Metastability in the BCS-model

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Abstract. We discuss metastable states in the mean-field version of the strong coupling BCS-model and study the evolution of a superconducting equilibrium state subjected to a dynamical semi-group with Lindblad generator in detailed balance w.r.t. another equilibrium state. The intermediate states are explicitly constructed and their stability properties are derived. The notion of metastability in this genuine quantum system, is expressed by means of energy-entropy balance inequalities and canonical coordinates of observables.

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1. Introduction

One of the most well-known phenomena in physics, is metastability. Phenomena like supercooled water or hysteresis in magnetic systems are easily observed and identified with metastability. But in spite of its clear appearance, the development of a complete theory of metastability is still a hard and unresolved problem, for an overview, see e.g. [1]. The basic concept of metastability could be formulated in the following way: a thermodynamic system is prepared in a special initial state different from the equilibrium state. If the initial conditions are suitably chosen, the system will not relax immediately to equilibrium, but it persists a longer period of time away from the equilibrium state, until some large fluctuation or an external disturbance occurs driving the system to equilibrium. The key problem is to formulate an expression for the size of the perturbation characterising the metastable regime [1–4].

Metastability has intensively been studied for classical models, and interesting results are obtained for the metastable relaxation in kinetic Ising models [1–4], we will not try to give a full overview of this field but refer to one of these papers for more references. It was conjectured (see e.g. [1]) that the metastable evolution is governed by the growth of droplets of the stable phase in a background of the (initial) metastable phase. Small droplets are probable to disappear again, but bigger droplets tend to grow, ultimately driving the system to equilibrium. The lifetime of the metastable
phase should then be linked to the probability of creating a droplet-excitation of critical volume \[3\]. A rigorous result pointing in that direction was obtained in a paper by Schonmann and Shlosman \[4\] where they proved that the ‘exit-time’ could be expressed as a function of the equilibrium surface-tension of a Wulff-droplet of volume one. A Wulff-droplet is a typical droplet excitation, for which the shape is found minimizing the surface terms in the free-energy. This activity and success for classical models is in sharp contrast with the situation for quantum mechanical models where little is known. In a recent paper \[5\], droplet states were constructed for the quantum mechanical XXZ-Heisenberg model.

In this note, we want to develop ideas of \[4\] in order to approach the phenomenon of metastability for quantum systems. We put forward that the underlying concept for exit-times and the metastable evolution is situated in the behaviour of non-extensive terms such as fluctuations of relevant observables, like the non-extensive (equilibrium) surface-tension of droplet excitations determines the metastable evolution in Ising models \[4\]. For the BCS-model \[4,6,7\] studied in this paper, we find a characterisation for metastability and define exit-times for different observables, expressed as a function of the equilibrium expectation values of the ‘normal coordinates’ of the observable under consideration. The metastable evolution at an arbitrary temperature between two extremal superconducting phases is studied. The evolution is driven by a semigroup with Lindblad generator \[8,9\]. In fact we consider a detailed balance dynamics between two different fixed phase states and realise the evolution from one equilibrium state to another equilibrium state with a different phase. The intermediate states are explicitly constructed and their thermodynamic properties are derived. These states are not invariant under the Hamiltonian evolution, but the correlation inequalities (section \[3\]) are satisfied for the normal coordinates of observables. We present a simple criterion to distinguish observables exhibiting monotone relaxation or metastable relaxation, and in the latter case, an expression for the exit-time is given. The exit-time is the time necessary to leave the initial state on the basis of having reached the maximum value of the observable under consideration. In the BCS-model, the observables which are invariant under the gauge transformation group of the broken symmetry \[10,12\], come over as relevant observables. They all exhibit metastable relaxation and all have the same exit-time.

2. The BCS-model

The strong-coupling BCS-model is described by the local Hamiltonians \[3,4\]

\[
H_N = -\frac{1}{N} \sum_{i \neq j=1}^{N} \sigma_i^+ \sigma_j^- + \epsilon \sum_{i=1}^{N} \sigma_i^z, \quad \epsilon > 0
\]

where \(\sigma^+, \sigma^-\) and \(\sigma^z = \sigma^+ \sigma^- - \sigma^- \sigma^+\) are the well-known Pauli matrices. \(H_N\) acts on the Hilbert space \(\bigotimes_{i=1}^{N} \mathbb{C}_i^2\).
The equilibrium states $\omega_\beta$ studied here are elements of the set of $(\tau_t, \beta)$-KMS states in the thermodynamic limit ($N \uparrow \infty$) of this model, i.e. the states satisfying the equilibrium conditions of Kubo, Martin and Schwinger [13]:

$$\omega_\beta(BA) = \omega_\beta(A\tau_\beta B) \quad \forall A, B \in \mathcal{B},$$

on the infinite tensor product algebra $\mathcal{B} = \bigotimes_{i=1}^\infty M_2$ at an inverse temperature $\beta$ and with the reversible Heisenberg dynamics:

$$\tau_t(\cdot) = w - \lim_{N \to \infty} = e^{itH}e^{-itH}.$$

The extremal points of the set of equilibrium states are given by the symmetric product states [14]:

$$\omega_\lambda(\cdot) = \prod_{i=1}^\infty \text{tr} \rho_\lambda,$$

on the infinite tensor product algebra $\mathcal{B} = \bigotimes_{i=1}^\infty M_2$; $\rho_\lambda$ is a $2 \times 2$ density matrix, given by the solutions of the gap-equation:

$$\rho_\lambda = \frac{\exp[-\beta h_\lambda]}{\text{tr} \exp[-\beta h_\lambda]},$$

