Quasispin dynamics beyond the Bloch sphere: Exact versus time-dependent Hartree-Fock evolution

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We examine the complementary types of motion induced by the time-dependent mean field and the related residual interaction in the frame of quasispin systems. The time-dependent Hartree-Fock law of motion is used to generate an instantaneous basis, where the residual interaction induces transitions that deviate the exact motion with respect to the simple Slater determinant evolution. Geometric images of both kinds of dynamics are given and definite time scales are extracted for the validity of the time-dependent Hartree-Fock description, its second order correction, and the building up of a noticeable relative polarization of the exact wave function. It is seen that in addition to the time-dependent Hartree-Fock motion over the Bloch sphere, the exact dynamics contains an "inwards" component as well as additional rotations.

[NUCLEAR STRUCTURE Time-dependent Hartree-Fock; moving basis; residual interaction; complementary motions; quasispin systems; Slater determinant; time scales; rotations and nonrotations on Bloch sphere; polarization.]

I. INTRODUCTION

The motion of antisymmetrized, uncorrelated many-fermion wave functions in a nonlinear mean field exerts a strong fascination on nuclear theorists. A Slater determinant of single particle (sp) orbits, subject to nonlocal forces that adjust themselves to the changing quality of the space where their sources are located, satisfies most claims of simplicity and elegance for a zero-order model of many body evolution. The success of mean field or time-dependent Hartree-Fock (TDHF) calculations in describing and giving a deep understanding of several features of nuclear dynamics[1] follows the consideration of some difficulties,[2-4] inherent to either the sp picture or the determinantal way of thinking. Comparisons of TDHF with the exact Schrödinger dynamics have been performed in several workable situations[5-7] and attempts to go beyond the uncorrelated particle model have come into sharp focus.[8,9] It is nowadays customary to speak of "collisional TDHF dynamics" with reference to a frame that incorporates irreversibility as a consequence of two-body scattering processes induced by the residual interaction. However, the numerical complexity of these approaches, that bring the time evolution of the many fermion system close to the kinetic decay to equilibrium of a quantum Boltzmann gas,[10] postpones any criticism of its predictions.

A finite nucleus is far from a system in the thermodynamic limit [$N\rightarrow\infty$, $V\rightarrow\infty$, $\lim(N/V)=\rho_0$] that undergoes irreversible evolution and approches a thermal equilibrium situation described by a Fermi distribution. As a matter of fact, it is a rather localized object, its Hamiltonian spanning a discrete spectrum, and its "not-so-many" body density matrix would oscillate over the eons, should one build it in an arbitrary initial condition. The exact dynamics of discrete spectra, say, poses a problem that cannot be tackled by resorting to kinetic, i.e., collisional TDHF, equations. Of course, we firmly believe that much interesting physics can be learned from nuclear "half-matter" encounters or slab collisions, a theme that currently enjoys high popularity. But, in the present work, we accept the challenge of trying again a comparison between TDHF and exact dynamics of a small N, finite discrete spectrum, interacting fermion system. We focus our attention on the complementary types of

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motion induced by the time-dependent mean field and by the related residual interaction, and give quantitative views of their rates of competition. The geometrical frame in which quasispin systems are inscribed allows a simple interpretation of the dynamics and we are able to measure the departure of the exact wave function from the TDHF, as well as from an arbitrary Slater determinant. We find that several peculiarities of determinantal dynamics as compared to the full evolution could be traced to the law of motion, rather than to the selection of an uncorrelated wave function, and we suggest a few alternatives, each of them deserving a separate analysis.

In Sec. II, we briefly review some current knowledge about TDHF and confront several points of view. The separation of the exact motion in mean-field and residual interaction paths is carried out in Sec. III, where we also define what we call "a TDHF moving basis." Section IV contains the description of the dynamics of quasispin systems and the calculations performed in this work are detailed in Sec. V. The summary and final conclusions are the subject of Sec. VI.

II. THE TDHF EQUATIONS OF MOTION

Many derivations of the TDHF equations are available from the literature.[1,11–24] Far from attempting to summarize them all, we are going to discuss briefly three different insights. In one version, the TDHF evolution may be regarded as the first approach to the motion of a many-body interacting system insofar as the collective effects are the most important ones, as it is often argued. From this point of view, one averages the two-body Hamiltonian with respect to the one-body density ρ,[13–16]

$$h_{\mathrm{HF}}(1)=\mathrm{Tr}_2 H_1(1,2)\rho(2)+H_0(1)\ , \tag{2.1}$$

while the total energy contained in the collective path reads

$$\mathscr{E}_{\mathrm{HF}}=\mathrm{Tr}_1 h_{\mathrm{HF}}(1)\rho(1)\ . \tag{2.2}$$

The full many-body Hamiltonian is written as

$$H=\sum_{i=1}^{N} h_{\mathrm{HF}}(i)+V_{\mathrm{res}}=\mathscr{H}_{\mathrm{HF}}+V_{\mathrm{res}}\ , \tag{2.3}$$

where the residual interaction V_{res} is usually negligible with respect to $\mathscr{H}_{\mathrm{HF}}$. The TDHF equation is

$$i\dot{\rho}=[\mathscr{H}_{\mathrm{HF}}(\rho),\rho] \tag{2.4a}$$

or

$$i\,|\dot{\psi}\rangle=\mathscr{H}_{\mathrm{HF}}(\,|\psi\rangle)\,|\psi\rangle\ , \tag{2.4b}$$

with

$$\rho=|\psi\rangle\langle\psi|\ . \tag{2.5}$$

This formulation of the TDHF picture suggests that it may give rise to a zeroth-order approach to the time propagator in a time dependent perturbation theory.

