Dynamics of the Hubbard model: A general approach by the time-dependent variational principle

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We describe the quantum dynamics of the Hubbard model at the semiclassical level, by implementing the time-dependent variational principle (TDVP) procedure on appropriate macroscopic wave functions constructed in terms of SU(2)-coherent states. Within the TDVP procedure, such states turn out to include a time-dependent quantum phase, part of which can be recognized as Berry's phase. We derive two semiclassical model Hamiltonians for describing the dynamics in the paramagnetic, superconducting, antiferromagnetic and charge-density wave phases and solve the corresponding canonical equations of motion in various cases. Noticeably, a vortexlike ground-state phase dynamics is found to take place for $U>0$ away from half filling. Moreover, it appears that an oscillatorylike ground-state dynamics survives at the Fermi surface at half filling for any U. The low-energy dynamics is also exactly solved by separating fast and slow variables. The role of the time-dependent phase is shown to be particularly interesting in the ordered phases. [S0163-1829(97)02806-3]

I. INTRODUCTION

Interest in strongly correlated itinerant electron systems has been constantly growing in the last three decades. Especially since the discovery (almost ten years ago) of high-T_c superconductors, an enormous amount of work has been devoted to such systems, aimed both at investigating their macroscopic thermodynamical properties via experimental measurements, and to disclose—by employing the standard methods of statistical mechanics—what type of macroscopic collective order is responsible for the frictionless regime.

Nevertheless, due to the high number of variables naturally involved in the models proposed for investigating these many-electron systems, and probably to the background of the community of physicists who first considered these models, to the best of our knowledge very little effort has been made in order to investigate their dynamical behavior. On the other hand, this type of analysis is known to lead to interesting properties of superfluidity when applied, for instance, to the BCS Hamiltonian.[1]

Two circumstances, at least, prompt us to attempt the dynamical approach and to carefully consider its possible developments. First of all, standard theoretical techniques such as the time-dependent variational principle (TDVP) procedure and its path-integral version, the stationary phase approximation method, have been remarkably developed in the recent years, by exploiting the notion of the generalized coherent state[2] (GCS) and the spectrum generating (or dynamical) algebra method. At the formal level, such group-theoretical tools have greatly simplified and provided of a systematic character the TDVP procedure, which essentially consists of reducing the system quantum dynamics to a semiclassical Hamiltonian form. The procedure, formulated, for example, in the form of Refs. 3 and 4, was introduced for studying the low-lying collective states in nuclei, but it is easily extended also to any systems endowed with a large number of degrees of freedom.

Furthermore the special role assigned to the quantum phase of the macroscopic trial wave function involved within the TDVP framework makes the procedure even more attractive. Such a quantum phase, in fact, is structured so as to have a memory of the entire dynamical behavior. It is thus natural to expect some kind of correlation between the type of microscopic order which possibly characterizes the medium and the phase time behavior. Such effects have been, for instance, investigated in Ref. 5, where the study of quantum dynamics of solitons in ferromagnets was shown to have remarkable consequences on Berry phase behavior.

This aspect, in turn, directly leads to the second circumstance which motivates our interest for the dynamical viewpoint. At low temperature, one can reasonably think of performing current measurements or superconductive quantum interference measurements based on experimental devices similar to the ones employed to investigate the *Josephson effect*.[6,7] It is essential recalling that, in that case, the time dependence of the order parameter (the macroscopic wave function of the system) has a crucial role in allowing for the detection of microscopic phenomena occurring in the medium. Although the TDVP approach is able to take into account a large number of dynamical degrees of freedom, and is thus able to describe a strongly correlated electron gas, one can expect that low excited states actually involve a restricted number of dynamical variables. Under such conditions the quantum phase could retain a nonrandom character which makes it suitable for experimental measurements.

A further quality of the TDVP approach must be still pointed out. Such a scheme, in fact, involves the construction of semiclassical Hamiltonians which are obtained in a completely independent way with respect to the model Hamiltonians derived by standard mean-field techniques of statistical mechanics (for instance, Hartree-Fock). The ground state of the semiclassical Hamiltonian reproduces, as we shall see, the same results of the Hartree-Fock approach from the set of dynamical fixed points. Moreover, as opposite to the mean-field cases, here also the excited states at low energy are

expected to be a realistic description of those of the original model Hamiltonian. This character is related with the fact that TDVP Hamiltonians, even though affected by the approximations imposed by the method, generally preserve a structure rather faithful to the second quantized Hamiltonian. Comparison with statistical mechanics approximate models is thus interesting in any case.

In this paper we propose the implementation of an appropriate generalization of TDVP to itinerant interacting electron systems. This amounts to applying the TDVP to a trial wave function representing a semiclassical macroscopic state constructed by generalized coherent states of the dynamical algebra of the model Hamiltonian.[2,3] From the semiclassical picture of the system obtained in this way one can derive canonical equations of motion, and a classical description of the system's dynamics. A key role within this approach is played by a time-dependent phase, which has to be fixed so as to satisfy, at least in average, the Schrödinger equation. In Ref. 4 it was shown that, under appropriate assumptions, the latter is nothing but the dynamical plus geometric phases[9] beyond the adiabatic approximation.

Here we apply the above method to the Hubbard model,[8] described by the Hamiltonian

$$H_{\mathrm{Hub}}=-T\sum_{\langle \mathbf{i},\mathbf{j}\rangle}\sum_{\sigma} c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma}+U\sum_{\mathbf{i}} n_{\mathbf{i},\uparrow}n_{\mathbf{i},\downarrow}-\mu\sum_{\mathbf{i}}(n_{\mathbf{i},\uparrow}+n_{\mathbf{i},\downarrow})$$

$$=\sum_{\mathbf{k},\sigma}(\epsilon_{\mathbf{k}}-\mu)n_{\mathbf{k},\sigma}+U\sum_{\mathbf{k},\mathbf{l},\mathbf{m}} a^{\dagger}_{\mathbf{k},\uparrow}a^{\dagger}_{\mathbf{m},\downarrow}a_{\mathbf{l},\downarrow}a_{\mathbf{k}+\mathbf{m}-\mathbf{l},\uparrow}, \quad (1)$$

where, on the first line, $c^{\dagger}_{\mathbf{i},\sigma}, c_{\mathbf{j},\sigma}$ are fermionic creation and annihilation operators $(\{c_{\mathbf{j},\sigma},c_{\mathbf{i},\sigma'}\}=0,\{c_{\mathbf{j},\sigma},c^{\dagger}_{\mathbf{i},\sigma'}\}=\delta_{\mathbf{i},\mathbf{j}}\,\delta_{\sigma,\sigma'}\mathbb{I}$, $n_{\mathbf{i},\sigma}\doteq c^{\dagger}_{\mathbf{i},\sigma}c_{\mathbf{i},\sigma})$ on a d-dimensional lattice Λ $(\mathbf{i},\mathbf{j}\in\Lambda,\ \sigma\in\{\Uparrow,\Downarrow\})$ with N sites, and $\langle \mathbf{i},\mathbf{j}\rangle$ stands for nearest neighbors in Λ. In the second line the same Hamiltonian is rewritten in the reciprocal space $\tilde{\Lambda}$, with $a_{\mathbf{k},\sigma}\doteq\Sigma_{\mathbf{j}}e^{i\pi\mathbf{j}\cdot\mathbf{k}}c_{\mathbf{j},\sigma}$, $\epsilon_{\mathbf{k}}\doteq -2T\sum_{r=1}^{d}\cos k_r$. In Eq. (1) the first term represents the tight-binding band energy of the electrons (T being the hopping amplitude), the U term describes their on-site Coulomb interaction, and μ is the chemical potential, which will allow us to fix the conserved quantity $\mathcal{N}_e=\Sigma_{\mathbf{i}}(n_{\mathbf{i},\uparrow}+n_{\mathbf{i},\downarrow})$, i.e., the total electron number operator on the lattice.

Since the GCS of the dynamical algebra of Hamiltonian (1) is quite complex to deal with, we choose as trial GCS's for constructing the semiclassical macroscopic state the SU(2) coherent states which are exact for the corresponding Hartree-Fock Hamiltonian. This is done for two different cases, namely that describing superconducting (SC) and paramagnetic phases, and, at half-filling, that describing antiferromagnetic (AF) and charge-density-wave (CDW) phases. The approximate equations of motion we obtain for the full Hamiltonian in the two cases are then solved in some integrable cases, and by approximate methods in other interesting limits. This gives rise to a variety of different dynamical behaviors, from vortexlike dynamics in the ground state for the $U>0$, $n\neq 1$ regime, to oscillations of the number of electrons around the Fermi surface and possible laser effect at low energy, and to single-mode collective frequency dynamics, which should reflect the occurrence of macroscopic order in the medium. In particular, the time-dependent phase, which—due to its macroscopic nature—can be considered as an observable quantity, exhibits a behavior which is shown to be related to the nonvanishing of order parameters, and is evaluated exactly in several situations.

The paper is organized as follows. In Sec. II we review the generalized TDVP approach and its connections with the quantum geometric phase. In Sec. III we treat explicitly the SC-paramagnetic case, by constructing first the macroscopic trial wave function and the corresponding semiclassical Hamiltonian, and deriving then the canonical equations of motion with the time-dependent phase factor. Section IV is devoted to studying the fixed points of these equations and in particular the ground-state solutions and metastable states; obtaining for the ground state the Hartree-Fock results as well as a nontrivial vortexlike dynamics in the so-called paramagnetic phase, and topological excitations for the metastable states. In Sec. V we analyze an integrable case, which exhibits collective order and nonzero pairing induced by the k-mode interactions. In Sec. VI we investigate the global dynamics by comparing slow with fast degrees of freedom. We show how slow variables tend to constitute an autonomous subsystem which drives fast variable dynamics on large time scales. An integrable case where the slow subsystem is reduced to a two-level system representing k modes close to the Fermi level, is explicitly solved in Sec. VII. In Sec. VIII we repeat some of the above analysis for the AF phase at half-filling, finding in particular an oscillating behavior at the Fermi surface. The final section is devoted to some conclusions.

II. GENERALIZED TDVP METHOD

Knowledge of the dynamical algebra $\mathcal{G}$ of a given (time-independent) Hamiltonian H allows the construction of an over-complete set of states known as generalized coherent states,

$$|\Phi_0\rangle=\exp\left[\sum_{\alpha}(\theta_{\alpha}E_{\alpha}-\theta^{*}_{\alpha}E_{-\alpha})\right]|0\rangle,$$

where $\{E_{\alpha},E_{-\alpha}\}$ are the raising and lowering operators in the Cartan representation of $\mathcal{G}$, and $|0\rangle$ is the highest weight of the representation, defined by $E_{-\alpha}|0\rangle=0$ for all positive α's. The state $|\Phi(t)\rangle$, which is the obvious time-dependent generalization of $|\Phi_0\rangle$,

$$|\Phi(t)\rangle=\exp\left[\sum_{\alpha}(\theta_{\alpha}(t)E_{\alpha}-\theta_{\alpha}(t)^{*}E_{-\alpha})\right]|0\rangle,$$

is related to the time evolution of $|\Phi_0\rangle$, described by the state $|\Psi(t)\rangle\doteq e^{-(i/\hbar)Ht}|\Phi_0\rangle$, through

$$|\Psi(t)\rangle\equiv e^{i[\varphi(t)/\hbar]}|\Phi(t)\rangle, \quad (2)$$

where

$$\varphi\doteq -\mathcal{H}t+i\hbar\int_0^t d\tau\left\langle\Phi(\tau)\left|\frac{\partial}{\partial\tau}\right|\Phi(\tau)\right\rangle, \quad (3)$$

and $\mathcal{H}=\langle\Phi(t)|H|\Phi(t)\rangle$.