where

$$h_\lambda = \epsilon \sigma^z - \lambda \sigma^- - \lambda^* \sigma^+,$$

and with order parameter $\lambda$, given by,

$$\lambda = \text{tr} \rho_\lambda(\sigma^+) = \omega_\lambda(\sigma^+).$$

This equation can be transformed into the equation

$$\lambda(1 - \frac{1}{2k} \tanh[\beta k]) = 0,$$

where $k = \sqrt{\epsilon^2 + |\lambda|^2}$; $\{-k, k\}$ is the spectrum of the effective Hamiltonians $h_\lambda$, which is independent of the phase of the order parameter $\lambda \in \mathbb{C}$. It can readily be seen that this equation (7) has always a solution $\lambda = 0$. This corresponds to the normal phase state. Solutions with $\lambda \neq 0$ exist if the following conditions are satisfied:

$$\begin{cases}
\epsilon < 1/2, \\
\beta > \beta_c = \frac{1}{2\epsilon} \log \left(\frac{1+2\epsilon}{1-2\epsilon}\right).
\end{cases}$$

These solutions $\lambda \neq 0$, are understood to describe the superconducting phase states. The inverse temperature $\beta > \beta_c$, fixes only $|\lambda|$, the norm of the order parameter. The phase of the order parameter $\phi$, defined by $\lambda = |\lambda|e^{i\phi}$, $\phi \in [0, 2\pi]$, remains free to choose. This leads to an infinite degeneracy of the states in the superconductive regime and is due to spontaneous symmetry breaking [11,11]. As this phase becomes important in the remainder of this article, it will from now on explicitly be labelled, i.e. we denote the order parameter as $\lambda e^{i\phi}$, with a phase $\phi \in [0, 2\pi]$, and norm $\lambda \in \mathbb{R}^+$. Furthermore, we fix now a certain subcritical temperature $\beta > \beta_c$, and hence the norm of the order
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parameter, which will now be labelled by \( \lambda \in \mathbb{R}^+ \). The superconducting pure phase states \((4)\) are therefore from now on denoted by \( \omega_{\phi} \) instead of \( \omega_{\lambda e^{i\phi}} \).

The mechanism of spontaneous symmetry breaking can be explicitly seen as follows: The Hamiltonian \( H_N \) is invariant under the norm-continuous gauge transformation automorphism group \( G = \{ \alpha_\psi \mid \psi \in [0, 2\pi] \} \) on \( B \), defined by the action:

\[
\alpha_\psi(\sigma_i^+) = e^{i\psi} \sigma_i^+.
\]

On finite subsets \( \Lambda \subset \mathbb{N} \), these transformations \( \alpha_\psi \) are implemented by the unitaries

\[
U_\Lambda^\psi = e^{i\psi Q_\Lambda/2}
\]

where \( Q_\Lambda \) is the (local) infinitesimal generator:

\[
Q_\Lambda = \sum_{i \in \Lambda} \sigma_i^z.
\]

Clearly \( \alpha_\psi(H_N) = U_\Lambda^\psi H_N U_\Lambda^{\psi} = H_N \) with \( \{1, \ldots, N\} \subset \Lambda \), but this symmetry is broken in the equilibrium states of the superconducting phase, we have:

\[
\omega_{\phi} \left( \alpha_\psi(\sigma_i^+) \right) = \lambda e^{i(\phi + \psi)} \neq \lambda e^{i\phi} = \omega_{\phi}(\sigma_i^+).
\]

In fact the gauge group \( G \) establishes a relation between the superconducting pure phase states with different phase-factors:

\[
\omega_{\phi}(\alpha_\phi(X)) = \omega_{\phi+\psi}(X), \quad \forall X \in B, \text{ and } \phi, \psi \in [0, 2\pi].
\]

In the following we learn that the observables \( X \in B \) which are invariant under the gauge transformations, i.e. \( \alpha_\phi(X) = X \), are relevant in order to determine the metastable evolution between two superconducting states.

We conclude this paragraph by remarking that a common method to single out an equilibrium state with fixed phase \( \phi \), consists of adding a thermodynamic unimportant term to the local Hamiltonians \((1)\), such as a vanishing external field:

\[
- \frac{1}{N} \sum_{i=1}^{N} \sigma_i^+ e^{-i\phi} + \sigma_i^- e^{i\phi},
\]

forcing the system in the limiting Gibbs state \( \omega_{\phi} \) of the superconducting phase. This fixes the phase to \( \phi \).

3. Thermodynamic stability

An alternative way to characterise equilibrium states, is given by the correlation inequalities \((13)\). These represent conditions, which have been proven to be equivalent to the \( \beta \)-KMS condition \((2)\), while their interpretation is related to the principle of minimum free energy. In other words, they are an expression for the thermodynamic stability of the KMS (equilibrium) states \((13)\).

Energy-Entropy Balance Inequalities

Let \( \tau_t(.) = \lim_N e^{\imath tH_N} e^{-\imath tH_N} \) be the Heisenberg dynamics, (defined in a weak limit sense)
and $\beta$ the inverse temperature. A state $\omega$ is a $(\tau_\beta, \beta)$-KMS state if and only if for all $X \in \text{Dom}(\delta)$

$$-i\beta\omega(X^*\delta X) \geq \omega(X^*X) \log \frac{\omega(X^*X)}{\omega(XX^*)},$$

(12)

with $\delta(\cdot)$ the infinitesimal generator of the dynamics $(\tau_\beta)$.

