Symmetry-conserving variational dynamics: Application to quasispin systems

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A time-dependent variational procedure is proposed that possesses the same constants of the motion as the exact many-body Schrödinger dynamics. The class of trial wave functions is larger than the manifold of Slater determinants that supports the time-dependent Hartree-Fock dynamics. These wave functions can be regarded as superpositions of the eigenfunctions of the conserved observable of interest and the variational equations display the usual parametric structure, with properly admixed energy gradients and the symplectic metric tensor. In an application to the Lipkin-Meshkov-Glick model, significant improvements over the usual mean-field or determinantal dynamics can be achieved.

[NUCLEAR STRUCTURE Mean field symmetry breaking; symmetry restoration; nondeterminantal wave function; time-dependent variational principle; parametric equations of motion; mean energy metric tensor; canonical coordinates; quasispin models; comparison with time-dependent Hartree-Fock dynamics.]

I. INTRODUCTION

The realm of nuclear phenomena has received enriching contributions thanks to the observation, over finite time intervals, of the motion of several (yet few) degrees of freedom in a nucleus. Experiments involving the coherent dynamics of many nucleons have been carried out in present-day heavy ion accelerators, giving rise to a wealth of data that manifests the fascinating dance of both single-particle (sp) and collective coordinates.[1-3] Among the various theoretical models proposed to explain most features of the observed dynamics, the time-dependent Hartree-Fock (TDHF) procedure occupies a honored site. A recent review of the TDHF achievements and its current range of applications to heavy ion collisions can be found in Ref. 4, where room is devoted as well to commenting on the most prominent limitations of the approach, which can be traced back to its being a one-body theory. Inclusion of two-body residual coupling gives rise to a fairly complicated problem of quantal kinetics[5-9] that remains so far computationally unsolved.

Recently, the verisimilitude of the TDHF version of the many-body wave function has been examined from a different viewpoint—in the frame of a solvable quasispin model.[10] In that work we traced the motion of both the exact and the TDHF wave function—the latter being a Slater determinant—over a lengthy time interval, compared to typical microscopic periods of a system with N interacting quasispins. The shortness of the overlapping time between both the wave functions has become evident, coincidentally with the observation posed in another recent related work on a simplified model.[11] Furthermore, the computation of a proper one-body observable—namely, the expectation value of the quasispin vector $\vec{J}$, denoted as the wave function polarization[10]—showed indications of a kind of recurrence phenomenon. Indeed, it has been observed that although the exact and TDHF polarizations, starting from identical initial conditions, grow rather rapidly apart, the modulus of $\vec{J}_{\text{exact}}$ approaches again the TDHF value on a long, i.e., macroscopic, time scale. It must be remembered that the angle between the exact and TDHF polarizations is, in this case, different from zero, in correspondence with the fact that the respective wave functions do not overlap to a respectable amount. This quasiparticle behavior has been interpreted as a recurrence of the determinantal structure of the many body wave function evolved from a Slater determinant at $t=0$. It has been suggested (see Ref. 12, and also Ref. 13) that this quasiparticle phenomenon could be traced to quantal tunneling of the exact wave function between the two degenerate sets of librations[14] or local trajectories[15] in the TDHF phase portrait for the quasispin system.

In the many-body model under consideration, namely, the so-called Lipkin-Meshkov-Glich (LMG) model[16] the generator of exact evolution commutes with the parity operator.[17,18] However, the TDHF motion is not labeled by a constant parity, this being a typical example of symmetry breaking in the mean field. Our purpose in this work is to examine the problem of dynamical symmetry breaking on general grounds, raising the restriction to quasispin models, and to prescribe a variational procedure that does not suffer from such a limitation. In this spirit we indicate a choice of nondeterminantal trial wave functions for the time-dependent variational principle, whose evolution ensures symmetry conservation at all times. The equations of motion thus obtained describe what we denote as the symmetry conserving variational dynamics (SCVD); they are canonical on a symplectic manifold and display the standard parametric structure[19,20] with a proper mean Hamiltonian and a similarly adequate metric tensor that contains the admixture of parity eigenstates. Application of the SCVD prescription to the LMG model permits a discussion of the situations in which it yields a significant improvement over the TDHF procedure as one regards the proximity to the exact wave function and the one-body dynamics.

In Sec. II, the ingredients and hypothesis of our problem of interest are set and the general formalism is derived and discussed. The particular case of the LMG model in the present frame is worked out in Sec. III. The calculations performed to illustrate the applications are described in Sec. IV, while the corresponding discussion and summary constitute the final section.

