B we review briefly the generalization of the theory suggested by our previous study of the monopole model and indicate how it applies to the more general cases.

II. ALGEBRAIC AND DYNAMICAL PRELIMINARIES

A. The algebra of $\text{Sp}(n, \mathcal{R})$

The defining algebra of the group $\text{Sp}(n, \mathcal{R})$ is given most simply in terms of n boson pairs, $a_i, a^i, i = 1 \cdots n$,

where the subscript identifies the destruction and the superscript the creation operators. One standard set of generators is composed of three distinct bilinear forms in these operators,

$$A_{ij} = a_i a_j, \quad (2.1)$$

$$A^{ij} = a^i a^j, \quad (2.2)$$

$$B_j^i = a^i a_j + \frac{1}{2} \delta_j^i. \quad (2.3)$$

An equivalent set of generators, more useful for the purposes of this paper is given in terms of single-particle coordinate and momentum operators, x_i and p_i , respectively, related to the boson operators in the standard way, namely,

$$a_i = \frac{1}{\sqrt{2}}(x_i + ip_i), \quad (2.4)$$

$$a^i = \frac{1}{\sqrt{2}}(x_i - ip_i). \quad (2.5)$$

The alternative set of generators takes the form

$$Q_{ij} = x_i x_j, \quad (2.6)$$

$$K_{ij} = p_i p_j, \quad (2.7)$$

$$L_{ij} = \frac{1}{2}(x_i p_j - x_j p_i), \quad (2.8)$$

$$S_{ij} = \frac{1}{2}(x_i p_j + x_j p_i) - \frac{1}{2} i \delta_{ij}, \quad (2.9)$$

satisfying the set of commutation relations,

$$[Q_{ij}, K_{kl}] = i(\delta_{jk} S_{il} + \delta_{jl} S_{ik} + \delta_{ik} S_{jl} + \delta_{il} S_{jk}) + i(\delta_{jk} L_{il} + \delta_{jl} L_{ik} + \delta_{ik} L_{jl} + \delta_{il} L_{jk}), \quad (2.10)$$

$$[Q_{ij}, L_{kl}] = \frac{1}{2} i(\delta_{lj} Q_{ik} - \delta_{jk} Q_{il} + \delta_{il} Q_{jk} - \delta_{ik} Q_{jl}), \quad (2.11)$$

$$[Q_{ij}, S_{kl}] = \frac{1}{2} i(\delta_{lj} Q_{ik} + \delta_{jk} Q_{il} + \delta_{il} Q_{jk} + \delta_{ik} Q_{jl}), \quad (2.12)$$

$$[K_{ij}, L_{kl}] = \frac{1}{2} i(\delta_{il} K_{jk} + \delta_{jl} K_{ik} - \delta_{ik} K_{jl} - \delta_{jk} K_{il}), \quad (2.13)$$

$$[K_{ij}, S_{kl}] = -\frac{1}{2} i(\delta_{il} K_{jk} + \delta_{jl} K_{ik} + \delta_{ik} K_{jl} + \delta_{jk} K_{il}), \quad (2.14)$$

$$[L_{ij}, S_{kl}] = \frac{1}{2} i(\delta_{ik} S_{jl} - \delta_{jl} S_{ik} + \delta_{il} S_{jk} - \delta_{jk} S_{il}), \quad (2.15)$$

$$[L_{ij}, L_{kl}] = \frac{1}{2} i(\delta_{ik} L_{jl} + \delta_{jl} L_{ik} - \delta_{il} L_{jk} - \delta_{jk} L_{il}), \quad (2.16)$$

$$[S_{ij}, S_{kl}] = -\frac{1}{2} i(\delta_{ik} L_{jl} + \delta_{jl} L_{ik} + \delta_{il} L_{jk} + \delta_{jk} L_{il}). \quad (2.17)$$

In terms of these generators, the second-order Casimir invariant is given by the expression

$$C_2 = -\frac{1}{2} \{Q_{ij}, K_{ij}\} + S_{ij} S_{ij} - L_{ij} L_{ij}. \quad (2.18)$$

B. Dynamical preliminaries

In the body of this paper we shall find it convenient to assign a different meaning to the upper-case symbols

used above to denote the various generators. We shall therefore refer to these quantities in the text below by the corresponding lower-case letters, $Q_{ij} \rightarrow q_{ij}$, etc. We shall be concerned with a many-body realization of the algebra, for which we shall use the second-quantized formalism. Thus, if $\psi(\mathbf{x})$, $\psi^\dagger(\mathbf{x}')$ satisfy the anticommutation relations,

$$\{\psi(\mathbf{x}), \psi^\dagger(\mathbf{x}')\} = \delta(\mathbf{x} - \mathbf{x}'), \quad (2.19)$$

where \mathbf{x} stands for the n -dimensional vector $(x_1 \cdots x_n)$ and any additional intrinsic variables such as spin and isospin that are included in the dynamics, then the operators \hat{Q}_{ij} , \hat{K}_{ij} , etc., where, for example,

$$\hat{Q}_{ij} = \int d\mathbf{x} \psi^\dagger(\mathbf{x}) q_{ij} \psi(\mathbf{x}), \quad (2.20)$$

are the set of generators of $\text{Sp}(n, R)$ relevant to the fermion many-body problem. Below we shall also suppress the boldface for the quantity \mathbf{x} .

We shall be concerned further with studying the classical limit of Hamiltonian operators belonging to the enveloping algebra of $\text{Sp}(n, R)$ for $n=1,2,3$, i.e., Hamiltonians that are polynomials in the generators of these algebras. Consider the one-dimensional case, where we have just three generators, \hat{Q}_{11} , \hat{K}_{11} , and \hat{S}_{11} , that we rename by dropping the subscripts. We then study a Hamiltonian,

$$\hat{H} = \frac{1}{2}(\hat{K} + \hat{Q}) + \frac{1}{2}\kappa\hat{Q}\hat{Q}, \quad (2.21)$$

that is the sum of an harmonic oscillator part and of a "monopole-monopole" interaction. The considerations to be applied to this Hamiltonian can be generalized to one in which we add any polynomial in the operator \hat{Q} , but we shall quote detailed results only for the Hamiltonian (2.21).

Consider an arbitrary Slater determinant describing N fermions. We shall be interested in the expectation value of (2.21) in this state, evaluated in Hartree approximation, i.e., to the leading order in N , the number of particles. Using angular brackets to denote this average, we have in this approximation

$$\langle \hat{H} \rangle \equiv H_C = \frac{1}{2}(K + Q) + \frac{1}{2}\kappa Q^2, \quad (2.22)$$

where, e.g.,

$$Q = \langle \hat{Q} \rangle, \quad (2.23)$$

i.e., the Hartree average of any generator will be denoted by the same symbol without a hat. As a further instance, the Hartree approximation to the Casimir invariant of $\text{Sp}(1, R)$ is

$$\langle C_2 \rangle = C_2 = -QK + S^2. \quad (2.24)$$

The most important idea that informs the next section is that we consider Q to be a classical collective coordinate and associate it with a corresponding canonical momentum, P . The Hartree approximation to the generators then defines a classical limit of the algebra in which the commutators are replaced by Poisson brackets. These are a set of partial differential equations for the classical generators, Q , K , and S , that determine the latter as functions of Q and P . This mapping will not only determine the Hartree average as a function of Q and P , but will allow us to associate this classical boson mapping with a solution of the time-dependent Hartree equation. The concepts mentioned here will be rendered precise in the next section and then extended to two and three dimensions in the following sections.