A second point of view is contained in the variational description[1,18–22]: One takes the trajectory $|\Psi\rangle$ of the many-body system as the solution of

$$\delta\int_0^t \langle\Psi|\,i\frac{\partial}{\partial t'}-H\,|\Psi\rangle dt'=0\ , \tag{2.6}$$

while the collective path corresponds to a given class of trial vectors, i.e., to the Slater determinants. The extremal principle is not too easy to understand by itself, as pointed out by several authors (Ref. 25 and the references therein). If one examines the variational formulation in the context of a path-integral approach to the time propagator, it follows that the principle just states the stationary phase condition and thus gives rise to the classical path.[23,24] In this sense, improvements upon the predictions of the TDHF method will be furnished by semiclassical, higher order approaches.

The third insight is provided by the kinetic equation theory.[8,10,26–28] It briefly tells that TDHF equations are collisionless kinetic ones. Now, an arbitrary kinetic equation may be written as

$$i\dot{\rho}=[\mathscr{H}_{\mathrm{HF}},\rho]+K(\rho)\ , \tag{2.7}$$

where $[\mathscr{H}_{\mathrm{HF}},\rho]$ is the conservative flow term and $K(\rho)$ is the so-called collision term. In this picture, there are two ways for the many-body system to propagate from one uncorrelated (sp) state to another. One way of evolution is reversible oscillation induced by the mean field, that acts upon a sp state as an external force would do. The other way is represented by the collision term and takes place via two-particle scattering, on the assumption that such a process is very fast and essentially instantaneous, as compared with a typical period for the HF flow. However, an important requirement for the existence of a kinetic regime is the decay of any two-body correlation other than those created as a consequence of the dynamical evolution. This implies that the two-body Hamiltonian is of such a kind that the particles become asymptotically free for large times and is only consistent with a continuous spectrum for the full H and the asymptotic

H_0.[29–31] Systems with a pure point spectrum do not admit a kinetic improvement of the TDHF equations.

III. TDHF VERSUS EXACT EVOLUTION

In order to analyze the rate of departure of the TDHF Slater determinant with respect to the true many-body state vector, it will be useful to utilize a time-dependent basis that includes the Hartree-Fock state as one of its vectors. First we note that the equation for the TDHF propagator is

$$i\dot{U}_{\rm HF}(t)=\mathscr{H}_{\rm HF}(t)U_{\rm HF}(t)\ , \tag{3.1}$$

with $\mathscr{H}_{\rm HF}=\mathscr{H}^{\dagger}_{\rm HF}$. In general, $[\mathscr{H}_{\rm HF},U_{\rm HF}]\neq 0$. It is interesting to introduce a "residual interaction representation" through the removal of the HF motion from the exact one, i.e., let $\hat{U}(t)$ be the evolution operator in an interaction representation,

$$\hat{U}(t)=U^{\dagger}_{\rm HF}(t)U(t)\ , \tag{3.2}$$

where U is the true propagator. One easily finds

$$\begin{aligned} i\dot{\hat{U}}(t)&=U^{\dagger}_{\rm HF}V_{\rm res}U_{\rm HF}\\ &=\hat{V}_{\rm res}(t)\hat{U}(t)\ , \end{aligned} \tag{3.3}$$

with

$$\hat{V}_{\rm res}(t)=\hat{U}^{\dagger}_{\rm HF}(t)V_{\rm res}(t)U_{\rm HF}(t)\ . \tag{3.4}$$

It follows that

$$U(t)=U_{\rm HF}(t)-i\int_0^t dt'U_{\rm HF}(t)U^{\dagger}_{\rm HF}(t')\times V_{\rm res}(t')U(t')\ . \tag{3.5}$$

We now select a basis

$$\{\,|\,\Phi_0\rangle,\ldots,|\,\Phi_M\rangle\}$$

for the Hilbert space of the system, where $|\,\Phi_0\rangle$ is a Slater determinant representing the initial state for the motion under consideration. Let us define a "TDHF moving basis" as the set

$$\{\,|\,0\rangle,\ldots,|\,M\rangle\}\ ,$$

where

$$|\,i\,\rangle=U_{\rm HF}(t)\,|\,\Phi_i\,\rangle\ . \tag{3.6}$$

Then, if

$$|\,\Psi\,\rangle=U(t)\,|\,\Phi_0\rangle$$

is the true state vector at time t, the one predicted by the TDHF equation of motion is $|\,0\rangle$, while the expansion of $|\,\Psi\rangle$ in the moving basis is given by the amplitudes

$$a_j(t)=\langle j(t)\,|\,\Psi(t)\rangle=\langle j\,|\,U_{\rm HF}(t)\,|\,\Phi_0\rangle-i\int_0^t dt'\langle j(t')\,|\,U_{\rm HF}(t)U^{\dagger}_{\rm HF}(t')V_{\rm res}(t')\,|\,\Psi(t')\rangle\ . \tag{3.7}$$

We now use $\{\,|\,j(t')\rangle\}$ as an intermediate basis to decouple the operators in (3.7) and take advantage of the somehow obvious properties,

$$\langle j(t)\,|\,U_{\rm HF}(t)=\langle\Phi_j\,|\ , \tag{3.8a}$$

$$\langle j(t)\,|\,U_{\rm HF}(t)U^{\dagger}_{\rm HF}(t')=\langle j(t')\,|\ . \tag{3.8b}$$