II. VARIATIONAL DYNAMICS OF A SYMMETRY-CONSERVING STATE VECTOR

In this section we will develop and discuss a general prescription for the parametric dynamics, induced by the variational condition, of a nondeterminantal, symmetry-conserving state vector. We formulate the problem as follows. Let $\hat{\vec{X}}=\{\hat{X}_\mu\}$ be a basis for a Lie algebra, $\hat{H}(\hat{\vec{X}})$ a generator of evolution that commutes with the Casimir operator of the algebra and $\hat{I}$ a Hermitian constant of the motion, $[\hat{H},\hat{I}]=0$, with an orthogonal (not necessarily orthonormal) set of eigenvectors $\{|s\rangle\}$. Let $g=[\hat{U}(x)=\exp\vec{x}\cdot\hat{\vec{X}}]$ be a dynamical group on the Grassmann manifold of Slater determinants, or generalized coherent states[21,22] (GCS),

$$|\vec{x}\rangle=\hat{U}(\vec{x})\,|\,\mathrm{ref}\rangle\ , \tag{2.1}$$

with $|\,\mathrm{ref}\rangle$ a given reference state and $\vec{x}$ a complex vector. Let $\{\hat{P}_s\}$ be a set of eigenprojectors,

$$\hat{I}\hat{P}_s=\hat{P}_s I_s \tag{2.2}$$

(I_s being the time-independent eigenvalue of $\hat{I}$), we can extract the eigenvector $|s\rangle$, parametrized on the manifold, as a linear combination of GCS's,

$$\begin{aligned}|s(\vec{x})\rangle&=\hat{P}_s\,|\vec{x}\rangle\\&=\int d\mu(\vec{y})\langle\vec{y}\,|\hat{P}_s|\,\vec{x}\rangle\,|\,\vec{y}\rangle\ .\end{aligned} \tag{2.3}$$

Here $d\mu(\vec{y})$ is the invariant measure on the manifold.[23]

Single determinantal (TDHF) dynamics assigns, via the variational principle, a Hamiltonian evolution law to the parameters x^μ of a trial wave function of the form (2.1). According to the variational formulation of quantum dynamics discussed by Rowe,[19,20] these equations of motion respond to the general law (summation convention for Greek indices is hereafter used)

$$\sigma_{\mu\nu}\dot{x}^\nu=\frac{\partial}{\partial x^\mu}\langle\vec{x}\,|H|\,\vec{x}\rangle\ , \tag{2.4}$$

where $\sigma_{\mu\nu}$ is the symplectic metric tensor,

$$\sigma_{\mu\nu}=i\left[\left\langle\frac{\partial}{\partial x^\mu}\vec{x}\,\middle|\,\frac{\partial}{\partial x^\nu}\vec{x}\right\rangle-\left\langle\frac{\partial}{\partial x^\nu}\vec{x}\,\middle|\,\frac{\partial}{\partial x^\mu}\right\rangle\right]\ . \tag{2.5}$$

We note that Eq. (2.4) has been extracted as well by Kan *et al.*[24] as a prescription for a two-parameter TDHF model.

Now, we are especially concerned with the case in which the expectation value

$$\hat{I}(\vec{x})=\langle\vec{x}\,|\hat{I}|\,\vec{x}\rangle$$

does not remain constant on the trajectory (2.4). We propose an alternative to the single determinantal dynamics (2.4) and (2.5) allowing the initial single determinant $|\vec{x}(0)\rangle$ to admix configurations in the course of evolution,

$$|\vec{x}(0)\rangle\rightarrow|\Psi(t)\rangle=\sum_s a_s(t)\,|\,s(\vec{x}(t))\rangle\ , \tag{2.6}$$

in such a way as to keep the action integral

$$S=\int_{t_1}^{t_2}dt'\left\langle\Psi(t')\,\middle|\,\hat{H}-i\frac{\hat{\partial}}{\partial t'}\,\middle|\,\Psi(t')\right\rangle \tag{2.7}$$

at an extremum. The variational prescription reads[19,20]

$$\delta\mathscr{H}(\Psi)=i\langle\delta\Psi\,|\,\dot{\Psi}\rangle-i\langle\dot{\Psi}\,|\,\delta\Psi\rangle\ , \tag{2.8}$$

where, having defined

$$\mathscr{H}_s=\langle s\,|\hat{H}|\,s\rangle/\langle s\,|\,s\rangle \tag{2.9a}$$

and

$$\alpha_s=|\,a_s\,|^2\langle s\,|\,s\rangle\ , \tag{2.9b}$$

we can write

$$\mathscr{H}(\Psi)=\sum_s\alpha_s\mathscr{H}_s\ . \tag{2.10}$$

In addition, the time derivative reads

$$\begin{aligned}|\dot{\Psi}\rangle&=\sum_s\dot{a}_s\,|\,s\rangle+\sum_s a_s\,|\,\dot{s}\rangle\\&=\sum_s\dot{a}_s\,|\,s\rangle+\sum_s a_s\dot{x}^\nu\,|\,s_\nu\rangle\ .\end{aligned} \tag{2.11}$$

