Time-dependent Hartree-Fock-Bogoliubov approximation and nonintegrable quantum phase

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We shall show how the so-called Berry's or quantum nonintegrable phase appears in the context of the time-dependent Hartree-Fock-Bogoliubov equations. It is shown that the right requantization of the time-dependent Hartree-Fock-Bogoliubov equations is achieved only when Berry's phase is properly taken into account.

I. INTRODUCTION

It is one of the oldest questions in the many-body theory: "How should one proceed in analyzing a complex system?" The standard procedure is to start with the identification of slow or collective degrees of freedom and the fast ones. Often, the physical system under scrutiny suggests a very natural separation of such degrees of freedom. Typical examples are molecules, where the role of slow and fast degrees of freedom is played by nuclear and electronic coordinates, respectively. It seems natural to initially solve the electron problem for a fixed nuclear configuration, since the two times scales are so dramatically different that practically nobody questions the validity of such an approach. One ends up with a widely known Born-Oppenheimer approximation.[1] Although the total wave function for a molecule is written as a product between the nuclear wave function (w.f.) (which depends only on nuclear coordinates) and the electronic wave function (which however depends on both sets of coordinates, though only parametrically on nuclear ones) there is a constant exchange of energy between the nuclear and electron systems. The electronic Hamiltonian depends adiabatically on the nuclear coordinates; and due to this, the electronic energy is not conserved but changes at a slow rate. The averaged value of the electronic Hamiltonian, over the instantaneous electronic configuration, plays the role of the potential energy for the nuclear motion. Effectively, the nuclear motion is described through a Hamiltonian characterized by a standard kinetic energy and a potential term. In spite of the great success of the Born-Oppenheimer picture for molecules, there is a whole class of phenomena, which did not fit into such an approach and which were dubbed nonadiabatic effects, such as dissociation, Landau-Zener-Stückelberg effect, etc., when during the slow evaluation of the nuclear system, the electronic configuration changes suddenly. However, nobody ever questioned whether the structure of the effective nuclear Hamiltonian was really that simple, a kinetic plus a potential term only. Could it be, that the interaction among nuclei in a molecule contains a *magnetic* type of force? It is truly amazing to find that during the long period of evolution of the quantum theory of molecules, nobody addressed this question. Only relatively recently were physicists[2] forced to accept such a possibility as a hard fact. It was Berry,[3] who recognized the true generality of such a situation and who showed that such an *esoteric* concept as a *magnetic monopole,* envisaged by Dirac, but never observed, could be useful for the description of the effective interaction among nuclei in a molecule. The gauge fields, both Abelian and non-Abelian, are often unavoidable in molecules[4] and in almost any other field in physics.[5] The origin or source of such fields are the so-called *diabolical*[3] points or funnels.[6] They correspond to such nuclear configurations, when two or more electronic terms become degenerate. If the nuclei, during their time evolution approach such a configuration, then the electronic w.f.'s are ill defined there. There is a high probability for the electrons to rearrange and for the nuclei to *jump* from one potential sheet to another. The nuclei do not have to come close to such a configuration in order for the *diabolical* point or *funnel* to have a non-negligible influence on nuclear motion. It is enough to go around such a point, at a *safe* distance, such that the adiabaticity is never violated, and one will observe the molecular analogue of the Aaranov-Bohm effect.[2,3,7] This means that at a degeneracy in the electronic spectrum one has the analogue of a *magnetic monopole,* which is the source of an effective *gauge field.* Such an effective gauge field has nothing to do with the fact that the interaction in molecules is electromagnetic in nature and therefore is a gauge type of interaction. Neither can this fact be traced down to some inherent deficiencies of the adiabatic approach. The appearance of such effective gauge fields is a result of reducing the number of degrees of freedom, by *integrating* some of them out[8] and these effective gauge fields appear as naturally as does the common effective potential term.

In nuclei the definition of slow or collective degrees of freedom and fast or noncollective or intrinsic ones is not such a simple matter as in molecular physics; and it is still an unsolved problem, despite the tremendous effort of a few generations of nuclear theorists. It is unquestionable, however, that in the case of nuclear motion one has collective and noncollective branches of the spectra and such a concept allows one to understand an enormous body of experimental data. One can then rationally address the question of whether in nuclear collective Hamiltonians there are effective gauge fields. In spite of

the great variety of collective models formulated in terms of kinetics and potential energy terms or bosons for a large body of phenomena (starting with low-energy spectra, giant resonances, fission, heavy-ion interactions, and so on) in none of these models has anyone ever introduced an effective gauge field. And the explanation why is as simple as in the case of molecules: "Nobody ever suspected them to be present there." There are a couple of late exceptions to this rule, due to the advent of effective gauge potentials in other fields.[9,10] Since the situations where such fields could appear are now relatively easy to pinpoint, namely, when in the spectrum of the fast variables, regarded as a function of the collective variables there are degeneracies, *diabolical points* or *funnels* (depending on the terminology one would like to adopt) it is highly desirable to assess their relevance.

