Nonequilibrium cooper pairing in the nonadiabatic regime

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We obtain a complete solution for the mean-field dynamics of the BCS paired state with a large, but finite number of Cooper pairs in the nonadiabatic regime. We show that the problem reduces to a classical integrable Hamiltonian system and derive a complete set of its integrals of motion. The condensate exhibits irregular multifrequency oscillations ergodically exploring the part of the phase space allowed by the conservation laws. In the thermodynamic limit, however, the system can asymptotically reach a steady state.

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The study of the dynamics of the BCS superconductors has a long history. Early attempts to describe nonstationary superconductivity were based on the time-dependent Ginzburg-Landau (TDGL) equation,2-4 which reduces the problem to the time evolution of a single collective order parameter $\Delta(t)$. The TDGL approach is valid only provided the system quickly reaches an equilibrium with the instantaneous value of $\Delta(t)$, i.e., a local equilibrium is established faster than the time scale of the order parameter variation, $\tau_{\Delta} \simeq 1/\Delta$. This requirement limits the applicability of the TDGL to special situations where pair breaking dominates, e.g., due to a large concentration of magnetic impurities. An alternative to TDGL is the Boltzmann kinetic equation^{5,6} for the quasiparticle distribution function coupled to a selfconsistent equation for $\Delta(t)$. This approach is justified only when external parameters change slowly on the au_{Δ} time scale, so that the system can be characterized by a quasiparticle distribution.

Is it possible to describe theoretically the dynamics of a BCS paired state in the nonadiabatic regime when external parameters change substantially on the τ_{Δ} time scale? In particular, an important question is whether, following a sudden perturbation, the condensate reaches a steady state on a τ_{Δ} time scale or on a much longer quasiparticle energy relaxation time scale τ_{ϵ} . In the nonadiabatic regime both TDGL and the Boltzmann kinetic equations fail and one has to deal with the coupled coherent dynamics of individual Cooper pairs. Recent studies 7-10 of this outstanding problem were motivated by experiments on fermionic pairing in cold atomic alkali gases. 11,12 The strength of pairing interactions in these systems can be fine tuned rapidly by a magnetic field, making it easier than in metals to access the nonadiabatic regime experimentally.

The main result of the present paper is an explicit general solution for the *dynamics* of the BCS model, which describes a spatially homogenous condensate at times $t \ll \tau_\epsilon$. We employ the usual BCS mean-field approximation, which is accurate when the number of Cooper pairs is large. ^{13,14} It turns out that the mean-field BCS dynamics can be formulated as a nonlinear *classical Hamiltonian* problem. We obtain the

exact solution for all initial conditions and a complete set of integrals of motion for the mean-field BCS dynamics.

In this paper we assume that the number of Cooper pairs in the system is arbitrary large, but *finite*. In this case the typical evolution at times $t \ll \tau_{\epsilon}$ is quasiperiodic with a large number of incommensurate frequencies. The condensate exhibits irregular multifrequency oscillations ergodically exploring the part of the phase space allowed by the conservation laws. The system returns arbitrarily close to its initial state at irregular time intervals. However, the return time diverges in the thermodynamic limit for physical initial conditions, while the solution asymptotically reaches a *steady* state on the τ_{Δ} time scale. The system thermalizes on a much larger energy relaxation time scale τ_{ϵ} .

The dynamics of the BCS condensate following a sudden change of external parameters has been previously discussed by a number of authors. 7-10,14,16-18 Most notably, a linear analysis around the BCS ground state has been performed 14,16 and some simple particular solutions for the nonlinear mean-field dynamics in the context of superconductivity have been reported. 7 We discuss below how these results fit into the general picture.