As a first realization of Eq. (2.8) we find, choosing the coefficients of δa_s^*,

$$i\dot{a}_s\langle s\,|\,s\rangle=a_s\langle s\,|\,s\rangle\mathscr{H}_s-i\sum_{s'}a_{s'}\langle s\,|\,\dot{s}'\rangle\ . \tag{2.12}$$

Because $|s\rangle$ is an eigenvector of $\hat{I}$, and assuming that the latter is not explicitly time dependent (i.e., $id\hat{I}/dt=[\hat{I},\hat{H}]$), it is easy to verify that

$$\langle s\,|\,\dot{s}'\rangle=\langle s\,|\,\dot{s}\rangle\delta_{ss'}\ . \tag{2.13}$$

Thus,

$$i\dot{a}_s=\mathscr{L}_s a_s\ , \tag{2.14}$$

where

$$\mathscr{L}_s=\mathscr{H}_s-i\langle s\,|\,\dot{s}\rangle/\langle s\,|\,s\rangle \tag{2.15}$$

is the Lagrangian for the configuration $|s\rangle$. Equation (2.12) expresses the fact that the positive number α_s denoting the probability for configuration $|s\rangle$ to occur in $|\Psi\rangle$ is a constant of the motion, and, consequently,

$$\langle \Psi | I | \Psi \rangle = \sum_s \alpha_s I_s \tag{2.16}$$

remains constant as well, as required by the exact dynamics. This property suggests the denomination symmetry-conserving variational dynamics (SCVD) for the present trial. We realize that the state vector (2.6) represents a true improvement with respect to the single-determinant ansatz. Notice that no restriction to norm-conserving variations has been imposed anywhere; indeed, the conservation of α_s indicates that

$$\langle \Psi(t) | \Psi(t) \rangle = \sum_s \alpha_s = 1 , \tag{2.17}$$

provided that $\langle \Psi(0) | \Psi(0) \rangle = 1$.

As a further consequence of (2.13) we obtain, for the total Lagrangian

$$\mathscr{L}(\Psi) = \mathscr{H}(\Psi) - i \langle \Psi | \dot{\Psi} \rangle = \sum_s \alpha_s \mathscr{L}_s . \tag{2.18}$$

It is now a trivial exercise to demonstrate that the Hamiltonian dynamics possesses the same form as in (2.4), namely,

$$\sigma_{\mu\nu} \dot{x}^\nu = \frac{\partial}{\partial x^\mu} \mathscr{H}(\Psi) , \tag{2.19}$$

where the tensor of the sympletic metric exhibits the configuration mixing,

$$\sigma_{\mu\nu} = \sum_s \alpha_s \sigma_{\mu\nu}(s) = i \sum_s \alpha_s (\langle s_\mu | s_\nu \rangle - \langle s_\nu | s_\mu \rangle) . \tag{2.20}$$

The short-hand notation $| s_\mu \rangle = \partial | s \rangle / \delta x^\mu$ is hereafter used.

An illustration of the dynamics in Eqs. (2.18) and (2.19) will be given in the next two sections in the frame of the two-level quasispin model. It is interesting to remark that, opposite to what happens in TDHF evolution, multideterminantal dynamics cannot be expressed in terms of a nonlinear generator of motion. In other words, we cannot write, in general,

$$i | \dot{\Psi} \rangle = \hat{\mathfrak{H}}(\Psi) | \Psi \rangle , \tag{2.21}$$

except for very specific situations. This fact contrasts with single-determinantal dynamics; we can show that Eq. (2.4) provokes a time variation of $| \vec{x} \rangle$ as follows,

$$i \frac{\partial}{\partial t} | \vec{x} \rangle = i \dot{x}^\nu \frac{\partial}{\partial x^\nu} | \vec{x} \rangle = i (\sigma^{-1})_{\nu\mu} \frac{\partial \mathscr{H}}{\partial x^\mu} \hat{X}_\nu | \vec{x} \rangle . \tag{2.22}$$

The latter expression is locally valid, i.e., it can be stated in a neighborhood of $| \text{ref} \rangle$ where one may not bother at all about the nonvanishing commutators $[\hat{X}_\mu, \hat{X}_\nu]$. Equation (2.22) is thus a typical mean-field evolution law,

$$i \frac{\partial}{\partial t} | \vec{x} \rangle = \hat{\mathfrak{H}}^{\text{HF}}(\vec{x}) | \vec{x} \rangle , \tag{2.23}$$

where

$$\hat{\mathfrak{H}}^{\text{HF}}(\vec{x}) = \Omega^{\text{HF}}(\vec{x}) \cdot \underline{\hat{X}} , \tag{2.24}$$

and the mean-field frequency is proportional to the Hamiltonian vector field $\partial \mathscr{H} / \partial x^\mu$,

$$\Omega_\nu^{\text{HF}} = (\sigma^{-1})_{\nu\mu} \frac{\partial \mathscr{H}}{\partial x^\mu} . \tag{2.25}$$

Thus,

$$\Omega_\nu^{\text{HF}} = \frac{\partial \mathscr{H}}{\partial x^\nu} , \tag{2.26}$$

if the x's are canonical coordinates.