In the present paper we show how Berry's phase appears in the treatment of pairing correlations. As we shall show, in this case one deals with the nonadiabatic manifestation of this phenomenon. However, the framework is generic in our opinion. In the case of pairing, the role of collective degrees of freedom is played by the single-particle (s.p.) field (pairing in particular). The s.p.w.f.'s will play the role of the fast degrees of freedom; and the degeneracies in the s.p. spectrum, as a function of collective variables, will be the sources of the effective gauge field in the collective Hamiltonian. Equally well can one consider the deformation of the s.p. field as another set of collective variables, separately or in conjunction with pairing. The collective rotation of deformed nuclei, mass or charge asymmetry, and so on are other examples of *slow* nuclear motions, which can lead to collective Hamiltonians with effective gauge fields.

II. DERIVATION OF TIME-DEPENDENT HARTREE-FOCK-BOGOLIUBOV EQUATIONS

It might sound inappropriate to give a rederivation of the time-dependent Hartree-Fock-Bogoliubov (TDHFB). However, it seems that in the literature there is some confusion concerning this subject.[11] The time-dependent Hartree-Fock (TDHF) equations seem to be well established. By analogy, the TDHFB equations are usually written in the commutator form as ($\hbar=1$),

$$i\partial_t \mathcal{R}=[\mathcal{H},\mathcal{R}] , \tag{1a}$$

$$\mathcal{H}=\begin{bmatrix} h-\lambda & \Delta \\ \Delta^\dagger & -(h^*-\lambda) \end{bmatrix} , \tag{1b}$$

$$\mathcal{R}=\begin{bmatrix} \rho & \kappa \\ \kappa^\dagger & 1-\rho^* \end{bmatrix} , \quad \mathcal{R}=\mathcal{R}^2 , \tag{1c}$$

where h and Δ stand for the Hartree-Fock and pairing operators, respectively, and λ for the chemical potential. To understand that there really is a problem with such a form of the equations, imagine that one would like to describe the collision between two superconducting nuclei. Obviously when the two systems are far apart, prior to any interaction, there are two independent chemical potentials entering into the problem, which by no means should be equal. Upon time evolution, when the two nuclei come into contact, one would expect to have only one such quantity entering into the equations. On the other hand, the single-particle Hamiltonian, the 2×2 matrix operator (1b) cannot contain two chemical potentials at the same time and this must be a unique and well-defined quantity.

In order to resolve these seemingly contradictory facts, we shall sketch a rederivation of the TDHFB equations. One way to do this is to use the Green function method.[12] Let us introduce the notations and define the relevant quantities. Let $|0\rangle$ represent the initial configuration, which is a generalized Slater determinant, the total many-body Hamiltonian

$$H=H_0+V , \tag{2a}$$

$$H_0=\int dx\, \psi^\dagger(x)\left[-\frac{1}{2m}\Delta\right]\psi(x) , \tag{2b}$$

$$V=\tfrac{1}{4}\int dx_1 dx_2 dx_3 dx_4 \psi^\dagger(x_1)\psi^\dagger(x_2) \times\Gamma(x_1,x_2,x_3,x_4)\psi(x_4)\psi(x_3) , \tag{2c}$$

where $\psi(x),\psi^\dagger(x)$ are the annihilation and creation operators and x stands for spatial, spin (and isospin) coordinates. As in the standard approach,[12] we shall work in the Heisenberg representation and introduce the normal and anomalous single-particle Green's functions

$$G(x,t;x',t')=-i\langle 0|T\{\psi(x,t)\psi^\dagger(x',t')\}|0\rangle , \tag{3a}$$

$$F(x,t;x',t')=-i\langle 0|T\{\psi(x,t)\psi(x',t')\}|0\rangle , \tag{3b}$$

where

$$\tilde{\psi}^\dagger(x,t)=\exp(iHt)\psi^\dagger(x)\exp(-iHt) , \tag{4a}$$

$$\tilde{\psi}(x,t)=\exp(iHt)\psi(x)\exp(-iHt) . \tag{4b}$$

Proceeding in a straightforward manner one can easily show that

$$(i\partial_t-h)G(x,t;x',t')=\delta(x,t;x',t') +\Delta F^*(x,t;x',t') , \tag{5a}$$