We begin our description of the nonequilibrium Cooper pairing in the nondissipative regime, $t \le \tau_{\epsilon}$, with the BCS model.^{19–21}

$$\hat{H}_{BCS} = \sum_{j,\sigma} \epsilon_j \hat{c}_{j\sigma}^{\dagger} \hat{c}_{j\sigma} - g \sum_{j,q} \hat{c}_{j\uparrow}^{\dagger} \hat{c}_{j\downarrow}^{\dagger} \hat{c}_{q\downarrow} \hat{c}_{q\uparrow}, \qquad (1)$$

where ϵ_j are single-particle energies. The pairing is between time reversed states $|j\uparrow\rangle$ and $|j\downarrow\rangle$.²² Our goal is to determine the evolution of a state that was driven out of equilibrium at, say, t=0.

There are several equivalent ways to derive mean-field equations of motion. One can start with the BCS product state, $\Pi_j[U_j(t)+V_j(t)c_{j\uparrow}^{\dagger}\hat{c}_{j\downarrow}^{\dagger}]|0\rangle$, and use Bogoliubov–de Gennes equations for the time-dependent amplitudes $U_j(t)$ and $V_j(t)$. Alternatively, one can study the evolution of the normal, $G_j(t)=-i\langle[\hat{c}_{j\uparrow}(t),\hat{c}_{j\uparrow}^{\dagger}(t)]\rangle$, and anomalous, $F_j(t)=-i\langle[\hat{c}_{j\uparrow}(t),\hat{c}_{j\downarrow}(t)]\rangle$, Green's functions at coinciding times. 16

The most convenient way for us approach to the BCS mean-field dynamics is based on the Anderson pseudospin representation. Within this approach the mean-field equations are Hamiltonian equations of motion for a classical spin chain. Pseudospin-1/2 operators are related to fermion creation and annihilation operators via $\hat{K}_j^z = (\hat{n}_{j\uparrow} + \hat{n}_{j\downarrow} - 1)/2$ and $\hat{K}_j^- = \hat{c}_{j\downarrow}\hat{c}_{j\uparrow} = (\hat{K}_j^+)^{\dagger}$. Pseudospins are defined on empty and doubly occupied (unblocked) single-particle orbitals ϵ_j . Singly occupied orbitals are decoupled from the dynamics. For n unblocked orbitals the Hamiltonian has the form

$$\hat{H}_{BCS} = \sum_{j=0}^{n-1} 2\epsilon_j \hat{K}_j^z - g \sum_{j,q} \hat{K}_j^+ \hat{K}_q^-.$$
 (2)

The mean-field approximation is accurate 13,14 in the thermodynamic limit due to the infinite range of interactions between spins in the Hamiltonian (2). Therefore, the effective field seen by each pseudospin in (2) can be replaced with its quantum mechanical average, $\mathbf{b}_j(t) = (-2\Delta_x(t), -2\Delta_y(t), 2\epsilon_j)$, where $\Delta(t) \equiv \Delta_x(t) - i\Delta_y(t) \equiv g\Sigma_j\langle\hat{K}_j^-(t)\rangle$ is the BCS gap function. In this approximation, each spin evolves in the self-consistent field: $\hat{\mathbf{K}}_j = i[\hat{H}_{BCS}, \hat{\mathbf{K}}_j] \approx \mathbf{b}_j \times \hat{\mathbf{K}}_j$. Taking the quantum mechanical average of these equations with respect to the time-dependent state of the system, we obtain for $\mathbf{s}_i(t) = \langle \hat{\mathbf{K}}_i(t) \rangle$,

$$\dot{\mathbf{s}}_j = \mathbf{b}_j \times \mathbf{s}_j, \quad \mathbf{b}_j = (-2gJ_x, -2gJ_y, 2\epsilon_j), \quad \mathbf{J} = \sum_{q=0}^{n-1} \mathbf{s}_q.$$
 (3)

The components of the classical spins $s_j^z(t)$ and $s_j^\pm = s_j^\pm \pm i s_j^v$ are related to Bogoliubov amplitudes and equal times Green's functions as $2s_j^z = |V_j|^2 - |U_j|^2$, $s_j^- = \bar{U}_j V_j$ and $G_j(t) = i s_j^z(t)$, $F_j(t) = i s_j^-(t)$, respectively. Evolution equations (3) conserve the square of the average for each spin: $d s_j^2 / d t = 0$. If the spins initially were in a product state, $s_j^2 = 1/4$. Note also that $\Delta(t) = g J_-(t)$.