We readily obtain the coupled equation

$$a_j(t)=\delta_{j0}-i\sum_k\int_0^t dt'\langle j(t')\,|\,V_{\rm res}(t')\,|\,k(t')\rangle a_k(t')\ . \tag{3.9}$$

In particular, it is interesting to examine the evolution of the coefficient $a_0=\langle 0\,|\,\Psi\rangle$, since $|\,a_0\,|^2$ measures the overlap between the true and the TDHF state, at any time. We also recall here that the residual interaction does not connect the TDHF state with any other vector differing from it by the action of a one body operator. Then

$$a_0(t)=1-i\sum_k\int_0^t dt'\langle 0(t')\,|\,V_{\rm res}(t')\,|\,k(t')\rangle a_k(t') \tag{3.10}$$

gives straightforwardly a means of measuring the departure of the exact wave function from a determinant, at the expense of populating the moving orthogonal subspace $\{\,|\,k\neq 0\rangle\}$.

A final remark for this section is the following. The residual interaction representation (3.2) might be considered as giving a description of the overall evolution with two complementary sorts of motion, namely the TDHF collective path "dragging" the propagated state $\hat{U}(t)\,|\,\Phi_0\rangle$. Expression (3.5) indeed is

$$\begin{aligned} U(t)&=U_{\rm HF}(t)\hat{U}(t)\\ &=U_{\rm HF}(t)\left\{1-i\int_0^t dt'\hat{V}_{\rm res}(t')\hat{U}(t')\right\}\ . \end{aligned} \tag{3.11}$$

We clearly see that the TDHF path is a good approximation to the full evolution of the many-body system, provided $\hat{U}(t)$ differs only slightly from the identity. An obvious first-order estimate,

$$\hat{U}(t) \sim 1 - i \int_0^t dt' \hat{V}_{\rm res}(t') \sim 1 - i\Omega_{\rm res} t \ , \quad (3.12)$$

relates the correction to a typical magnitude $\Omega_{\rm res}$ representing the residual strength over the time interval of interest. If such a quantity $\Omega_{\rm res}$ exists for times $t \sim T_{\rm HF}$, where $T_{\rm HF}$ is a characteristic period of the collective orbit, the correction is proportional to $T_{\rm HF}/T_{\rm res}$. This figure is, of course, much smaller than unity if the residual interaction is weak enough as compared to the mean field energy and implies that the collective motion is fast, with respect to the "collision time" $T_{\rm res}$. In this sense, this decomposition of the evolution could be regarded as complementary to the usual adiabaticity assumption[32] that demands that the TDHF motion be slow compared to the unperturbed, intrinsic particle motion.

IV. TIME SCALES IN QUASISPIN SYSTEMS

In the spirit of the preceding section, we believe it is stimulating to study in some detail the decomposition of the full time evolution into TDHF and complementary motions. We have found it useful to work with a model that accomplishes a twofold purpose. On one hand, it allows a fast classification of relevant orders of magnitude of the admixture rates

$$\langle j(t') \,|\, V_{\rm res}(t') \,|\, k(t') \rangle$$

of Eq. (3.9). This fact permits a straightforward interpretation of the calculated figures and illustrates a more general method. On the other hand, an appealing, geometrical description of the competition between both types of motion is possible, due to some simple topological properties of compact Lie groups.

We then consider one of the simplest, nontrivial many-body Hamiltonians proposed by Lipkin, Meshkov, and Glick.[33] It describes an assembly of N fermions with two allowed states separated by a jump of height ϵ, that interact through a force able to scatter two particles across the gap. The Hamiltonian is usually written as

$$H = \epsilon J_z + \frac{V}{2}(J_+{}^2 + J_-{}^2) \ , \quad (4.1)$$

where $\vec{J} = (J_z, J_+, J_-)$ is the quasispin operator whose components, related to the fermions through

$$J_z = \tfrac{1}{2} \sum_{p,\sigma=\pm} \sigma a^\dagger_{p\sigma} a_{p\sigma} \ , \quad (4.2a)$$

$$J_+ = \sum_p a^+_{p+} a_{p-} \ , \quad (4.2b)$$

$$J_- = (J_+)^\dagger \ , \quad (4.2c)$$

generate an SU(2) algebra.

The completely symmetric representation $J = N/2$ of the SU(2) group is the one of interest provided that the unperturbed ground state belongs to it. In such a case, rotations of the ground-state $|J_z = -J\rangle$ give rise to the Slater determinants, that are in one-to-one correspondence with the atomic coherent states.[34,35]

$$|\Phi(\tau)\rangle = R(\tau)\,|-J\rangle \ , \quad (4.3)$$

where

$$J_z\,|-J\rangle = -J\,|-J\rangle \ , \quad (4.4)$$

and

$$R(\tau) = \exp\left\{ \frac{\tan^{-1}|\tau|}{|\tau|}(\tau J_+ - \tau^* J_-) \right\} . \quad (4.5)$$

The parameter $\tau = \tan(\theta/2)e^{-i\varphi}$ may be represented by points on a differentiable manifold, actually the Bloch sphere, to which we assign the radius J equal to the modulus of the vector

$$\langle \Phi(\tau) \,|\, \vec{J} \,|\, \Phi(\tau) \rangle \ .$$

Any state $|\Psi\rangle$ such that

$$|\langle \Psi | \vec{J} | \Psi \rangle| < J$$

cannot be a Slater determinant; we will say that it belongs to the "interior" of the sphere.