$$(i\partial_t-h)F(x,t;x',t')=\Delta^\dagger G(x,t;x',t') , \tag{5b}$$

where h is the usual HF operator and Δ is the pairing field and $|0\rangle$ is the vacuum with respect to the annihilation operators β_k defined through the generalized TD Bogoliubov transformation

$$\tilde{\psi}^\dagger(x,t)=\sum_k[u^*(x,t)\beta_k^\dagger+v_k(x,t)\beta_k] , \tag{6a}$$

$$\tilde{\psi}(x,t)=\sum_k[v^*(x,t)\beta_k^\dagger+u_k(x,t)\beta_k] . \tag{6b}$$

Now, it is a standard exercise to obtain the TDHFB equations for the single-particle wave functions $u_k(x,t),v_k(x,t)$ from Eqs. (5)

$$i\partial_t\begin{bmatrix} u_k(x,t) \\ v_k(x,t) \end{bmatrix}=\begin{bmatrix} h & \Delta \\ \Delta^\dagger & -h^* \end{bmatrix}\begin{bmatrix} u_k(x,t) \\ v_k(x,t) \end{bmatrix} . \tag{7}$$

It seems that up to here we did not do anything new. However, the careful reader will surely remark that no

chemical potential or Lagrange multiplier has entered into the above derivation. Does one really need one? In the case of stationary HFB equations one obviously has to introduce the chemical potential, since one desires to minimize the total energy of the system by having a given expectation value for the total number of particles. In the case of TDHFB equations however, the initial wave function $|0\rangle$ is characterized by an average number of particles. Since the number operator obviously commutes with the total Hamiltonian under consideration, under the time evolution in the TDHFB approximation the average value of this one-body operator is conserved and this can be shown in a manner completely similar to the TDHF case. One does not have to enforce it by introducing a constraint, and consequently the chemical potential does not appear explicitly in the above form of the TDHFB equations. In a similar fashion, in TDHF equations one does not need to enforce at every moment in time the orthonormality of the s.p.w.f.'s through Lagrange multipliers, as one will do in a static calculation. The overlaps among s.p.w.f.'s, the total linear and angular momenta, the total number of particles, etc., are in integrals of motion.

In order to obtain the stationary HFB equations as a particular case of the TDHFB equations one has to consider the following ansatz:

$$u_k(x,t)=u_{0k}(x)\exp(-i\lambda t-iE_k t)\ , \tag{8a}$$

$$v_k(x,t)=v_{0k}(x)\exp(i\lambda t-iE_k t)\ . \tag{8b}$$

Then, the Hartree-Fock and pairing potentials read

$$V_{HF}(x,y)=\tfrac{1}{2}\int dx'dy'\Gamma(x,y;x',y')\times\sum_k v^*_{0k}(x')v_{0k}(y')\ , \tag{9a}$$

$$\Delta(x,y;t)=\Delta_0(x,y)\exp(-2i\lambda t)=\tfrac{1}{2}\int dx'dy'\Gamma(x,y;x',y')\sum_k v^*_{0k}(x')v_{0k}(y')\times\exp(-2i\lambda t) \tag{9b}$$

and for a stationary state the TDHFB equations have the form

$$i\partial_t\begin{bmatrix}u_k(x,t)\\ v_k(x,t)\end{bmatrix}=\begin{bmatrix}h & \Delta_0\exp(-2i\lambda t)\\ \Delta_0^\dagger\exp(2i\lambda t) & -h^*\end{bmatrix}\times\begin{bmatrix}u_k(x,t)\\ v_k(x,t)\end{bmatrix}\ , \tag{10}$$

or after removing the trivial time dependence

$$E_k\begin{bmatrix}v_{0k}(x)\\ v_{0k}(x)\end{bmatrix}=\begin{bmatrix}h-\lambda & \Delta_0\\ \Delta_0^\dagger & -(h^*-\lambda)\end{bmatrix}\begin{bmatrix}u_{0k}(x)\\ v_{0k}(x)\end{bmatrix}\ , \tag{11}$$

which is the textbook formulation of the HFB approximation.