One can check that Eqs. (3) are equations of motion for a *classical* spin Hamiltonian

$$H_{BCS} = \sum_{j=0}^{n-1} 2\epsilon_j s_j^z - g \sum_{j,q} s_j^+ s_k^-.$$
 (4)

It means that Eqs. (3) are Hamilton equations $\dot{\mathbf{s}}_j = \{H_{BCS}, \mathbf{s}_j\}$ derived from Hamiltonian (4) using the usual angular momentum Poisson brackets

$$\{s_j^a, s_k^b\} = -\varepsilon_{abc}\delta_{jk}s_j^c,\tag{5}$$

where a, b, and c stand for spatial indexes x, y, and z. The classical model (4) can be obtained from its quantum counterpart (2) by replacing operators with classical dynamical variables and commutators with Poisson brackets.

Both the classical (4) and quantum models (1) and (2) are integrable $^{23-25}$ (see also Ref. 26 and references therein). To show this, one can introduce a vector function (Lax vector) of an auxiliary parameter u

$$\mathbf{L}(u) = -\frac{\hat{\mathbf{z}}}{g} + \sum_{i} \frac{\mathbf{s}_{i}}{u - \epsilon_{i}},\tag{6}$$

where $\hat{\mathbf{z}}$ is a unit vector along the z axis. Poisson brackets between components of $\mathbf{L}(u)$ at different values of u can be evaluated using Eq. (5).

$$\{L^{a}(v), L^{b}(w)\} = \varepsilon_{abc} \frac{L^{c}(v) - L^{c}(w)}{v - w}.$$
 (7)

[Relations (7) hold for each term in (6) separately; all terms Poisson commute with each other.] It follows from Eq. (7) that the lengths of the Lax vector at different values of u Poisson commute are

$$\{\mathbf{L}^2(v), \mathbf{L}^2(w)\} = 0. \tag{8}$$

The scalar function $L^2(u)$ can be represented in the form

$$\mathbf{L}^{2}(u) = \frac{1}{g^{2}} + \sum_{j=0}^{n-1} \left(\frac{2H_{j}}{u - \epsilon_{j}} + \frac{\mathbf{s}_{j}^{2}}{(u - \epsilon_{j})^{2}} \right), \tag{9}$$

where

$$H_{j} = \sum_{k=0}^{n-1} \frac{\mathbf{s}_{j} \cdot \mathbf{s}_{k}}{\epsilon_{i} - \epsilon_{k}} - \frac{s_{j}^{z}}{g}.$$
 (10)

Since Eq. (8) holds for any v and w, all H_j Poisson commute with each other. Therefore, each H_j , as well as any algebraic combination of H_j , defines a classical model²⁷ that has n degrees of freedom (n classical spins) and n integrals of motion (including itself) and thus is integrable in the usual sense.²⁸ Note that the sum of H_j is proportional to the z component of the total spin \mathbf{J} , therefore J_z is conserved by all H_j and their combinations. Moreover, the following identity follows from Eqs. (4) and (10):

$$H_{BCS} = -g \sum_{j} \epsilon_{j} H_{j} + \text{const.}$$
 (11)

This implies that the classical BCS model (4) Poisson-commutes with all H_j 's and thus is also integrable. Equations (10) and (11) can be straightforwardly quantized by replacing $\mathbf{s}_j \rightarrow \hat{\mathbf{K}}_j$. The resulting operators \hat{H}_j all pairwise commute, thus showing the integrability of quantum models (1) and (2).

To obtain the general solution for the mean-field dynamics of the BCS model (1), we follow the method of Ref. 29 and introduce n-1 separation variables u_k as zeros of $L_-(u) = L_x(u) - iL_y(u)$, i.e., $\sum_j s_j^- / (u_k - \epsilon_j) = 0$.