In this paper we concentrate on the BCS-model. Since this model is of mean-field type, we only need to consider product states (see section 2). For such states the correlation inequalities for operators $X \in \mathcal{B}$ of the form $X = X_1 \otimes X_2 \otimes \ldots \otimes X_n$ with $X_1, X_2, \ldots, X_n \in M_2$ follow from the correlation inequalities for $X_1, X_2, \ldots, X_n$. Therefore it is sufficient to consider only one-point operators, and (12) is reduced to:

**Energy-Entropy Balance Inequalities in the BCS-model**

A product state $\rho$ on $\mathcal{B} = \bigotimes_{i=1}^{\infty} M_2$ is a $(\tau_\beta, \beta)$-KMS state for the BCS-model (1) if and only if for every one-point operator $X \in M_2$ the following inequality holds:

$$\beta \rho(X^*[h_\rho, X]) \geq \rho(X^*X) \log \frac{\rho(X^*X)}{\rho(XX^*)},$$

(13)

with $h_\rho$ the effective Hamiltonian in this state, i.e. $h_\rho = \epsilon \sigma^z - \rho(\sigma^+)\sigma^- - \rho(\sigma^-)\sigma^+$.

The interpretation of these inequalities is the following: the l.h.s. of (12) or (13) reflects the change in energy if we alter the state with a ‘perturbation $X$’. The r.h.s. of inequalities (12) or (13) originates from the corresponding change in entropy $S(\rho) = -\text{tr} \rho \log \rho$ under the ‘perturbation $X$’. For example, if the criterion (13) is applied to unitaries $U \in M_2$, with $U^*U = 1 = UU^*$, and we substitute $U$ for $X$ in (13), it is reduced to:

$$\rho(U^*[h_\rho, U]) \geq 0.$$

This inequality expresses the fact that the the local state $\text{tr}(\rho \cdot)$ must have a lower internal energy than the perturbed states $\text{tr}(U\rho U^* \cdot)$, while the entropy of these states remain unchanged: $S(\rho) = S(U\rho U^*)$.

If a state $\omega$ satisfies condition (12) for an operator $X$, we say that $\omega$ is stable under the ‘perturbation $X$’.

**4. The perturbed states**

In classical kinetic models [1–4] the metastable evolution is introduced by a dynamical semigroup of dissipative maps (e.g. Glauber dynamics), satisfying the detailed balance conditions w.r.t. the asymptotic equilibrium measure. The notion of detailed balance and dissipative evolutions are generalised for quantum systems [8, 9]. The quantum dynamical semigroups as well as the classical Glauber dynamics do share the same physical background, in the sense that they can be constructed as the result of a weak coupling of the system with a temperature reservoir system [10].

A continuous 1-parameter group $\{\gamma(t) \mid t \geq 0\}$ of linear maps $\gamma(t)$ on the algebra $\mathcal{B} = \bigotimes_{i=1}^{\infty} M_2$, is called a dynamical semigroup if for every $t \geq 0$, $\gamma(t)$ is a completely positive, unity preserving map on $\mathcal{B}$ and $\gamma(0)$ is the identity map.
Let $L$ be the (densely defined) infinitesimal generator of such a dynamical semigroup, i.e.

$$\gamma(t) = e^{tL}, \quad \forall t \geq 0.$$ 

The dynamical semigroup is then called dissipative if the generator $L$ is self-adjoint, i.e. $L(A^*) = L(A)^* \forall A \in \mathcal{B}$, and satisfies the following inequalities:

$$L(A^*A) \geq A^*L(A) + L(A^*)A, \quad \forall A \in \mathcal{B}. \quad (14)$$

Let $\omega$ be a state on $\mathcal{B}$, the dynamical semigroup $(\gamma(t))_{t \geq 0}$ is said to satisfy the detailed balance conditions w.r.t. the state $\omega$ if the following duality property holds:

$$\omega(XL(Y)) = \omega(L(X)Y), \quad \forall X, Y \in \mathcal{B}. \quad (16)$$

Consider now one of the extremal superconducting phase states $\omega_{\phi}$ (4), we can construct a dynamical semigroup $\{\gamma_{\phi}(t)\}_{t \geq 0}$ with generator $L_{\phi}$, satisfying the condition of detailed balance w.r.t. this state. Because we are dealing with product states, the generator $L_{\phi}$ of $(\gamma_{\phi}(t))$ is globally defined if it is defined on the local sites, i.e.

$$L_{\phi} : M_2 \to M_2.$$ 

It is given by (3,4):

$$L_{\phi}(.) = \sum_{i,j} \exp[-\beta(\epsilon_i - \epsilon_j)/2] \left( E_{ij}^* [., E_{ij}] + [E_{ij}^*, .]E_{ij} \right), \quad (15)$$

where $E_{ij} = |\psi_i\rangle\langle\psi_j|$ stands for the matrix units in the base of eigenvectors $\{|\psi_i\rangle| i \in \{-, +\}\}$ of $h_{\phi}$, the effective Hamiltonian (3) of the $(\tau_1, \beta)$-KMS state $\omega_{\phi}$ (4); $|\psi_i\rangle$ is the eigenvector corresponding to the eigenvalue $\epsilon_i$ of $h_{\phi}$. It is immediately checked that $L_{\phi}$ is dissipative (14) and satisfies the detailed balance conditions in the state $\omega_{\phi}$ with fixed phase $\phi$, i.e.

$$\omega_{\phi}(XL_{\phi}(Y)) = \omega_{\phi}(L_{\phi}(X)Y) \quad \forall X, Y \in M_2. \quad (16)$$

The action of this generator (15) is naturally extended to operators $X \in \mathcal{B}$ of the form $X = X_1 \otimes X_2 \otimes \ldots \otimes X_n$ with $X_1, X_2, \ldots, X_n \in M_2$ by

$$L_{\phi}(X_1 \otimes X_2 \otimes \ldots \otimes X_n) = \sum_{i=1}^{n} X_1 \otimes \ldots \otimes L_{\phi}(X_i) \otimes \ldots \otimes X_n.$$ 

Since $\omega_{\phi}$ is a symmetric product state (4), the dissipativity and the detailed balance properties (14) are preserved for these more general operators and follow from the properties of their one-site factors. The dynamical semigroup $(\gamma_{\phi}(t))_{t \geq 0}$ is then defined by:

$$\gamma_{\phi}(t) = e^{tL_{\phi}}, \quad \forall t \geq 0. \quad (17)$$

Remark that the detailed balance properties (16) guarantee that $\omega_{\phi}$ is stationary under this dynamical semigroup, while any other $(\tau_1, \beta)$-KMS state with a different phase-factor is not invariant.