The time dependence of the parameters $\theta_{\alpha}(t)$'s is determined by imposing that $|\Psi(t)\rangle$, as given by Eq. (2), satisfies

the Schrödinger equation. It turns out that this amounts to requiring the $\theta_\alpha(t)$'s obey the canonical equation of motion (see below). An alternative parametrization for the state $|\Phi(t)\rangle$ can be used, namely

$$|\Phi(t)\rangle = \mathcal{N}^{-1/2}\exp\left(\sum_{\alpha>0} z_\alpha(t) E_\alpha\right)|0\rangle, \tag{4}$$

$\mathcal{N}$ being the normalization factor, such that $\langle\Phi(t)|\Phi(t)\rangle = 1$. In this case the canonical equations of motion read[4]

$$i\hbar\sum_\beta g_{\alpha,\beta}\dot{z}_\beta = \frac{\partial\mathcal{H}}{\partial z_\alpha^*}\ , \quad i\hbar\sum_\beta g_{\alpha,\beta}^*\dot{z}_\beta^* = -\frac{\partial\mathcal{H}}{\partial z_\alpha}\ , \tag{5}$$

where $g_{\alpha,\beta} = \partial^2 \ln\mathcal{N}/\partial z_\alpha^* \partial z_\beta$ is the metric of the phase space spanned by $\{z_\alpha, z_\alpha^*\}$, and determines its symplectic structure. The metric $g_{\alpha,\beta}$ indeed determines the explicit form of Poisson's brackets,

$$\{A,B\}_{\mathrm{PB}} = \sum_{\alpha,\beta} i\hbar (g^{-1})_{\alpha,\beta}\left(\frac{\partial A}{\partial z_\alpha^*}\frac{\partial B}{\partial z_\beta} - \frac{\partial A}{\partial z_\beta}\frac{\partial B}{\partial z_\alpha^*}\right), \tag{6}$$

where g^{-1} represents the inverse matrix of g.

If the algebra $\mathcal{G}$ is the full dynamical algebra of H (i.e., if $H \in \mathcal{G}$ for any choice of the physical parameters) the above procedure is exact. In particular, it gives the exact quantum ground state of H as the fixed point of equations (5). Nevertheless, in a many-body problem like the one described by the Hamiltonian (1) the dimension of the dynamical algebra is exponentially growing with N, and infinite in the thermodynamical limit. Even though one may still work out the canonical equations of motion,[12] their explicit solution becomes then quite hard to handle. It is therefore reasonable to inquire to which extent the above scheme can be used in the case where the GCS are built in a subalgebra $\mathcal{A} \subset \mathcal{G}$ for which the equations of motion become tractable. In this case, of course, $|\Psi(t)\rangle$ as given by Eq. (2), differs from $e^{-(i/\hbar)Ht}|\Phi_0\rangle$, and the Schrödinger equation is in general not satisfied. Nevertheless, the answer given by the generalized TDVP approach[4] is that in fact the above scheme still holds also in this case, if one just requires that at least the inner product of the Schrödinger equation for $|\Psi(t)\rangle$ with $\langle\Psi(t)|$ vanishes, i.e.,

$$\left\langle \Psi(t)\left|\left(i\hbar\frac{\partial}{\partial t} - H\right)\right|\Psi(t)\right\rangle = 0. \tag{7}$$

Notice that now $|\Psi(t)\rangle$ is to be built only with the raising operators $E_\alpha \in \mathcal{A}$. Hence the analogy with the exact solution (2)–(5) (where $E_\alpha \in \mathcal{G}$) is complete at a formal level, but approximate in the results, $\mathcal{H}$ being evaluated on a subspace of the whole dynamical algebra $\mathcal{G}$. Nevertheless, as for the reliability of the method, one should recall that in the limit $\hbar \to 0$ the results obtained within TDVP become exact (to second order in $\hbar$), meaning that one obtains the classical description of the system dynamics.

Both in the exact case, and in the TDVP approximation, the role of phase $\varphi(t)$ given by Eq. (3) is particularly simple at the fixed points of Eq. (5). In fact in this case $|\Phi(t)\rangle$ is independent of t, and the second term at the right-hand side (rhs) of Eq. (3) (the so-called kinetic term) is vanishing. This implies that $|\Psi(t)\rangle = \exp(-(i/\hbar)\mathcal{H}t)|\Phi_0\rangle$ is uniquely determined by the energy pertaining to the initial state $|\Phi_0\rangle$. Such behavior is very reminiscent of what is called the dynamical phase for a time-dependent Hamiltonian in the adiabatic approximation. More generally, by inserting Eq. (3) into the expression (2) for the state $|\Psi(t)\rangle$, the latter can be written as

$$|\Psi(t)\rangle = \exp\left[\frac{i}{\hbar}\int dt\left(-\mathcal{H} + i\hbar\left\langle\Phi(t)\left|\frac{\partial}{\partial t}\right|\Phi(t)\right\rangle\right)\right]|\Phi(t)\rangle, \tag{8}$$

and we recognize a formal analogy between the phase $\varphi(t)$ and the dynamical plus geometric phase in the adiabatic approximation (for a derivation of the quantum phase beyond the adiabatic approximation, see for instance Ref. 10). More precisely, in Eq. (8) we can identify the first term in the exponential with the dynamical phase, and the other (kinetic) term as the geometric phase obtained by relaxing some of the hypotheses of the adiabatic approximation. We recall that the latter is nothing but the so-called Berry[11] phase. In fact in some simple exactly solvable case[4] it was shown that—by imposing appropriate quantization condition—the phase (3) does coincide with the geometric plus dynamical phases even if evaluated within the generalized TDVP approximation scheme. This leads us to expect that the present approach, apart from leading to a simplified, if approximate, description of the dynamics of the Hubbard model, may give a precise physical information, i.e., which is the Berry phase of the states we are studying. If this is the case, we expect that whenever we shall obtain states with the same energy $\mathcal{H}$ but different phases $\varphi(t)$, an appropriate physical device should be able to observe their interference.

A further investigation of this relationship for the model discussed here is beyond the purpose of the present paper. Here we want just to emphasize that the state $|\Psi(t)\rangle$, thanks to its phase $\varphi(t)$, is able in principle to approximate the wave function of the full model Hamiltonian, no matter how small the subalgebra $\mathcal{A}$ of $\mathcal{G}$. However, we expect in general that the results will be more reliable the more $\mathcal{A}$ is a reasonable description of $\mathcal{G}$, i.e., the more the Hamiltonian is in a (thermodynamical) phase in which the relevant operators are contained in $\mathcal{A}$. It will turn out that precisely $\varphi(t)$ will measure how far the system is from the states generated by $\mathcal{A}$. In particular, we expect that the system is correctly described by $\mathcal{A}$ whenever $\varphi(t)$ happens to be linearly increasing with time, in that the wave function $|\Psi(t)\rangle$ which satisfies Eq. (7) results to differ by the one we constructed in $\mathcal{A}$ $(|\Phi(t)\rangle)$ just for an oscillating phase factor.

III. SEMICLASSICAL EQUATIONS OF MOTION IN SC PHASE

The model described by Eq. (1), has been intensively studied in the literature.[13] However, as for most many-electron problems, it is quite difficult to obtain rigorous results (for a recent review, see Ref. 14). In particular, only the one-dimensional zero-temperature energy is known exactly.[15] Therefore, different approximation schemes have been used in order to deal with Eq. (1). Among them, a standard one is the Hartree-Fock decoupling procedure,

which amounts to approximating the interaction term by reducing it to a sum of its bilinear parts, weighted by coefficients which have to be fixed self-consistently. There are of course different ways of decoupling the interaction term, depending on the phase which has to be investigated.[6,17]. The dimension of the dynamical algebra of the resulting ''decoupled'' Hamiltonian turns out to be greatly reduced, and to all effects one is lead to deal with a subalgebra of the spectrum generating algebra of the original Hamiltonian. It is our purpose to construct the GCS involved by the TDVP scheme in these subalgebras.

In order to identify the subalgebra, we explicitly need the reduced Hamiltonian. Neglecting for the moment the possibility of an AF or a CDW phase (which will be investigated in a later section) and of a ferromagnetic phase (which is not to be expected at low U), it turns out that such a Hamiltonian coincides with the linearized Hamiltonian $H_l^{(\mathrm{sc})}=\Sigma_k H_k^{(\mathrm{sc})}$ where

$$H_k^{(\mathrm{sc})}=(\epsilon_k-\mu)n_k+U\left[\frac{n}{2}n_k+(\Delta a_k^\dagger a_{-k}^\dagger+\mathrm{H.c.})\right]-U\left(\frac{n^2}{4}N+|\Delta|^2\right)N.$$

Here, as customary, k stays for the multi-index $(\mathbf{k},\sigma)$ $[k\equiv(\mathbf{k},\uparrow),\ -k\equiv(-\mathbf{k},\downarrow)]$, and $n_k\doteq a_k^\dagger a_k$. Moreover n is the average electron number per site, $n=\langle\mathcal{N}_e\rangle/N$, and $\Delta\doteq\langle\Sigma_k a_{-k}a_k\rangle/N$ is the average pairing per site, where $\langle\bullet\rangle$ denotes the expectation value of operator $\bullet$ over appropriate states.

It is important noticing that $H_l^{(\mathrm{sc})}$, contrary to H_{Hub}, for any $\Delta\neq0$ does not commute with the electron-number operator per site $\mathcal{N}_e$. This is justified by observing that $H_l^{(\mathrm{sc})}$ is a faithful approximation of H_{Hub} in an ordered phase which does not conserve such quantity (namely, the superconducting phase). On the other hand, for $\Delta=0$ $\mathcal{N}_e$ is still conserved, and $H_l^{(\mathrm{sc})}$ describes in that case the system in a paramagnetic phase, which is known to be the case for the ground state, at least for low positive U, away from half filling (i.e., $n\neq1$).

The Hamiltonians $H_k^{(\mathrm{sc})}$'s have the property that $[H_k^{(\mathrm{sc})},H_{k'}^{(\mathrm{sc})}]=0$, and hence can be diagonalized simultaneously. More precisely, $H_l^{(\mathrm{sc})}$ turns out to be an element of the dynamical algebra $\mathcal{A}_{\mathrm{sc}}=\oplus_k\mathcal{A}_k^{(\mathrm{sc})}$, where $\mathcal{A}_k^{(\mathrm{sc})}$ is the local SU(2) generated by

$$\mathcal{A}_k^{(\mathrm{sc})}=\left\{J_3^{(k)}\equiv\frac{1}{2}(n_k+n_{-k}-1),J_+^{(k)}\equiv a_k^\dagger a_{-k}^\dagger,J_-^{(k)}\equiv a_{-k}a_k\right\}. \tag{9}$$

Any eigenstate of the Hamiltonian $H_l^{(\mathrm{sc})}$ can then be expressed as superposition of the GCSs of $\mathcal{A}_{\mathrm{sc}}$, namely

$$|\eta\rangle=\Pi_k(1+\overline{\eta_k}\eta_k)^{-1/2}\exp(\eta_k J_+^{(k)})|0\rangle_{\mathrm{sc}},$$

where the coefficients $\eta_k\in\mathbb{C}$ parametrize the (overcomplete) set of exact GCS of $H_k^{(\mathrm{sc})}$ and $|0\rangle_{\mathrm{sc}}$ is the electron vacuum.