Equations of motion for the variables u_k are 30

$$\dot{u}_k = 2i\sqrt{Q_{2n}(u_k)} \prod_{m \neq k} (u_k - u_m)^{-1},$$
 (12)

where $Q_{2n}(u)$ is the spectral polynomial defined as

$$Q_{2n}(u) = g^2 \mathbf{L}^2(u) \prod_i (u - \epsilon_i)^2. \tag{13}$$

By Eq. (9), the coefficients of $Q_{2n}(u)$ depend only on the integrals of motion H_i .

Equations (12) constitute the well-known Jacobi's inversion problem solvable in terms of hyperelliptic theta functions.³¹ Here we outline the final answer; the details will be reported elsewhere.³⁰ Klenian σ and ζ functions of *genus* G (in our case G=n-1) are defined as

$$\zeta_l(\mathbf{x}) = \frac{\partial \ln \sigma(\mathbf{x})}{\partial x_l}, \quad \sigma(\mathbf{x}) = \sum_{\mathbf{m} \in Z^G} \exp[S_{\mathbf{m}}(x)/2],$$

$$S_{\mathbf{m}}(x) = \mathbf{x} \cdot \eta \omega^{-1} \mathbf{x} + 2i\pi (\mathbf{m} \cdot \tau \mathbf{m} + \omega^{-1} \mathbf{x} \cdot \mathbf{m}), \quad (14)$$

where the sum is over all G-dimensional integer vectors \mathbf{m} , $\tau = \omega' \omega^{-1}$, and ω , ω' , and η are $G \times G$ matrices of periods (see below). The solution is

$$s_{j}^{-}(t) = \langle \hat{c}_{j\downarrow}(t)\hat{c}_{j\uparrow}(t)\rangle = J_{-}(t)r(\epsilon_{j},t)\prod_{k\neq j}\frac{\epsilon_{j}}{\epsilon_{j}-\epsilon_{k}}, \qquad (15)$$

$$\Delta(t) = gJ_{-}(t) = g\sum_{j} s_{j}^{-}(t) = c_{n}e^{-i\beta t}\frac{\sigma(\mathbf{x} + \mathbf{d})}{\sigma(\mathbf{x} - \mathbf{d})}.$$
 (16)

Here $\mathbf{x}^T = i(c_1, \dots, c_{n-2}, 2t + c_{n-1})$; **d** is a vector of constants; $\beta = gJ_z + \sum_j \epsilon_j$; c_1, \dots, c_n are constants fixed by the initial conditions, and

$$r(u,t) = 1 - \sum_{k=1}^{n-1} \left[\zeta_k(\mathbf{x} + \mathbf{d}) - \zeta_k(\mathbf{x} - \mathbf{d}) + a_k \right] u^{k-n}.$$
 (17)

Constants a_k , the matrices of periods, constant vector **d**, are all uniquely determined³² by the spectral polynomial $Q_{2n}(u)$, i.e., by integrals of motion.

The evolution of $\mathbf{s}_j(t) = \langle \hat{\mathbf{K}}_j(t) \rangle$ described by the general solution is typical of an integrable system. It is characterized by n frequencies, which in our case can be determined in terms of integrals of motion, and are typically incommensurate. Note that $|\Delta(t)|$ contains only n-1 frequencies. The typical dynamics is stable against perturbations destroying integrability. The system of t

Now let us discuss some particular solutions. There are two types of equilibrium states that play an important role in the dynamics. In *normal* states all spins are parallel to the z axis, $2\mathbf{s}_j^z = \pm 1$. Since $2\mathbf{s}_j = \langle \hat{n}_j \rangle - 1$, these states correspond to the ground state and excitations of the single-particle part of the Hamiltonian (1) (Fermi gas). They are stationary within the mean-field dynamics (3). For a finite system, they are nonstationary for the quantum Hamiltonian (1) and their short time dynamics is entirely driven by quantum corrections (cf. Refs. 33 and 34).

