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FAST TRACK COMMUNICATION

Lindblad master equation approach to superconductivity in open quantum systems

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Abstract

We consider an open quantum Fermi system which consists of a single degenerate level with pairing interactions embedded into a superconducting bath. The time evolution of the reduced density matrix for the system is given by the Linblad master equation, where the dissipators describe exchange of Bogoliubov quasiparticles with the bath. We obtain fixed points of the time evolution equation for the covariance matrix and study their stability by analyzing full dynamics of the complex order parameter.

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(Some figures may appear in colour only in the online journal)

The Bardeen, Cooper and Schrieffer (BCS) theory of superconductivity [1] is based on the simple Hamiltonian but it captures the essential physics not only for superconductivity of electrons in metals, but also the superconductivity of atomic nuclei, nuclear matter, neutron stars [2] and cold atomic Fermi gases [3]. Here, based on the Lindblad master equation, we propose the extension of the BCS theory to the open quantum system. We determine the order parameter—the density of Cooper pairs, and optionally the order parameters of a superconducting reservoir, self-consistently. A simple model of a single degenerate fermionic level embedded into a fermionic reservoir is proposed. For a self-consistent treatment of the reservoir, we recover the standard mean-field superconducting phase transition in the grand-canonical (equilibrium) state, whereas for a fixed state of the reservoir, we find that the state of the system follows the state of the reservoir, being either superconducting or normal.

Let us consider a quantum impurity connected to the superconducting bath. The impurity Hamiltonian consists of a single degenerate level with BCS-type pairing interaction

$$H = \epsilon \left(a_{\uparrow}^{\dagger} a_{\uparrow} + a_{\downarrow}^{\dagger} a_{\downarrow} \right) + U a_{\uparrow}^{\dagger} a_{\downarrow}^{\dagger} a_{\downarrow} a_{\uparrow} a_{\uparrow}.$$
⁽¹⁾

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Here $a^{\dagger}_{\sigma}(a_{\sigma})$ denote creation (annihilation) operators for a fermion with spin $\sigma = \uparrow, \downarrow$ in the impurity. The superconducting bath is described by the Bogoliubov-de Gennes Hamiltonian and the system-bath interaction is given by the tunneling Hamiltonian $\sim (a^{\dagger}_{\sigma}a_{b\sigma} + h.c.)$, where $a_{b\sigma}$ is an annihilation operator for a bath fermion in mode b. We write the Liouville equation for the total density matrix and project out the bath degrees of freedom. Then, under the standard assumptions (Markovian approximation, factorization of the (initial) system-bath density matrix and rotating wave approximation) [4], we obtain the Lindblad master equation for the reduced (impurity) density matrix $\rho(t)$:

$$\frac{d\rho}{dt} = -i[H,\rho] + \sum_{\nu=1}^{M} \left(2L_{\nu}\rho L_{\nu}^{\dagger} - \{L_{\nu}^{\dagger}L_{\nu},\rho\} \right),$$
(2)

where L_{μ} are some Lindblad operators [5] which will be specified later.

Introducing the (time-dependent) averages $\langle A \rangle = tr A \rho(t)$, and using the Wick theorem, we approximate (1) by the mean-field Bogoliubov-de Gennes Hamiltonian

$$H = \epsilon \left(a_{\uparrow}^{\dagger} a_{\uparrow} + a_{\downarrow}^{\dagger} a_{\downarrow} \right) + \Delta \left(e^{i\chi} a_{\downarrow} a_{\uparrow} + e^{-i\chi} a_{\uparrow}^{\dagger} a_{\downarrow}^{\dagger} \right), \tag{3}$$

where

$$\Delta e^{i\chi} = U \left\langle a_{\uparrow}^{\dagger} a_{\downarrow}^{\dagger} \right\rangle \tag{4}$$

is the complex order parameter.

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Hamiltonian (3) can be diagonalized by the canonical Bogoliubov transformation

$$\alpha_1 = -e^{i\chi}\cos(\phi)a_{\uparrow} + \sin(\phi)a_{\downarrow}^{\dagger}, \qquad (5)$$

$$\alpha_2^{\dagger} = e^{-i\chi} \cos(\phi) a_{\downarrow}^{\dagger} + \sin(\phi) a_{\uparrow}, \tag{6}$$

where $\tan(2\phi) = -\frac{\Delta}{\epsilon}$, and α_i are Bogoliubov quasiparticles, which satisfy standard anticommutation relations. The diagonal form of the Hamiltonian is

$$H = \sqrt{\epsilon^2 + \Delta^2 \left(\alpha_1^{\dagger} \alpha_1 + \alpha_2^{\dagger} \alpha_2\right)}.$$
(7)