A Slater determinant fulfills the eigenvalue equation

$$I_z(\tau)\,|\Phi(\tau)\rangle = -J\,|\Phi(\tau)\rangle \ , \quad (4.6)$$

where $I_z(\tau)$ is the z component of the rotated quasispin vector

$$\vec{I} = R(\tau)\vec{J}R^{-1}(\tau) \ ,$$

i.e.,

$$\begin{bmatrix} I_z \\ I_+ \\ I_- \end{bmatrix} = \frac{1}{1+|\tau|^2} \begin{bmatrix} 1-|\tau|^2 & -\tau^* & -\tau \\ 2\tau & 1 & -\tau^2 \\ 2\tau^* & -\tau^{*2} & 1 \end{bmatrix} \begin{bmatrix} J_z \\ J_+ \\ J_- \end{bmatrix} . \quad (4.7)$$

The rotated Hamiltonian reads

$$H=\left\{\epsilon[(1-|\tau|^2)I_z+\tau^* I_+ +\tau I_-]\right.$$
$$+\frac{V}{1+|\tau|^2}[(\tau^2+\tau^{*2})(2I_z{}^2-\tfrac{1}{2}I_+I_- -\tfrac{1}{2}I_-I_+)+(\tau^{*3}-\tau)(I_+I_z+I_zI_+)$$
$$\left.+(\tau^3-\tau^*)(I_-I_z+I_zI_-)+\tfrac{1}{2}(1+\tau^{*4})I_+{}^2+\tfrac{1}{2}(1+\tau^4)I_-{}^2]\right\}\frac{1}{1+|\tau|^2}\ . \quad (4.8)$$

The equation of motion for the TDHF Slater determinant is simply [here $\chi=V(N-1)/\epsilon$]

$$\dot{\tau}=i\epsilon\left[\tau+\chi\frac{\tau^*-\tau^3}{1+|\tau|^2}\right], \quad (4.9)$$

while the Hartree-Fock Hamiltonian can be written, as a function of the one-body generator $\vec{\mathrm{I}}$,

$$\mathscr{H}_{\mathrm{HF}}=\Omega_0 J+\vec{\Omega}_{\mathrm{HF}}\cdot\vec{\mathrm{I}}$$
$$=\Omega_0 J+\Omega_z I_z+\Omega_+ I_+ +\Omega_- I_-\ , \quad (4.10)$$

where

$$\Omega_+=\Omega_-^*=\frac{\epsilon}{1+|\tau|^2}\left[\tau^*+\chi\frac{\tau-\tau^{*3}}{1+|\tau|^2}\right]. \quad (4.11)$$

Furthermore, the energy contained in the HF trajectory

$$|0\rangle=R(\tau(t))\,|-J\rangle$$

is

$$\langle 0|\mathscr{H}_{\mathrm{HF}}|0\rangle=J(\Omega_0-\Omega_z)$$
$$=\frac{J\epsilon}{1+|\tau|^2}\left\{|\tau|^2-1+\chi\frac{\tau^2+\tau^{*2}}{1+|\tau|^2}\right\}. \quad (4.12)$$

The TDHF moving basis (see Sec. III) depends upon the choice of the stationary basis $|\Phi_j\rangle$ and the Lipkin model yields at least two possibilities:

(i) $|\Phi_j\rangle=N_j(J_+)^j\,|-J\rangle$

is a Dicke state containing j 1 particle-1 hole excitations. In this case,

$$|j(t)\rangle=U_{\mathrm{HF}}(t)\,|\Phi_j\rangle$$
$$=N_j[I_+(t)]^j\,|0(t)\rangle\ ; \quad (4.13)$$

(ii) $|\Phi_\xi\rangle=R(\xi)\,|-J\rangle$

is a Slater determinant or atomic coherent state for some position ξ on the Bloch sphere. In this case, the states $|\xi(t)\rangle$ are TDHF Slater determinants for different intitial conditions of the system; in Eq. (3.9), the summation

$$\sum_k |k(t')\rangle\langle k(t')|$$

ought to be replaced by

$$\frac{2J+1}{4\pi}\int d\xi\,|\xi(t')\rangle\langle\xi(t')|\ ,$$

(see Refs. 34 and 35). For a given initial condition τ_0, the complementary subspace in the moving framework,

$$\{\,|\xi(t)\rangle=U_{\mathrm{HF}}(t)\,|\xi\rangle\,,\ \ \xi\neq\tau_0\}$$

is not orthogonal to $|\tau(t)\rangle\equiv|0\rangle$. Owing to this feature inherent to coherent states we prefer to select (i) as our TDHF moving basis.