The second type of equilibrium states are *anomalous* ones, which correspond to the BCS ground state and excitations. These states are obtained by aligning each spin in (4) self-consistently along the effective magnetic field acting on it. The self-consistency condition is the BCS gap equation. As $\mathbf{s}_j = \langle \hat{\mathbf{K}}_j \rangle$, one can obtain the BCS wave function and energy spectrum from anomalous equilibrium configurations of classical spins \mathbf{s}_j .

It turns out that equilibrium states are a part of a more general scheme when the dynamics of n spins degenerates to that of m < n collective spins (m-spin solutions) governed by

the same Hamiltonian (4) only with m spins and new parameters μ_i instead of ϵ_i . Normal and anomalous states correspond to zero- and one-spin solutions, respectively. To construct m-spin solutions one has to take the Lax vector (6) to be proportional to that of a system with m spins \mathbf{t}_k , $\mathbf{L}(u) = [1 + \sum_i b_i / (u - \epsilon_i)] \mathbf{L}_{\mathbf{t}}(u)$, where b_i are time-independent constants, and $\mathbf{L}_{\mathbf{t}}(u) = -\hat{\mathbf{z}}/g + \sum_{k} \mathbf{t}_{k}/(u - \mu_{k})$. Then, 2(n-m) of 2n, typically distinct, roots of the spectral polynomial $Q_{2n}(u)$ become doubly degenerate and n-m separation variables u_k are frozen in these double roots, which automatically solves the equations of motion for these n-m variables. The dynamics is obtained by replacing $n \rightarrow m$ and $\epsilon_k \rightarrow \mu_k$ in Eqs. (14)–(17) and is characterized by m < n typically incommensurate frequencies. For m=2 the solution is in terms of hyperelliptic functions of genus G=m-1=1, i.e., in terms of ordinary elliptic functions.

Now let us discuss the connection of our results with the previous work. The solutions for the mean-field BCS dynamics obtained in Ref. 7 are two-spin solutions in the above classification. They were used in Ref. 7 to describe the evolution beginning from a state infinitesimally close to the normal ground state. In our view, the dynamics in the vicinity of this state can have additional features and deserves further analysis.

The two-spin solutions resemble the TDGL approach in that they describe the dynamics of all pairs in terms of only two collective degrees of freedom resulting in large amplitude single frequency (periodic) oscillations of the order parameter magnitude $|\Delta(t)|$. Mathematically, they lie on a onedimensional curve of points in a multidimensional (infinite dimensional in the thermodynamic limit) space of possible values of integrals of motion. The situation with other few spin solutions is similar.³⁵ In contrast, the general solution we obtained here typically has a large (infinite in the thermodynamic limit) number of incommensurate frequencies and a substantially reduced amplitude. The difference between the general and few spin solutions is clear in a linear analysis 14,16 around the BCS ground state that displays normal modes with frequencies $\omega_k = 2\sqrt{\epsilon_k^2 + \Delta_0^2}$, where ϵ_k are single-particle energies and Δ_0 is the equilibrium order parameter. In the linear regime, the general solution becomes an arbitrary superposition of all normal modes, while few spin solutions single out all, but few modes. For example, two-spin solutions of Ref. 7 correspond to a single normal mode with a frequency $2\Delta_0$.

In conclusion, we have obtained the explicit general solution for the mean-field dynamics of the BCS paired state and discussed a number of special cases including two types of equilibrium states and few spin solutions. A still open problem is to fully analyze the solution in the thermodynamic limit. It is also desirable to better understand the dynamics in the vicinity of normal states where quantum effects become important. Finally, it is interesting to identify experimental setups where peculiar features of the nonequilibrium Cooper pairing in the nonadiabatic regime can be observed in realistic systems such as, e.g., cold Fermi gases.

Note Added. Recently, we became aware of a publication³⁶ that is in agreement with some of our conclusions—that the initial dynamics of the normal ground state is driven by quantum corrections and that $\Delta(t)$ can decay to a constant value at large times.

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