III. THE MONOPOLE MODEL ASSOCIATED WITH THE ALGEBRA OF $\text{Sp}(1, R)$

A. Classical mapping and Hartree solution

As stated in the Introduction, the results to be presented in this section have appeared in our previous work [6]. What we aim for here is a more systematic presentation with enhanced emphasis on the significance of the results. We do this by collecting the results into a theorem.

Theorem: For a class of many-Fermion Hamiltonians belonging to the enveloping algebra of $\text{Sp}(1, R)$, of which Eq. (2.21) is a prototype, there exists a two-parameter family of Slater determinants, defined by density matrices $\rho(x|x'|Q, P)$ that describe states belonging to an irreducible representation. These states (i) induce a mapping of $\text{Sp}(1, R)$ onto a symplectic manifold (Q, P) in which the generators, \hat{G} , are mapped as classical dynamical variables, i.e.,

$$\hat{G} \rightarrow G(Q, P), \quad (3.1)$$

and in particular,

$$\hat{Q} \rightarrow Q. \quad (3.2)$$

The Hartree expectation value of any member of the enveloping algebra is thereby also mapped.

(ii) The associated density matrices have the diagonal form

$$\rho(x, x'|Q, P) = \sum_h \psi_h(x|Q, P) \psi_h^*(x'|Q, P), \quad (3.3)$$

where the sum is over the N occupied orbitals, h . Furthermore $\psi_h(x|Q, P)$ can be written as a product

$$\psi_h(x|Q, P) = \exp(iPx^2) \phi_h(x, Q), \quad (3.4)$$

and ϕ_h is the solution of a constrained Hartree equation

$$\epsilon_h \phi_h = (\mathcal{H} - \lambda x^2) \phi_h, \quad (3.5)$$

$$\mathcal{H} = \frac{1}{2}(p^2 + x^2) + \kappa Q x^2, \quad (3.6)$$

$$\lambda = \frac{dH_C(Q, P=0)}{dQ} \equiv \frac{dV}{dQ}. \quad (3.7)$$

Here \mathcal{H} is the Hartree Hamiltonian and H_C is the classical collective Hamiltonian defined in (2.22). These results identify the density matrix (3.3) as a solution of the time-dependent Hartree equation

$$i\dot{\rho} = [\mathcal{H}, \rho]. \quad (3.8)$$

We turn to the proof of part (i) of the theorem. The Hartree average of a product of two generators, \hat{G}_1 and \hat{G}_2 ,

$$\langle \hat{G}_1 \hat{G}_2 \rangle = G_1(Q, P) G_2(Q, P) \quad (3.9)$$

can be identified as the leading term in the convolution of these two operators under a Wigner transform with

respect to the collective variables Q, P . For a consistent evaluation of commutators, however, we need the next term in the convolution,

$$\langle [\hat{G}_1, \hat{G}_2] \rangle \rightarrow i[G_1(Q, P), G_2(Q, P)]_{PB}, \quad (3.10)$$

where the Poisson bracket is to be evaluated with respect to the single canonical pair (Q, P) . From Eqs. (2.10)–(2.17) we thereby obtain the Poisson bracket algebra

$$[Q, S] = \frac{\partial S}{\partial Q} = 2Q, \quad (3.11)$$

$$[Q, K] = \frac{\partial K}{\partial Q} = 4S, \quad (3.12)$$

$$[K, S] = -2K. \quad (3.13)$$

Treated in turn, these differential equations yield the relations

$$S = 2QP, \quad (3.14)$$

$$K = 4QP^2 + \chi(Q), \quad (3.15)$$

with

$$Q \frac{d\chi}{dQ} = -\chi(Q). \quad (3.16)$$

Thus

$$\chi(Q) = C/Q. \quad (3.17)$$

The constant C can be obtained by evaluating the second-order Casimir invariant in the Hartree approximation. We find

$$\langle \hat{C}_2 \rangle = -C = -N^4/4, \quad (3.18)$$

where the pair of equalities express the results of two separate procedures. On the one hand the value $-C$ is obtained by direct substitution of the mapped generators. On the other hand the specific value $-N^4/4$ is obtained by calculating the Casimir invariant for a simple state in the irreducible representation, as explained in Appendix A. Finally, we record that the collective Hamiltonian, which is the Hartree value of the many-particle Hamiltonian, maps to

$$\begin{aligned} H_C &= 2QP^2 + \frac{1}{2}Q + \frac{1}{2}\kappa Q^2 + N^4/8Q, \\ &\equiv 2QP^2 + V(Q), \end{aligned} \quad (3.19)$$

and we have also displayed the collective potential energy. Note, however, that the singular term in the latter, that has a tantalizing resemblance to the scalar Berry potential [2], originates in the many-particle kinetic energy.

We turn next to part (ii) of the theorem, which provides a construction of the manifold of density matrices associated with the classical mapping just given. We show first that the single-particle wave functions of which the density matrix is composed are of the form

$$\psi_h(x|Q, P) = \exp[i\mathcal{S}(x, P)]\phi_h(x, Q), \quad (3.20)$$

i.e., the dependence on the collective momentum is inde-

pendent of the orbit label. To see this, let us calculate the time derivative of the classical variable Q in two ways, directly from the classical equations of motion,

$$\dot{Q} = \frac{\partial H_C}{\partial P} = 4PQ, \quad (3.21)$$

and by actually evaluating the Hartree approximation of the quantum equations of motion,

$$\begin{aligned} \dot{Q} &= -i\langle [\hat{Q}, \hat{H}] \rangle = 2\langle \hat{S} \rangle \\ &= 2 \int dx x \frac{\partial \mathcal{S}}{\partial x} \rho(x, x). \end{aligned} \quad (3.22)$$

In obtaining this last result, we have assumed that the orbitals ϕ_h are real. Equations (3.21) and (3.22) yield the solution

$$S = Px^2. \quad (3.23)$$

To find the orbitals ϕ_h introduced in Eq. (3.20), we back up a notch by defining

$$\tilde{\psi}_h = \exp\left(-i \int_0^t dt' \epsilon_h[Q(t')]\right) \psi_h. \quad (3.24)$$

The extra adiabatic phase in (3.24) drops out of the density matrix, but must be included in order that $\tilde{\psi}$ satisfy the time-dependent Hartree equation,

$$i \frac{d\tilde{\psi}}{dt} = \mathcal{H}\tilde{\psi}. \quad (3.25)$$

Taking into account both the explicit and the implicit time dependence contained in (3.25), the latter is replaced by the equation

$$\epsilon_h \psi_h + i\dot{P} \frac{\partial \psi_h}{\partial P} + i\dot{Q} \frac{\partial \psi_h}{\partial Q} = \mathcal{H}\psi_h. \quad (3.26)$$

Substituting the classical equations of motion for the time derivatives and inserting the form of ψ_h , the resulting equation has terms of zero, first, and second order in the momentum P . The terms of second order are found to cancel, whereas the terms of zero and first order give, respectively, the equations

$$\epsilon_h \phi_h = (\mathcal{H} - \lambda x^2)\phi_h, \quad (3.27)$$

$$4Q \frac{\partial \phi_h}{\partial Q} = -\phi_h - 2x \frac{\partial \phi_h}{\partial x}. \quad (3.28)$$

We deal first with (3.27). By means of the definitions

$$\tilde{\mathcal{H}} = \frac{1}{2}(p^2 + \bar{\omega}^2 x^2), \quad (3.29)$$

$$\bar{\omega}^2 = 1 + 2(\kappa Q - \lambda), \quad (3.30)$$

(3.27) becomes

$$\epsilon_h \phi_h = \tilde{\mathcal{H}}\phi_h, \quad (3.31)$$

with the normalized solution, in terms of solutions $\phi_h^{(\text{sho})}$ for the simple harmonic oscillator with unit mass and unit frequency,

$$\phi_h(x) = \bar{\omega}^{1/4} \phi_h^{(\text{sho})}(\sqrt{\bar{\omega}}x). \quad (3.32)$$

It remains only to verify (3.28). This can be done, using the explicit form of $\bar{\omega}^2$, derived from Eq. (3.30) by substituting the value of $\lambda = (dV/dQ)$ from Eq. (3.19), namely,

$$\bar{\omega}^2 = C/Q^2. \quad (3.33)$$

This completes the proof of the theorem.