We note, however, that if we select the spanning space $| s(t) \rangle$ of Eq. (2.6) as

$$| s(t) \rangle^{\text{new}} = | s(t) \rangle^{\text{true}} \exp \left[i \int_0^t dt' \mathscr{L}_s(t') \right] , \tag{2.27}$$

[where $| s \rangle^{\text{true}}$ is the one in Eq. (2.3)], the time derivative $| \dot{\Psi} \rangle$ in Eq. (2.11) changes into

$$| \dot{\Psi} \rangle^{\text{new}} = \sum_s a_s \, (t=0) | \dot{s}(t) \rangle^{\text{true}} , \tag{2.28}$$

and, utilizing the same local criterion as in (2.22), we obtain

$$i | \dot{\Psi} \rangle^{\text{new}} = \hat{\mathfrak{H}}(a_s(0), \vec{x}) | \Psi \rangle^{\text{new}} . \tag{2.29}$$

Here the nonlinear generator $\hat{\mathfrak{H}}$ possesses the same structure as (2.24) with the frequency (2.25), referred to the Hamiltonian $\mathscr{H}(\Psi)$ and the configuration mixing metric in (2.20). This indicates that $| \Psi \rangle^{\text{new}}$, where we have removed all relative phases other than the initial ones and those provoked by the motion of the states $| s(\vec{x}(t)) \rangle$, does evolve as a single determinant would, but under a modified, configuration-mixed generator of motion. The true state vector $| \Psi \rangle$ undergoing the variational dynamics can be generated from $| \Psi \rangle^{\text{new}}$ as

$$| \Psi \rangle = \exp \left[-i \sum_s \hat{P}_s \Psi_s \right] | \Psi \rangle^{\text{new}} , \tag{2.30}$$

where

$$\Psi_s = \int_0^t dt' \mathscr{L}_s(t') . \tag{2.31}$$

Thus, the projection indicated in (2.30) is meant to restore the relative phases among the amplitudes $a_s(t)$, as demanded by the Lagrange equation (2.14).

III. AN APPLICATION TO QUASISPIN DYNAMICS

The Lipkin-Meshkov-Glick[16] (LMG) model consists of a set of N particles in two energy levels ($\sigma = \pm 1$) of sufficient degeneracy, interacting through a two-body force that can scatter two particles across the gap of width ϵ. The LMG Hamiltonian reads

$$\hat{H} = \epsilon \hat{J}_Z + \tfrac{1}{2} V (\hat{J}_+^2 + \hat{J}_-^2) , \tag{3.1}$$

where the quasispin operators

$$\hat{J}_+ = \sum_p a_{p+}^+ a_{p-} , \tag{3.2a}$$

$$\hat{J}_- = (J_+)^\dagger , \tag{3.2b}$$

$$\hat{J}_Z = \frac{1}{2}\sum_{p,\sigma} \sigma a_{p\sigma}^+ a_{p\sigma} \tag{3.2c}$$

expand an SU(2) algebra. The Hamiltonian is block diagonal in the irreducible representations of SU(2), the unperturbed ground state belonging to the completely symmetric one ($J = N/2$), which turns out to be the most interesting representation.

It is well known that the N-fermion Slater determinants are in one-to-one correspondence with the GCS's of the SU(2) group[10,14,21,22] defined as the rotations of the extremal state $|J_Z = -J\rangle$,

$$|\tau\rangle = \hat{R}(\tau)\,|-J\rangle , \tag{3.3}$$

where

$$\hat{R}(\tau) = \exp\left[\frac{\tan^{-1}|\tau|}{|\tau|}(\tau\hat{J}_+ - \tau^*\hat{J}_-)\right] . \tag{3.4}$$

The complex parameter

$$\tau = \tan\frac{\theta}{2}e^{-i\varphi}$$

corresponds to points on a Grassmann manifold—actually the Bloch sphere.