It is clear now that the problem we have mentioned at the beginning, when considering the collision between two superconducting nuclei, is solved in a very transparent way. When the two systems are well apart and do not interact, both the HF and pairing potentials are represented as sums of two operators acting in different regions of the space; and the chemical potentials of the two systems determine the time dependence of the corresponding parts of the pairing potential. The subsequent time evolution is completely determined by the TDHFB Eq. (7) and there is no ambiguity whatsoever.

The fact that the pairing field is not time independent, even in the case of the ground state, brings to mind an analogy with a rotating nucleus.[13] In the *laboratory reference frame* the ground state corresponds to a *rotating* pairing field with an *angular frequency* 2λ in the gauge space. One can go from the *laboratory frame* to the *body-fixed frame,* as one does in the usual cranking model, applying the *boost* operator $\exp[-i\hat{N}\lambda t]$ to the many-body wave function. In the *body-fixed frame* the pairing field will be time independent then, but in complete analogy with usual rotations, a term analogous to ωJ_x will appear in the single-particle Hamiltonian, namely $\lambda\hat{N}$. In the case of pairing, there is an *absolute reference frame,* the physical vacuum. The wave function of the vacuum is time independent in the Schrödinger representation and this fixes the *laboratory frame* for gauge rotations. For processes in which the particle number is conserved, it will make no difference which *reference frame* one is using. When considering particle transfer from one nucleus to another the relevant quantity will be of course the *relative angular velocity* in the gauge space, or in more familiar terms, the difference between the chemical potentials in the two considered nuclei.

III. BERRY'S PHASE IN THE CASE OF TDHFB EQUATIONS

We shall now establish the relation between the TDHFB approximation and the quantum phase. Berry showed[3] that the adiabatic evolution of a quantum system often has some unexpected features. Under certain conditions, a quantum state transported along a closed trajectory acquires an additional phase (early unnoticed), which can be linked with the appearance of an effective gauge field. This effective gauge field has a nonvanishing *curl* and consequently cannot be gauged away. Due to this a certain nonvanishing closed-loop integral appears. This is the nonintegrable Berry's phase and at the same time can be identified with the flux of this effective magnetic field through the surface subtended by the collective trajectory.[3] In a similar way the renowned Aaronov-Bohm effect manifests itself for a charged particle in a magnetic field.[7] The presence of such effective gauge fields leads to completely astonishing features sometimes—systems expected to behave like bosons suddenly acquire fermionic characteristics or vice versa.[4,5] The reason for this is that the gauge field carries an angular momentum of its own; and the conserved quantity is the total angular momentum, which is the sum of the angular momentum of the particle and of the gauge field.

Now let us turn to the canonical example of a physical

system which displays the Berry's phase, namely the Schrödinger equation for a spin-$\frac{1}{2}$ particle in a magnetic field precessing uniformly around the Oz-axis,[3,8]

$$i\partial_t\varphi = H(t)\varphi = \mu B \begin{bmatrix} \cos\theta & \sin\theta\exp(-i\omega t) \\ \sin\theta\exp(i\omega t) & -\cos\theta \end{bmatrix}\varphi , \tag{12a}$$

$$\mathbf{B}(t) = B(\sin\theta\cos(\omega t),\sin\theta\sin(\omega t),\cos\theta) . \tag{12b}$$

Obviously, $H(0)=H(T)$, where $\omega T = 2\pi$. The general solution to the above equation is a combination between two linearly independent solutions, which have the form

$$\varphi_\pm(t) = \begin{bmatrix} a_\pm \exp\left[-\frac{i\omega t}{2} - i\epsilon_\pm t\right] \\ b_\pm \exp\left[\frac{i\omega t}{2} - i\epsilon_\pm t\right] \end{bmatrix} , \tag{13}$$

where

$$\epsilon_\pm = \pm\left[\left(\mu B\cos\theta - \frac{\omega}{2}\right)^2 + (\mu B\sin\theta)^2\right]^{1/2} ,$$
$$a_\pm^2 + b_\pm^2 = 1 , \tag{14}$$

and the constants $a_\pm$, $b_\pm$ can be chosen real such that

$$\epsilon_\pm \begin{bmatrix} a_\pm \\ b_\pm \end{bmatrix} = \begin{bmatrix} \mu B\cos\theta - \frac{\omega}{2} & \mu B\sin\theta \\ \mu B\sin\theta & -\left(\mu B\cos\theta - \frac{\omega}{2}\right) \end{bmatrix} \begin{bmatrix} a_\pm \\ b_\pm \end{bmatrix} . \tag{15}$$

This solution was first obtained by Rabi[14] and as one can easily see it does not assume adiabaticity.