B. Application of the theory of large amplitude collective motion

It is not the purpose of this section to review yet again the theory of large amplitude collective motion. It has been described exhaustively in the works referred to in the Introduction. In so far as the present discussion is concerned the principal aim is to find the collective Hamiltonian from this theory. The first step of the procedure is to assume that the collective variable is the expectation value of a one-body operator. For the model Hamiltonian, Eq. (2.21), with a separable interaction, the logical starting choice is always determined by the ingredients of that interaction. In the present instance, the choice is the Hartree expectation value of \hat{Q} , or in other words it is determined by the mapping $\hat{Q} \rightarrow Q$. This leads automatically to the constrained Hartree equation solved in part (ii) of the theorem.

The next step is to compute the many-particle Hartree energy associated with the filling of these orbits with N particles. We outline the calculation, in which this Hartree energy is identified as the potential energy, $V(Q)$, of the system. We have first

$$V(Q) \equiv \langle \hat{H} \rangle = \text{tr}[\frac{1}{2}(p^2 + x^2)\rho] + \frac{1}{2}\kappa Q^2. \quad (3.34)$$

This equation can be transformed into a more useful version, as follows: We first calculate the sum of the single-particle energies,

$$\begin{aligned} \sum_h \epsilon_h &= \text{tr}(\bar{\mathcal{H}}\rho) \\ &= \text{tr}[\frac{1}{2}(p^2 + x^2)\rho] + \kappa Q^2 - Q(dV/dQ). \end{aligned} \quad (3.35)$$

We then invoke the virial theorem, in the form

$$\sum_h \epsilon_h = \bar{\omega}^2 \text{tr}(x^2 \rho) = \bar{\omega}^2 Q, \quad (3.36)$$

which allows us to replace (3.35) by the expression

$$\text{tr}[\frac{1}{2}(p^2 + x^2)\rho] = \bar{\omega}^2 Q - \kappa Q^2 + Q \frac{dV}{dQ}. \quad (3.37)$$

When the latter is now substituted into (3.34), the result is a differential equation for the potential energy,

$$V(Q) = Q + \frac{3}{2}\kappa Q^2 - Q \frac{dV}{dQ}, \quad (3.38)$$

of which the solution is

$$V(Q) = \frac{1}{2}Q + \frac{1}{2}\kappa Q^2 + C/Q. \quad (3.39)$$

The last term is the solution of the homogeneous version of (3.38), depending on the same constant that appeared in Eq. (3.17).

The next stage in this procedure is to calculate the collective mass, B , defined by writing the collective kinetic energy in the form $\frac{1}{2}BP^2$. We shall calculate B in two (equivalent) ways. The first, that we have not used in our previous work, is connected to the work done in proving the theorem of the previous section. Its deceptive simplicity carries special instruction to which we shall return below. The procedure is to make use once more of the two values of \hat{Q} found in Eqs. (3.21) and (3.22), without assuming that we know the coefficient of P^2 . This yields the equality

$$BP = 2\langle \hat{S} \rangle = 2S. \quad (3.40)$$

Since we have already solved for the value of S from the PB form of the algebra, we may substitute from (3.14) into (3.40) and verify the value $B = 4Q$ found previously. (We are not depending on the theorem. If we did not know S as a classical dynamical variable we would calculate it now.) According to the general theory, the fact that B depends only on Q verifies that we are dealing with an exactly decoupled mode. This means that we have chosen the collective coordinate correctly, i.e., self-consistently.

We shall next attempt to convince the reader that we have not engaged in slight of hand. We can do this by complicating the model in what appears to be a minimal way, but taking it outside of the algebra $\text{Sp}(1, R)$. We do this by adding to \hat{H} a term $\frac{1}{2}\kappa_4 \hat{Q}_4^2$, where \hat{Q}_4 is the many-body version of the operator $q_4 = x^4$. Even if we crank only with x^2 , we now find that the *potential* energy is a function both of Q and of Q_4 , so that the minimum number of collective variables that we can introduce is two. We must therefore apply the procedure followed above to calculate the mass to the two-dimensional domain with kinetic energy, T , given by

$$T = \frac{1}{2}B^{00}P^2 + B^{04}PP_4 + \frac{1}{2}B^{44}P_4P_4. \quad (3.41)$$

We shall not carry this through in detail, but, in fact, it is a perfectly straightforward exercise and yields the mass matrix

$$B^{00} = 4Q, \quad (3.42)$$

$$B^{04} = 8Q_4, \quad (3.43)$$

$$B^{44} = 16Q_6, \quad (3.44)$$

where Q_6 is the Hartree average of x^6 . The point is that in the classical collective Hamiltonian, Q_6 is independent of the two variables introduced previously. Thus the effort to decouple a finite symplectic manifold has failed. There is no cure for this ailment. Thus we might try to introduce Q_6 as an additional collective variable by cranking on x^6 and thus bringing it into the potential energy. By extension with what has been found above, however, the augmented kinetic energy will bring in still

higher powers of x .

The method of calculating the collective mass developed in our previous work [6] that gives the same result as above is described in Appendix B.

IV. MONOPOLE PLUS TWO-DIMENSIONAL MODEL ASSOCIATED WITH THE ALGEBRA OF $\text{Sp}(2, \mathcal{R})$

A. Classical mapping and Hartree solution

We turn to the problem of stating and proving a theorem that generalizes the results of the previous section. We first specify the model to be studied. Here it is convenient to replace the coordinate generators, \hat{Q}_{ij} by a monopole \hat{Q}_0 , and a two-dimensional quadrupole, \hat{Q}_i , $i = 1, 2$, where

$$\hat{Q}_0 = \int \psi^\dagger(x) \frac{1}{2}(x_1^2 + x_2^2) \psi(x), \quad (4.1)$$

$$\hat{Q}_1 = \int \psi^\dagger(x) \frac{1}{2}(x_1^2 - x_2^2) \psi(x), \quad (4.2)$$

$$\hat{Q}_2 = \int \psi^\dagger(x) x_1 x_2 \psi(x). \quad (4.3)$$

The Hartree expectation values of these operators will be interpreted as their classical maps. We consider one further definition, namely,

$$\hat{K}_0 = \frac{1}{2}(\hat{K}_{11} + \hat{K}_{22}). \quad (4.4)$$

As the model Hamiltonian we choose

$$\hat{H} = (\hat{K}_0 + \hat{Q}_0) + \frac{1}{2}\kappa_0 \hat{Q}_0 \hat{Q}_0 + \frac{1}{2}\kappa_2 (\hat{Q}_1 \hat{Q}_1 + \hat{Q}_2 \hat{Q}_2). \quad (4.5)$$

As in the previous section, the Hartree approximation of any generator, the corresponding classical variable, will be denoted by the same symbol without a hat, the map of a product will be the product of the maps, but the map of a commutator will be i times the Poisson bracket of the two maps in the same order. We can now state the theorem that generalizes the one for $n = 1$.

