Flow-Equation method for a superconductor with magnetic correlations

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Abstract

The flow equation method has been used to calculate the energy of single impurity in a superconductor for the Anderson model with \( U \neq 0 \). We showed that the energy of the impurity depends only of the \( \Delta_R^2 \) (renormalized order parameter) which depends of the renormalized Hubbard repulsion \( U_R \). For a strong Hubbard repulsion \( U_R = U \) and \( \Delta_R = \Delta_I \) the effect of the \( s-d \) interactions are nonrelevant, a result which is expected for this model.

Key Words: 2D superconductors, flow equations, magnetic correlations
1 Introduction

The flow equation method given by Wegner [1] has been successfully applied for the many-body problem by Kehrein and Mielke [2], for the Anderson Hamiltonian. In a previous paper the present authors [4] showed that this method can be used to calculate the energy of a superconductor containing magnetic impurities describe by the Anderson Hamiltonian, with $U = 0$. We studied (See ref.[4]) the influence of the density of states on the single impurity energy for the case of a van-Hove density of states. In this case the energy is reduced by the superconducting state and corrections depends on $\Delta^2$. In this paper we consider a superconductor with a constant density of states but for the impurity we take the Hubbard repulsion $U \neq 0$.

2 Model

We consider a superconductor containing magnetic impurities describe by the model Hamiltonian.

$$H = H_{BCS} + H_A$$

where $H_{BCS}$ is

$$H_{BCS} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^+ c_{k,\sigma} + \sum_k \Delta(c_{k,\uparrow}^+ c_{-k,\downarrow} + c_{k,\uparrow} c_{-k,\downarrow})$$

$\Delta$ being the order parameter and $H_A$ the Anderson Hamiltonian, describing the impurity in a metal,as:

$$H_A = \sum_d \epsilon_d d_d^+ d_d + \sum_{k,\sigma} V_{k,d}(c_{k,\sigma}^+ d_d + d_d^+ c_{k,\sigma}) + Ud_\uparrow^+ d_\downarrow d_\uparrow$$

In equation (3) the first term is the energy of the impurities, the second term is the interaction between the itinerant-electron and impurity and the last term in the Hubbard repulsion between the d-electrons of the impurity. In order to make the problem analytically tractable we consider the case of a one impurity problem.

This problem has been treated using the flow-equation method by Crisan et.al. for $U = 0$ and a van-Hove density of states. In the next section we consider the case $U \neq 0$ which is a more realistic case.
3 The Flow Equations

The flow equations method, which is in fact a renormalization procedure applied in the Hamiltonian formalism has been applied in the solid-state theory by the Wegner[1], Kehrein and Mielke [3] and has the main point the diagonalization of the Hamiltonian which describes the system by a continuous unitary transformation $\eta(l)$ which lead to a Hamiltonian $H(l)$ with the parameters functions of the flow parameter $l$. This transformation satisfies:

$$\frac{dH(l)}{dl} = [\eta(l), H(l)]$$

(4)

where $\eta(l)$ can be calculated from:

$$\eta(l) = [H_0(l), H_{int}(l)]$$

(5)

In order to solve the differential equations using the Hamiltonian. (1) we introduce, following [2] the initial values:

$$\epsilon^I_k(l) = \epsilon_k(l = 0)$$

$$\epsilon^I_d(l) = \epsilon_d(l = 0)$$

$$V^I(l) = V(l = 0)$$

$$U^I(l) = U(l = 0)$$

(6)

and the renormalized value for $l \rightarrow \infty$

$$\epsilon^R_k(l) = \epsilon_k(\infty)$$

$$\epsilon^R_d(l) = \epsilon_d(\infty)$$

$$V^R(l) = V(\infty)$$

$$U^R(l) = U(\infty)$$

(7)

Using the Eq. (5) and the general method (see Ref.[1]) we calculate $\eta(l)$ as:

$$\eta(l) = \eta^{(0)}(l) + \eta^{(1)}(l) + \eta^{(2)}(l) + \eta^{(3)}(l) + \eta^{(4)}(l)$$