Suppose now that our system is prepared in a $\beta$-KMS state $\omega_{-\phi}$ at time $t = 0$. Based on ideas from classical models (1–4), we apply at $t \geq 0$, an evolution $(\gamma_{\phi}(t))$ (17)
with phase $\phi$, and the system is forced to evolve accordingly. This implies that the system will ultimately relax to the equilibrium state $\omega_\phi$. The intermediate states $\omega_t$ are introduced by:

$$\omega_t(\cdot) = \omega_{-\phi}(e^{t\gamma_{\phi}}),$$

where the intermediate states $\omega_t$ are constructed by applying the dynamical semigroup $(\gamma_{\phi}(t))_{t \geq 0}$ \textsuperscript{17} with phase $\phi$ to the initial equilibrium state $\omega_{-\phi}$ with phase $-\phi$. These states $\omega_t$ are, by construction, again product states, and their density matrices can explicitly be calculated. They are understood to describe a metastable regime. For $t$ small enough, the state $\omega_t$ will still be close to the initial state $\omega_{-\phi}$, while if $t$ becomes large enough, the system will be relaxing to the equilibrium state $\omega_\phi$, where the words “close” and “almost” have to get a precise meaning.

We proceed now with the explicit construction of the metastable states $\omega_t$ \textsuperscript{18}. The spectral decomposition of the generator $L_\phi$ \textsuperscript{13} and the dissipative evolution $\gamma_{\phi}(t)$ is given in terms of the matrix units $(E_{ij}^\phi)$ of the corresponding asymptotic effective Hamiltonian, which can be written as $h_\phi = kE_{++}^\phi - kE_{--}^\phi$. We compute that:

$$L_\phi(1) = 0; \quad L_\phi(D) = -dD; \quad L_\phi(E_{+-}^\phi) = -cE_{+-}^\phi; \quad L_\phi(E_{-+}^\phi) = -cE_{-+}^\phi,$$

where $d = 4\cosh(\beta k), c = 2 + 2\cosh(\beta k)$ and $D = e^{\beta k}E_{++}^\phi - e^{-\beta k}E_{--}^\phi$. Hence, the expectation values for the operators \textsuperscript{19} in the state $\omega_t$ \textsuperscript{18} are given by:

$$\begin{align*}
\omega_t(1) &= 1; \\
\omega_t(D) &= e^{-td}\omega_{-\phi}(D); \\
\omega_t(E_{+-}^\phi) &= e^{-tc}\omega_{-\phi}(E_{+-}^\phi); \\
\omega_t(E_{-+}^\phi) &= e^{-tc}\omega_{-\phi}(E_{-+}^\phi).
\end{align*}$$

(20)

From these equations \textsuperscript{20} and linearity, all expectation values in $\omega_t$, and hence the density matrix $\rho_t$ at time $t$, can be calculated.

4.1. Exit-times and normal coordinates

Remark that any observable $X \in M_2^{sa}$ can be developed in its normal coordinates for the asymptotic equilibrium state $\omega_{-\phi}$ \textsuperscript{16}, i.e.

$$X = \omega_{-\phi}(X)1 + a_\phi^+(X) + a_\phi^-(X) + a_\phi^0(X).$$

(21)

The operators $a_\phi^+(X)$ and $a_\phi^-(X)$ are understood to be the creation, resp. annihilation operator of the normal modes determined by $X$, they are given in terms of $X$ and the projection operators $E_{++}^\phi$ and $E_{--}^\phi$ on the eigenspaces of the asymptotic effective Hamiltonian $h_\phi$, corresponding to positive, resp. negative energy:

$$\begin{align*}
a_\phi^+(X) &= E_{++}^\phi X E_{--}^\phi; \\
a_\phi^-(X) &= E_{--}^\phi X E_{++}^\phi,
\end{align*}$$

(22)

(23)

while $a_\phi^0(X)$ is the canonical constant of motion determined by $X$:

$$a_\phi^0(X) = E_{++}^\phi X E_{++}^\phi + E_{--}^\phi X E_{--}^\phi - \omega_{-\phi}(X)1.$$

(24)
Indeed, $a_0^0(X)$ is a constant of motion in the state $\omega_0$, since it commutes with the effective Hamiltonian $h_0$ and:

$$\frac{d}{dt} \omega_0(A\tau_i(a^0_\phi(X))B) = i\omega_0(A[h_0, \tau_i(a^0_\phi(X))]B) = 0, \quad \forall A, B, X \in M_2.$$  

Note that these operators (22, 23, 24) all have expectation value zero in the asymptotic state $\omega_0$. They are an expression for the fluctuations of $X$ around its asymptotic equilibrium value $\omega_\phi(X)$ (see also below). Using (20) and (21) we get an expression for the expectation value of $X$ in $\omega_t$:

$$\omega_t(X) = \omega_0(X) + \omega_\phi\left(a_\phi^+(X) + a_\phi^-(X)\right)e^{-tc} + \omega_-\phi\left(a_\phi^0(X)\right)e^{-td}. \quad (25)$$

The time limits $t \rightarrow 0$ and $t \rightarrow \infty$ of expression (25) yield clearly the equilibrium expectation values $\omega_-\phi(X)$ resp. $\omega_\phi(X)$:

$$\lim_{t \rightarrow 0} \omega_t(X) = \omega_-\phi(X);$$
$$\lim_{t \rightarrow \infty} \omega_t(X) = \omega_\phi(X),$$

i.e. this time evolution describes the transition between the two states under consideration, i.e. the transition from $\omega_-\phi$ to $\omega_\phi$.