Theorem: For a class of many-Fermion Hamiltonians belonging to the enveloping algebra of $\text{Sp}(2, \mathcal{R})$, of which Eq. (4.5) is a prototype, there exists a six-dimensional family of Slater determinants, defined by density matrices, $\rho(\mathbf{x}, \mathbf{x}' | Q_0, P_0, Q_1, P_1, Q_2, P_2)$, that describe states belonging to an irreducible representation, which (i) induce a mapping of $\text{Sp}(2, \mathcal{R})$ onto a symplectic manifold $(Q_0, P_0, Q_1, P_1, Q_2, P_2) \equiv (Q, P)$ in which the generators, \hat{G} , are mapped as classical dynamical variables, i.e.,

$$\hat{G} \rightarrow G(Q, P). \quad (4.6)$$

The mapping of products and commutators is as previously specified.

(ii) The density matrices have the diagonal form

$$\rho(x, x' | Q, P) = \sum_h \psi_h(x | Q, P) \psi_h^*(x' | Q, P), \quad (4.7)$$

where the sum is over occupied orbitals, h . Furthermore $\psi_h(x | Q, P)$ has the form

$$\begin{aligned} \psi_h(x | Q, P) &= \exp[i\mathcal{S}(x, P)] \phi_h(x, Q), \\ \mathcal{S}(x, P) &= \frac{1}{2}(x_1^2 + x_2^2)P_0 + \frac{1}{2}(x_1^2 - x_2^2)P_1 \\ &\quad + x_1 x_2 P_2, \end{aligned} \quad (4.8)$$

and ϕ_h is the solution of a constrained Hartree equation that will be specified and solved in the course of the demonstration. Altogether, these results will establish that the density matrix (4.7) is a solution of the time-dependent Hartree equation in the density-matrix form.

We turn to the proof of this theorem. Since the technique is a relatively straightforward generalization of the proof given in the previous section, we shall be sparing of details, except in so far as these bring in something novel compared to the previous case. The first step is to replace the commutator algebra by a Poisson-bracket (PB) algebra. One new aspect is that we have an angular-momentum generator, L_{12} . The PB relations between the coordinates and this quantity determine it to have the (not surprising) value

$$L_{12} = Q_1 P_2 - Q_2 P_1. \quad (4.10)$$

Next we consider the PB relations of the coordinates with the ‘‘deformation’’ generators, S_{ij} . We thereby obtain nine differential equations which have the solutions

$$S_{11} = (P_1 + P_0)(Q_1 + Q_0) + P_2 Q_2, \quad (4.11)$$

$$S_{22} = (P_1 - P_0)(Q_1 - Q_0) + P_2 Q_2, \quad (4.12)$$

$$S_{12} = Q_0 P_2 + Q_2 P_0. \quad (4.13)$$

A simple check on these results is that the sum of S_{11} and S_{22} must be a rotational invariant. We find

$$S_{11} + S_{22} = 2P_0 Q_0 + 2P_1 Q_1 + 2P_2 Q_2. \quad (4.14)$$

With the above results, we can determine the momentum generators, K_{ij} , by considering the nine PB relations of the coordinates with these generators, which are determined by the known values for S_{ij} and L_{12} . We thus find

$$\begin{aligned} P_{11} &= (Q_0 + Q_1)(P_0 + P_1)^2 + (Q_0 - Q_1)P_2^2 \\ &\quad + 2Q_2 P_2 (P_0 + P_1) + \chi_{11}(Q), \end{aligned} \quad (4.15)$$

$$\begin{aligned} P_{22} &= (Q_0 - Q_1)(P_0 - P_1)^2 + (Q_0 + Q_1)P_2^2 \\ &\quad + 2Q_2 P_2 (P_0 - P_1) + \chi_{22}(Q), \end{aligned} \quad (4.16)$$

$$\begin{aligned} P_{12} &= 2Q_0 P_0 P_2 + 2Q_1 P_1 P_2 + Q_2 (P_0^2 - P_1^2 + P_2^2) \\ &\quad + \chi_{12}(Q). \end{aligned} \quad (4.17)$$

Here, $\chi_{ij}(Q)$ are three unknown functions of Q that remain to be determined for a completion of the mapping. Notice in passing that the classical kinetic energy,

$$\begin{aligned} K &= \frac{1}{2}(P_{11} + P_{22}) = Q_0(P_0^2 + P_1^2 + P_2^2) \\ &\quad + 2P_0(Q_1 P_1 + Q_2 P_2) + \frac{1}{2}(\chi_{11} + \chi_{22}), \end{aligned} \quad (4.18)$$

is rotationally invariant, provided the sum of the last two terms on the right-hand side has this property.

For the determination of the unknown functions, χ_{ij} , we study the PB relations of the deformation generators S_{ij} with the momentum generators K_{ij} . As an example, the three relations involving S_{ij} and P_{12} yield the differential equations

$$(Q_0 + Q_1) \left(\frac{\partial \chi_{12}}{\partial Q_0} + \frac{\partial \chi_{12}}{\partial Q_1} \right) + Q_2 \frac{\partial \chi_{12}}{\partial Q_2} = -\chi_{12}, \quad (4.19)$$

$$(Q_1 - Q_0) \left(\frac{\partial \chi_{12}}{\partial Q_0} - \frac{\partial \chi_{12}}{\partial Q_1} \right) - Q_2 \frac{\partial \chi_{12}}{\partial Q_2} = \chi_{12}, \quad (4.20)$$

$$-Q_2 \frac{\partial \chi_{12}}{\partial Q_0} - Q_0 \frac{\partial \chi_{12}}{\partial Q_2} = \chi, \quad (4.21)$$

where $\chi = \frac{1}{2}(\chi_{11} + \chi_{22})$. These equations have the solutions

$$\chi_{12} = \frac{CQ_2}{Q_0^2 - Q_1^2 - Q_2^2}, \quad (4.22)$$

$$\chi = \frac{-CQ_0}{Q_0^2 - Q_1^2 - Q_2^2}, \quad (4.23)$$

whereas the remaining differential equations are compatible with the above and in addition yield

$$\chi_- \equiv \frac{1}{2}(\chi_{11} - \chi_{22}) = \frac{CQ_1}{Q_0^2 - Q_1^2 - Q_2^2}. \quad (4.24)$$

In order, finally, to determine the constant C , we calculate the map, \mathcal{C}_2 , of the second-order Casimir invariant in two ways. On the one hand we substitute the maps of the individual generators into the appropriate expression and thus find

$$\mathcal{C}_2 = 2C. \quad (4.25)$$

On the other hand, we calculate the Hartree value of the invariant directly, as done in Appendix A. We thereby obtain (for a special representation)

$$C = \frac{2}{9}N^3. \quad (4.26)$$

We complete part (i) of this demonstration by displaying the collective Hamiltonian that emerges from these considerations:

$$H_C = Q_0(P_0^2 + P_1^2 + P_2^2) + 2P_0(Q_1P_1 + Q_2P_2) + V(Q), \quad (4.27)$$

$$V(Q) = Q_0 + \frac{1}{2}\kappa_0Q_0^2 + \frac{1}{2}\kappa_2(Q_1^2 + Q_2^2) + \frac{CQ_0}{Q_0^2 - Q_1^2 - Q_2^2}. \quad (4.28)$$