In line with the general approach discussed in the previous section we can think of the η_k's as time-dependent parameters, and construct the approximate trial time-dependent wave function of the full Hamiltonian H_{Hub}, $|\psi(t)\rangle_{\mathrm{sc}}$, as

$$|\psi(t)\rangle_{\mathrm{sc}}=e^{(i/\hbar)\varphi_{\mathrm{sc}}(t)}|\eta(t)\rangle. \tag{10}$$

We are now ready for evaluating the expectation value of H_{Hub} over $|\psi(t)\rangle_{\mathrm{sc}}$, namely the semiclassical Hamiltonian $\mathcal{H}_{\mathrm{sc}}$, which reads

$$\mathcal{H}_{\mathrm{sc}}=2\sum_k(\epsilon_k-\mu)\frac{\overline{\eta_k}\eta_k}{1+\overline{\eta_k}\eta_k}+U\left[\left(\sum_k\frac{\overline{\eta_k}\eta_k}{1+\overline{\eta_k}\eta_k}\right)^2+\sum_{k,l}\frac{\overline{\eta_k}\eta_l}{(1+\overline{\eta_k}\eta_k)(1+\overline{\eta_l}\eta_l)}\right], \tag{11}$$

where η_k, $\overline{\eta_k}$ obey the Poisson-bracket relations obtained from Eq. (6), $i\hbar\{\eta_k,\overline{\eta_k}\}=(1+\overline{\eta_k}\eta_k)^2$.

Instead of proceeding directly to the derivation of the canonical equations of motion, we notice that Hamiltonian (11) can be fruitfully rewritten in terms of the following semiclassical pseudospin variables

$$S_3^{(k)}\doteq\frac{1}{2}\frac{\overline{\eta_k}\eta_k-1}{\overline{\eta_k}\eta_k+1}\equiv{}_{\mathrm{sc}}\langle\phi(t)|J_3^{(k)}|\phi(t)\rangle_{\mathrm{sc}},$$

$$S_+^{(k)}\doteq\frac{\overline{\eta_k}}{1+\overline{\eta_k}\eta_k}\equiv{}_{\mathrm{sc}}\langle\phi(t)|J_+^{(k)}|\phi(t)\rangle_{\mathrm{sc}}, \tag{12}$$

and $S_-^{(k)}=(S_+^{(k)})^*$, whose Poisson brackets recover for each k a SU(2)$_k$ algebra. Explicitly

$$i\hbar\{S_+^{(k)},S_-^{(k)}\}=2S_3^{(k)},\quad i\hbar\{S_\pm^{(k)},S_3^{(k)}\}=\mp S_\pm^{(k)}. \tag{13}$$

Moreover, one can define the related ''mesoscopic'' variables $S_\alpha^{(a)}\doteq\Sigma_{k\in\tilde{\Lambda}_a}S_\alpha^{(k)}$, with $\alpha=3,+,-$, $\tilde{\Lambda}_a\doteq\{k\in\tilde{\Lambda};\ \epsilon_k=\epsilon_a\}$ denoting the mesoscopic (kinetic energy) levels. One can easily verify that the $S_\alpha^{(a)}$'s form a SU(2) algebra like Eq. (13) (with $k\to a$), which we identify by SU(2)$_a$. Hamiltonian (11), when written in terms of $S_\alpha^{(a)}$, reduces to a genuine one-dimensional problem, in that the index a (contrary to k) is strictly one-dimensional, numbering the different mesoscopic levels. Indeed

$$\mathcal{H}_{\mathrm{sc}}=2\sum_a(\epsilon_a-\mu)\left(S_3^{(a)}+\frac{N_a}{2}\right)+u\left[\left(S_3+\frac{N}{2}\right)^2+\left|S_+\right|^2\right]. \tag{14}$$

Here $S_\alpha\doteq\Sigma_a S_\alpha^{(a)}\equiv\Sigma_k S_\alpha^{(k)}$, and $u=U/N$. The Casimir operators of both SU(2)$_k$ and SU(2)$_a$ algebras, $I_k\doteq|S_+^{(k)}|^2+|S_3^{(k)}|^2$ (and the same definition for I_a with k replaced by a) are conserved quantities for $\mathcal{H}_{\mathrm{sc}}$. In view of the definitions (12), $I_k=1/4$, and $I_a\leq N_a^2/4$, depending on the initial conditions.

Noticeably, Hamiltonian (14), like H and unlike $H_l^{(\mathrm{sc})}$, commutes also with S_3, i.e., the semiclassical variable corresponding to the total electron number operator. S_3 is thus, as it should be, a conserved quantity, for which the relation holds

$$S_3=\frac{N}{2}(n-1). \tag{15}$$

In this sense we can therefore claim that the $1-d$ Hamiltonian $\mathcal{H}_{\rm sc}$ obtained by means of the present semiclassical approach is a more accurate approximation of H than $H_l^{(\rm sc)}$, In particular, in Eq. (14) the k modes are coupled dynamically through $|S_+|^2$, while in $\mathcal{H}_l^{(\rm sc)}$ they are not. This feature in turn keeps track in the present scheme of the nonlinearity of $H_{\rm Hub}$, thus making $\mathcal{H}_{\rm sc}$ a good candidate for giving an approximate description of the physics of the Hubbard model in the whole phase space. Of course, the results obtained by using instead $H_l^{(\rm sc)}$ will be reproduced by the present approximation, as we shall see in the next section.

From Eqs. (13) and (14) we can now derive the equations of motion for the mesoscopic variables $S_\alpha^{(a)}$, which read

$$\mp i\hbar \dot{S}_\pm^{(a)} = \delta_a S_\pm^{(a)} - 2u S_3^{(a)} S_\pm$$

$$i\hbar \dot{S}_3^{(a)} = u(S_- S_+^{(a)} - S_+ S_-^{(a)}). \tag{16}$$

Here $\delta_a = 2(\epsilon_a - \mu) + unN$, where the constant factor $unN - 2\mu$ in δ_a is vanishing at half-filling ($\mu = U/2$, $n=1$), and in any case does not affect the dynamics described by $S_\pm^{(a)}$, apart from an overall phase factor $e^{\pm i/\hbar(Un-2\mu)\tau}$. Notice that of the three equations (16) only two are independent, whereas the third one is obtained from the Casimir constraint. For instance, one could use as independent variables $S_3^{(a)}$, which fixes also the absolute value of $S_\pm^{(a)}$, and the phase λ_a of $S_\pm^{(a)} = |S_\pm^{(a)}| e^{\pm i\lambda_a}$. This alternative representation of the pseudospin variables will also be considered, when useful, in the text.

Let us emphasize that the true dynamical variables are, of course, the microscopic canonical variables $S_\alpha^{(k)}$, which satisfy the same equations of motion (16) with a replaced by k. Here we preferred to write them only for the mesoscopic variables $S_\alpha^{(a)}$ because the Hamiltonian $\mathcal{H}_{\rm sc}$ given by Eq. (11) was shown to be degenerate with respect to the inner dynamics of the mesoscopic variables. Moreover every solution we will be able to find for the $S_\pm^{(a)}$'s holds straightforwardly also for the $S_\pm^{(k)}$'s, as $\delta_k \equiv \delta_a$. In fact, apart from this simple case, every solution for the microscopic variables can be, in principle, worked out once we have found the mesoscopic solutions, and consequently $S_\pm$, as in this case equations (16) with $a \to k$ reduce to a linear system with time-dependent coefficients. Interestingly, it is easily verified from Eq. (16) that the scalar product of any two microscopic pseudospin vectors $\mathbf{S}^{(k)}$ belonging to the same mesoscopic level is constant. This observation implies that in fact the time evolution of every microscopic vector in a given mesoscopic level is identical, the relative orientation of different $\mathbf{S}^{(k)}(t)$ depending only on the initial conditions.

According to the generalized TDVP approach introduced in previous section, and by means of Eqs. (3), (12), (14), and (16), we are finally able to obtain the time derivative of the time-dependent phase $\varphi_{\rm sc}(t)$,

$$\begin{aligned}\dot{\varphi}_{\rm sc} &= -\mathcal{H}_{\rm sc} + i\hbar \sum_k \frac{\dot{S}_-^{(k)} S_+^{(k)} - \dot{S}_+^{(k)} S_-^{(k)}}{1 - 2S_3^{(k)}} \\ &= u\left[n^2 \frac{N^2}{4} - \left(S_+ \sum_k S_-^{(k)} \frac{1 + 2S_3^{(k)}}{1 - 2S_3^{(k)}} + \text{c.c.} \right) \right] \\ &= -\mathcal{H}_{\rm sc} + \frac{1}{2}\hbar \sum_k (1 + 2S_3^{(k)}) \dot{\lambda}_k \ , \end{aligned} \tag{17}$$

where the last expression was explicitly written to make evident that a nonvanishing geometric contribution to $\varphi_{\rm sc}$ is expected whenever the phase λ_k of $S_\pm^{(k)}$ is not constant.

Equation (17) has some other relevant features which it is worth underlying:

(i) it vanishes for vanishing u, as can be recognized from the second line form. In fact we know that if this is the case the wave function given by Eq. (10) becomes exact, and according to the discussion developed in the previous section this implies that $\varphi_{\rm sc}(t)$ must reduce to the exact value given by Eq. (3), which can be shown to be zero;

(ii) it reduces to the constant $un^2(N^2/4)$ for $S_+ = 0$. Since S_+ is related through Eq. (12) to the semiclassical analog of the total pairing operator, it must be inferred that a nonlinear time behavior of $\varphi_{\rm sc}(t)$ is closely connected to the possible superconductivity of the state;

(iii) contrary to both $\mathcal{H}_{\rm sc}$ and the equations of motion (16), $\varphi_{\rm sc}(t)$ cannot be expressed only in terms of the one-dimensional mesoscopic variables $S_\alpha^{(a)}$. This means that it maintains the memory of the inherent complexity of the original Hamiltonian, and gives information about the time evolution of its wave function which goes beyond that implicit in its semiclassical approximation (14), in particular depending on the inner dynamics of the mesoscopic levels a.

IV. FIXED POINTS AND STATIONARY POINTS

The first step in investigating the dynamical behavior of any nonlinear Hamiltonian system usually consists of finding its fixed points, that is those points in phase space where the equation of motions involve vanishing time derivatives of the dynamical variables. The stability analysis of such a set of points leads to revealing their topological nature (by resorting, for example, to standard methods such as Routh-Hurwitz criterion) and, in conclusion, to structuring the phase space in regions where the dynamical behavior of the system exhibits well defined features.[18]

A complete stability analysis is beyond the scope of present work. In fact, in this section we shall simply work out all the solutions to fixed-point equations, in particular showing that indeed those among them which minimize the energy $\mathcal{H}_{\rm sc}$ give the same energy and the same self-consistency equation as the Hartree-Fock approximation, both for $u \leqslant 0$ and for $u \geqslant 0$. Apart from that, the knowledge of the fixed points allows us, in principle, to look for other solutions of Eq. (16) by means of standard perturbative methods in their proximity.