Now by simply comparing Eqs. (8)–(11) with the corresponding ones (12)–(15) it becomes evident that both sets of equations have a remarkable similarity. The role of the *magnetic field* in the case of TDHFB equations is played by $[\mathrm{Re}(\Delta),\mathrm{Im}(\Delta),h]$, while 2λ is the *precision frequency*. The Hartree-Fock and pairing operators play the role of the *slow* variables; and the single-particle degrees of freedom are the *fast* ones, in complete analogy with the case of a spin and in an external magnetic field. However, the adiabatic assumption does not hold in the present case, since the *precession frequency* $\omega = 2\lambda$ of the single-particle field is not small in comparison with the single-particle excitation energies. Consequently, if one desires to derive the corresponding collective Hamiltonian one has to rely on the general prescriptions.[8]

As a simple and very illustrative example let us consider N particles in a 2Ω-fold degenerate level, interacting by a pure pairing force only.[15] The total Hamiltonian for such a system can be taken as

$$H = -G\sum_{m,m'=1}^{\Omega} a_m^\dagger a_{-m}^\dagger a_{-m'} a_{m'} . \tag{16}$$

The s.p. Hamiltonian in this case reads

$$H_0 = \sum_{m>0}\left[\epsilon(a_m^\dagger a_m + a_{-m}^\dagger a_{-m}) + \Delta a_m^\dagger a_{-m}^\dagger + \Delta^* a_{-m} a_m\right] ,$$
$$\epsilon = -G|v|^2, \quad \Delta = -G\Omega u v^*, \quad |u|^2+|v|^2 = 1 \tag{17}$$

and the wave function is (in the Schrödinger representation)

$$|\mathrm{BCS}\rangle = \prod_{m>0}(u^* + v^* a_m^\dagger a_{-m}^\dagger)|0\rangle , \tag{18}$$

which is a vacuum state for the quasiparticle destruction operators $a_{\pm m}$

$$\alpha_m^\dagger = u a_m^\dagger - v a_{-m}, \quad \alpha_{-m}^\dagger = u a_{-m}^\dagger + v a_m ,$$
$$\alpha_m = -v^* a_{-m}^\dagger + u^* a_m, \quad \alpha_{-m} = v^* a_m^\dagger + u^* a_{-m} .$$

The easiest way to find the equations for the time dependence of the coefficients u,v is by applying the s.p. operator H_0, which determines the time evolution in this approximation, to the w.f. $|\mathrm{BCS}\rangle$. In this way one readily obtains that

$$i\partial_t \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} 0 & \Delta \\ \Delta^* & -2\epsilon \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} , \tag{19}$$

with the stationary solution

$$u = u_0\exp[-i(-\epsilon+E)t - i\lambda t] , \tag{20a}$$

$$v = v_0\exp[-i(-\epsilon+E)t + i\lambda t] , \tag{20b}$$

where u_0, v_0 are time independent and without any loss of generality can be considered real, and

$$\Delta = \Delta_0\exp[-2i\lambda t] ,$$
$$v_0^2 = \frac{N}{2\Omega}, \quad u_0^2 = 1 - \frac{N}{2\Omega},$$
$$\Delta_0 = -G\Omega u_0 v_0 ,$$
$$\epsilon = -G v_0^2 ,$$
$$E = \pm[(\epsilon-\lambda)^2 + \Delta_0^2]^{1/2}$$

and consequently the time dependence of the total w.f. reads

$$|\mathrm{BCS}\rangle = \exp[i\Omega(-\epsilon+E+\lambda)t] \times\prod_m(u_0 + \exp(-2i\lambda t)v_0 a_m^\dagger a_{-m}^\dagger)|0\rangle . \tag{21}$$

The period of the *rotation* is

$$T = \frac{2\pi}{2\lambda} . \tag{22}$$

The nonintegrable quantum or Berry's (nonadiabatic in this case) phase is defined as the difference between the actual phase of the w.f. after one period

$$\Phi_{\mathrm{actual}} = \Omega[(\epsilon-E)-\lambda]T$$

and the expected one, also called the dynamical phase, which is given by

$$\Phi_{\mathrm{dynamical}} = \langle\mathrm{BCS}|H_0|\mathrm{BCS}\rangle T = \Omega[(\epsilon-E)-\lambda(u_0^2-v_0^2)]T.$$