For part (ii) of the theorem, we must construct the density matrix that solves the time-dependent Hartree equation. The first step is to separate $\psi(x|Q, P)$ into two factors, as done in Eq. (4.8). From the time derivatives of the coordinates, calculated in two equivalent ways, from the classical equations of motion and from the Hartree averages of the quantum equations of motion, we obtain three equations, one for each coordinate, that generalize the single equation obtained by combining (3.21) and (3.22). These yield the solution

$$S(x, P) = \frac{1}{2}(x_1^2 + x_2^2)P_0 + \frac{1}{2}(x_1^2 - x_2^2)P_1 + x_1x_2P_2. \quad (4.29)$$

In analogy with Eqs. (3.24) and (3.25), we introduce the orbital that is the solution to the time-dependent Hartree equation, $\tilde{\psi}_h$, leading to the equation

$$\epsilon_h \psi_h + i \sum_{\mu=0,1,2} \left(\dot{P}_\mu \frac{\partial \psi_h}{\partial P_\mu} + \dot{Q}_\mu \frac{\partial \psi_h}{\partial Q_\mu} \right) = \mathcal{H} \psi_h, \quad (4.30)$$

where the time derivatives are to be replaced by the classical equations of motion and the Hartree Hamiltonian, \mathcal{H} , has the form

$$\mathcal{H} = k_0 + q_0 + \kappa_0 q_0 Q_0 + \kappa_2 (q_1 Q_1 + q_2 Q_2). \quad (4.31)$$

As before terms of second order in the classical momentum variables cancel. The zero-order terms yield the constrained Hartree equation

$$\epsilon_h \phi_h = \left(\mathcal{H} - \sum \lambda_\mu q_\mu \right) \phi_h, \quad (4.32)$$

$$\lambda_\mu = \frac{\partial V}{\partial Q_\mu}. \quad (4.33)$$

The first-order terms yield three equations that state, in analogy with Eq. (3.28), the identity, when acting on ϕ_h , between certain linear operators in the collective coordinates and corresponding linear operators in the single-particle coordinates. The statement and proof of these identities is given in Appendix C in order not to interfere with the flow of the main argument.

We turn then to the solution of the constrained Hartree equation (4.32). The operator that appears on the right-hand side of this equation will be called $\tilde{\mathcal{H}}$. The cross terms in the potential energy can be eliminated by an orthogonal transformation to the intrinsic system,

$$x_1 = \cos \theta \bar{x}_1 + \sin \theta \bar{x}_2, \quad (4.34)$$

$$x_2 = -\sin \theta \bar{x}_1 + \cos \theta \bar{x}_2, \quad (4.35)$$

$$\cos 2\theta = -(\tilde{\omega}_1^2 - \tilde{\omega}_2^2)/D_1, \quad (4.36)$$

$$\sin 2\theta = -4\lambda_{12}/D_1, \quad (4.37)$$

$$\tilde{\omega}_1^2 = \frac{C}{D_0} - \frac{CQ_0(Q_0 - Q_1)}{D_0^2}, \quad (4.38)$$

$$\tilde{\omega}_2^2 = \frac{C}{D_0} - \frac{CQ_0(Q_0 + Q_1)}{D_0^2}, \quad (4.39)$$

$$\lambda_{12} = -\frac{CQ_0Q_2}{D_0^2}, \quad (4.40)$$

$$D_0 = Q_0^2 - Q_1^2 - Q_2^2, \quad (4.41)$$

$$D_1 = \left| \sqrt{16\lambda_{12}^2 + (\tilde{\omega}_1^2 - \tilde{\omega}_2^2)^2} \right|. \quad (4.42)$$

These equations transform $\tilde{\mathcal{H}}$ to the form

$$\tilde{\mathcal{H}} = \frac{1}{2}(\tilde{p}_1^2 + \tilde{\omega}_1^2 \tilde{x}_1^2) + \frac{1}{2}(\tilde{p}_2^2 + \tilde{\omega}_2^2 \tilde{x}_2^2), \quad (4.43)$$

where

$$\tilde{\omega}_1^2 = |C|/(Q_0 + Q)^2, \quad (4.44)$$

$$\tilde{\omega}_2^2 = |C|/(Q_0 - Q)^2, \quad (4.45)$$

$$Q = \sqrt{Q_1^2 + Q_2^2} = \bar{Q}_1. \quad (4.46)$$

The last of these expressions shows that the intrinsic system is the one in which \bar{Q}_2 vanishes.

In consequence of the above transformation, the solution of the constrained Hartree equation is

$$\phi_h(x, Q) = (\bar{\omega}_1 \bar{\omega}_2)^{1/4} \phi_{h_1}^{(\text{sho})}(\sqrt{\bar{\omega}_1} \bar{x}_1) \phi_{h_2}^{(\text{sho})}(\sqrt{\bar{\omega}_2} \bar{x}_2). \quad (4.47)$$

Together with the material relegated to Appendix C this completes the proof of the theorem.

B. Application of the theory of large amplitude collective motion

Following the procedure outlined for the one-dimensional case, the first step is to compute the collective potential energy. Because in the intrinsic frame the Hartree Hamiltonian is a sum of two harmonic-oscillator contributions (with different frequencies), the procedure, including the use of the virial theorem, for obtaining a differential equation for the potential energy follows through without a hitch. Here it yields the partial differential equation

$$V = 2Q_0 + \frac{3}{2}(\kappa_0 Q_0^2 + \kappa_2 \bar{Q}_1^2) - Q_0 \frac{\partial V}{\partial Q_0} - \bar{Q}_1 \frac{\partial V}{\partial \bar{Q}_1}, \quad (4.48)$$

with the solution

$$V = Q_0 + \frac{1}{2}(\kappa_0 Q_0^2 + \kappa_2 \bar{Q}_1^2) + \frac{|C|Q_0}{Q_0^2 - \bar{Q}_1^2}. \quad (4.49)$$

In a general coordinate system, we should replace \bar{Q}_1 by $\sqrt{Q_1^2 + Q_2^2}$. Thus we recognize also in the present context that V is a scalar.

Consider next the kinetic energy, in the form

$$T = \frac{1}{2} B^{\mu\nu} P_\mu P_\nu, \quad (4.50)$$

where the indices take the values 0, 1, 2. We illustrate the two steps that enter into the calculation of the mass matrix elements $B^{\mu\nu}$. As one of three equations for the time derivatives of the coordinates, calculated in two ways, we have

$$\dot{Q}_1 = S_{11} - S_{22} = \frac{\partial H_C}{\partial P_1} = B^{1\mu} P_\mu. \quad (4.51)$$

As one of six equations necessary to complete the calculation, we have

$$[Q_1, S_{11} - S_{22}] = \frac{\partial(S_{11} - S_{22})}{\partial P_1} = 2Q_0 = B^{11}, \quad (4.52)$$

that combines a known PB relation with a derivative of (4.51). The completion of the procedure just exemplified yields the mass matrix previously determined by the

theorem, that we display in matrix form,

$$\mathbf{B} = \begin{pmatrix} 2Q_0 & 2Q_1 & 2Q_2 \\ 2Q_1 & 2Q_0 & 0 \\ 2Q_2 & 0 & 2Q_0 \end{pmatrix}. \quad (4.53)$$

As explained in the previous section, this establishes once more that we have an exactly decoupled manifold. Again the alternative calculation within the framework of our theory of collective motion is summarized in Appendix B.