Minimum energy points are contained among the stationary points of $\mathcal{H}_{\rm sc}$, which are easily shown to coincide with fixed points of Eq. (16) first by rewriting the equations of

motions in terms of canonical variables $(S_3^{(a)},\lambda_a)$, and by setting then $\dot{\lambda}_a=0,\dot{S}_3^{(a)}=0$. Since this is equivalent to $\dot{S}_+^{(a)}=0$ and $\dot{S}_3^{(a)}=0$, Eqs. (16) furnish the stationary point equations

$$0=\delta_a S_+^{(a)}-2uS_3^{(a)}S_+ ,$$

$$0=S_+^{(a)}S_- -S_-^{(a)}S_+ . \tag{18}$$

The case in which $S_+^{(a)}=0$ for any a represents the simplest possible solution. We observe that $S_3^{(a)}$, thanks to the Casimir's constraint, can be chosen in a fully arbitrary way within the interval $-N_a/2\leqslant S_3^{(a)}\leqslant N_a/2$, so that an enormous number of stationary points characterizes the mesoscopic pseudospin dynamics.

It is important noticing that the solution $S_\pm^{(a)}=0$, when inserted in the equations for the microscopic variables, makes them immediately integrable, and the solution shows that in general a microscopic, inner dynamics for k pseudospins $\in\tilde{\Lambda}_a$ can take place, according to

$$S_+^{(k)}(t)=S_+^{(k)}(0)e^{it(\delta_a/\hbar)} , \tag{19}$$

provided $\Sigma_{k\in\tilde{\Lambda}_a}S_+^{(k)}(0)\doteq\Sigma_{k\in\tilde{\Lambda}_a}Re^{i\lambda_k(0)}=0$. Such a constraint in $d=2$ is naturally obeyed by those configurations where the initial phase $\lambda_k(0)$ is topologically nontrivial, while R is independent of k. Indeed this is the case when $\lambda_k(0)$—regarded as a function of k along the 1-d closed paths associated with each ath mesoscopic level—undergoes a variation of $2\pi p$, with $p\in\mathbb{N}$. For paths with energy $\epsilon_a\simeq 0$ the number of modes N_a is great enough to allow $e^{i\lambda_k(0)}$ to be twisted many times in a quasicontinuous way. Let us underline that solution (19), which, being consistent with $S_\pm^{(a)}=0$, corresponds to a stationary point of $\mathcal{H}_{\rm sc}$, is not a fixed point of the microscopic dynamics when $S_\pm^{(k)}(0)\neq 0$.

The energy associated with the solution $S_+=0$ has the form $E=-u(S_3+N/2)^2+\Sigma_a\delta_a(S_3^{(a)}+N_a/2)$. For $u>0$ it is easy to check that an absolute minimum endowed with the energy

$$E_{\rm sc}^{(+)}=-un^2\frac{N^2}{4}-\sum_{a>F}|\delta_a|N_a \tag{20}$$

is reached when $S_3^{(a)}=+(-)N_a/2$ for $a>F$ $(a<F)$ is imposed, F being that particular value of a for which $\delta_F=0$, which implies $\mu=\epsilon_F+U(n/2)$, $\Sigma_{a>F}N_a-\Sigma_{a<F}N_a=N(n-1)-2S_3^{(F)}$, and $\delta_a=2(\epsilon_a-\epsilon_F)$. This absolute minimum corresponds to $|S_\pm^{(k)}|=0$ for each k. Noticeably, the latter constraint does allow the ground state to still have a phase dynamics. In fact, on the one hand, by rewriting the equations of motions in terms of the canonical variables $\lambda_a,S_3^{(a)}$ introduced in previous section, it is straightforwardly verified that in the limit where $|S_\pm^{(k)}|\to 0$ uniformly the equation for the angle variables reduces to

$$\hbar\dot{\lambda}_k=\delta_k-2uS_3^{(k)}\sum_{l\in\tilde{\Lambda}}\cos(\lambda_k-\lambda_l), \tag{21}$$

where, to second order in $|S_\pm^{(k)}|$, $S_3^{(k)}=\pm\frac{1}{2}$ for $k\in\tilde{\Lambda}_\mp$. On the other hand, for $|S_\pm^{(k)}|\equiv 0$ the phase is totally free, as one can check from equations (18). Hence, by a continuity argument, we expect that also in this case the dynamics of $\lambda_k(t)$ evolves according to Eq. (21). Equation (21) has already been investigated in a different context (see, for instance, Ref. 19). In particular, it was shown[20] that for XY-like models it allows for vortexlike excitations. Moreover, in the continuum limit it can be recognized as a Bernoulli-like equation, the latter being known to describe once more a vortex dynamics. Finally, let us observe that the solution of Eq. (21) contains as a particular case the (topological) one discussed after Eq. (19), which requires $S_\pm^{(k)}\neq 0$, and reduces to it only in the (exact) noninteracting case, i.e., for $u=0$.

The absolute minimum Eq. (20) corresponds to the paramagnetic phase within the Hartree-Fock approximation, and gives the same ground-state energy. Contrary to that approximation, here it was possible to make evident a nontrivial dynamical behavior of the paramagnetic ground state. Such behavior implies in particular the appearance of a nonvanishing geometric phase in the ground state, as can be understood from the third of equations (3). Let us recall that this should happen at any filling but half. We shall see in fact that at half-filling $(n=1)$ states built with antiferromagnetic order can provide lower energy for the corresponding semiclassical Hamiltonian, again in agreement with the Hartree-Fock approximation.

Moreover, let us stress that stationary points characterized by $S_+^{(a)}=0$—even when not identifying an absolute minimum—indeed can be shown to be local minima of the Hamiltonian when the geometric constraints represented by the Casimir's are taken into account. A simple first-order expansion of $\mathcal{H}_{\rm sc}$ in the variables $|S_+^{(a)}|^2$, where $S_3^{(a)}$'s are now expressed as $S_3^{(a)}=+(-)(I_a-|S_+^{(a)}|^2)^{-1/2}$ for $a>F(a<F)$, shows that the variation $\delta\mathcal{H}_{\rm sc}$ is positive provided u is positive and sufficiently small. In summary, we conclude that such stationary points are minimum energy points for $u>0$, possibly possess inner dynamics and topological structure, but do not involve superconductive situations, being $S_+=0$.

The remaining set of fixed points, which are still solutions of Eqs. (18), can be fruitfully parametrized through the parameters I_a and S_+. Explicitly

$$S_3^{(a)}=-s_a\delta_a\sqrt{\frac{I_a}{\delta_a^2+4u^2|S_+|^2}},$$

$$S_+^{(a)}=2s_a|u|\sqrt{\frac{I_a}{\delta_a^2+4u^2|S_+|^2}}|S_+| , \tag{22}$$

with $s_a=\pm 1$. S_+ does not play the role of a free parameter, but it turns out to be constrained by the equation

$$1=-2u\sum_a s_a\sqrt{\frac{I_a}{\delta_a^2+4u^2|S_+|^2}} . \tag{23}$$

By substituting Eq. (22) in Eq. (14), and choosing the values of s_a and I_a which minimize $\mathcal{H}_{\rm sc}$ $(s_a=1$ and $I_a=N_a^2/4)$, it is

seen from Eq. (23) that such a solution exists only for $u<0$, and corresponds to an energy

$$E_{\rm sc}^{(-)}=|u|\frac{N^2}{4}n(2-n)-\frac{1}{2}\sum_a N_a\sqrt{\delta_a^2+4u^2|S_+|^2}+|u||S_+|^2 \ . \tag{24}$$

This result is once more in agreement with the ground-state result for the superconducting regime within the Hartree-Fock approximation, as can be seen by identifying the variational parameter Δ with the semiclassical pairing operator S_+. In particular, the constraint equation (23) coincides with the self-consistency equation for Δ.

Let us notice that, opposite to the mesoscopic fixed points $S_\pm^{(a)}=0$ case, here the insertion of the solutions (22) into the equations of motion for the variables $S_\pm^{(k)}$'s does not allow any microscopic dynamics, as the constraint $S_\pm^{(a)}\neq 0$ has to be satisfied.

V. COLLECTIVE FREQUENCY DYNAMICS

The dynamical system described by semiclassical Eqs. (16) is integrable in the special case when the pseudospin variables $S_3^{(a)}$ are supposed to be time independent. The main effect of such an assumption is, in fact, of halving the number of the system degrees of freedom. This can be easily seen by observing that $|S_+^{(a)}|$ cannot depend on time consistently with the fact that the Casimir's I_a are constants of motion, so that only the phases of the pseudospin projection variables $S_+^{(a)}$ are allowed to depend on time. Further restrictions on the dynamics are due to the equations of motion which take the form

$$-i\hbar\dot{S}_+^{(a)}=\delta_a S_+^{(a)}-2uS_3^{(a)}S_+,$$

$$S_+^{(a)}S_-=S_-^{(a)}S_+ . \tag{25}$$

The first of Eqs. (25) show how the system formally reduces to an ensemble of interacting oscillators with coupling constants $2uS_3^{(a)}$. Moreover, together with the second, rewritten as

$$S_+^{(a)}/S_-^{(a)}=S_+/S_-, \tag{26}$$

state that a unique, time-dependent phase $(W/\hbar)\tau$ characterizes the system dynamics. Namely, for any a,

$$S_+^{(a)}(\tau)=V_a e^{i\alpha}e^{i(W/\hbar)\tau}, \tag{27}$$

with $V_a,\alpha,W\in\mathbb{R}$. Both the constant phase α and V_a are fixed by assigning the initial conditions $S_+^{(a)}(0)$. The linear character of Eqs. (25) allows one to recast them in the matrix form

$$(\mathbf{M}\{\mathcal{S}\}-W\mathbb{I})\cdot\mathbf{S_+}=0, \tag{28}$$

where the vector $\mathbf{S_+}$ has components $S_+^{(a)}$ and the dynamical matrix $\mathbf{M}$, whose elements can be obtained by system (25), explicitly depends on the set $\mathcal{S}=\{S_3^{(a)}\}$. The associated secular equation, which in turn provides the eigenvalue equation,

$$\det(\mathbf{M}-W\mathbb{I}) \ =\left[1+2u\sum_b\frac{S_3^{(b)}}{W-\delta_b}\right]\Pi_a(W-\delta_a)=0, \tag{29}$$

is polynomial in W. The eigenvector components V_a can now be expressed in terms of W, $V=\Sigma_a V_a$ and $S_3^{(a)}$ as

$$V_a=\frac{2uS_3^{(a)}}{\delta_a-W}V. \tag{30}$$

It should be noticed that in fact V is itself a function of the initial conditions $S_3^{(a)}$ and energy $\mathcal{H}_{\rm sc}$, through the relations (14) and (27), which give $V=\pm[(\mathcal{H}_{\rm sc}+un^2N^2/4-2t\ \Sigma_a\delta_a S_3^{(a)})/u]^{1/2}$.

Moreover the eigenvalues fulfilling Eq. (29) are obtained, after assigning the initial condition set $\{S_3^{(a)}\}$, by solving

$$1=2u\sum_b\frac{S_3^{(b)}}{\delta_b-W} \ . \tag{31}$$

It turns out that the factor $\Pi_a(W-\delta_a)$ in Eq. (29) does not play a role unless $S_3^{(a)}=0$ for some a. When this is the case some of the eigenvalues coincide with the system proper frequency δ_a. The total number of eigenvalues, corresponding to the number of different mesoscopic levels, is however kept constant.