We assume that our system is embedded into a superconducting bath described by a macroscopic gas of Bogoliubov quasiparticles, which can be exchanged with the system. This process is quite generally described by a combination of the following M = 4 Lindblad operators:

$$L_{1} = \sqrt{\Gamma_{1}} \Big(-e^{i\eta} \cos(\theta) a_{\uparrow} + \sin(\theta) a_{\downarrow}^{\dagger} \Big),$$

$$L_{2} = \sqrt{\Gamma_{2}} \Big(-e^{-i\eta} \cos(\theta) a_{\uparrow}^{\dagger} + \sin(\theta) a_{\downarrow} \Big),$$

$$L_{3} = \sqrt{\Gamma_{1}} \Big(e^{i\eta} \cos(\theta) a_{\downarrow} + \sin(\theta) a_{\uparrow}^{\dagger} \Big),$$

$$L_{4} = \sqrt{\Gamma_{2}} \Big(e^{-i\eta} \cos(\theta) a_{\downarrow}^{\dagger} + \sin(\theta) a_{\uparrow} \Big).$$
(8)

The superconducting properties of the bath are not necessarily the same as those of the embedded system, so the angles θ , and η , may be different from ϕ , and χ , respectively. The coupling constants $\Gamma_{1,2}$ are connected to the Fermi–Dirac distribution of the normal modes of the Bogoliubov-de Gennes Hamiltonian (3):

$$\Gamma_1 = \gamma (1 - f), \qquad \Gamma_2 = \gamma f, \qquad f = \frac{1}{1 + e^{\beta \sqrt{\epsilon^2 + \Delta^2}}},$$
(9)

where γ is a parameter controlling the strength of system–bath coupling.

It is convenient to rewrite the Lindblad equation in terms of Hermitian Majorana fermions

$$w_1 = a_{\uparrow} + a_{\uparrow}^{\dagger}, \qquad w_2 = i(a_{\uparrow} - a_{\uparrow}^{\dagger}), \qquad w_3 = a_{\downarrow} + a_{\downarrow}^{\dagger}, \quad w_4 = i(a_{\downarrow} - a_{\downarrow}^{\dagger}), \tag{10}$$

satisfying $\{w_j, w_k\} = 2\delta_{j,k}$, j, k = 1, ..., 4. Since our master equation is quadratic in terms of w_j , we obtain a closed set of equations for the covariance matrix $\langle w_j w_k \rangle = \delta_{j,k} - iZ_{j,k}(t)$:

$$\frac{\mathrm{d}\mathbf{Z}}{\mathrm{d}t} = -\mathbf{X}^{\mathrm{T}}\mathbf{Z} - \mathbf{Z}\mathbf{X} + \mathbf{Y}.$$
(11)

Here $\mathbf{Z}(t)$ is a real, anti-symmetric 4 × 4 matrix, and **X** and **Y** are real matrices

$$\mathbf{X} = \begin{pmatrix} \gamma & -\epsilon & -\Delta \sin \chi & \Delta \cos \chi \\ \epsilon & \gamma & \Delta \cos \chi & \Delta \sin \chi \\ \Delta \sin \chi & -\Delta \cos \chi & \gamma & -\epsilon \\ -\Delta \cos \chi & -\Delta \sin \chi & \epsilon & \gamma \end{pmatrix},$$
(12)

$$\mathbf{Y} = 2\gamma (1 - 2f) \begin{pmatrix} 0 & \cos 2\theta & -\sin \eta \sin 2\theta & \cos \eta \sin 2\theta \\ -\cos 2\theta & 0 & \cos \eta \sin 2\theta & \sin \eta \sin 2\theta \\ \sin \eta \sin 2\theta & -\cos \eta \sin 2\theta & 0 & \cos 2\theta \\ -\cos \eta \sin 2\theta & -\sin \eta \sin 2\theta & -\cos 2\theta & 0 \end{pmatrix}.$$
 (13)

Note that equation (11) is nonlinear, as Δ and χ depend again on covariances through relation (4). If in addition, we determine the Lindblad operators self-consistently, which means that the bath has the same properties as the embedded system; then we should also set $\tan 2\theta = -\frac{\Delta}{\epsilon}$, $(\theta \equiv \phi)$ and $\eta \equiv \chi$.