V. MONOPOLE PLUS QUADRUPOLE MODEL ASSOCIATED WITH THE ALGEBRA OF $\text{Sp}(3, \mathbf{R})$

A. Classical mapping and Hartree solution

In this section, that indeed quotes the results of most future interest to us, we shall drop the pretensions of formality adhered to in the previous sections. Except for very few points emphasized below, the results to be proved as well as the techniques used to carry out the demonstrations should be evident by now. We divide the generators into monopole and quadrupole parts. In order to keep better track of the significance of the variables, we adopt an alphanumeric subscript notation, illustrated by means of the one-particle operators,

$$q_s = \frac{1}{3}(x_1^2 + x_2^2 + x_3^2), \quad (5.1)$$

$$q_{d1} = -\frac{1}{3}(x_1^2 + x_2^2 - 2x_3^2), \quad (5.2)$$

$$q_{d2} = \frac{1}{2}(x_1^2 - x_2^2), \quad (5.3)$$

$$q_{o1} = x_1 x_2, \quad (5.4)$$

$$q_{o2} = x_1 x_3, \quad (5.5)$$

$$q_{o3} = x_2 x_3, \quad (5.6)$$

$$s_s = \frac{1}{3}(x_1 p_1 + x_2 p_2 + x_3 p_3), \quad (5.7)$$

$$s_{d1} = -\frac{1}{3}(x_1 p_1 + x_2 p_2 - 2x_3 p_3), \quad (5.8)$$

etc.,

$$k_s = \frac{1}{3}(p_1^2 + p_2^2 + p_3^2), \quad (5.9)$$

$$k_{d1} = -\frac{1}{3}(p_1^2 + p_2^2 - 2p_3^2), \quad (5.10)$$

etc.

Associated with these one-particle operators are second quantized operators, designated by the same symbols in the upper case and carrying hats, and the Hartree maps of these, designated by the upper case but hatless. By means of the PB algebra these are expressed as functions of six canonical pairs, $(Q_s, P_s), \dots, (Q_{o3}, P_{o3})$. The resulting expressions, which were calculated with the aid of the program, MATHEMATICA, are too long to quote in their raw form. To obtain more concise expressions, we revert to a spherical tensor notation

$$\hat{Q}_0 = \frac{\sqrt{3}}{2} \hat{Q}_{d1}, \quad (5.11)$$

$$\hat{Q}_1 = -\frac{1}{\sqrt{2}}(\hat{Q}_{o2} + i\hat{Q}_{o3}), \quad (5.12)$$

$$\hat{Q}_{-1} = \frac{1}{\sqrt{2}}(\hat{Q}_{o2} - i\hat{Q}_{o3}), \quad (5.13)$$

$$\hat{Q}_2 = \frac{1}{\sqrt{2}}(\hat{Q}_{d2} + i\hat{Q}_{o1}), \quad (5.14)$$

$$\hat{Q}_{-2} = \frac{1}{\sqrt{2}}(\hat{Q}_{d2} - i\hat{Q}_{o1}), \quad (5.15)$$

for Q , and similar definitions for S and K . In the following expressions, the classical limit of \hat{Q}_m is denoted by Ξ_m , and the conjugate momenta are denoted by Π_m . We use Q_s and P_s for the monopole coordinate and its momentum. The spherical components of S are denoted by Σ , etc. Finally, L_m will refer below to the standard spherical components of the angular momentum vector.

We thus find that

$$L_m = i\sqrt{10}[\Xi \times \Pi]_m^{(1)}, \quad (5.16)$$

$$S_s = \frac{2}{3}(\Xi \cdot \Pi + Q_s P_s), \quad (5.17)$$

$$\Sigma_m = -\sqrt{\frac{7}{6}}[\Xi \times \Pi]_m^{(2)} + \frac{2}{3}P_s \Xi_m + Q_s \Pi_m, \quad (5.18)$$

$$K_s = -\frac{\sqrt{42}}{9}[\Pi \times \Pi]^{(2)} \cdot \Xi + \frac{8}{9}P_s \Xi \cdot \Pi + \frac{4}{3}Q_s \Pi \cdot \Pi + \frac{4}{9}Q_s P_s^2 + \chi_s, \quad (5.19)$$

$$K_m = \frac{\sqrt{5}}{15}[\Pi \times \Pi]^{(0)} \times \Xi_m^{(2)} - \frac{1}{3}[\Pi \times \Pi]^{(2)} \times \Xi_m^{(2)} + \frac{6\sqrt{5}}{5}[\Pi \times \Pi]^{(4)} \times \Xi_m^{(2)} - \frac{2\sqrt{42}}{9}P_s [\Xi \times \Pi]_m^{(2)} + \frac{4}{9}P_s^2 \Xi_m + X_m, \quad (5.20)$$

$$\chi_s = -C\partial_{Q_s} \ln(4Q_s^3 - 4\Xi \cdot \Xi Q_s - I_3(\Xi)), \quad (5.21)$$

$$X_m = -\frac{3}{2}C\partial_{\Xi_m} \ln(4Q_s^3 - 4\Xi \cdot \Xi Q_s - I_3(\Xi)), \quad (5.22)$$

$$I_3(\Xi) = \frac{8}{3\sqrt{3}}\sqrt{\frac{35}{2}}[[\Xi \times \Xi]^{(2)} \times \Xi]^{(0)}, \quad (5.23)$$

$$C_2 = -3\phi_s Q_s - 2 \sum_m \Phi_m \Xi_m = 9C, \quad (5.24)$$

$$H_C = \frac{3}{2}(K_s + Q_s) + \frac{1}{2}\kappa_0 Q_s^2 + \frac{1}{2}\kappa_2 \Xi \cdot \Xi + \frac{1}{2}\kappa_L L \cdot L. \quad (5.25)$$

The above expressions contain the standard notation for angular momentum coupling. We recognize χ_s and X_m as the singular functions that arise in the determination of the momentum generators. Here the partial signs represent derivatives with respect to the variables written, and C is the integration constant that has appeared analogously in the calculations for lower dimensionality. A complication that has *not* appeared previously is the occurrence of the cubic invariant, I_3 , constructed from the tensor Ξ_m . Finally, from the given form of the collective Hamiltonian, H_C , it is obvious what starting many-body Hamiltonian was used. Compared to the corresponding two-dimensional case, we have only added an angular momentum coupling.