(8)

and obtain:

$$\eta^{(0)} = \sum_{k,\sigma} \eta_k(c^+_k\sigma d_\sigma - d^+_\sigma c_{k,\sigma})$$

$$+ \sum_{k,\sigma} \xi_k(d^+_\sigma c^+_{k,\sigma} + c^+_{k,\sigma}d_{-\sigma})$$

(9)
where:

$$\eta_k = (\epsilon_k - \epsilon_d)V_{k,d} \quad (10)$$

and:

$$\xi_{k,\sigma} = -\Delta V_{-k}\sigma \quad (11)$$

In Eq.(11) \(\sigma = \uparrow, \downarrow\) correspond to \(\sigma = \pm 1\) in the right side. The higher order contributions will be given as functions of expressions given by Eqs.(10) and (11) and by:

$$\Theta_{k,\sigma} = \eta_{-k}\Delta\sigma + \xi_{k,\sigma}\epsilon_d \quad (12)$$

as:

$$\eta^{(1)}_{k,\sigma} = (\epsilon_k V_k - \epsilon_d V_k - \Delta\Theta_{-k,\sigma}) \quad (13)$$

$$\eta^{(1)}_{k,k_1,\sigma} = \epsilon_k (\eta_{k,\sigma} V_{k_1} + \eta_{k_1,\sigma} V_k) - \Delta (\xi_{-k,\sigma} V_{k_1} - \xi_{k_1,\sigma} V_{-k}) \quad (14)$$

$$\eta^{(2)}_{k,\sigma} = (-\Delta V_{-k}\sigma - \epsilon_k \Theta_{k,\sigma} - \epsilon_d \Theta_{-k,\sigma}) \quad (15)$$

$$\eta^{(1)}_{k,k_1,\sigma} = \Delta (\eta_{k_1,\sigma} V_k + \eta_{k\sigma} V_{k_1})\sigma + \epsilon_k (\xi_{k_1,\sigma} V_{-k} + \xi_{-k,\sigma} V_{k_1}) \quad (16)$$

$$\eta^{(3)}_{k,\sigma} = (\epsilon_k \eta_{k,\sigma} U - \epsilon_d \eta_{k,\sigma} U + \Delta U \xi_{-k,\sigma}\sigma) \quad (17)$$

$$\eta^{(4)}_{k,\sigma} = (\Delta \eta_{-k,\sigma} U\sigma - \epsilon_k \xi_k U - \epsilon_d \xi_k U) \quad (18)$$

If we take the spin orientation as \(\sigma = 1\) (the non-magnetic states) the flow equations are:

$$\frac{d\epsilon_d}{dl} = -2 \sum_k \eta^{(1)}_k V_k + 2 \sum_k \eta^{(3)}_k V_k n_k$$

$$\frac{dV_k}{dl} = \eta^{(1)}_k [\epsilon_k - \epsilon_d + \frac{U \Delta^2}{[U(1 - n_k) + \epsilon_d + \epsilon_k][\epsilon_d - \epsilon_k + U] - \Delta^2}]$$

$$\frac{dU}{dl} = -4 \sum_k \eta^{(3)}_k V_k$$

$$\frac{d\Delta}{dl} = \frac{1}{N(0)} \sum_k \eta^{(2)}_k V_{-k}$$

where \(n_k\) is the Fermi function.
4 Solutions of the flow equations

Using the spectral function

\[ J(\epsilon, l) = \sum_k V_k^2 \delta(\epsilon - \epsilon_k(l)) \]  

(20)

and the factorization \( \eta_k^{(1)}(l) = V_k f(\epsilon_k, l) \) the Eqs. (17) becomes as follows:

\[
\frac{de_d}{dl} - \int d\epsilon \frac{\partial J(\epsilon, l)}{\partial l} \left[ \frac{\epsilon_d - \epsilon + U_1}{\epsilon_d + \epsilon + U_2} \right] - \Delta^2 = \frac{\epsilon_d - \epsilon + U_1}{U_2 + \epsilon_d + \epsilon} - \Delta^2(\epsilon_d - \epsilon - U) \]  