At this point we notice that there exists an arbitrariness regarding an overall time dependent phase for the TDHF state and the remaining vectors of the moving basis (see Sec. III). More precisely, since the one body density ρ is linear in I_z (Ref. 7), the TDHF equation of motion $i\dot{\rho}=[\mathscr{H}_{\mathrm{HF}},\rho]$ turn into an equation of evolution for I_z of the type

$$i\dot{I}_z=\Omega_+I_+ +\Omega_-I_-\ . \quad (4.14)$$

Thus, any term of the form $\Omega_z I_z$ in (4.10) introduces a phase $e^{-i\Omega_z(j-J)t}$ in each vector $|j(t)\rangle$, without modifying Eq. (4.14). We choose to lift this arbitrariness requiring that the matrix elements $\langle j'|I_+|j\rangle$ remain constants of the motion

$$i\frac{d}{dt}\langle j'|I_+|j\rangle=\langle j'|\,i\dot{I}_+-[\vec{\Omega}_{\mathrm{HF}}\cdot\vec{\mathrm{I}},I_+]\,|j\rangle$$
$$=0\ . \quad (4.15)$$

The local variation of I_+ is obtained with (4.7) and

(4.9). From condition (4.15) together with (4.12) we obtain

$$\Omega_z=-\frac{\epsilon}{1+|\tau|^2}\left[2|\tau|^2+\chi(\tau^2+\tau^{*2})\times\frac{1-|\tau|^2}{1+|\tau|^2}\right] \tag{4.16}$$

and

$$\Omega_0=-\epsilon\left[1-\chi|\tau|^2\frac{\tau^2+\tau^{*2}}{(1+|\tau|^2)^2}\right] . \tag{4.17}$$

The total Hamiltonian can then be written as

$$\begin{aligned} H&=\mathcal{H}_{\mathrm{HF}}+V_{\mathrm{res}}\\ &=\vec{\Omega}_{\mathrm{HF}}\cdot\vec{\mathrm{I}}+\vec{\mathrm{I}}^T\cdot\overleftrightarrow{\alpha}\cdot\vec{\mathrm{I}} , \end{aligned} \tag{4.18}$$

where $\overleftrightarrow{\alpha}$ denotes a 3×3 matrix,

$$\overleftrightarrow{\alpha}=\begin{bmatrix} 2h_0 & Nh_1 & (2-N)h_1^* \\ (2-N)h_1 & h_2 & \frac{1}{2}(\epsilon-h_1)+\frac{1}{2}(N-1)\ (1-|\tau|^2)h_1 \\ Nh_1^* & -\frac{1}{2}(\epsilon+h_1)-\frac{1}{2}(N-1)(1-|\tau|^2)h_1 & h_2^* \end{bmatrix} , \tag{4.19}$$

where

$$h_0=V\frac{\tau^2+\tau^{*2}}{(1+|\tau|^2)^2} , \tag{4.20a}$$

$$h_1=V\frac{\tau^{*3}-\tau}{(1+|\tau|^2)^2} , \tag{4.20b}$$

$$h_2=\frac{V}{2}\frac{1+\tau^{*4}}{(1+|\tau|^2)^2} . \tag{4.20c}$$

The matrix elements of the residual interaction in the moving basis are

$$\langle k\,|\,V_{\mathrm{res}}\,|\,k\rangle=\epsilon k+h_0[3k^2-4Jk-k-(N-1)k\,|\tau|^2] , \tag{4.21a}$$

$$\langle k\,|\,V_{\mathrm{res}}\,|\,k+1\rangle=2kh_1^*[(2J-k)(k+1)]^{1/2} , \tag{4.21b}$$

$$\langle k\,|\,V_{\mathrm{res}}\,|\,k+2\rangle=h_2^*[(2J-k)(k+1)(2J-k-1)(k+2)]^{1/2} . \tag{4.21c}$$

It is clear from these formulas that the TDHF state is not connected with the "first excited" configuration $|1\rangle$ by the residual Hamiltonian

$$\langle 0\,|\,V_{\mathrm{res}}\,|\,1\rangle=0 . \tag{4.22}$$

On the other hand, one can recognize that the elements in Eqs. (4.21) represent different characteristic rates for the motion of the components of the true wave function on the TDHF basis. Indeed, deriving Eqs. (3.9) one gets

$$i\dot{a}_j(t)=\sum_{p=-2}^{2}\Omega_{j,j+p}a_{j+p}(t) , \tag{4.23}$$

with

$$\Omega_{j,j+p}=\langle j\,|\,V_{\mathrm{res}}\,|\,j+p\rangle . \tag{4.24}$$

Equations (4.21) display the dependence between the frequencies in (4.23) and the particle number. In addition, it is worthwhile to recall that the time dependence of $\Omega_{j,j+p}$ is twofold, as seen in (4.24); it arises from both the instantaneous definition of the residual interaction between the HF independent particles [see Eqs. (4.18)-(4.20)] and from the motion of the selected basis. In particular, the amplitude of the TDHF determinant in the true state evolves according to

$$i\dot{a}_0(t)=\Omega_{02}(t)a_2(t) . \tag{4.25}$$

The parameter $\Omega_{02}(t)$ then measures the rate of departure of the exact wave function from the surface of the Bloch sphere, to which $|0(t)\rangle$ belongs, into its interior, Its value is

$$\Omega_{02}=4Vh_2^*J=2VNh_2^* . \tag{4.26}$$

We observe that the order of magnitude here is VN, comparable to the characteristic frequency χ of the TDHF motion as seen in Eq. (4.9).

V. NUMERICAL EXAMPLES

We have performed the evaluation of the amplitudes given in Eq. (3.9) for the Lipkin model as described in the previous section. The results displayed in Figs. 1 to 3 correspond to an initial condition $|\tau_0|=0.3$, $\varphi_0=0$ and to a mean-field strength $\chi=1.5$. The TDHF trajectory $\tau(t)$ is obtained after numerical integration of Eq. (4.9) and it has been found that it is periodic with $T_{\rm HF}\sim 4.2$ in units $\hbar/\epsilon$. The maximum $|\tau|$ is about 0.58, while φ stays in the interval [0.17, −0.17].