To construct the density matrix, we write

$$\psi_h(x|Q, P) = \exp[i\mathcal{S}(x, P)]\phi_h(x, Q), \quad (5.26)$$

and find

$$\mathcal{S}(x, P) = P_s q_s + \Pi \cdot q. \quad (5.27)$$

For the real orbitals, ϕ_h , we find

$$\phi_h = \prod_{i=1}^3 (\bar{\omega}_i)^{1/4} \phi_{h_i}^{(\text{sho})}(\sqrt{\bar{\omega}_i} \bar{x}_i), \quad (5.28)$$

as the solution of a constrained Hartree equation, referred to the intrinsic or barred system [cf. (4.44)]. For the constrained Hamiltonian we write

$$\bar{\mathcal{H}} = \frac{1}{2} \sum_i (\bar{p}_i^2 + \bar{x}_i^2) + q_s \left(\kappa_0 \bar{Q}_s - \frac{\partial V}{\partial \bar{Q}_s} \right) + q_0 \left(\kappa_2 \bar{Q}_0 - \frac{\partial V}{\partial \bar{Q}_0} \right) + q_{d_2} \left(\kappa_2 \bar{Q}_{d_2} - \frac{\partial V}{\partial \bar{Q}_{d_2}} \right) \quad (5.29)$$

$$= \frac{1}{2} \sum_i (\bar{p}_i^2 + \bar{\omega}_i^2 \bar{x}_i^2), \quad (5.30)$$

$$\bar{\omega}_1^2 = 1 + \frac{2}{3} \left(\kappa_0 \bar{Q}_s - \frac{\partial V}{\partial \bar{Q}_s} \right) - \frac{1}{\sqrt{3}} \left(\kappa_2 \bar{Q}_0 - \frac{\partial V}{\partial \bar{Q}_0} \right) + \left(\kappa_2 \bar{Q}_{d_2} - \frac{\partial V}{\partial \bar{Q}_{d_2}} \right), \quad (5.31)$$

$$\bar{\omega}_2^2 = 1 + \frac{2}{3} \left(\kappa_0 \bar{Q}_s - \frac{\partial V}{\partial \bar{Q}_s} \right) - \frac{1}{\sqrt{3}} \left(\kappa_2 \bar{Q}_0 - \frac{\partial V}{\partial \bar{Q}_0} \right) - \left(\kappa_2 \bar{Q}_{d_2} - \frac{\partial V}{\partial \bar{Q}_{d_2}} \right), \quad (5.32)$$

$$\bar{\omega}_3^2 = 1 + \frac{2}{3} \left(\kappa_0 \bar{Q}_s - \frac{\partial V}{\partial \bar{Q}_s} \right) + \frac{2}{\sqrt{3}} \left(\kappa_2 \bar{Q}_0 - \frac{\partial V}{\partial \bar{Q}_0} \right). \quad (5.33)$$

Alternative expressions for the frequencies that may be found by substituting the derivatives of the potential energy will not be recorded here.

In addition to the above relations and conditions, there are also equations that relate certain linear differential operators with respect to the collective coordinates to linear differential operators with respect to the intrinsic coordinates. These were discussed for the two-dimensional case in Appendix C, but will not be discussed at all for this case.

B. Application of the theory of large amplitude collective motion

Following the procedure developed for the one-dimensional case and previously also applied to the two-dimensional case, we obtain a partial differential equation for the potential energy. In stating this equation and its solution we shall suppress the bar notation, understanding that the collective coordinates refer to the intrinsic system. We thus find

$$V = 3Q_s + \frac{3}{2}[\kappa_0 Q_s^2 + \kappa_2(Q_0^2 + Q_{d_2}^2)] - Q_s \frac{\partial V}{\partial Q_s} - Q_0 \frac{\partial V}{\partial Q_0} - Q_{d_2} \frac{\partial V}{\partial Q_{d_2}}. \quad (5.34)$$

This equation has the solution

$$V = \frac{3}{2}Q_s + \frac{1}{2}\kappa_0 Q_s^2 + \frac{1}{2}\kappa_2(Q_0^2 + Q_{d_2}^2) + \chi_s, \quad (5.35)$$

where χ_s is the singular scalar function displayed in Eq. (5.21). In the present calculation, the quadratic and cubic scalars I_2 and I_3 are found in the versions to which they reduce in the intrinsic system, namely,

$$I_2 = Q_0^2 + Q_{d_2}^2, \quad (5.36)$$

$$I_3 = -\frac{8}{3\sqrt{3}}(Q_0^3 - 3Q_0 Q_{d_2}^2). \quad (5.37)$$

There remains only the problem of computing the mass tensor. This remains a simple algebraic task, if one applies the method first described for the one-dimensional case. The calculation is simplest to carry out in terms of Cartesian variables, but the equivalence of the result to that given by Eqs. (5.19) and (5.25) can then be verified. Nothing new is learned by repeating either the calculation or the results.

VI. CONCLUDING REMARKS

In this paper we have developed a new exactly solvable example for the theory of large amplitude collective motion by looking at the classical limit of the algebra of $\text{Sp}(3, R)$ and a Hamiltonian defined within the enveloping algebra of the algebra. Possibilities exist both for the application and for theoretical refinement of the results of this paper. A natural first application would involve the requantization of the classical collective Hamiltonian and comparison of the results of diagonalizing the resultant Bohr Hamiltonian with the results of an exact diagonalization of the corresponding many-particle Hamiltonian [14]. A theoretical refinement would be to attempt to upgrade the classical mapping to a full quantum boson mapping [15]. This is probably not difficult for the one- and two-dimensional cases, but might prove laborious for the interesting $n = 3$ case.

It would be inappropriate to conclude this paper without mentioning possible connections with other work. For instance there has been extensive research on the unitary representations of the non-compact symplectic algebras considered in this paper [16–18], that can be viewed as exact boson mappings of these algebras. The relation of our special mapping to this work may be worth pursuing. Along a different line, we may be said to have produced soliton solutions to a highly simplified class of field theories, using Hamiltonian methods. It would be interesting to investigate if our methods can teach us something about the Hamiltonian approach to other soliton models [19].

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APPENDIX A: EVALUATION OF SECOND-ORDER CASIMIR INVARIANT

Consider the one-dimensional case. The evaluation is based on the idea that since the monopole-monopole interaction belongs to the enveloping algebra, changing its strength does not change the irreducible representation. In particular, we may set the strength to zero. In that case the ground state, that defines the representation of interest to us, is the Slater determinant obtained by filling the lowest orbitals. Since in this state the Hartree value of \hat{S} vanishes, we have from Eq. (2.18)

$$\begin{aligned} C_2(1d) &= -\left(\sum_h \epsilon_h\right)^2 = -\left(\sum_0^{N-1} n\right)^2 \\ &\cong \frac{1}{4}N^4. \end{aligned} \quad (A1)$$

In this evaluation, as in the ones that occur below, it is strictly the definition of the classical variables as Hartree averages that intervene. Furthermore, we have utilized the virial theorem for the harmonic oscillator described by the Hamiltonian $\frac{1}{2}(p^2 + x^2)$.

For the two- and three-dimensional cases we shall evaluate the Casimir invariant only for the closed shell and for the representation containing the ground state. This allows us to take the fullest advantage of circular and spherical symmetries, respectively. We provide a few details for three dimensions only. We have

$$\begin{aligned} C_2(3d) &= -\sum_{i=1}^3 Q_{ii} P_{ii} \\ &= -\frac{1}{3}\left(\sum_i Q_{ii}\right)^2. \end{aligned} \quad (A2)$$

For N particles, this becomes

$$\begin{aligned} C_2(3d) &= -\frac{1}{3}\left(\sum_0^{(6N)^{1/3}} \frac{1}{2}n^3\right)^2 \\ &= -\frac{3}{16}6^{2/3}N^{8/3}. \end{aligned} \quad (A3)$$

Here we have used the fact that the level with energy n has degeneracy $\frac{1}{2}n^2$ and that the number of shells needed for N particles is $(6N)^{1/3}$. These, of course, are approximate values needed to get the answer to leading order in N .