Fixed points of flow (11), which are solutions of the continuous Lyapunov equation

$$\mathbf{X}^T \mathbf{Z} + \mathbf{Z} \mathbf{X} = \mathbf{Y},\tag{14}$$

determine the stationary states of the system. These stationary states may not be unique because of the nonlinearity. However, one can show that a stable fixed point is unique. It follows from the fact that all linear relaxation rates, i.e. eigenvalues of the matrix **X** (12), $x_{1,2,3,4} = \gamma \pm i\sqrt{\Delta^2 + \epsilon^2}$, have strictly positive real parts for $\gamma > 0$. One can further show that all solutions of equation (14) are of the form

$$\mathbf{Z} = \begin{pmatrix} 0 & z_1 & z_2 & z_3 \\ -z_1 & 0 & z_3 & -z_2 \\ -z_2 & -z_3 & 0 & z_1 \\ -z_3 & z_2 & -z_1 & 0 \end{pmatrix},$$
(15)

which is specified by only three real variables z_1, z_2, z_3 . The Lyapunov equation should be solved self-consistently (4), i.e.

$$z_2 = -\frac{2\Delta}{U}\sin\chi, \qquad z_3 = \frac{2\Delta}{U}\cos\chi.$$
 (16)

Let us now consider two possible cases of the bath, i.e. two possible choices of angles θ , η .

(i) *Fixed bath.* If the bath is considered fixed, we can set $\eta := 0$ without loss of generality, so equation (16) together with the Lyapunov equation (14) results in the conditions

$$(\gamma \sin \chi - \epsilon \cos \chi) \sin 2\theta = \Delta \cos 2\theta,$$

$$U(1 - 2f) \left(\left(\left(\gamma^2 + \Delta^2 \right) \cos \chi + \gamma \epsilon \sin \chi \right) \sin 2\theta - \Delta \epsilon \cos 2\theta \right) = 2\Delta \left(\gamma^2 + \Delta^2 + \epsilon^2 \right).$$
(17)

For a normal, non-superconducting bath, $\sin 2\theta = 0$, and there exists only a trivial solution $\Delta = 0$ for the system. For a superconducting bath, $\sin 2\theta \neq 0$, the system is always superconducting as well, for all inverse temperatures β , as the only solution of (17) has $\Delta \neq 0$. In other words, for a superconducting bath, the embedded system cannot be in the normal state no matter how small the parameter γ is.

(ii) *Self-consistent bath.* If the superconducting properties of the bath are not known *a priori* and it is assumed that the bath has the same order parameter as the system, then the bath can be considered self-consistent in the following way. We associate the Lindblad operators with the normal mode creation and annihilation operators such that $\theta = \phi$, $\eta = \chi$. Inserting these assumptions into the Lyapunov equation (14), we obtain

$$z_{1} = \frac{\epsilon \tanh\left(\frac{1}{2}\beta\sqrt{\Delta^{2} + \epsilon^{2}}\right)}{\sqrt{\Delta^{2} + \epsilon^{2}}},$$

$$z_{2} = \frac{\Delta \sin(\chi) \tanh\left(\frac{1}{2}\beta\sqrt{\Delta^{2} + \epsilon^{2}}\right)}{\sqrt{\Delta^{2} + \epsilon^{2}}},$$

$$z_{3} = -\frac{\Delta \cos(\chi) \tanh\left(\frac{1}{2}\beta\sqrt{\Delta^{2} + \epsilon^{2}}\right)}{\sqrt{\Delta^{2} + \epsilon^{2}}}.$$
(18)

The consistency conditions (16) now result in

$$\left(\frac{U\tanh\left(\frac{1}{2}\beta\sqrt{\Delta^2 + \epsilon^2}\right)}{2\sqrt{\Delta^2 + \epsilon^2}} + 1\right)\Delta = 0.$$
(19)

We always have the trivial solution $\Delta = 0$; however, for temperatures smaller than $1/\beta_c$, where

$$\beta_{\rm c} = -\frac{2}{\epsilon} \operatorname{artanh}\left(\frac{2\epsilon}{U}\right),\tag{20}$$

we also find a superconducting solution with $\Delta \neq 0$. Obviously, the critical temperature only exists for $-U > 2\epsilon$. Equations (19) and (20) are exactly the result that we obtain in the standard grand canonical ensemble. The bath-self-consistency conditions completely eliminate the dependence of the properties of the stationary state on the system–bath coupling γ .

The self-consistency condition implies that the bath consists of a macroscopic number of (other) single-particle levels with the same or very similar superconducting properties; however, in our open-system's description, we trace out everything but one level. Perhaps such a model might appear trivial at first sight; however, we believe that it becomes very important and even practical when applied to out-of-equilibrium systems. For example, let us consider a lattice described by the Bogoliubov–de Gennes Hamiltonian with local site-dependent order parameter. The edges of the lattice are attached to different superconducting thermal baths held at different temperatures and chemical potentials. In this case, the edges would be treated self-consistently with corresponding thermal baths which would enforce the edge sites to have the same dynamics and the same superconducting properties as the corresponding baths.

In figure 1, we plot a phase diagram $\Delta(\beta)$, for both cases (i) and (ii). Note that only if $\Delta_{\text{bath}} := -\epsilon \tan 2\theta$ is smaller than $\sqrt{\frac{1}{4}U^2 - \epsilon^2}$, then we may have $\Delta = \Delta_{\text{bath}}$ for some temperature $1/\beta$.