In general, the evolution of $\omega_t(X)$ (25) can express two types of behaviour as a function of the time $t$. This is easily derived from the analysis the functions

$$f_X(t) : \mathbb{R}^+ \rightarrow \mathbb{R} : t \mapsto \omega_t(X), \quad \forall X \in M_2^{sa}, \quad (26)$$

and their time derivatives.

Let us illustrate this with two pictures (Fig. 4.1):

(a) $f_{X_1}(t) : t \mapsto \omega_t(X_1)$

(b) $f_{X_2}(t) : t \mapsto \omega_t(X_2)$

**Figure 1.** Typical pictures of monotone (a) and metastable (b) relaxation

Firstly, $\omega_t(X)$ can relax monotonically to its asymptotic value $\omega_\phi(X)$, and thus behaves qualitatively as shown in figure 4.1(a). This behaviour is met if the function $f_X(t)$ (26) has only an extremum at $t = 0$. Calculating the time derivative of $f_X(t)$ (26), we see that this happens whenever

$$-\frac{\omega_-\phi(a^0_\phi(X))}{\omega_-\phi(a^+_\phi(X)) + \omega_-\phi(a^-_\phi(X))} \leq c/d, \quad (27)$$
where
\[ c = 1 + \cosh(\beta k), \quad d = \frac{2 \cosh(\beta k)}{2 \cosh(\beta k)}. \]

This condition is satisfied if e.g. the second and the third term on the r.h.s. of expression (25) have the same sign. The relaxation is exponentially fast and is determined by the constants \( c = 2 + 2 \cosh(\beta k) \) and \( d = 4 \cosh(\beta k) \) (19).

The second possibility is that condition (27) is violated, i.e. if
\[ -\omega_t - \phi(a_0) + \omega_t - \phi(a_0(X)) > 1 + \cosh(\beta k) \frac{2 \cosh(\beta k)}{2 \cosh(\beta k)}. \]

In this case the function \( f_X(t) : t \mapsto \omega_t \) (26) has an extremum, reached at a time \( t^*_X \) which may depend on the observable \( X \). A typical picture of such a behaviour is shown figure 4.1(b).

The interpretation of this extremum is the following. The time \( t^*_X \) is a time-scale which indicates where the expectation value \( \omega_t(X) \) leaves the metastable regime and the relaxation to the asymptotic equilibrium value \( \omega_\phi(X) \) starts. For \( t < t^*_X \), \( \omega_t(X) \) moves away from the original equilibrium value \( \omega_{-\phi}(X) \), this behaviour with an increasing distance from equilibrium corresponds to the metastable regime. At time \( t = t^*_X \), this evolution comes to an end since \( \omega_t(X) \) is now at its maximum distance from the equilibrium value \( \omega_{-\phi}(X) \). For \( t > t^*_X \), we see another type of behaviour. The system is again approaching equilibrium, but \( \omega_t(X) \) is not returning to the initial equilibrium value \( \omega_{-\phi}(X) \), it relaxes now (monotonically) to its new equilibrium value \( \omega_\phi(X) \).

Since the time \( t^*_X \) marks where \( \omega_t(X) \) leaves metastability and the relaxation to the asymptotic value is started, we call \( t^*_X \) the exit-time for the observable \( X \). The exit-time \( t^*_X \) can be found calculating the extrema of function (26), i.e. \( t^*_X \) is the time \( t \) for which \( \frac{d}{dt}f_X(t) \big|_{t = 0} = 0 \), it is readily computed being:
\[ t^*_X = \frac{1}{d - c} \left( \log \frac{d}{c} + \log \left| \frac{\omega_{-\phi}(a_0^+(X))}{\omega_{-\phi}(a_0^+(X)) + \omega_{-\phi}(a_0^-(X))} \right| \right). \]

In this expression, it is clear that the exit-time for the expectation value of an observable \( t^*_X \) is determined by the constants \( c, d \) (19) and the ratio between the initial-state expectation values of the normal coordinates of \( X \) (22), (23) and (24).

In general we can formulate the following statement:

**Metastable Relaxation for the BCS-model**

A system prepared in a initial product state \( \omega_{-\phi} \) on \( \mathcal{B} = \bigotimes_{i=1}^\infty M_2 \) will relax to a superconducting equilibrium state \( \omega_\phi \) at subcritical temperature \( \beta \) (8) according to the evolution induced by a dynamical semigroup (17) with a dissipative generator \( L_\phi \) (14), satisfying the quantum detailed balance conditions in state \( \omega_\phi \). The behaviour of this relaxation depends on the chosen observables \( X \in M_2^{sa} \):

- Monotone Relaxation
The relaxation of the expectation value of an observable \( X \in M_2^{sa} \) is monotone if the following holds:

\[
\frac{\omega_{-\phi}(a^0_\phi(X))}{\omega_{-\phi}(a^+_\phi(X)) + \omega_{-\phi}(a^-_\phi(X))} \leq \frac{1 + \cosh(\beta k)}{2 \cosh(\beta k)},
\]

where \( a^+_\phi(X) \), \( a^-_\phi(X) \) and \( a^0_\phi(X) \) are the normal coordinates of \( X \) in the equilibrium state \( \omega_\phi \) as defined by equation (21), and \( k = \sqrt{\epsilon^2 + \lambda^2} \), the positive eigenvalue of the effective Hamiltonians at inverse temperature \( \beta \) [3].