The LMG model possesses an important symmetry, since the Hamiltonian (3.1) preserves the parity of the difference between excited ($\sigma = 1$) and unexcited ($\sigma = -1$) particle numbers. The parity operator may be written as[18]

$$\hat{\mathcal{P}} = e^{i\pi\hat{J}_Z}e^{i\pi J} . \tag{3.5}$$

Since $\hat{\mathcal{P}}$ is a cyclic operator of order 2 ($\hat{\mathcal{P}}^2 = 1$), the projectors associated with the symmetric and the skew-symmetric subspaces are

$$\hat{\mathcal{P}}_s = \frac{1}{2}(1 + \hat{\mathcal{P}}) , \tag{3.6a}$$

$$\hat{\mathcal{P}}_A = \frac{1}{2}(1 - \hat{\mathcal{P}}) . \tag{3.6b}$$

The action of $\hat{\mathcal{P}}$ on a GCS is easily determined,

$$\hat{\mathcal{P}}\,|\tau\rangle = |-\tau\rangle , \tag{3.7}$$

and its expectation value reads

$$\langle\tau|\,\hat{\mathcal{P}}\,|\tau\rangle = \left[\frac{1-|\tau|^2}{1+|\tau|^2}\right]^N$$
$$= \cos^N\theta \le 1 . \tag{3.8}$$

It is also clear that the TDHF Hamiltonian presents the symmetry

$$\langle\tau|\hat{H}|\tau\rangle = \langle-\tau|\hat{H}|-\tau\rangle \tag{3.9a}$$

and

$$\langle\tau|\hat{H}|-\tau\rangle = \langle-\tau|\hat{H}|\tau\rangle . \tag{3.9b}$$

The TDHF equations of motion have been studied by Kan *et al.*,[14] who performed a detailed analysis of the orbits $\tau(t)$ and the energy surface in a canonical phase space $\{(p,q)\}$. When the order parameter $\chi = V(N-1)/\epsilon$ is zero, the only allowed orbits are straight lines (p=cte) in phase space, or circumferences parallel to the equator on the Bloch sphere (quasispin rotations). As χ increases from zero to unity, the perturbation manifests on the orbits as oscillations around the original circles. When χ becomes larger then unity, a new kind of orbit appears in addition to these global trajectories—actually a class of librations or closed paths in the neighborhood of each extremum on the variational energy surface. A similar analysis recently has been presented in Ref. 15.

Now, in view of Eq. (3.8), it is clear that the TDHF equations of motion $\dot{\tau}(t)$ [or $\dot{\theta}(t)$, $\dot{\varphi}(t)$] are parity violating, but the magnitude of this effect may differ from one orbit to another. The amount of symmetry breaking is measured by the difference, on a given trajectory,

$$\Delta(\langle\hat{\mathcal{P}}\rangle) = \max[\cos^N\theta(t)] - \min[\cos^N\theta(t)] , \tag{3.10}$$

so it is expected to play an important role for strongly deformed orbits ($\chi > 1$) and low particle number. This is precisely the case examined in Ref. 10.

In order to utilize the SCVD prescription for the trial wave function (2.26), we write the parity eigenvectors

$$|+\rangle = \frac{1}{\sqrt{2}}(|\tau\rangle + |-\tau\rangle) , \tag{3.11a}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|\tau\rangle - |-\tau\rangle) , \tag{3.11b}$$

and the corresponding Hamiltonian in (2.10),

$$\mathcal{H} = \alpha_+\mathcal{H}_+ + \alpha_-\mathcal{H}_- , \tag{3.12a}$$

$$\alpha_\pm = \frac{1}{2}[1 \pm \cos^N\theta(0)] , \tag{3.12b}$$

$$\mathcal{H}_\pm = \epsilon J(-\cos\theta + \chi\sin^2\theta\cos2\varphi)\frac{1\pm\cos^{N-2}\theta}{1\pm\cos^N\theta} . \tag{3.12c}$$

The mean parity $\pi = \langle\Psi|\,\hat{\mathcal{P}}\,|\Psi\rangle$ is

$$\pi = \alpha_+ - \alpha_- = \cos^N\theta(0) , \tag{3.13}$$

and it is a constant of the motion as shown in the previous section. Owing to wave function normalization ($\alpha_+ + \alpha_- = 1$) the energy surface is actually parametrized by three real variables, i.e.,

$$\mathcal{H}(\Psi) \equiv \mathcal{H}(\pi,\theta,\varphi) .$$

The sympletic metric tensor in (2.20) reads

$$\sigma_{\theta\varphi} = \frac{d}{d\theta}p(\theta) , \tag{3.14}$$

where

$$p(\theta) = \alpha_+p_+(\theta) + \alpha_-p_-(\theta) , \tag{3.15a}$$

$$p_\pm(\theta) = (1-\cos\theta)\frac{1\mp\cos^{N-1}\theta}{1\pm\cos^N\theta} , \tag{3.15b}$$

and the Hamiltonian equations in (2.19) read

$$\dot{\theta}(t) = -[p'(\theta)]^{-1}\frac{\partial\mathcal{H}}{\partial\varphi} , \tag{3.16a}$$

$$\dot{\varphi}(t)=[p'(\theta)]^{-1}\frac{\partial \mathscr{H}}{\partial \theta} \ . \tag{3.16b}$$