In the present case, the expectation value of the single-particle Hamiltonian is time independent, despite the fact that the Hamiltonian itself is time dependent. The resulting (nonadiabatic) Berry's phase is

$$\Phi_{\text{Berry}}=\Omega\pi(1-u_0^2+v_0^2)$$
$$=\Omega\pi\left[1-\frac{(\epsilon-\lambda)}{\sqrt{(\epsilon-\lambda)^2+\Delta^2}}\right]$$
$$=\Omega\pi\frac{N}{\Omega}=\pi N\ , \tag{23}$$

which means that every pair of particle and hole m states contributed an amount $\pi N/\Omega$ to the overall quantum phase. In the present case the collective variables are ϵ, Δ, and Δ^* and the *monopole*, responsible for the appearance of this additional phase, sits at

$$\epsilon-\lambda=\Delta=0\ ,$$

i.e., at the degeneracy of the paired s.p. states, and has a *total charge* equal to $\Omega\times(-\frac{1}{2})$, i.e., $-\frac{1}{2}$ for every such pair. The trajectory of a single quasiparticle state is a circle and the solid angle under which the *monopole* sees the trajectory is $2\pi[1-u_0^2+v_0^2]=2\pi N/\Omega$. The *magnetic field* created by such a *monopole* is *radial* in the collective space[3]

$$\mathbf{B}=\frac{\mathbf{R}}{2R^3}\ ,\quad \mathbf{R}=(\text{Re}\Delta,\text{Im}\Delta,\epsilon-\lambda)\ .$$

The *force* acting on the system point, due to one quasiparticle only,

$$\mathcal{F}=\mathbf{v}\times\mathbf{B},\quad \mathbf{v}=\frac{d}{dt}\mathbf{R}$$

bends the trajectory out of the *reaction plane*, i.e., the system point does not remain in the plane normal to the *angular momentum*. This happens because the *monopole* modifies the *conserved angular momentum* by $-g\mathbf{R}/R$, where $g=-\frac{1}{2}$ is the *magnetic charge of the monopole* in the present case.[16,17] One must remark also that this *magnetic* force is long ranged, as a Coulomb force would be, and consequently, the presence of a *monopole* will be felt by the system point even when this will be relatively far from the degeneracy. (We emphasize *magnetic monopole, magnetic interaction, magnetic force, reaction plane, angular momentum*, etc., in order to underline the fact that there is no actual monopole but an effective gauge field, which has all the formal properties of a monopole in the corresponding collective space.)

The case of an N-particle system in a degenerate shell is an idealization. Different quasiparticle states do not have to become degenerate simultaneously. Allowing for other collective degrees of freedom to become active new effective gauge fields will come into play and the position of different *diabolical points* or *funnels* will depend on deformation, rotation frequency, pairing, and any other collective degrees of freedom relevant to the problem at hand. The role of deformation has already been put in evidence and pretty well understood,[10,16,18–20] even though none of these authors explicitly considered the Hartree-Fock problem. The corresponding formulas can be simply rewritten for such a case. For example, in the generic Hamiltonian for the interaction between the quadrupole (slow) and dipole (fast) oscillations considered in Ref. 10 one has simply to replace (rename) the dipole variables with s.p.w.f.'s and one obtains a Nilsson type of s.p. Hamiltonian. As Jackiw[19] showed, the form of the corresponding effective fields can be deduced by simply requiring invariance under the action of the rotation group. It is likely that this is a general result, namely, knowing the broken symmetry simply from invariance under the action of the corresponding symmetry group one would be able to deduce the form of the effective gauge field. However, in the case of a nuclear many-body wave function, the number of different symmetries which can be broken is so large, that such an approach could prove to be useless. It is enough to look at a Nilsson diagram, in order to realize that the positions of level crossings cannot be linked with the breaking of the rotational or any other simple symmetry. Most of the level crossings which appear in a Nilsson scheme occur between two levels only, except the case of vanishing deformation, when the degeneracy is $2j+1$. The effective gauge field determined in Refs. 10, 16, and 18–20 is generated by the breaking of the rotational symmetry and the corresponding gauge potential, either Abelian or non-Abelian, take values in a given representation of the SO(3) algebra. However, they do not provide the most general solution to the problem. The gauge potentials determined in Ref. 10 (which seems to be the most complete treatment of the rotational symmetry breaking) have components in the collective variables only along the three Euler angles, which determine the orientation of the nucleus. The β and γ components (β,γ are the usual deformation variables, which define the intrinsic shape of the nucleus) of the effective field are vanishing, only because these authors[10] did not allow the "s.p.w.f.'s" (the dipole variables in their case) to have components across a shell (they suppressed the $\Delta N\geq 2$ transitions). Allowing for such terms will give rise to SO(5) gauge potentials, instead of only SO(3), which is the symmetry group of the five-dimensional harmonic oscillator.