- Metastable Relaxation

The expectation value of an observable \( X \in M_2^{sa} \) relaxes metastably if the following is true:

\[
\frac{\omega_{-\phi}(a^0_\phi(X))}{\omega_{-\phi}(a^+_\phi(X)) + \omega_{-\phi}(a^-_\phi(X))} > \frac{1 + \cosh(\beta k)}{2 \cosh(\beta k)}.
\]

In this case we define the exit-time for the observable \( X \), \( t^*_X \) as the time when the expectation value of \( X \) has past its extremal value and the relaxation to equilibrium starts. \( t^*_X \) is then given by the expression:

\[
t^*_X = \frac{1}{2 \cosh(\beta k) - 2} \left( \log \frac{2 \cosh(\beta k)}{1 + \cosh(\beta k)} + \log \left| \frac{\omega_{-\phi}(a^0_\phi(X))}{\omega_{-\phi}(a^+_\phi(X)) + \omega_{-\phi}(a^-_\phi(X))} \right| \right).
\]

An interesting point of these considerations is that the decomposition (21) and the construction of the exit-times is in terms of operators which are closely related to quantum fluctuations. Quantum fluctuations \( F_\omega(X) \) are the limits \( n \to \infty \) of operators \( F_n(X) \) defined by:

\[
F_n(X) = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} X_i - \omega(X),
\]

where \( X \) is a local observable and \( X_i \) is a copy of \( X \), translated to site \( i \). In [17,18] one has proved the existence of the limit:

\[
\lim_{n \to \infty} \omega \left( F_n(X)^2 \right) = \tilde{\omega} \left( F_\omega(X)^2 \right),
\]

defining a dynamical system on the level of the algebra of fluctuations \( \{ F_\omega | X \} \), and defining a state \( \tilde{\omega} \) on the algebra of fluctuations. Also a dynamics \( (\tilde{\tau}_t) \) of fluctuations induced by the original one \( (\tau_t) \), is defined by the formula

\[
\tilde{\tau}_t F_\omega(X) = F_\omega(\tau_t X).
\]

In [17,18] it is proved this dynamical system is always a bosonic system. This is worked out in great detail. We refer to [17,18] for more details and more precise information on this subject. The point is that the exit-times (29) can formally be expressed in term of fluctuations, as follows:

\[
t^*_X = \frac{1}{d - c} \left( \log \frac{d}{c} + \log \left| \frac{\omega_{-\phi}(F_\phi(X_0))}{\omega_{-\phi}(F_\phi(QX))} \right| \right),
\]
where

\[ F_\phi(Q_X) = \lim_{n \to \infty} \frac{1}{\sqrt{n}} \sum_{i=1}^n (a_\phi^+(X) + a_\phi^-(X))_i; \]

\[ F_\phi(X_0) = \lim_{n \to \infty} \frac{1}{\sqrt{n}} \sum_{i=1}^n (a_0^\phi(X))_i, \]

and \( \tilde{\omega}_{-\phi} \) is the limiting state with phase \(-\phi\) on the fluctuation algebra. The thermodynamic limit in nominator and denominator is taken jointly. Although the mathematical formulation of this computation is far from completely coherent with the general theory of quantum fluctuations [17, 18], we are tempted to conjecture that this construction might be the key to the understanding of metastability in a broader class of quantum systems.

**4.2. Invariant observables under the gauge transformation group**

Let us now continue the study of the metastable relaxation in the BCS-model between two equilibrium states, in particular the evolution from \( \omega_{-\phi} \) to \( \omega_\phi \) for gauge invariant observables. As explained, these superconducting states are not invariant under the gauge-symmetry \( \alpha_\psi, \psi \in [0, 2\pi] \) (9) of the BCS-Hamiltonians (1), in particular:

\[ \omega_\phi = \omega_{-\phi} \circ \alpha_2 \phi. \]

Observables \( X \in M_2 \) which are invariant under this gauge transformation group \( \mathcal{G} \) (9) i.e. satisfying

\[ \alpha_\psi(X) = X \text{ or } [\sigma^z, X] = 0, \]

have the same expectation value in all superconducting phase states, hence

\[ \omega_{-\phi}(X) = \omega_\phi(X). \]

Developing the observable \( X \) in normal coordinates w.r.t. \( \omega_\phi \) (21) yields

\[ \omega_{-\phi} \left( a_\phi^+(X) \right) + \omega_{-\phi} \left( a_\phi^-(X) \right) + \omega_{-\phi} \left( a_0^\phi(X) \right) = 0. \]

Hence we can rewrite equation (22) yielding:

\[ \alpha_t(X) = \omega_\phi(X) - \omega_{-\phi} \left( a_0^\phi(X) \right) \left( e^{-tc} - e^{-td} \right). \]

This implies that the relaxation for observables invariant under the gauge transformation group \( \mathcal{G} \) (9) is of the metastable type. The transition between the metastable regime and the relaxation regime happens at the same moment i.e. the invariant observables \( \alpha_\psi(X) = X \) share the same exit-time (29):

\[ t_* = \frac{\log d - \log c}{d - c} = \frac{\sqrt{1 - 4k^2}}{2\sqrt{1 - 4k^2}} \log \left( \frac{1}{2} + \sqrt{\frac{1 - 4k^2}{2}} \right). \]

The time \( t_* \) gives a time-scale for the transition between the metastable regime \( t < t_* \) during which the system evolves away from equilibrium and the relaxation regime \( t > t_* \), where the system evolves towards the new equilibrium state.
4.3. Explicit computations

Let us now illustrate the metastability in the BCS-model with a few special observables: using (20) or (25) we calculate the expectation values in the intermediate states (18) of some typical observables:

\[ \omega_t(\sigma^+ e^{-i\phi} + \sigma^- e^{i\phi}) = 2\lambda \left( 1 - 2\sin^2(\phi) \frac{\lambda^2 e^{-td} + \epsilon e^{-tc}}{k^2} \right) ; \]  