Both eigenvalues and eigenvectors can be easily obtained in an (approximate) explicit way when $|u|/t$ is suitably small. Looking at the structure of Eq. (31), it appears clear that the values of W close enough to δ_a are reasonably expected to fulfill it. In order to check this we first replace W with $W_a=\varepsilon+\delta_a$ in Eq. (31) which becomes

$$1=-\frac{2uS_3^{(a)}}{\varepsilon}+2u\sum_{b\neq a}\frac{S_3^{(b)}}{\delta_b-\delta_a-\varepsilon},$$

then, by taking $|\varepsilon|\ll|\delta_b-\delta_a|$, for any pair (a,b), one easily finds that $\varepsilon\simeq -2uS_3^{(a)}$ thus obtaining

$$W_a\simeq\delta_a-2uS_3^{(a)}.$$

On the other hand, the condition $|\varepsilon|\ll|\delta_b-\delta_a|$ is satisfied if it holds in the less favorable case $a=0,b=\pm 1$. Since $|\delta_0-\delta_1|=2t\epsilon_1\simeq 8t\pi^2/N$ (for $d=2$), then the condition on ε becomes $|\varepsilon|\ll 8t\pi^2/N$, which finally leads to

$$|U|\ll 8t\pi^2/N_a$$

for the greatest possible $S_3^{(a)}$ given by $N_a/2$. The present approximation scheme, based on considering $W_a\simeq\delta_a$, is thus permitted for reasonably small values of $|U|/t$. In particular, if $|U|\ll 8t\pi^2/N_0$ all the eigenvalues can be obtained from this scheme, whereas if $|U|\geqslant 8t\pi^2$ none of the W_a's is well approximated by it. The ath eigenvector associated with eigenvalue W_a is readily obtained from Eqs. (30) and exhibits components $V_c(W_a)$ given by

$$V_c(W_a)\simeq\frac{2uS_3^{(c)}}{\delta_c-\delta_a}\ V \ \text{ for } \ c\neq a,$$

$$V_a(W_a)\simeq V\left(1-\sum_{b\neq a}\frac{2uS_3^{(b)}}{\delta_b-\delta_a}\right).$$

The above equations show how the ath eigenvector $\mathbf{S_+}(W_a)$ in this approximate case is characterized by the fact that only the component V_b with $b=a$ is strongly nonzero, being in fact $V_a \simeq V$. This implies that each eigenvector can be regarded as describing a superconductive situation where the superconductive order parameter $S_+ = \langle \Sigma_k J_+^{(k)} \rangle = \Sigma_k S_+^{(k)}$ is essentially given by $S_+ \simeq S_+^{(a)}$ and the u-dependent contribution to the energy $\mathcal{H}_{sc}$ is mainly given by the k modes with $\epsilon_k = \epsilon_a$.

Some general observations are now in order. First we notice that the eigenvector problem is completely solved provided $\{S_3^{(a)}\}$ and $\mathcal{H}_{sc}$—the quantities which, at this stage, describe the initial system configuration—have been assigned, and the eigenvalues W_a have been worked out from Eq. (31). No restriction constrains $\mathcal{H}_{sc}$ and $\{S_3^{(a)}\}$ except for the filling condition (15) and the condition $V \neq 0$. The latter allows one to consider eigenvectors with arbitrarily small components V_a but excludes the solutions characterized by $\mathbf{S_+}=\mathbf{0}$ ($V_a=0$ for any a) representing a subset of the solution of the fixed-point equation (18). The single-mode solution set is thus completely disjoint from such a fixed-point subset in the space of solutions of Eqs. (25), even if the former is dense around any element of the latter. On the contrary, the other fixed points of Eq. (25), given by Eq. (22), are a (time-independent) subset of Eq. (27), corresponding to $W=0$.

Moreover we point out that the nonlinear nature of pseudospin dynamics survives our initial assumption $S_3^{(a)} = \text{const}$ because of the second of Eqs. (25). In fact the linear system of coupled oscillators described by Eqs. (25) should have an arbitrary superposition of eigenvectors related to Eq. (28) as a general solution. This is no longer possible when Eqs. (26) are taken into account in that any superposition of single-mode solutions (eigenvectors) violates the request that pseudospins exhibit the same phase.

Furthermore we observe that $S_+^{(k)}(\tau)$ can be easily obtained from Eqs. (25), where the term $S_+(\tau)$ is now playing the role of an external forcing term. Since $S_+^{(k)}(\tau)$ results to be proportional to $S_+^{(a)}$ up to a constant factor $e^{i\theta}$, then it follows that the equation for quantum phase $\varphi_{sc}(\tau)$ has form

$$\hbar \dot{\varphi}_{sc}(\tau) = W(S_3 + N/2) - \mathcal{H}_{sc}. \tag{32}$$

Hence, already in this simple integrable case within our approximation there is a nonvanishing contribution of the geometric phase (equal to $WnN/2$ times t), at any energy but the ground state. Such a contribution should, in principle, be observable by appropriate experiments. Finally it is remarkable that these single-mode solutions, exhibiting some form of collective order through the unique time-dependent phase $(W/\hbar)t$, correspond to nonvanishing superconductive order parameter S_+.

VI. SLOW DYNAMICS VS FAST DYNAMICS

A standard procedure for tackling many-body system dynamics consists in simplifying the equation of motions by separating fast degrees of freedom from slow degrees of freedom.[4,9,21] Such a procedure is profitable in that it leads the slow variable system to become an autonomous system and sometimes reduces the complexity of its equations of motion. These features are, of course, appealing here because the slow variables dynamics is the one surviving at a macroscopic level (and thus it might be observable), while the dynamics of high-frequency degrees of freedom disappears on large time scales.

For the pseudospin system a classification of pseudospins either as fast variables or as slow variables is naturally established by the fact that either $\delta_a \simeq 0$ or $\delta_a \neq 0$, respectively. We recall that such reference parameter depends on n and is associated with the mesoscopic a level of the ground-state configuration where $S_3^{(a)}$ changes its sign.

The effect of such a distinction is made evident by performing the substitutions $S_+^{(a)} = \exp[i\delta_a(t/\hbar)]\Psi_a$, which turn Eqs. (16) into the form

$$-i\hbar\dot{\Psi}_a = -2uS_3^{(a)}\Psi_a - 2uS_3^{(a)}\sum_{b\neq a} e^{i(\delta_b-\delta_a)t/\hbar}\Psi_b,$$

$$i\hbar\dot{S}_3^{(a)} = u\left(\Psi_a \sum_{b\neq a} \Psi_b^* e^{i(\delta_a-\delta_b)t/\hbar} - \text{c.c.}\right), \tag{33}$$

explicitly exhibiting dependence on the frequencies δ_a. Introducing the parameter δ_* as the frequency distinguishing slow frequencies (defined by $|\delta_a| \leqslant \delta_*$) from fast frequencies (defined by $|\delta_a| > \delta_*$), it clearly results that those time-dependent oscillating terms of Eqs. (33) where $|\delta_b| > \delta_*$ can be neglected on a time-scale greater than $\hbar/\delta_*$, since their rapid oscillations make their time-average vanishing.

This fact has remarkable implications. In fact, upon denoting fast pseudospin variables and slow pseudospin variables by $F_\pm^{(b)}$, $F_3^{(b)}$ and $Q_\pm^{(b)}$, $Q_3^{(b)}$, respectively, we are now able to separate the dynamical equation set into two almost independent subsets, the first one of which describes short-time-interval processes ($t < \hbar/\delta_*$), and reads

$$-i\hbar\dot{F}_+^{(a)} = \delta_a F_+^{(a)} - 2uF_3^{(a)}(F_+ + Q_+),$$

$$i\hbar\dot{F}_3^{(a)} = u(F_+^{(a)}(F_- + Q_-) - \text{c.c.}). \tag{34}$$

while the second concerns long-time processes ($t > \hbar/\delta_*$) involving the slow variables, and is given by

$$-i\hbar\dot{Q}_+^{(a)} = \delta_a Q_+^{(a)} - 2uQ_3^{(a)}Q_+,$$

$$i\hbar\dot{Q}_3^{(a)} = u(Q_+^{(a)}Q_+ - \text{c.c.}). \tag{35}$$

Here $Q_+ = \Sigma_a' Q_+^{(a)}$ and $F_+ = \Sigma_a'' F_+^{(a)}$ where the prime and the double prime remind us that a must range within selected intervals ($|\delta_a| > \delta_*$ and $|\delta_a| < \delta_*$, respectively). We notice that in Eqs. (34) $Q_\pm$ can be regarded as time-independent terms (adiabatic approximation), since their evolution takes place on the time scale of slow variables, whereas in Eqs. (35) fast variables are absent because of the effects of rapid oscillations discussed above. Also, when $t > \hbar/\delta_*$, such oscillations makes $F_\pm$ negligible with respect to $Q_\pm$ in terms like $(Q_\pm + F_\pm)$ of Eqs. (35), so that F-variable dynamics turn out to be driven by $Q_\pm$. On the other hand, the Q system can be considered as an almost isolated system which exhibits the same features of the initial N-pseudospin system except for the fact that now the pseudospin number is $N_* = \Sigma_a' N_a < N$ and the effective Hamiltonian is

$$H_Q=\sum_a 2(\epsilon_a-\mu)Q_3^{(a)}+u_*(N_*/2+Q_3)^2+u|Q_+|^2 \ , \tag{36}$$

where $u_*=U/N_*$. Two remarks are now in order. First we note that the long-time dynamics is weakly influenced by those k modes for which $|\delta_a-\delta_F|>\delta_*$, so that the complexity of the dynamical behavior now issues from the Q system, as manifestly suggested by the fact that the restricted Q system has inherited the same structure the N-pseudospin system. This is the main consequence of the adiabatic approach. Secondly, we recall that the density of states of the noninteracting system has in two dimensions a logarithmic divergence for $\epsilon\simeq 0$[16], which implies that the levels $\tilde{\Lambda}_a$ with $\epsilon_a\simeq 0$ are the most populated ones. For situations where the value of n involves $\epsilon_F\simeq 0$ (near half-filling) such a fact well matches the first observation since it turns out that the Q system, whose dynamics is complex, is also the subsystem involving the most part of k modes.

From the above observations, one is led to restricting the number of interacting levels in order to work out the simplest yet still significant dynamics. The corresponding model turns to be a three-level system, namely the pseudospin model where the Q system is endowed with three levels. A simple calculation allows one to establish that the number of constants of motion is not sufficient to make the system integrable. In this sense three-level dynamics still is far from being trivial, yet it is physically meaningful in several circumstances.

At first, for example, one can take into account just the three innermost levels of the k space, i.e., those around $\epsilon_a=0$, which in the following we shall label by $a=-1,0,+1$. This is natural when investigating the low-energy dynamics of $\mathcal{H}_{sc}$ at half-filling with $u>0$. In this case, in fact, it is reasonable to expect that increasing the energy from the ground-state value of small amounts (recall that $S_3^{(0)}=0$ and $S_3^{(\pm)}=\pm N_{\pm 1}/2$ with $N_1=N_{-1}$) makes interacting just the levels with the smallest energy, i.e., those with $a=-1,0,+1$. In view of the fact that $|\epsilon_{a+1}-\epsilon_a|\ll 4t$, expressing the almost continuous character of ϵ_a vs a, one can replace both the upper level and the lower level of the three-level model with two sheaves constituted by those levels with $\epsilon_a\simeq\epsilon_{+1}$ and $\epsilon_a\simeq\epsilon_{-1}$, respectively. This allows one to enlarge the number of modes participating in the dynamics as well as to treat the situation where excited states are more than small perturbations. We recall however that this case is mainly pedagogic, as at half-filling the ground state of Hamiltonian H has antiferromagnetic order.