In Fig. 1, we display the quantity $|a_0|^2 = |\langle 0|\Psi\rangle|^2$ as a function of $t\epsilon/\hbar$ for $N=6$. The solid line corresponds to the complete calculation, while the dashed line gives a second-order correction to TDHF ($|a_0|^2=1$ for all t) obtained as the solution of the coupled equations

$$\dot{a}_0(t) = -i\Omega_{02}(t)a_2(t) \ , \tag{5.1a}$$

$$\dot{a}_2(t) = -i\Omega_{20}(t)a_0(t) - i\Omega_{22}(t)a_2(t) \ . \tag{5.1b}$$

One can easily see that the integrals of these equations reproduce those of the complete system (4.23) to the order $(\Delta t)^2$, i.e., for

$$\Omega_{02}\Omega_{20}(\Delta t)^2 = |\langle 2|V_{\rm res}|0\rangle \Delta t|^2 \ll 1 \ .$$

Since the modulus of the quantity h_2 given by Eq. (4.20c) lies within the interval $[\frac{1}{2},1]$, as can be easily verified, we realize that the second-order correction is valid for

$$\Delta t \ll (1/VN) \sim T_{\rm HF} \ .$$

This is what we see in Fig. 1, that, in addition, gives a quantitative estimate for Δt of about $T_{\rm HF}/8$.

The time interval displayed in this figure approximately corresponds to a full period of the exact motion and to about $5T_{\rm HF}$. One can recognize three different rates of variation of $|a_0|^2$: (i) slow, associated with the exact evolution ($T_{\rm exact}\sim 5T_{\rm HF}$); (ii) medium, associated with the decay of $|a_0|^2$ to about 5 to 6 percent of the TDHF value, ($T_{\rm decay}\sim T_{\rm HF}$) and; (iii) fast, related to the short-time evolution governed by the second-order correction ($T_{\rm short}\sim 0.1T_{\rm HF}$). As mentioned at the end of Sec. IV, the latter measures the rate of departure of $|\Psi(t)\rangle$ with respect to the TDHF state.

A second illustration of the above discussed features of TDHF vs exact dynamics is given in Fig. 2, the same as in Fig. 1, but for a system of $N=10$ fermions. The strength χ, being the same as in the preceding case, implies that we attend to the same TDHF trajectory $\tau(t)$. The decay of the determinant component of the exact wave function occurs at a slower rate ($T_{\rm decay}\sim 2T_{\rm HF}$), while the descriptions based on the second-order approximation are identical in both figures. A possible quantitative explanation of the difference in decay trends, related to the particle number, could be given as follows. We have seen that the short-time evolution of the system is ruled by the second-order correction, actually by the admixture of two particle-two hole

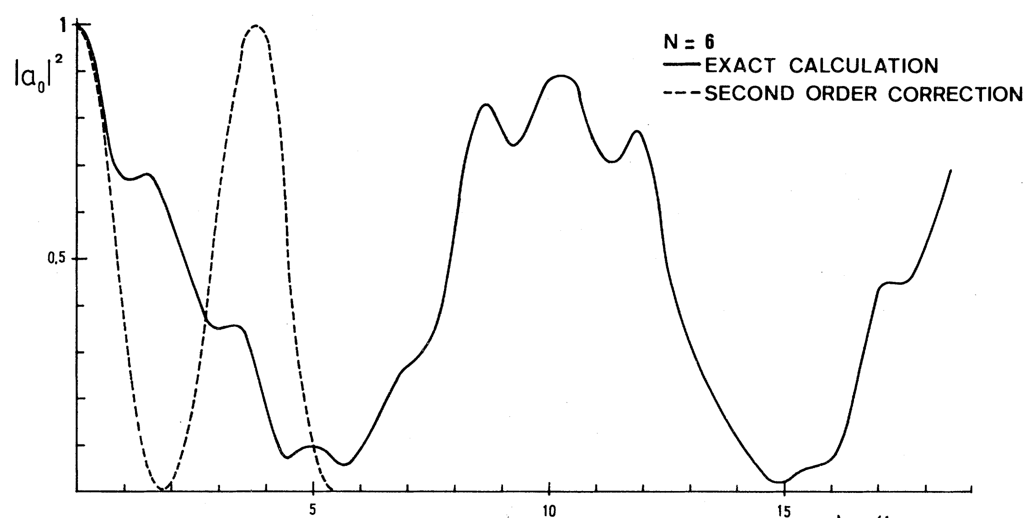

FIG. 1. The weight $|a_0|^2 = |\langle 0|\Psi\rangle^2$ of the TDHF Slater determinant in the exact state vector as a function of time. The solid and dashed lines correspond to the exact calculation and to the second order correction described in Sec. V, respectively. The time unit is $\hbar/\epsilon$ and the particle number is $N-6$.