(33)

\[ \omega_t(i\sigma^+ e^{-i\phi} - i\sigma^- e^{i\phi}) = 2\lambda \sin(2\phi) e^{-tc}. \]  

(34)

In equations (33,34), the monotone exponential relaxation towards the state \( \omega_\phi \) is clear. The limits \( t \to 0(\infty) \) of the expectation values give again the equilibrium values in the states \( \omega_{-\phi}(\omega_\phi) \), in particular one computes also:

\[ \lim_{t \to 0} \omega_t(\sigma^+) = \lambda e^{-i\phi} = \omega_{-\phi}(\sigma^+); \]

\[ \lim_{t \to \infty} \omega_t(\sigma^+) = \lambda e^{i\phi} = \omega_\phi(\sigma^+). \]

Note that we have the following bound on the time evolution of the ‘condensate’: \( \lambda(t) = |\omega_t(\sigma^+)| \leq \lambda \), indicating that the ‘condensation’ is suppressed in the intermediate states.

The situation is different for the evolution of the expectation value of \( \sigma^z \), the generator of the gauge group (3):

\[ \omega_t(\sigma^z) = -2\epsilon - 4\sin^2(\phi) \frac{\epsilon\lambda^2}{k^2} (e^{-tc} - e^{-td}); \]  

(35)

Clearly, this is an example of an observable invariant under the gauge transformation group \( G \) (31), and its relaxation is metastable. In the time limits \( t \to 0(\infty) \), \( \omega_t(\sigma^z) \) (35) tends to the equilibrium value \( -2\epsilon \), but \( |\omega_t(\sigma^z) - \omega_{\pm\phi}(\sigma^z)| \) goes through a maximum, attained at \( t_*(\sigma^z) \), the exit-time for invariant observables.

4.4. Temperature Dependence

To conclude this section about the relaxation behaviour, we give some remarks on the dependence on the temperature. At the critical point (3), i.e. if \( T \uparrow T_c \) or \( \beta \downarrow \beta_c \), the order parameter \( \lambda \) vanishes. This also implies the following equalities for \( T = T_c \):

\[ \omega_{-\phi}(X) = \omega_t(X) = \omega_\phi(X), \quad t \geq 0, \forall X \in \mathcal{B}, \]

and the metastability effects disappears completely. The constants \((c,d)\), governing the speed of relaxation decrease to the values \( c_c = 2 + 2 \cosh(\beta \epsilon) \) resp. \( d_c = 4 \cosh(\beta \epsilon) \). Since the expression for the exit-times \( t_*(X) \) (29) depends on the ratio of the expectation values \( \omega_{-\phi}(a_\phi^0(X)) \) and \( \omega_{-\phi}(a_\phi^\pm(X)) \), the behaviour in limit \( \lambda \to 0 \) of \( t_*(X) \) can be different for different observables \( X \in M_2^a \). Both \( \omega_{-\phi}(a_\phi^0(X)) \) and \( \omega_{-\phi}(a_\phi^+(X)) \) tend to zero at the critical point \( \lambda \to 0 \), but the speed at which they decay to zero can be different. This depend on the observable \( X \) under consideration.
If we consider the metastable evolution between two groundstates \( T = 0, \beta = \infty \), we find that there are no intermediate states, since the constants \( c, d \) governing the relaxation speed blow up to infinity as \( \beta \) tends to infinity, hence

\[
\omega_t = \begin{cases} 
\omega_{-\phi} & \text{for } t = 0; \\
\omega_{\phi} & \text{for } t > 0.
\end{cases}
\]

This results from the fact that the dynamical semigroup which we consider becomes trivial for groundstates. The detailed analysis of the dynamics when \( T \to 0 \) indicates the existence of a non-trivial evolution only on a different time-scale.

Hence, if one would like to compare the dynamics at different temperatures, one has to rescale the time with an appropriate, temperature dependent, scaling factor. This scaling and the resulting dynamics ask for an independent analysis and is out of the scope of our considerations here.

5. Stability-instability properties of the intermediate states

Here we consider the stability properties of the intermediate states \( \omega_t(\cdot) \) on the basis of the correlation inequalities (13), i.e. we consider the equilibrium or stability conditions:

\[
\beta \omega_t(X^*[h_t, X]) \geq \omega_t(X^*X) \log \left( \frac{\omega_t(X^*X)}{\omega_t(XX^*)} \right),
\]

where \( h_t \) stands for the effective Hamiltonian in the state \( \omega_t \):

\[
h_t = \epsilon \sigma^z - \omega_t(\sigma^+)\sigma^- - \omega_t(\sigma^-)\sigma^+.
\]

From section 3 we know that \( \omega_t \) is a \( \beta \)-KMS state if and only if equation (36) is satisfied for all operators \( X \in \mathcal{B} \). In this section we analyse to what extent the intermediate states are still stable, i.e. we check for which operators \( X \in M_2 \) these states satisfy the inequalities (36). The meaningful operators in this context are the matrix units in the base of the spectral decomposition of \( h_t \), denoted by \( \{ E(t)_{++}, E(t)_{+-}, E(t)_{-+}, E(t)_{--} \} \). Compute first the expectation values

\[
\omega_t(E(t)_{--}) = \frac{1}{2} + k_t + \epsilon f_t/(2k_t);
\]

\[
\omega_t(E(t)_{++}) = -\lambda_t f_t/k_t,
\]

with \( \lambda_t = |\omega_t(\sigma^+)| \), \( k_t = \sqrt{\epsilon^2 + \lambda_t^2} \), the positive eigenvalue of \( h_t \) and \( f_t = 4\sin^2(\phi)\epsilon^2 (e^{-tc} - e^{-td}) / k^2 \). The expectation values of the other matrix units can be determined from the expressions (38), since \( \omega_t(E(t)_{++}) = 1 - \omega_t(E(t)_{--}) \) and \( \omega_t(E(t)_{-+}) = \omega_t(E(t)_{+-}) \).