Such observations readily extend to those situations where $n\neq 1$. In these cases, in fact, the minimum energy configuration is not symmetric with respect to $a=0$, but with respect to the level $a=F$, where $S_3^{(a)}$ change from negative to positive so as to minimize the energy. Then the three-level construction must be referred to the new central level thus obtained.

The further reduction to a two-level scenario immediately makes the Q system integrable. Again by replacing the two levels with two *effective* levels one can reasonably expect to still represent the main features of Q dynamics, in particular when the energy is low enough to make interacting a limited number of levels situated around the level with $a=F$.

VII. TWO-LEVEL DYNAMICS

In the previous section we noted that the three-level system is nonintegrable, although it is the oversqueezed version of a multilevel system that was dramatically more complex. A thorough investigation of its dynamics, where the occurrence of a chaotic behavior indeed is expected due to its similitude with the dynamical model of Refs. 22 and 23, requires a separate, extended analysis that will be pursued elsewhere. Nevertheless we shall start with the three-level model equations, so as to make the approximations performed to achieve the two-level scenario evident.

Let us express the three-level system equations in the form given by Eqs. (35) by renaming $S_\alpha^{(\nu)}$ ($\alpha=+,-,3$) for $\nu=F+1,F,F-1$ by P_α, $\mathcal{Z}_\alpha$, and M_α, respectively, and by setting $\delta_\pm=\delta_{F\pm 1}$, in order to simplify the notation and to recall the interpretation of the levels as level sheaves. The equations then read

$$-i\hbar\dot{M}_+=\delta_- M_+-2uM_3Q_+,$$

$$i\hbar\dot{M}_3=u(M_+Q_--M_-Q_+), \tag{37}$$

$$-i\hbar\dot{\mathcal{Z}}_+=-2u\mathcal{Z}_3Q_+,$$

$$i\hbar\dot{\mathcal{Z}}_3=u(\mathcal{Z}_+Q_--\mathcal{Z}_-Q_+), \tag{38}$$

$$-i\hbar\dot{P}_+=\delta_+P_+-2uP_3Q_+,$$

$$i\hbar\dot{P}_3=u(P_+Q_--P_-Q_+). \tag{39}$$

For $u>0$ the two-level model is readily obtained by freezing the $\mathcal{Z}$ variables at the values $\mathcal{Z}_3=0=\mathcal{Z}_+$. From the physical viewpoint, such an assumption is not particularly restrictive because it allows one to switch on dynamics through M variables and P variables starting from the ground-state configuration. One should recall, in fact, that $P_+=M_+=\mathcal{Z}_+=0$ characterize the ground state, while the further condition $\mathcal{Z}_3=0$ can be implemented by suitably selecting n [see the discussion following Eq. (20)]. The fact that set δ_a is almost continuous still ensures the possibility of choosing n almost arbitrarily.

For $u<0$, instead, the fact that $P_+,M_+,\mathcal{Z}_+\neq 0$ in connection with the minimum energy state, prevents the system from developing a dynamics in which $\mathcal{Z}_+$ and $\mathcal{Z}_3$ keep their ground-state values. Thereby the presence of the central level, even if as a nondynamical level reminiscent of three-level scenary, is prohibited and the central level must be embodied within one of the two sheaves, unless one is facing the nonintegrable version of pseudospin dynamics. At this point the two-level scenario is restored and one can proceed to integrate the equations of motion.

We construct now the solutions of two-level dynamics by solving simultaneously the systems of Eqs. (37) and (39). The main variable of the system is $D_3=P_3-M_3$ which will be shown to obey a nonlinear equation completely decoupled from the other variables. Indeed the knowledge of $D_3(t)$, together with the constant of motion Q_3 allows one to integrate such a system,[24] which becomes linear with time-dependent coefficients. To work out the equation for D_3 one needs to exploit all the constants of motion. Explicitly,

the energy $H_2=\delta_+P_3+\delta_-M_3+u_*(N_*/2+Q_3)^2+u|P_+ +M_+|^2$, $N_*=N_++N_-$ counting the active modes of two-level dynamics, must be used to eliminate the variables $P_\pm$ and $M_\pm$ from the equation

$$\hbar^2\dot{D}_3{}^2=4u^2|P_+M_--P_-M_+|^2, \tag{40}$$

obtained via the second equation in Eq. (37) and in Eq. (39). This is done by exploiting first the identity $|P_+M_--P_-M+|^2=4|P+|^2|M+|^2-(|P++M_+|^2-|P_+|^2 -|M_+|^2)^2$, which leads us to rewrite the rhs of Eq. (40) as

$$4u^2|P_+M_--P_-M_+|^2=16u^2|P_+|^2|M_+|^2-4[h_2-\sigma D_3 -u(|P_+|^2+|M_+|^2)]^2, \tag{41}$$

where $h_2=H_2-\gamma Q_3-u_*(Q_3+N_*/2)^2$, $\gamma=(\delta_++\delta_-)/2$, and $\sigma=(\delta_+-\delta_-)/2$. Then, by using the pseudospin Casimir's $I_M=M_3^2+|M_+|^2$, $I_P=P_3^2+|P_+|^2$ and the further identities $P_3^2+M_3^2=(Q_3^2+D_3^2)/2$, $P_3^2-M_3^2=Q_3D_3$, one reduces the D_3 equation to the closed form

$$\frac{\hbar^2}{2}\dot{D}_3{}^2=-2(h_2-\sigma D_3)^2+2u(h_2-\sigma D_3)(2I-Q_3^2-D_3^2) -2u^2(I_P-I_M-Q_3D_3)^2, \tag{42}$$

with $I=I_P+I_M$.

Equation (42), which expresses the integrable character of the two-level system, presents several interesting features. First of all it shows that the D_3 dynamics is as complex as that of a 1-d potential problem. Indeed, upon introducing the potential

$$\mathcal{U}(D_3)=-2aD_3^3+2bD_3^2+2cD_3+2d,$$

where $a=u\sigma$, $b=\sigma^2+uh_2+u^2Q_3^2$, $c=u\sigma(2I-Q_3^2) -2\sigma h_2-2u^2Q_3(I_P-I_M)$, and $d=(h_2-uI)^2+uh_2Q_3^2 -4u^2I_MI_P$, Eq. (42) simply becomes $\hbar^2\dot{D}_3{}^2/2=-\mathcal{U}(D_3)$. Therefore the dynamical behavior of the two-level system can be completely specified by identifying the regions where the cubic $\mathcal{U}(D_3)$ is negative and finding the value of the derivative of $\mathcal{U}(D_3)$ when D_3 approaches an inversion point. Such regions actually are identified by the compact interval in the potential well of $\mathcal{U}(D_3)$ whose extremes coincide with two of the three roots of the cubic equation $\mathcal{U}(D_3)=0$. The remaining semi-infinite interval where $\mathcal{U}(D_3)$ tends to $-\infty$ must be excluded, in that D_3 there would assume infinitely large values, while its range is finite: $-N_-\leq D_3\leq N_+$.

The two other points which play some role in characterizing the dynamics through $\mathcal{U}(D_3)$ are, of course, the potential stationary points

$$R_\pm=\frac{1}{3a}[b\pm(b^2+3ac)^{1/2}],$$

furnished by $d\mathcal{U}/dD_3=0$. In fact, upon denoting the minimum and the maximum coordinates by D_m and D_M, respectively, it is possible to identify the fixed points as those configurations of the two-level system with $\mathcal{U}(D_m)=0$ so that the D_3 interval reduces to the point $D_3=D_m$. It is easily checked that D_m is consistent with the general result given by Eqs. (20)–(22) for the exact minimum energy points. On the other hand, when the initial conditions imply $\mathcal{U}(D_m)<0$ and $\mathcal{U}(D_M)>0$, then the system oscillates between two extreme states. From the physical point of view this property has the interesting consequence that the filling of each of the two mesoscopic levels near the Fermi surface $(F\pm1)$ varies periodically with time, while the sum of the two fillings remains constant.

On the other hand, it is worth noticing that such periodic behavior of the mesoscopic levels filling ceases to exist for appropriate initial conditions. In fact when $\mathcal{U}(D_M)=0$ the system exhibits a *laser*like effect, namely it tends, employing an infinitely long time, to an asymptotic stationary state in which (depending on the sign of u) a mesoscopic level is totally empty while the other is full. Moreover one should recall that each choice of the constants of motion h_2, Q_3, I_M, and I_P embodied in a, b, c, and d selects a different cubic potential. Two solutions are associated with the same potential when they differ just for the choice of the initial position $D_3(0)$.

The nice feature of Eq. (42) is that it can be reduced to the equation for the Weierstrass $\mathcal{P}$ function,[25] which reads

$$\left(\frac{d\mathcal{P}}{d\tau}\right)^2=4\mathcal{P}^3-g_2\mathcal{P}-g_3,$$

Any solution of Eq. (42) can then be given in explicit form. A straightforward calculation based on the substitution of D_3 with $D_3=\pm\mathcal{P}+b/3a$ [the plus (minus) corresponds to the case $a>0$ $(a<0)$] turns Eq. (42) into the above equation for $\mathcal{P}$ where $\tau=\sqrt{a}t/\hbar$ and the standard coefficients g_2, g_3 are identified as

$$g_2=\frac{4}{3a^2}(b^2+3ac),$$

$$g_3=\pm\frac{4}{27a^3}(2b^3+9abc+27a^2d).$$

Then, by exploiting the solution $\mathcal{P}$ in terms of Jacobi elliptic functions[26] $\mathcal{P}(\tau)=(1/3)\gamma^2(1+k^2)-\gamma^2k^2\mathrm{sn}^2(\gamma\tau+\alpha;k)$ where

$$g_2=\frac{4}{3}\gamma^4(1-k^2+k^4),$$

$$g_3=\frac{4}{27}\gamma^6(1-2k^2)(2-k^2)(1+k^2),$$

the explicit analytic expression of $D_3(t)$ is easily shown to be[24]

$$D_3(t)=\frac{b}{3a}\pm\left[\frac{1}{3}\gamma^2(1+k^2)-\gamma^2k^2\mathrm{sn}^2(\gamma\tau+\alpha;k)\right]. \tag{43}$$

Such a solution, as expected, shows that the dynamics is periodic around the point D_m with period

$$T_2=2\hbar\frac{K(k^2)}{\gamma|a|^{1/2}},$$

since the elliptic sine fulfills the equation $\mathrm{sn}(x+2K)=-\mathrm{sn}(x)$, where $K(k^2)$ is the elliptic integral of

the first kind.[26] As anticipated, a special case can be selected out when initial conditions allow the condition $\mathcal{U}(D_M)=0$ to occur. This condition states that one of the two $\mathcal{U}$ roots confining the oscillations of D_3 inside the potential well, coincides with the maximum coordinate D_M. Reaching D_M thus requires an infinitely long time provided the motion starts exactly at the other inversion point, that is the remaining root of $\mathcal{U}(D_3)=0$. When this is the case $k\to 1$ so that $\mathrm{sn}(x,k)\to th(x)$ and $D_3(t)$ describes indeed a transition for $t\to\infty$.