We remark here that $p(\theta)$ defined in Eqs. (3.15) is the canonical momentum conjugate to the coordinate $q=\varphi+\text{cte}$; indeed, it can be observed that Eqs. (3.16) are Hamilton's equations of motion,

$$\dot{p}=-\frac{\partial \mathscr{H}}{\partial q} \tag{3.17a}$$

$$\dot{q}=\frac{\partial \mathscr{H}}{\partial p} \ . \tag{3.17b}$$

It is easily verified that, for the Lagrangian in (2.18), we have, in this case,

$$\mathrm{Re}\mathscr{L}=\mathscr{H}-p\dot{q} \ . \tag{3.18}$$

The relative phase $\Psi=\Psi_+-\Psi_-$ between the symmetric and the skew-symmetric amplitudes $a_\pm(t)$ evolves in time according to

$$\begin{aligned}\dot{\Psi}&=\mathrm{Re}(\mathscr{L}_+-\mathscr{L}_-)\\&=\mathscr{H}_+-\mathscr{H}_--\dot{\varphi}(p_+-p_-) \ .\end{aligned} \tag{3.19}$$

It is easy to see from Eqs. (3.14) to (3.16) that the TDHF equations of motion[10,14] are recovered when $\Delta(\pi)\ll 1$. In addition, Eq. (3.18) indicates that local SCVD trajectories (librations) are expected to reflect the oscillation of the SCVD wave function between the two degenerate TDHF orbitals $|\tau\rangle$ and $|-\tau\rangle$. Indeed, one realizes that while $\mathscr{H}_+-\mathscr{H}_-$ does not change sign on an orbit, $\dot{\varphi}$ does; thus the relative phase oscillates with a typical frequency close to

$$\Omega=\frac{1}{T}\int_0^T[\mathscr{H}_+(t')-\mathscr{H}_-(t')]dt' \ , \tag{3.20}$$

where T is a period of the SCVD motion.

IV. NUMERICAL EXAMPLES

Equations (3.16) have been numerically solved for several initial conditions $\tau(0)$ and for different particle numbers N and order parameters χ. In Fig. 1 we show the SCVD phase portrait $\{(p,q)\}$ for $N=6$ and $\chi=1.5$, this being a selection of parameters that permits us to observe major differences between SCVD and TDHF descriptions (the latter being shown in Fig. 2). The orbits in both figures are in one-to-one correspondence, i.e., they have evolved from identical initial conditions. The phase coordinates are, in both cases, the TDHF canonical ones,[14] $P_{\text{HF}}=-N\cos\theta$ and $q_{\text{HF}}=\varphi$. This choice has been made in order to facilitate the comparison between both flows and it has been seen that the diagram $(p_{\text{SCVD}},q_{\text{SCVD}})$ with the coordinates $p_{\text{SCVD}}=p(\theta)$ [see Eqs. (3.14)] and $q_{\text{SCVD}}=q_{\text{AF}}$ differs only slightly from the one shown in Fig. 1. It is interesting to note that the 4th and 10th orbits are rotations in TDHF and librations in SCVD; this is a manifestation of the fact that critical points on the energy surface are not located at the same position in either description. Furthermore, one can see from the corresponding expressions of the mean energy that the so-called critical orbits, i.e., those containing the poles, bear different energy values in the two approaches. For example, the south polar orbits correspond to the TDHF energy $-\epsilon J$ and to the SCVD energy $-\epsilon J(1-\alpha_-/J)$.

Notice that, opposite to what happens in the TDHF case, the SCVD frame does not allow an analytic evaluation of stationary points. In the present context, it is not obvious that we must search for a "phase transition" like the well-known Hartree-Fock one.[14] The SCVD energy hypersurface is labeled by three parameters, namely, the coordinates θ and φ and the parity π, the latter being fixed by the chosen initial conditions. Thus, a phase transition, regarded as a qualitative change of the topology of the phase portrait $\{(\theta(t),\varphi(t))\}$ might be either observed or unobserved depending upon the specific projection of the three dimensional phase space that one selects for the drawing.

Larger values of particle number cause the two patterns to collapse into the single TDHF flow. Indeed, already for $N=25$, the SCVD phase portrait cannot be distinguished from its TDHF counterpart, insofar as χ remains not too much higher than unity. For low particle number, say $N=6$, and χ below the phase transition, a similar observation holds, except for the fact that SCVD rotations exhibit larger wiggling in the neighborhood of the poles.