5.1. \( \omega_t \) is not an invariant state

A first observation is that the states \( \omega_t, t > 0 \) are not invariant under the Hamiltonian evolution: this is easily derived from the expressions (38), calculating

\[
\omega_t([h_t, E(t)_{+-}]) = 2k_t \omega_t(E(t)_{+-}) \neq 0.
\]
5.2. Stability

The position $Q_X$ and momentum $P_X$ observables of a normal mode are constructed in the usual way, by means of the creation and annihilation operators:

$$a_t^+(X) = E(t)_{++} X E(t)_{--}; \quad (40)$$
$$a_t^-(X) = E(t)_{--} X E(t)_{++}, \quad (41)$$
yielding the following expression for $Q_X$ and $P_X$:

$$Q_X = \frac{1}{\sqrt{2}} (a_t^+(X) + a_t^-(X)); \quad (42)$$
$$P_X = \frac{i}{\sqrt{2}} (a_t^+(X) - a_t^-(X)). \quad (43)$$

These observables $(Q_X, P_X)$ satisfy the canonical dynamical equations:

$$i[h_t, Q_X] = 2k_t P_X;$$
$$i[h_t, P_X] = -2k_t Q_X,$$
justifying the name normal coordinates. For the sake of completeness we also give $a_t^0(X)$, the canonical constant of motion of $X$:

$$a_t^0(X) = E(t)_{++} X E(t)_{++} + E(t)_{--} X E(t)_{--} - \omega_t(X) 1 \quad (44)$$

These definitions are analogous to the ones in equations (22), (23) and, (24) in section 4 with an important difference. In section 4 we need the normal mode $\phi$ for the asymptotic equilibrium state $\omega$ (16), whereas the expressions (40), (41) and, (44) define the normal modes w.r.t. the intermediate state $\omega_t$. We can now formulate the following stability statements:

- **The correlation inequalities** (36) are satisfied for all linear combinations $aQ_X + bP_X$, with $a, b \in \mathbb{C}$ and $Q_X$ and $P_X$ as in (42) resp. (43).

For such an operators the correlation inequalities yield:

$$\omega_t(E(t)_{--}) \geq \omega_t(E(t)_{++}).$$

Since $k_t + \epsilon f_t/(2k_t) > 0$ (38), this condition is satisfied for every intermediate state $\omega_t$.

- **The constants of motion**, e.g. $a_t^0(X)$ (44) satisfy the correlation inequalities. An operator $C \in M_2$ is a constant of motion in $\omega_t$ if it satisfies $[h_t, C] = 0$, such operators can be written as $C = aE(t)_{++} + bE(t)_{--}$ with $a, b \in \mathbb{C}$. It is easy to check that the correlation inequalities (36) are trivially satisfied. Moreover, this stability property holds for any operator $C \in M_2$ satisfying $[h_\rho, C] = 0$ in a general symmetric product state with density matrix $\rho$ and effective Hamiltonian $h_\rho$, see e.g. (15).
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5.3. Instability

The instability of the intermediate states is reflected in the following statements: The correlation inequalities are satisfied for the creation operators \( a_t^+(X) \) (40), \( \forall X \in M_2 \), but not for the annihilation operators \( a_t^-(X) \) (41).

Substituting the operators \( a_t^+(X) \) (40) resp. \( a_t^-(X) \) (41) for \( X \) in the energy-entropy balance inequalities (36) yields:

\[
\text{if } X = a_t^+(X), \text{ then } \frac{\omega_t(E(t)_-)}{\omega_t(E(t)_{++})} \leq e^{\beta 2k_t}, \quad (45)
\]

\[
\text{if } X = a_t^-(X), \text{ then } \frac{\omega_t(E(t)_-)}{\omega_t(E(t)_{++})} \geq e^{\beta 2k_t}, \quad (46)
\]

i.e. \( \omega_t \) could only be stable under both \( a_t^+(X) \) and \( a_t^-(X) \), \( \forall X \in M_2 \), if the equality holds.

It follows from the gap-equation (7) that these equalities hold only for equilibrium states. The intermediate states are stable under the creation operators (45), but not under the annihilation operators (46). This can be seen as follows: using (38), it is readily computed that for all \( t > 0 \) the strict inequality (45) holds in the limit \( \epsilon \to 0 \).

Suppose now that there exists a point in parameter-space \( (t', \epsilon') \), with \( t' > 0, \epsilon' > 0 \), such that in that point the inequality (46) holds. By continuity of the state in parameter-space, we have continuity of the function \( f : (t, \epsilon) \mapsto \omega_t(E(t)_-) - e^{\beta 2k_t} \omega_t(E(t)_{++}) \). Since \( f(t', 0) < 0 \) and \( f(t', \epsilon') > 0 \), there must exist a point where this function is zero, this would imply that the intermediate state at that point is an equilibrium state, which cannot be true, see e.g. (39). This proves that condition (45) is always satisfied in the intermediate states, while (46) yields that the stability is violated for the annihilation operators \( a_t^-(X) \).

6. Outlook

All results in this paper concern the BCS-model, and rely very much on the mean-field character [14] of this model: all the states under consideration are chosen within the set of symmetric product states, the extension of these results to other mean-field models [12] is straight-forward. However, this work should be considered as a prototype model of a scheme which can be generalised to bona fide interacting systems. The main argument for this is that metastability is formulated in terms of fluctuation operators and their dynamics. Relying on the general theory of quantum fluctuations [17, 18] these fluctuation systems are quasi-free or generalised free systems, and therefore we are confident that our results have a much wider validity far beyond the model considerations of above. We reserve this generalisation to interacting systems for a future contribution.

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