The *diabolical points* or *funnels* are remarkable for a different reason too. As has been well known for more than half a century, they are the cause of the so-called Landau-Zener effect. It is not clear at the moment if there is a more direct connection between these two phenomena.

There is a direct analogy between the Berry's phase and a much older and known result. Almost anyone first coming across Berry's result wonders how such a simple fact was not observed earlier. This fact is even more astonishing, if one remarks that the adiabatic approximation is, at least at the formal level, nothing else but the old and well known WKB approach for solving the Schrödinger equation. Simply by calling the spatial coordinate the time, the linear local momentum the adiabatic energy and the turning points diabolical points one sees at once that the analogy is perfect. The adiabatic evolution corresponds to slow variation of the potential energy, the spin-up and spin-down states at a given time are

simply the forward or backward waves at a given position x, the adiabatic energies for the spin-up and spin-down states are the plus/minus local linear momentum, which become degenerate at a turning point. The phase acquired by the wave function, at least in the WKB approximation seems to be *dynamical* only in origin though. However, in order to have a *cyclic* evolution here, all one has to do is to go back and forth *around the turning point,* and in order to do this without *losing adiabaticity,* one must go around the turning point in the complex x plane at a *safe* distance from them.[1] Then the *Berry's* phase, after one *period* emerges as the factor -1, which is acquired by the wave function, due to the squared-root singularity at the turning points. The presence of turning points is known to modify the Bohr-Sommerfeld quantization rules. In a similar way, the presence of diabolical points or funnels will modify the quantization rules for collective modes. It is instructive to see how this will work in the case, analyzed above, N particles in a 2Ω-fold degenerate shell, interacting through a pure pairing force. Without taking into account the contribution from the *monopole,* the Bohr-Sommerfeld rule will read

$$\oint p\,dq=\oint p\frac{dq}{dt}dt=\oint\frac{N}{2}2\lambda dt=\pi N\ , \tag{24}$$

where the integral is over one period T, Eq. (22). It is known[13] that in the case of pairing $N/2$ plays the role of the momentum and 2λ is the velocity, i.e., the time derivative of the corresponding canonical conjugated coordinate. The above quantization rule fixes only the total number of particles to be an even integer. The additional contribution, due to the presence of the effective gauge field is equal to the (nonadiabatic) Berry's phase, Eq. (23), which by no accident is πN. The quantum phase takes this value only for a determined value of the chemical potential λ. Consequently, one can say that only the *exact* quantization rule

$$\oint(p-A)dq=2\pi\ \text{integer}\ , \tag{25}$$

where

$$\Phi_{\text{Berry}}=\oint A\,dq \tag{26}$$

and A is the effective gauge field solves the problem. Without the contribution from the gauge field, the standard quantization rule says that the total number of particles is an even integer, but the chemical potential remains to be determined from a logically unrelated condition (one has to enforce it *by hand).*

IV. CONCLUSIONS

We showed how a gauge structure appears in connection with the treatment of pairing correlations in the framework of the TDHFB approximations. The situation is new in at least two respects: (i) It demonstrates an explicit occurrence of the gauge effective fields in a many-body problem, where the s.p. degrees of freedom play the role of the fast variables while the s.p. field has to be associated with the slow variables. The effective gauge fields will manifest themselves in the effective Hamiltonian of these slow degrees of freedom. (ii) It is an example of the situation, when one has to go beyond the adiabatic approximation in treating the slow variables and their effect on the fast ones and where one has to apply the general prescription, in order to find the reduced Lagrangian.[8]

Even though it could seem that we dealt with a special case, the general framework for treating the effective gauge fields in a many-body problem is generic in our opinion. The TDHFB example can be generalized in a straightforward manner, in principle, to any collective variables and their corresponding reduced Hamiltonian. Since the action of the gauge fields on the time evolution of the collective degrees of freedom is sometimes so different from what one would expect from *usual conservative forces,* one could suspect the occurrence of a new whole class of phenomena. For example, when passing near a *monopole,* the collective trajectory will be bent out of what one will call loosely a *reaction plane.* The conservation laws of the collective momenta will be modified due to the presence of *monopoles* too. One could address the following question: "How will the trajectory of two heavy ions be influenced by the appearance of a *diabolical point?*" During the adiabatic evolution of the s.p. orbitals in the common field of the two ions, such *funnels* will certainly appear. One can expect the appearance of a more or less uniform distribution of *monopoles* in the collective space.[6] Due to the complexity of the problem and the fact that in analyzing experimental data one is usually relying on potential models, one can expect that new qualitative phenomena were overlooked. The list of potential problems is almost limitless and it is difficult to guess at the moment which problem could be the most interesting one.