In order to explicitly provide a situation where such transition happens we concisely examine the dynamics for $u>0$ when $Q_3=0$ and $I_M=I_P$. In this case the potential $\mathcal{U}$ manifestly exhibits its roots since it reduces to

$$\mathcal{U}(D_3)=-2(h_2-\sigma D_3)(h_2-2uI-\sigma D_3+uD_3^2). \quad (44)$$

Hence the circumstance where $\mathcal{U}(D_3)=0$ for $D_3=D_M$ is obtained by imposing the two roots of the quadratic factor in Eq. (44) to merge, i.e., to tend to D_M. As a result one finds first the constraint $4uh_2=\sigma^2+8u^2I$ on the energy, then that the limiting point of the transition is $D_3(\infty)=\sigma/2u=D_M$ when $D_3(0)=h_2/\sigma$, provided the condition $4\sqrt{I_P}<|\sigma|/u<2N_+$ holds ensuring that $-N+<D_M<D_3(0)$.

Returning to Eq. (43), one can now easily evaluate the phase $\varphi_{\mathrm{sc}}(t)$ given by expression (17) in the simplest case in which $S_+^{(k)}=S_+^{(a)}/N_a$ for any k. Since this involves that $S_3^{(k)}=\pm S_3^{(a)}/N_a$, then pseudospins populating a level at most differ one from the other by the sign of $S_3^{(k)}$. We shall choose the same sign for the k's of a given level so that the microscopic dynamics is just a copy of the mesoscopic dynamics. Here, we shall not consider the possibility of more structurated configurations of pseudospins, since they do not introduce any substantial novelty concerning the phase behavior.

Finally, by using the above assumption, $\varphi_{\mathrm{sc}}(t)$ can be written in the form

$$\dot{\varphi}_{\mathrm{sc}}=-\mathcal{H}_{\mathrm{sc}}+\hbar\sum_a (N_a/2+S_3^{(a)})\dot{\lambda}_a. \quad (45)$$

The latter expression is particularly useful for the dynamics of weakly excited states since the variables $S_3^{(a)}$'s are expected to undergo small variations in time, with respect to their ground-state values. The levels whose pseudospins are fast should therefore contribute to φ_{sc} principally through the phases $\dot{\lambda}_a$'s. On the other hand, after solving Eqs. (34) for the pseudospins labeled by $a=F+2$ and $a=F-2$ (namely pseudospins of the first two levels with fast variables) so as to have a four-level system mimicking the real system, a simple calculation shows the time average of $\dot{\lambda}_{F\pm 2}$ to be almost zero in the Q-time scale. Indeed the slow variables M_3 and P_3 and the phases of M_+ and P_+ provide the main contribution to $\dot{\varphi}_{\mathrm{sc}}$ even when the fast variables are included. The expression of such a contribution can be readily obtained by rewriting Eq. (45) in terms of M_3, P_3, and of the constants of motion. One thus finds

$$\dot{\varphi}_{\mathrm{sc}}\simeq-\mathcal{H}_{\mathrm{sc}}+u\left\{n^2N^2 4-4(M_+P_-+M_-P_+)\times\frac{N_-P_3-N_+M_3}{(N_+-2P_3)(N_--2M_3)}\right\}. \quad (46)$$

The slow variation in time of its variables makes it a good candidate for experimental detection.

VIII. EQUATIONS OF MOTIONS IN THE ANTIFERROMAGNETIC PHASE

When the possibility of a AF phase is considered, the natural order parameter which has to be nonzero is[16]

$$m\doteq\frac{1}{N}\left\langle\sum_{\mathbf{j}\in\Lambda} e^{i\mathbf{G}\mathbf{j}}(n_{\mathbf{j},\uparrow}-n_{\mathbf{j},\downarrow})\right\rangle=\frac{1}{N}\left\langle\sum_{\mathbf{k}\in\tilde{\Lambda}} a^\dagger_{\mathbf{k},\uparrow}a_{\mathbf{k}-\mathbf{G},\uparrow}-a^\dagger_{\mathbf{k},\downarrow}a_{\mathbf{k}-\mathbf{G},\downarrow}\right\rangle, \quad (47)$$

where $\mathbf{G}$ is a vector with all its components equal to π.

Also here, we look at the reduced Hartree-Fock Hamiltonian in the AF phase, $H_l^{(\mathrm{af})}$, in order to derive the dynamical algebra in which we shall subsequently construct our GCS's. It reads

$$H_l^{(\mathrm{af})}=-t\sum_{\langle\mathbf{i},\mathbf{j}\rangle}\sum_\sigma c^\dagger_{\mathbf{i},\sigma}c_{\mathbf{j},\sigma}+\frac{U}{2}m\sum_{\mathbf{j}} e^{i\mathbf{G}\mathbf{j}}(n_{\mathbf{i},\uparrow}-n_{\mathbf{i},\downarrow})-U\frac{N}{4}(1-m^2)$$

and it can be rewritten in reciprocal space as $H_l^{(\mathrm{af})}=\Sigma_{\mathbf{k}\in\tilde{\Lambda}_-,\sigma}H^{(\mathrm{af})}_{\mathbf{k},\sigma}$ where now

$$H^{(\mathrm{af})}_{\mathbf{k},\sigma}=\epsilon_{\mathbf{k}}\sum_\sigma (n_{\mathbf{k},\sigma}-n_{\mathbf{k}-\mathbf{G},\sigma})+U\frac{m}{2}(a^\dagger_{\mathbf{k},\uparrow}a_{\mathbf{k}-\mathbf{G},\uparrow}-a^\dagger_{\mathbf{k},\downarrow}a_{\mathbf{k}-\mathbf{G},\downarrow}+\mathrm{H.c.})+\frac{U}{4}(m^2-n^2),$$

and $\tilde{\Lambda}_-$ is that half of $\tilde{\Lambda}$ in which $\epsilon_{\mathbf{k}}$ is negative, e.g., for $d=2$ $\tilde{\Lambda}_-\equiv\{\mathbf{k}\in\tilde{\Lambda}|\,\epsilon_{\mathbf{k}}<0,$ or $\epsilon_{\mathbf{k}}=0$ and $0<k_1\leqslant\pi\}$.

$H_l^{(\mathrm{af})}$ can be recognized as an element of the dynamical algebra $\mathcal{A}_{\mathrm{af}}=\oplus_{\mathbf{k}\in\tilde{\Lambda}_+,\sigma}\boldsymbol{\mathcal{A}}^{(\mathrm{af})}_{\mathbf{k},\sigma}$ with

$$\boldsymbol{\mathcal{A}}^{(\mathrm{af})}_{\mathbf{k},\sigma}=\left\{K^{(+)}_{\mathbf{k},\sigma}=a^\dagger_{\mathbf{k}-\mathbf{G},\sigma}a_{\mathbf{k},\sigma},K^{(-)}_{\mathbf{k},\sigma}=[K^{(+)}_{\mathbf{k},\sigma}]^\dagger,K^{(Z)}_{\mathbf{k},\sigma}=\frac{1}{2}(n_{\mathbf{k}-\mathbf{G},\sigma}-n_{\mathbf{k},\sigma})\right\}\sim\mathrm{SU}(2)_{\mathbf{k},\boldsymbol{\sigma}}, \quad (48)$$

and $K^{(\pm)}_{\mathbf{k},\sigma}=K^{(X)}_{\mathbf{k},\sigma}\pm iK^{(Y)}_{\mathbf{k},\sigma}$ In full analogy with the case treated in Sec. III, we use as a trial approximate time-dependent wave function for studying the full Hamiltonian H in antiferromagnetic phase the time-dependent generalization of GCS's, which can be built in $\boldsymbol{\mathcal{A}}_{\mathrm{af}}$, i.e.,

$$|\psi(t)\rangle_{\rm af}=e^{(i/\hbar)\varphi_{\rm af}(t)}|\xi(t)\rangle$$
$$=e^{(i/\hbar)\varphi_{\rm af}(t)}\Pi_{\mathbf{k}\in\tilde{\Lambda}_-,\sigma}(1+\overline{\xi_{\mathbf{k},\sigma}}\xi_{\mathbf{k},\sigma})^{-1/2}$$
$$\times\exp(\xi_{\mathbf{k},\sigma}K^{(+)}_{\mathbf{k},\sigma})|0\rangle_{\rm af}, \tag{49}$$

where $|0\rangle_{\rm af}\equiv\Pi_{\mathbf{k}\in\tilde{\Lambda}_-,\sigma}|\sigma\rangle\Pi_{\mathbf{k}\in\tilde{\Lambda}_+,\sigma}|0\rangle$ $(\tilde{\Lambda}_+=\tilde{\Lambda}-\tilde{\Lambda}_-)$, and the parameters $\xi_{\mathbf{k},\sigma}$ have to be thought of as time dependent.

The semiclassical Hamiltonian $\mathcal{H}_{\rm af}$, identified as the expectation value of H over $|\psi(t)\rangle_{\rm af}$, can be fruitfully rewritten in terms of the semiclassical variables $\zeta_{\mathbf{k},\sigma}\doteq_{\rm af}\langle\psi(t)|K^{(\zeta)}_{\mathbf{k}\sigma}|\psi(t)\rangle_{\rm af}$, with $\zeta=X,Y,Z$, which still satisfy a SU(2) algebra Eq. (13). Also here it is useful to introduce a one-dimensional index a instead of $\mathbf{k}$, and to define the mesoscopic variables $\zeta_{a,\sigma}\doteq\Sigma_{\mathbf{k}\in\tilde{\Lambda}_a}\zeta_{\mathbf{k},\sigma}$. One obtains

$$\mathcal{H}_{\rm af}=-2\sum_{a\in\tilde{\Lambda}_-,\sigma}\epsilon_a Z_{a,\sigma}+4uX_\uparrow X_\downarrow-u\frac{N^2}{4}\ , \tag{50}$$

with $\zeta_\sigma=\Sigma_{a\in\tilde{\Lambda}_+}\zeta_{a,\sigma}$.

The semiclassical equations of motion for the $\zeta_{a,\sigma}$'s, can be easily derived from Eqs. (50) and (5), and read

$$\hbar\dot{X}_{a,\sigma}=2\epsilon_a Y_{a,\sigma}\ ,$$
$$\hbar\dot{Y}_{a,\sigma}=-2\epsilon_a X_{a,\sigma}-4uX_{-\sigma}Z_{a,\sigma}\ ,$$
$$\hbar\dot{Z}_{a,\sigma}=4uX_{-\sigma}Y_{a,\sigma}\ . \tag{51}$$

It is interesting to notice that the above equations do reduce to equations formally identical with those studied for the SC-paramagnetic phases for the special choice $Y_\sigma=0$, $X_\sigma=\pm X_{-\sigma}=(1/2)S_\pm$, so that at least in this case the dynamics can be derived from that obtained there. Moreover, let us notice that the choices $X_{a,\uparrow}=\pm X_{a,\downarrow}$, $Y_{a,\uparrow}=\pm Y_{a,\downarrow}$ reduce to a half the number of Eqs. (51). One can easily verify that such choices minimize the value of $\mathcal{H}_{\rm af}$ in the positive $(-)$ and negative $(+)$ u regime, respectively.