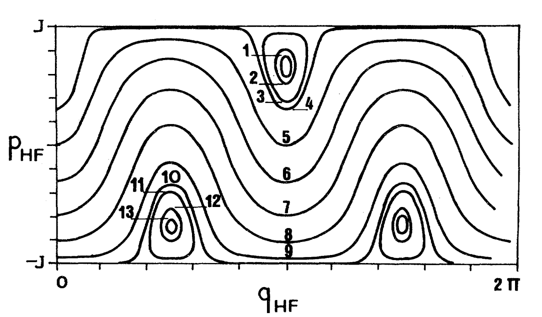

FIG. 1. The phase portrait $\{p(t),q(t)\}$ in the self-consistent variational dynamics (SCVD) description, for particle number $N=6$ and interaction strength $\chi=1.5$.

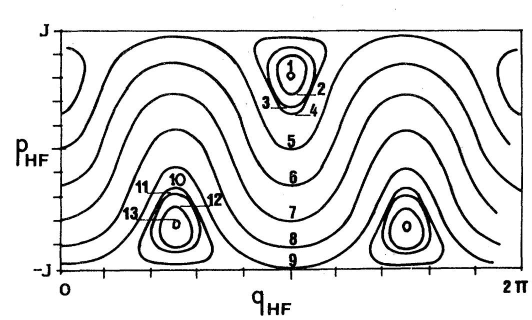

FIG. 2. The same initial conditions and parameters in Fig. 1, evolving according to the TDHF law.

In order to measure the quality of the different approaches to the exact dynamics, we have computed the values of the overlap between (a) exact and TDHF, (b) exact and SCVD, and (c) SCVD and TDHF wave functions. These quantities are shown in Fig. 3 for $N=6$, $\chi=1.5$, $\theta_0=\cos^{-1}(-0.8)$, and $\varphi_0=0$; the trajectory is a libration (orbit number 2 of Fig. 1). The improvement of SCVD upon TDHF is remarkable, since the former overlaps the exact wave function above 70% (0.84 is the minimum overlapping amplitude in Fig. 3) during several oscillations of the TDHF orbit. Indeed, it is well known[10,11,25] that TDHF is a short-time approximation to the true dynamics, due to its classical characteristics; by contrast, SCVD makes room for significant quantum effects like tunneling below the barrier between the two degenerate energy minima characteristic of this model. This feature is further illustrated in Fig. 4, where the same overlaps are displayed in the case of orbit number 7 ($\cos\theta_0=0.6$). This trajectory is a rotation in either portrait and it is seen that the SCVD pattern remains close enough to TDHF to yield no significant improvement with respect to the latter.

A second and important test consists of computing the mean values of one-body observables. In quasispin models, the observable of interest is the polarization $\vec{J}_\phi$ given by the expectation value of $\hat{\vec{J}}$ with respect to a given state vector $|\phi\rangle$, i.e.,

$$\vec{J}_\phi=\frac{\langle\phi|\hat{\vec{J}}|\phi\rangle}{\langle\phi|\phi\rangle}\ . \tag{4.1}$$

We have calculated $\vec{J}_\phi$ with the three selections for $|\phi\rangle$, namely, exact, SCVD, and TDHF state vectors. Indicative results of these calculations are the angle β between $\vec{J}_{\text{exact}}$ and either approximate polarization, and the modulus $|\vec{J}_\phi|$. Note that $|\vec{J}_{\text{TDHF}}|$ always equals the representation label J. In Fig. 5 we show the cosine of the angle β (corresponding to the same dynamics as in Fig. 3) and it is clearly seen that it remains close to unity during most of the interval displayed on the time axis; this is another indication of the already observed fact that the SCVD wave function approaches the exact one to a better extent than TDHF. The modulus of the polarization is displayed in Fig. 6.

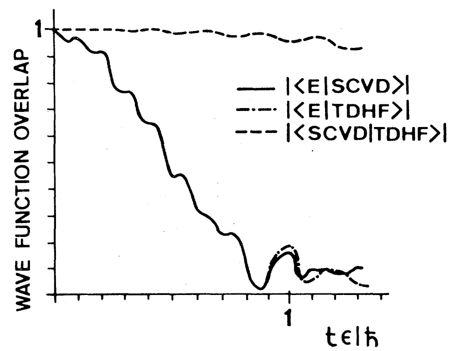

FIG. 4. Same as in Fig. 3, for the rotational orbit number 7.

Selections of parameters χ and N and initial conditions different from those here displayed (any χ smaller than unity, any N larger than 25, initial position on an SCVD rotation rather than on a libration) shows that (i) β_{SCVD} is always smaller than β_{TDHF} although they might differ slightly, and (ii) $|\vec{J}_{\text{SCVD}}|$ always remains closer to the exact figure than $|\vec{J}_{\text{TDHF}}|$. A long-time analysis shows that while all SCVD and TDHF quantities depart from the corresponding exact ones, the former approach does it at a much slower rate.