(21)

where:

\[
U_1 = U(1 + n(\epsilon)) \\
U_2 = U(1 - n(\epsilon)) \]

(22)

The equation for \( U \) becomes:

\[
\frac{dU}{dl} = 2 \int d\epsilon \frac{\partial J(\epsilon, l)}{\partial l} \left[ \frac{\epsilon_d - \epsilon + U}{\epsilon_d + \epsilon + U_2} \right] - \Delta^2(\epsilon_d - \epsilon - U) \]  

(23)

These equations contain \( \Delta^2 \) so we have to transform the equation for \( \Delta \) as:

\[
\frac{d\Delta^2}{dl} = \frac{1}{N(0)} \int d\epsilon \frac{\partial J(\epsilon, l)}{\partial l} \left[ \frac{\epsilon_d - \epsilon + U}{\epsilon_d + \epsilon + U_2} \right] - \Delta^2(\epsilon_d - \epsilon - U) \]  

(24)

In the Eqs. (22),(23),(24) we have \( \frac{\partial J(\epsilon, l)}{\partial l} \) which is obtained from Eqs. (18) as:

\[
\frac{\partial J(\epsilon, l)}{\partial l} = 2J(\epsilon, l)f(\epsilon, l)[\epsilon_d - \epsilon + \frac{U\Delta^2}{\epsilon_d + \epsilon + U_2}] - \Delta^2 \]

(25)

and because we have this relation, a supplementary equation for \( V_k(l) \) gives no more information about the system. The solutions of these equations will be obtained at \( T = 0 \) \( (n(\epsilon) = 1 - \Theta(\epsilon)) \) and if we take a concrete form for the \( J(\epsilon, l = 0) \) as

\[
J(\epsilon, l = 0) = \frac{2V^2}{\pi D} = \frac{\Gamma}{\pi} \]

(26)

\[ \Gamma = \frac{2\Delta^2}{\pi} \] where \( D \) is the bandwidth in the limit \( U >> D >> \epsilon_d^R \) we obtained from Eqs.(19) using conditions (6),(7):

\[
\epsilon_d^I = \epsilon_d^R - \frac{\Gamma}{2\pi \epsilon_d^R} \left[ 1 - \frac{\epsilon_d^R}{\epsilon_d^R + D} + \text{arctanh} \frac{D}{\epsilon_d^R} + \ln \frac{D}{\epsilon_d^R} \right] \]

\[
\Delta_f^2 = \Delta_f^2(1 + I_1) \]

\[
U_L = U^R + \frac{2\Gamma}{\pi} \left[ \ln \frac{\epsilon_d^R + D}{\epsilon_d^R} + \ln \frac{\epsilon_d^R + U^R - D}{\epsilon_d^R + U^R + D} \right] \]

(27)
where:

\[ I_1 = -\frac{1}{2U^R(\epsilon_d^R + U^R)} \left[ 2\ln \frac{\epsilon_d^R + U^R + D}{\epsilon_d^R + D} + \ln \frac{\epsilon_d^{R^2}}{\epsilon_d^R - D^2} \right] + \frac{2(\epsilon_d^R + U^R)}{2U^R(2\epsilon_d^R + U^R)} \text{arctanh} \frac{D}{\epsilon_d^R} \]

(28)

5 Conclusions

Using the flow equations method we showed that for a BCS superconductor with magnetic correlations described by the Anderson Hamiltonian with \( U \neq 0 \) we calculated the energy of impurity \( \epsilon_d \), the order parameter \( \Delta \), and the energy \( U \). For a large \( D \) we get

\[ \Delta_R = \Delta_I \quad U^R = U^I \]

(29)

and the energy of the impurity presents a small variation as function of \( D \).

References

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