From Eqs. (51) we also obtain the time-dependent phase characteristic of the TDVP approach,

$$\dot{\varphi}_{\rm af}=-\mathcal{H}_{\rm af}+\sum_{\mathbf{k}\in\tilde{\Lambda}_-}\frac{\dot{Y}_{\mathbf{k},\sigma}X_{\sigma,(\mathbf{k})}-\dot{X}_{\sigma,(\mathbf{k})}Y_{\mathbf{k},\sigma}}{1-2Z_{\mathbf{k},\sigma}}$$
$$=\phi-4u\sum_\sigma\left[X_{-\sigma}\sum_{\mathbf{k}\in\tilde{\Lambda}_-}X^{(\mathbf{k})}_\sigma\frac{1+2Z_{\mathbf{k},\sigma}}{1-2Z_{\mathbf{k},\sigma}}\right], \tag{52}$$

where $\phi=u(N^2/4)-2\Sigma_{\mathbf{k}\in\tilde{\Lambda}_-}\epsilon_{\mathbf{k}}$ is a constant. As in the superconducting case, also in Eq. (52) the time-dependent part of $\dot{\varphi}_{\rm af}$ is vanishing for vanishing u as well as for $X_\sigma=0$, which is related to the vanishing of the antiferromagnetic order parameter $X(X\doteq X_\uparrow-X_\downarrow)$.

As in the case treated in the previous sections, also here we first look for the fixed points of Eqs. (51). A first solution is of course the vanishing one, i.e., $X_{a,\sigma}=Y_{a,\sigma}=0$, and $Z_{a,\sigma}$ fixed by initial conditions. In particular, the configuration of $Z_{a,\sigma}$ minimizing the energy has energy $E^{(0)}_{\rm af}=-u(N^2/4)+2\Sigma_{a\in\tilde{\Lambda}_-}\epsilon_a N_a$, which is easily verified to coincide with that of the paramagnetic phase (20) in the positive u regime at half-filling.

The remaining set of fixed points can be parametrized by the Casimir's $\mathcal{I}_{a,\sigma}=X^2_{a,\sigma}+Z^2_{a,\sigma}$, which again are conserved quantities. It is characterized by $Y_{a,\sigma}=0$, and

$$X_{a,\sigma}=2s_{a,\sigma}u\sqrt{\frac{\mathcal{I}_{a,\sigma}}{\epsilon_a^2+4u^2X^2_{-\sigma}}}X_{-\sigma},$$
$$Z_{a,\sigma}=\epsilon_a s_{a,\sigma}\sqrt{\frac{\mathcal{I}_{a,\sigma}}{\epsilon_a^2+4u^2X^2_{-\sigma}}}\ , \tag{53}$$

where $s_{a,\sigma}=\pm1$. The X_σ's have to satisfy the constraint equations

$$X_\sigma=2u\sum_a\ s_{a,\sigma}\sqrt{\frac{\mathcal{I}_{a,\sigma}}{\epsilon_a^2+4u^2X^2_{-\sigma}}}X_{-\sigma}.$$

The corresponding energy $E_{\rm af}$ reads

$$E_{\rm af}=-u\frac{N^2}{4}+\sum_{a,\sigma}\ \epsilon_a^2 s_{a,\sigma}\sqrt{\frac{\mathcal{I}_{a,\sigma}}{\epsilon_a^2+4u^2X^2_{-\sigma}}}+4uX_\uparrow X_\downarrow\ . \tag{54}$$

In particular, the fixed points which minimize Eq. (54) are associated with the choices $s_{a,\sigma}=-1$, $\mathcal{I}_{a,\sigma}=N_a^2/4$, and $X_\uparrow=-\mathrm{sgn}(u)X_\downarrow$. In this case the constraint equations, apart from the solution $X_\sigma=0$, reduce to one, i.e.,

$$1=|u|\sum_a\ \frac{N_a}{\sqrt{\epsilon_a^2+4u^2X^2_\uparrow}}\ , \tag{55}$$

and the minimum energy is straightforwardly obtained from Eqs. (54) and (55) as

$$E^{(m)}_{\rm af}=-u\frac{N^2}{4}-2\sum_{a\in\tilde{\Lambda}_-}N_a\sqrt{\epsilon_a^2+4u^2X^2_\uparrow}+4|u|X^2_\uparrow\ . \tag{56}$$

As expected, this energy corresponds to a nonvanishing antiferromagnetic order parameter $X=2X_\uparrow$ only for $\mathrm{sgn}(u)=+$ (i.e., repulsive Coulomb interaction), whereas it gives $X=0$ for $\mathrm{sgn}(u)=-$. In the first case, the energy $E^{(m)}_{\rm af}$ coincides in fact with the one obtained within Hartree-Fock approximation, with X replaced by m satisfying the same self-consistency equation (55). On the contrary, in the attractive Coulomb interaction regime, even though $X=0$ the energy $E^{(m)}_{\rm af}$ is lower than the one obtained within Hartree-Fock approximation, which would be precisely given by $E^{(0)}_{\rm af}$ namely the energy corresponding to the trivial vanishing fixed point. This is not surprising, in that, while within the Hartree-Fock scheme the only parameter to be fixed self-consistently is m, here to all effect we have two related parameters, $X_\uparrow$ and $X_\downarrow$, which can separately be nonzero even

when their difference (i.e., X) is vanishing. Recalling that $X_\sigma = {}_{\rm af}\langle\psi|\Sigma_{\mathbf{j}}(-)^{\mathbf{j}} n_{\mathbf{j},\sigma}|\psi\rangle_{\rm af}$, this latter case ($X_\uparrow = X_\downarrow \neq 0$) can be recognized as a CDW phase.

Notice that in the absolute minimum energy point for $u<0$ both the conditions which reduce the equations of motion (51) to those of the superconducting case Eq. (16) were fulfilled [see the discussion following Eq. (51)]. A direct comparison with the result obtained for the negative u regime by means of the superconducting states Eq. (24) shows that in fact at half-filling $E_{\rm sc}^{(-)} \equiv E_{\rm af}^{(m)}$. Hence we derived within TDVP at $u<0$ two degenerate wave functions for the ground state, the superconducting and the charge-density-wave one. Indeed it is easily verified that the two wave functions are orthogonal, and that the expectation value of the order operator of one phase, when taken over the wave functions of the other phase, is identically vanishing.

Now let us analyze the equation of motions (51) away from the fixed points in some simple case. A first integrable case is obtained when the variable X_σ is kept constant. However this assumption is consistent only if $\Sigma_a \epsilon_a Y_{a,\sigma} = 0$, and such a condition in turn is satisfied only if $Y_{a,\sigma}$ is independent of time for $\epsilon_a \neq 0$. Then the solution for each $a \neq F$ reduces to Eq. (53), whereas for $a = F$ it turns out to be given by

$$Y_{F,\sigma} = A_\sigma \cos(\alpha_\sigma t) + B_\sigma \sin(\alpha_\sigma t),$$

$$Z_{F,\sigma} = A_\sigma \cos(\alpha_\sigma t) - B_\sigma \sin(\alpha_\sigma t) \quad , \tag{57}$$

and $X_{F,\sigma} = X_\sigma - \Sigma_{a \neq F} X_{a,\sigma}$, with $\alpha_\sigma = 4(u/\hbar) X_{-\sigma}$. Solution (57) survives in correspondence to stationary points of the Hamiltonian (when X_σ are chosen according to the self-consistency equations), as the system energy is not changed by the value of $Z_{F,\sigma}$ and $Y_{F,\sigma}$. Such a solution describes the periodic behavior of the mesoscopic Fermi level, holding even for the interacting ground state. In fact, due to the Casimir constraint the constants A_σ and B_σ turn out to be related by the equation $A_\sigma^2 + B_\sigma^2 = \mathcal{I}_F - X_{F,\sigma}^2$. The latter condition implies that $A_\sigma = B_\sigma = 0$ for $X_{F,\sigma} = \pm\sqrt{\mathcal{I}_F}$, which is the case only for the absolute minimum point of the noninteracting case [see Eq. (53)]. On the contrary, for any $|X_{F,\sigma}| < \sqrt{\mathcal{I}_F}$ from Eq. (57) we obtain this oscillatorylike behavior of the solution at the Fermi surface. Such a behavior affects neither the order parameter, nor the energy, but it turns out to affect the phase $\varphi_{\rm af}(t)$ characteristic of the TDVP approach, by adding to the term linear in time a structured periodic time-dependent contribution given by

$$\sum_{\mathbf{k} \in \tilde{\Lambda}_F} \tan^{-1}\left[\frac{B_{\mathbf{k},\sigma} + A_{\mathbf{k},\sigma} \tan\left(\frac{\alpha_\sigma}{2} t\right)}{\alpha_\sigma \sqrt{1 - 4X_{\mathbf{k}^*,\sigma}^2}} \right]. \tag{58}$$

Here we used the same dynamics for the local and the mesoscopic pseudospin variables. In summary, we obtained also in the AF and CDW phases a nontrivial phase dynamics for the ground state.

Apart from this simple case, more generally the system described by Eq. (51) has been investigated in the case where the mesoscopic levels which have fast dynamics are one or two.[22,23] Already within such a framework it appears to have very interesting chaotic properties.

IX. CONCLUSIONS

In the present paper we developed a consistent scheme for dealing with the dynamics of an itinerant interacting many-electron system described by the Hubbard Hamiltonian. Such a scheme is based on TDVP procedure, and has been applied for describing the dynamics of the model by means of macroscopic wave functions built in terms of the GCS of the dynamical algebras which generate the Hartree-Fock solution in SC, AF, CDW, and paramagnetic phases. Already for these simple cases a certain number of remarkable features related to the dynamical description rather than to the statistical-mechanical one was underlined.

First of all, a geometric phase—a macroscopic quantity which, in principle, is observable—occurs for appropriate values of the physical parameters in the ground state as well as for some low-energy excited states. Such a feature cannot be identified by solving the eigenvalue equation for the Hamiltonian (or related techniques, like the Bethe ansatz approach), as it is a consequence of the phase of the eigenfunction, which in the eigenvalue equation is free. Even more noticeably, away from half-filling in the repulsive regime, it was shown that such macroscopic behavior of the Berry phase is originated from a vortexlike dynamics of the phases of the microscopic variables. Both these features could be due to the approximations implied by our scheme, hence a first interesting point which is left open to future work is to study exactly the dynamics of the stationary points of H, by solving the Schrödinger equation near them. This could be done by using the Glauber GCS's, which map exactly the quantum Hamiltonian into its semiclassical form, and studying the fixed points of the resulting equations of motion.[12]

Other interesting dynamical properties of the system were stressed in the low-energy regime for some integrable cases. At half-filling, the ground state has been shown to exhibit an oscillatorylike behavior at the Fermi surface. Away from half-filling, for $u>0$ an analogous oscillating behavior for the mesoscopic density variable takes place near the Fermi surface. Such a feature is responsible for a nontrivial time dependence of the collective Berry phase. Again, this point should be further analyzed in different approximations. An alternative viewpoint could be furnished even by employing the same TDVP scheme starting from GCS's more realistic than the Hartree-Fock ones. For instance, in the $U \to \infty$ limit, a reliable basis is given by the Gutzwiller states.[27]

One more solution obtained exactly within the present scheme and exhibiting interesting features is the single-mode solution, characterized by the nonvanishing of the superconducting parameter, and by a unique time-dependent phase reflecting collective order. The possible relevance of this solution within the framework of superconductivity is related to the fact that it survives at $u>0$, and at any energy but the ground state, with a volume in the space of solutions increasing with energy.

All the above solutions, which are exact within the present approximation scheme, are interesting also in that

they could represent good starting points for studying more exhaustively the dynamics described by Eq. (16) in their neighborhood, by means of standard perturbative methods of classical dynamics. As a general conclusive observation let us notice that their validity beyond the present TDVP scheme could be tested by solving exactly the Schrödinger equation for H_{Hub} on small clusters of sites. Work is in progress along these lines.

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