V. DISCUSSION AND SUMMARY

In this work we have proposed a variational dynamics based on a larger set of trial functions than TDHF. The wave functions are admitted to be linear combinations of Slater determinants, but only in order to include the quantal effects related to the existence of N-body dynamical invariants (N-body symmetries). The evolution thus formulated keeps the value of any function of the invariant at a constant figure.

The state of the N-body system is no longer described by a Slater determinant, but rather by a superposition of them with amplitudes fixed by the initial conditions and relative phases determined by the trajectory. In this context, the motion of the system may be followed on the

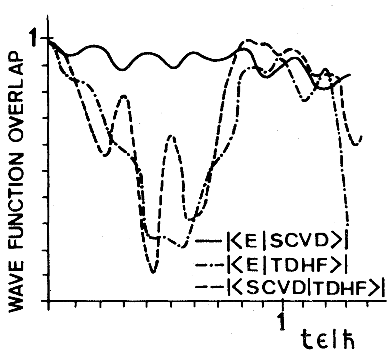

FIG. 3. The overlap between wave functions calculated with different methods for the librational orbit number 2 of Fig. 1.

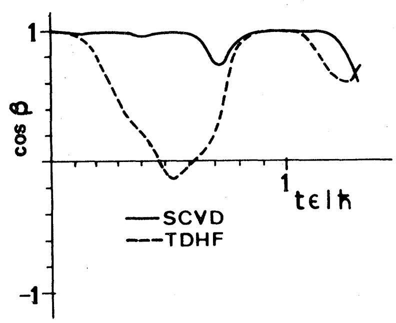

FIG. 5. The cosine of the relative polarization angle as a function of time, in the conditions of Fig. 3.

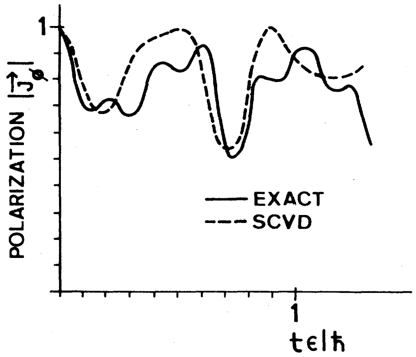

FIG. 6. The modules of the polarization vector as a function of time, in the conditions of Fig. 5.

manifold of the Slater determinants, although it must be kept in mind that both the symplectic metric that converts the Grassmann manifold into a phase space [Eqs. (2.20)] and the effective Hamiltonian [Eqs. (2.10)] depend on the initial symmetry conditions.

At first sight, one could assert that the larger the set of trial functions, the larger the accuracy of the approximated dynamics. This seems to be true, but it is seen that in some cases the improvement may be rather poor. In the light of SCVD, we can indicate two situations where it is necessary to include a quantal description of the symmetries in order to really improve the approximations. One of them is wherein TDHF dynamics depends strongly on the initial mean value of an observable $\hat{A}$ and the trial functions display an important quantal dispersion with respect to the $\hat{A}$ eigenfunctions; in other words, $(\langle\hat{A}^2\rangle-\langle\hat{A}\rangle^2)^{1/2}$ is not much smaller than $\langle\hat{A}\rangle$ at all times. In this case, it can be expected that different eigenspaces of $\hat{A}$ acquire significantly time-varying relative phases during the evolution. The other situation mentioned above is that in which the observable changes by an important amount over an interesting TDHF trajectory. In such a case, the SCVD trajectories on the symplectic manifold can differ considerably from the TDHF ones.

All these features have been examined on the LMG model. Regarding the overlap between approximated and exact wave functions as a measure of the quality of the description, the best fits are obtained for low particle numbers, moderate values of the interaction strength above the TDHF phase transition, and initial conditions associated to TDHF librations. In those situations, the two general reasons for the need of symmetry restoring are better fulfilled.

It is important to remark that, as SCVD phase portraits like the one shown in Fig. 1 are considered, one cannot associate their changes of shape with phase transitions since they are not simple projections of the full SCVD phase space $\{(p,q,\pi,|\Psi\rangle)\}$. The one-to-one correspondence between phase flows claimed in Sec. IV is related to the determinantal initial conditions that evolve on a hyperplane $\pi=$cte under SCVD dynamics. In other words, the SCVD phase portrait is built up picking just one SCVD orbit from each constant-π hyperplane and projecting them together on a p-q space. Notice that each of these orbits is labeled by a constant energy, the same as the corresponding TDHF path.

Since many interesting problems about symmetries and TDHF dynamics are to be formulated and discussed, it could be instructive to apply the SCVD method to other solvable models, especially to those possessing larger numbers of symmetry-related eigenspaces than LMG. It would be of interest as well to examine the case of systems where the amount of symmetry breaking is weak. The study of more realistic models will require suitable approaches for the projectors $\hat{P}_s$, in order to render the calculations feasible.

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