An analysis of the general structure of the collective effective action, which emerges in a path integral approach to the many-fermionic propagator, after applying the Hubbard-Stratonovich transformation[11] was done in Ref. 21. We show there that the effective collective Lagrangian has the following generic structure:

$$\mathcal{L}=\mathcal{A}_\alpha\dot{\sigma}_\alpha-\mathcal{E}(\sigma)\ , \tag{27}$$

where σ_α represents the "classical" limit of fermionic pair operators $a_j^\dagger a_k, a_j a_k, a_j^\dagger a_k^\dagger$, $\mathcal{A}_\alpha$ is a gauge field on the classical collective phase space and $\mathcal{E}(\sigma)$ is the total energy of the nucleus. The gauge potentials appear to play a fundamental role in the collective dynamics, since due to the way they enter into the theory, they govern the whole time evolution of the envisaged system. The corresponding terms in the collective effective Lagrangian are the only terms, which contain time derivatives of the collective variables and consequently, there is no dynamics once they are dropped. This result looks at least unexpected at the first sight, but a closer analysis shows that this is exactly what one should have expected. In Ref. 22 we showed that the classical limit of a Lie algebra is described by a Lagrangian which has exactly the same structure as (27). On the other side, the initial many-body Hamiltonian (2) can be represented through generators of the shell model algebra SO(2N) of pairs of creation and annihilation operators, where N is the total number of single-particle states. Consequently, the classical

counterpart of such a system is the classical limit of the corresponding Lie algebra. The reason why the gauge potentials emerged in the classical description of Lie algebras lies in the nontrivial topological structure of the corresponding phase space. If the Lie algebra is compact, the same applies to the corresponding classical phase space and the presence of gauge fields is merely a result of its curved character. Moreover, the presence of the gauge fields proves to be a necessary ingredient in order to find the correct quantum limit of the classical collective Lagrangian. In the special case of N particles in a degenerate level, see Eq. (16), the problem can be solved exactly once we recognize the SU(2) structure of this Hamiltonian.[15] In such a case, the pairing field Δ, Δ^* and the Hartree-Fock term ϵ (up to some additive and multiplicative constants) represent the classical limit of the generators of the SU(2) algebra generated by

$$S_+ = \sum_m a_m^\dagger a_{-m}^\dagger \ ,$$
$$S_- = \sum_m a_{-m} a_m \ , \tag{28}$$
$$S_0 = \tfrac{1}{2} \sum_m (a_m^\dagger a_m + a_{-m}^\dagger a_{-m} - 1) \ .$$

On the other side, the requantization of the Hartree-Fock-Bogoliubov solution must lead to the same exact result and to the fact that $\Delta, \Delta^*, \epsilon$ represents actually these generators. This is exactly what one obtains after applying in a consistent way the requantization procedure[22] and the presence of the gauge field, which generated the Berry's phase in this case, is an essential element of this procedure.

As a final remark we would like to point out some recent numerical results obtained by Wolf, Puddu, and Negele[23] of the symmetric fission of ^{32}S in the framework of TDHF theory. What these authors observed is that along the fission path the ^{32}S system manifestly "avoids" the diabolical point or funnel corresponding to a single-particle level crossing. The trajectory followed by the system in the neighborhood of this configuration looks very much like an approximate "circle," generated by a "magnetic" type of interaction. Near this diabolical point the s.p.w.f's change drastically from the configuration corresponding to one nucleus to one corresponding to two separated fragments. The "exact" TDHF time evolution shows that the system does not like to go through a diabolical point, but rather breaks the symmetry of the mean field in such a way as to avoid this configuration at a "safe" distance, as to ensure adiabaticity along the collective path. On the other side, the trajectory is not similar to the one one would expect in a standard cranking model, which would correspond to an effective Hamiltonian with a kinetic and potential energy terms only. It seems that this calculation is a clear example of the effect of a "magnetic force" on the time evolution of the system, which has to be taken into account in an effective collective Lagrangian.

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