So far we have investigated fixed points of the nonlinear flow (11). Let us now address the question of their stability by investigating the full dynamics. We shall only focus on case (ii) of self-consistently determined baths, which possesses a non-unique stationary solution below the critical temperature. The dynamical equations for $z_j(t)$, j = 1, 2, 3 follow directly from equation (11) with ansatz (15). By means of self-consistency equations (16), we replace $z_2(t)$, $z_3(t)$ by $\Delta(t)$, $\chi(t)$, resulting in a system of three non-linear differential equations,

$$\frac{\mathrm{d}\Delta}{\mathrm{d}t} = -2\gamma\Delta\left(\frac{U\tanh\left(\frac{\beta}{2}\sqrt{\epsilon^2 + \Delta^2}\right)}{2\sqrt{\epsilon^2 + \Delta^2}} + 1\right),\tag{21}$$

4



Figure 1. The phase diagram of the magnitude of the order parameter Δ versus the inverse temperature. $\Delta > 0$ signals the superconducting phase. The blue curve corresponds to the self-consistently determined bath, whereas the black and red curves correspond to fixed superconducting baths, with $\Delta_{\text{bath}} = -\epsilon \tan 2\theta$ (indicated by horizontal dashed lines), with $\theta = -\pi/20$ and $\theta = -\pi/7$, respectively. Other parameters are $\epsilon = 1$, $\gamma = 1$ and U = -3.

$$\frac{\mathrm{d}z_1}{\mathrm{d}t} = 2\gamma \left(\epsilon \frac{\tanh\left(\frac{\beta}{2}\sqrt{\epsilon^2 + \Delta^2}\right)}{\sqrt{\epsilon^2 + \Delta^2}} - z_1\right),\tag{22}$$

$$\frac{\mathrm{d}\chi}{\mathrm{d}t} = Uz_1 + 2\epsilon. \tag{23}$$

Note that the first equation (21) is independent of the other two and yields a closed first-order differential equation for the magnitude of the order parameter Δ . Writing it as $d\Delta/dt = G(\Delta)$, we can easily study the stability of two possible fixed points Δ_1 , and Δ_2 ($G(\Delta_j) = 0$, j = 1, 2, $\Delta_1 = 0$, and $\Delta_2 \neq 0$ if $\beta > \beta_c$). For the trivial fixed point, we find

$$G'(0) = -2\gamma \left(\frac{U}{2\epsilon} \tanh\left(\frac{\beta\epsilon}{2}\right) + 1\right),\tag{24}$$

which means that the non-superconducting state is stable, G'(0) < 0, if $\beta < \beta_c$ and unstable, G'(0) > 0, if $\beta > \beta_c$. As for the second, non-trivial fixed point Δ_2 , one can easily show that it is always stable, $G'(\Delta_2) < 0$, if $\beta > \beta_c$. The flow of the order parameter $\Delta(t)$ in different cases is illustrated in figure 2. We note that the other two phase-space variables $z_1(t)$ and $\chi(t)$ are completely *enslaved* by the order parameter $\Delta(t)$, so they again converge either to their trivial (non-superconducting) or non-trivial (superconducting) fixed point values.

In conclusion, based on the Lindblad master equation, we proposed the extension of the BCS theory to open Fermi systems exchanging Bogouliubov quasiparticles with the bath. We derived the equations of motion for the covariance matrix and found the fixed points of the flow equations. If the bath is considered self-consistently with the system, the results become equivalent to the grand canonical ensemble and all dependence on the Lindblad dissipators is eliminated. If the superconductivity of the bath is fixed, the system remains in the superconducting state for all values of temperature no matter how small the system—bath coupling is. We performed full nonlinear dynamic analysis of the fixed point and found that below the critical temperature, the fixed point which corresponds to the normal phase is not stable, whereas the superconducting solution is stable. Note that our results are closely related to an exact treatment of the open BCS model in quasi-spin formulation [6]. However, in [6], the (quasi-)particles cannot be exchanged with the system, so the study of the thermodynamic



Figure 2. Time-dependent order parameter $\Delta(t)$ as a function of time, for $\beta < \beta_c$ (red curves) and $\beta > \beta_c$ (black curves), and for an attractive potential U < 0 (full curves) and a repulsive potential U > 0 (dashed curves). We plot some typical trajectories starting from green points and ending in one of the two stable fixed points (blue). The numerical values of parameters are $\epsilon = 1, \gamma = 1$ and |U| = 3.

limit is more subtle. We thus believe that our single-level formulation provides a minimal model of open BCS quantum dynamics and should serve as the first step in approaching the non-equilibrium open BCS models with several different temperature/particle reservoirs.

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