The corresponding calculation for two dimensions yields

$$C_2(2d) = -\frac{4}{9}N^3. \quad (A4)$$

In future applications, we shall be interested in irreducible representations associated with open-shell nuclei. The generalization to such cases of the elementary calculations just presented will be deferred to the occasion when those applications are presented.

APPENDIX B: ALTERNATIVE COMPUTATION OF THE MASS TENSOR

In the body of the text we have described a new method for computing the mass tensor of a decoupled or approximately decoupled manifold. This method is particularly convenient when the cranking operator or operators can be represented in a basis of single-particle operators that depend only on the coordinates, though it can also be applied with a somewhat increased effort in more general cases. Nevertheless, it is important to show how the same results can be obtained by the methods developed in our previous work. In fact, the monopole model was instrumental in leading to a necessary generalization of the theory of the mass tensor as it had been presented and utilized by us. The generalization required is presented in some detail in [6]. We do not wish to repeat the technical details here, but rather we shall “remind” the reader of the basic idea and be content with the quotation and application of the final result.

The theory of large amplitude collective motion is based on the idea that starting from a Hamiltonian, quadratic in the momenta but otherwise arbitrary, one can introduce a point transformation chosen so that in the new coordinates the existence of a decoupled coordinate manifold is either apparent, or in more realistic cases can be demonstrated to be approximately true. The restriction to a coordinate or point transformation was based on the observation that this type of transformation maintained exactly the quadratic dependence on the momenta. However, the formulas derived from this procedure failed to reproduce the correct mass in the monopole example. Thereafter, it was discovered [6] that for consistency to second order in the momentum one had to replace point transformations by more general canonical transformations, correct to second order in the momenta. In the paper cited details were supplied only for the case of one collective coordinate, but for the separable Hamiltonians considered in the present paper it is straightforward to generalize the result to any number of collective coordinates. Below we describe the result of this generalization.

We suppose that there is a set of self-consistent cranking operators,

$$Q^i = \text{tr}(q^i \rho). \quad (\text{B1})$$

It follows then that the component B^{ij} of the mass tensor is given by the formula

$$B^{ij} = [q_{hp}^{(i)} \bar{\mathcal{H}}_{pp'} q_{p'h}^{(j)} + i \leftrightarrow j] - [q_{ph}^{(i)} \bar{\mathcal{H}}_{hh'} q_{h'p}^{(j)} + i \leftrightarrow j], \quad (\text{B2})$$

$$\bar{\mathcal{H}}_{ab} = \mathcal{H}_{ab} - \frac{\partial V}{\partial Q^i} q_{ab}^{(i)}. \quad (\text{B3})$$

Remarkably, where the present formula contains the cranked Hartree Hamiltonian, $\bar{\mathcal{H}}$, the previous, incorrect formula contains just the unconstrained Hartree Hamiltonian \mathcal{H} . Precisely because the single-particle orbits referred to in the above formula are the eigenmodes of the constrained operator, and using completeness as well, the

formula for the mass tensor can be transformed into the simple formula involving double commutators,

$$B^{ij} = \frac{1}{2} \text{tr}\{\rho[[q^i, \bar{\mathcal{H}}], q^j] + i \leftrightarrow j\}. \quad (\text{B4})$$

For the cases treated in the text, the q^i are coordinate operators. Consequently $\bar{\mathcal{H}}$ may be replaced by the single-particle kinetic energy. It is then a trivial calculation to show that all the results of the text are reproduced.

APPENDIX C: SOME ADDITIONAL DETAILS CONCERNING THE SOLUTION OF THE TIME-DEPENDENT HARTREE EQUATION

In the construction of the density matrix that solves the time-dependent Hartree equation for the two-dimensional case, we by passed the study of a set of conditions that must be satisfied by the real orbitals ϕ_h in addition to the constrained Hartree equation (4.32). These conditions, here three in number, arise from terms linear in the collective momenta in the time-dependent Hartree equation. They are of the form

$$2Q_0 \frac{\partial \phi}{\partial Q_0} + 2Q_1 \frac{\partial \phi}{\partial Q_1} + 2Q_2 \frac{\partial \phi}{\partial Q_2} = -x_1 \frac{\partial \phi}{\partial x_1} - x_2 \frac{\partial \phi}{\partial x_2} - \phi, \quad (\text{C1})$$

$$2Q_1 \frac{\partial \phi}{\partial Q_0} + 2Q_0 \frac{\partial \phi}{\partial Q_1} = -x_1 \frac{\partial \phi}{\partial x_1} + x_2 \frac{\partial \phi}{\partial x_2}, \quad (\text{C2})$$

$$2Q_2 \frac{\partial \phi}{\partial Q_0} + 2Q_0 \frac{\partial \phi}{\partial Q_2} = -x_2 \frac{\partial \phi}{\partial x_1} - x_1 \frac{\partial \phi}{\partial x_2}. \quad (\text{C3})$$

To show that each orbital, ϕ_h , given by Eq. (4.32) satisfies these conditions, it is convenient to transform them to the intrinsic system. In addition to the transformation equations (4.34), ..., we introduce polar coordinates

$$Q_1 = Q \cos \Theta, \quad (\text{C4})$$

$$Q_2 = Q \sin \Theta, \quad (\text{C5})$$

that are recognized as intrinsic coordinates, if we make the identifications $Q = \bar{Q}_1$ and $\Theta = -2\theta$. Straightforward calculation then permits us to replace Eqs. (C1)–(C3) by the equations

$$2Q_0 \frac{\partial \phi}{\partial Q_0} + 2Q \frac{\partial \phi}{\partial Q} = -\bar{x}_1 \frac{\partial \phi}{\partial \bar{x}_1} - \bar{x}_2 \frac{\partial \phi}{\partial \bar{x}_2} - \phi, \quad (\text{C6})$$

$$2Q \frac{\partial \phi}{\partial Q_0} + 2Q_0 \frac{\partial \phi}{\partial Q} = -\bar{x}_1 \frac{\partial \phi}{\partial \bar{x}_1} + \bar{x}_2 \frac{\partial \phi}{\partial \bar{x}_2}, \quad (\text{C7})$$

$$\frac{2Q_0}{Q} \frac{\partial \phi}{\partial \Theta} = -\bar{x}_2 \frac{\partial \phi}{\partial \bar{x}_1} - \bar{x}_1 \frac{\partial \phi}{\partial \bar{x}_2}. \quad (\text{C8})$$

To verify the last set of equations, we utilize the explicit form (4.48) of the orbitals, as well as Eqs. (4.45) and (4.46) that relate the barred frequencies to the collective coordinates. We must also remember that the barred coordinates are also functions of the collective coordinates, according to the equations that are the inverses of (4.34) and (4.35) and the relation between θ and Θ . After some algebra, we find that we can duplicate (C6) and (C7),

but in place of (C8), we deduce the result

$$2 \frac{\partial \phi}{\partial \Theta} = -\bar{x}_1 \frac{\partial \phi}{\partial \bar{x}_2} + \bar{x}_2 \frac{\partial \phi}{\partial \bar{x}_1}, \quad (\text{C9})$$

which obviously describes correctly the rotational prop-

erties of an orbital, in view of the connection between Θ and θ . To verify (C8), finally, we calculate the “commutator” of Eqs. (C7) and (C9) and indeed deduce the desired result.

The corresponding calculations for three dimensions will not be reproduced here.

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