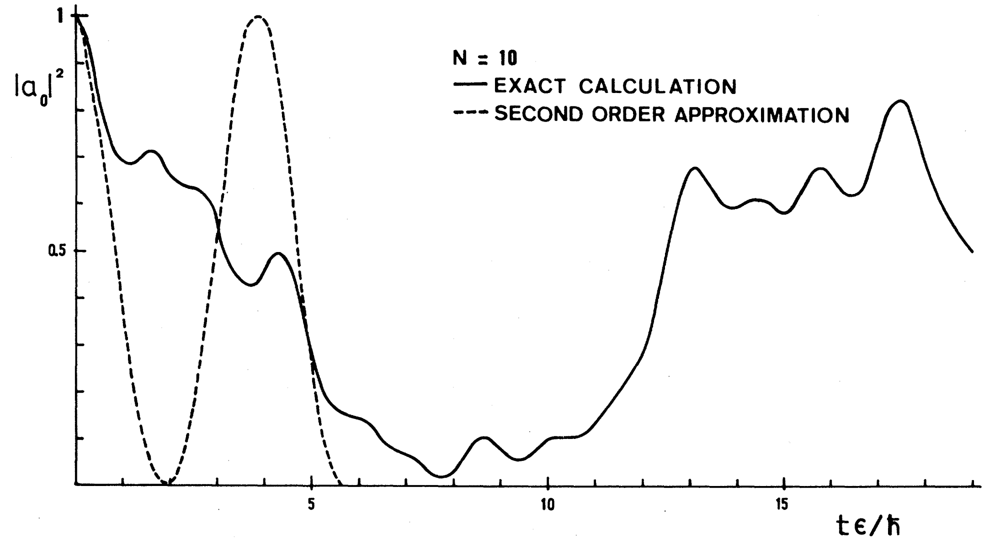

FIG. 2. The same as in Fig. 1, but for $N=10$ particles.

excited configurations in the moving basis into the initial Slater determinant. For even higher times, the "first neighbors" are admitted in the dynamics of $a_2(t)$ through the transition frequencies $\Omega_{2,2\pm2}$ and their effect is propagated into the remaining components. We notice from Eqs. (4.21) that in the vicinity of $k=0$, we have $\Omega_{k,k\pm1}\sim\chi/\sqrt{N}$. From Figs. 1 and 2 we find

$$\frac{T_{\text{decay}}(10)}{T_{\text{decay}}(6)}\sim\frac{1.86}{1.38}\sim1.34\ ,$$

while $\sqrt{10}/\sqrt{6}=1.29$. This estimate suggests that indeed $T_{\text{decay}}\sim\sqrt{N}$, bringing some support to the assertion that the drastic departure of the exact wave function, with respect to the TDHF determinant, is dominated by the excitation of one-particle—one-hole configurations (we always think of excitons in the moving frame). Such a trend would imply

$$T_{\text{decay}}\underset{N\to\infty}{\longrightarrow}\infty\ .$$

It is interesting to study the time evolution of the polarization vector $\langle\Psi|\vec{I}|\Psi\rangle$. Indeed, in the TDHF picture the tip of this vector always lies on the Bloch sphere, i.e.,

$$|\langle0|\vec{I}|0\rangle|=J=N/2\ .$$

In other words, $U_{\text{HF}}(t)$ could be regarded as the generator of tangent displacements. The exact time evolution contains as well those radial displacements directed towards the interior of the sphere, generated by $\hat{U}(t)$. From the preceding discussions we can learn that these radial displacements reflect the fact that the exact wave function, in the course of its evolution, admixes excitons of the moving frame [notice that at any t, the states $|j(t)\rangle$ are eigenstates of I_z, thus being instantaneously aligned with the TDHF state vector]. In Fig. 3, we show both the modulus $|\langle\Psi|\vec{I}|\Psi\rangle|$ and the relative angle

$$\beta=\tan^{-1}(\langle I_x\rangle^2+\langle I_y\rangle^2)^{1/2}/\langle I_z\rangle,$$

between $\langle\Psi|\vec{I}|\Psi\rangle$ and $\langle0|\vec{I}|0\rangle$. These calculations correspond to $N=6$. We can see that during most of the time evolution over about five TDHF periods, the expectation value of the quasispin vector lies on a shell of thickness unity below the surface of the Bloch sphere. On the other hand, an interesting observation is the following: We see from Fig. 1 that after $T_{\text{decay}}\sim5.8\epsilon/\hbar$ has elapsed we reach a minimum of $|a_0|^2$. Now, at this time we find

$$|\langle\vec{I}\rangle|\sim2.96=98.6\%J$$

and $\beta\sim85°$. We could possibly interpret that the proximity of the exact state to the surface of the Bloch sphere is an expression of its will to be a Slater determinant, although not precisely the TDHF one, to which it only assigns a weight of about 0.05 and from which it further distinguishes by orienting the quasispin vector in a quasiorthogonal direction.

As a summary of the inspection of this figure, we can say that, if one selects the parameter $|\langle\Psi|\vec{I}|\Psi\rangle|/J$ as a measure of the degree of

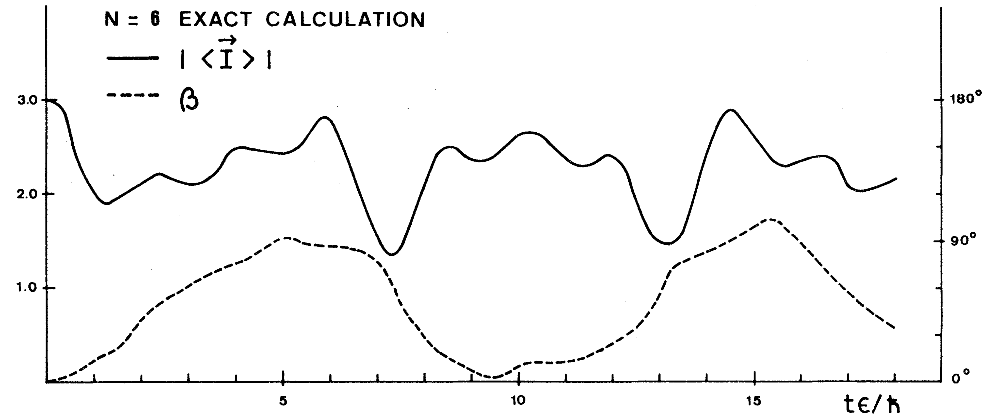

FIG. 3. The modulus and one of the angles relative to the current TDHF position of the exact polarization $\langle \Psi | \vec{I} | \Psi \rangle$. Details are the same as in Fig. 1.

"determinantality" of the exact wave function, it would yield a reasonable 70% for most of the time evolution. What this wave function rather dislikes is the law of motion that the TDHF approach assigns to determinants, since over a time length of the order of $T_{\rm decay}$, it builds up a 90° polarization in the moving TDHF frame. The scale for this process is proportional to $\sqrt{N}/\chi$, as compared to $1/\chi$ that is the typical TDHF period. As a consequence, when N increases towards the thermodynamic limit, it takes an infinite length of time to introduce a noticeable phase shift between exact and TDHF polarizations.

VI. SUMMARY

We have performed a comparison between TDHF and exact dynamics for a two-level system with a finite number of particles interacting via a two-body monopole force (Lipkin model). The exact time dependent wave function has been expanded as a superposition of the TDHF Slater determinant and its k-particle—k-hole excitations. The latter vectors expand a subspace that changes in time in order to keep orthogonality with respect to the former. The trajectory in the mean field is the locus of a point on the Bloch sphere, $\tau(t)$ while the TDHF state vector is an atomic coherent state obtained, at any time t, by a rotation $R(\tau(t))$ of the unperturbed quasispin vector whose tip lies on the south pole. Assuming that the initial state is a determinant or point on the Bloch sphere, deviations of the Schrödinger state vector from the predicted TDHF path are due to the increasing admixture of moving excitons and, from the geometrical point of view, provoke the motion of the average quasispin vector towards the interior of the sphere.

The evolution operator written as the product $U_{\rm HF}(t)\hat{U}(t)$, where $\hat{U}(t)$ is the propagator in the residual interaction representation, supports the geometrical picture and makes room for a quantitative estimate of the validity of the TDHF approach. Indeed, $U(t)$ does not differ significantly from the identity if $t \ll |\Omega_{02}|^{-1}$, where Ω_{02} measures the rate of admixture of two-exciton components. Thus the full motion is essentially a rotation on the Bloch sphere and the polarization $\langle \Psi | \vec{I} | \Psi \rangle$ of the exact wave function remains constant at the initial value (modulus J and direction τ_0). As the competition of 2-particle—2-hole moving excitations becomes important, the motion induced by $U(t)$ contains a large radial component that pulls the polarization towards the interior of the sphere. For even larger times, the total evolution consists of radial-plus-tangential motion due to the residual interaction and proceeding via $\hat{U}(t)$, times the pure tangential HF displacement.

The residual interaction is responsible for two effects with different rates. The frequencies Ω_{02}, Ω_{20} are related to the radial motion, as seen in Figs. 1 and 3, where one can appreciate the decreasing trend of $|\langle \vec{I} \rangle|$ during the interval of validity of the second-order correction. By contrast, the frequencies Ω_{12} (in general, $\Omega_{j,j\pm1}$) are associated with rotations of the polarization vector, taking place at a rate $\chi/\sqrt{N}$ and introducing a phase shift β between the exact and the TDHF quasipins. We pose special emphasis upon this issue since it reflects a general property of exact dynamics, as related to collective motion in the mean field. The Lipkin model is especially adequate to exhibit these two well defined, different ways of departure of full time evolution with respect to TDHF motion, namely, (i) the determinant decay[6] as a consequence of the second-order approximation, plus (ii), the building up of an angular correlation that does not exclude the possibility of determinant regeneration.

We have seen as well that the full wave function differs dramatically from the TDHF state vector after a typical oscillation period of the mean field, T_{HF}. This time could be regarded as an upper bound for the validity of a TDHF description of the motion of quasispin systems. A lower bound is given by the typical time for two-exciton admixture, $|\Omega_{02}|^{-1}$. This agrees with the estimate of the lifetime of a Slater determinant presented by Lichtner and Griffin.[6] The model discussed here possesses a peculiarity, namely that upper and lower bounds coincide. Consequently, severe doubts ought to be raised regarding the use of the Lipkin model for TDHF calculations. In more realistic cases, it would be beneficial to use a previous estimate of the leading admixture rate, before involving oneself in the use of Slater determinant dynamics.

We have illustrated the behavior of the exact polarization and showed that over a period of full motion, its modulus stays mostly above 70% of the Slater determinant parameter, while it can point 90° away from the TDHF trajectory. The fact that the polarization vector lies within a moderately thin shell near the surface of the Bloch sphere suggests that the true wave function is close to a determinant. Now, among the possible orientations of determinants the TDHF trajectory $\tau(t)$ is not the most favored. One is tempted to think of alternatives to the TDHF approximation that coincide in the determinantal picture but differ in the evolution law. In this spirit, several possibilities could be enumerated, whose deeper analysis we postpone for a later work in view of the increasing numerical complexity: (i) the multiconfigurational TDHF approximation, that substitutes the exact wave function by a linear superposition of determinants, and (ii) the maximum overlap criterium[36] to select a determinant, that has been proven to be identical to the variational criterium in the static case, if the bare interaction is replaced by a reaction matrix.

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