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The bipolaronic superconducting glass state in the random infinite-range interaction Hubbard model

T K Kopeć and P Wróbel
Institute for Low Temperature and Structure Research, Polish Academy of Sciences, 50–950 Wrocław 2, PO Box 937, Poland

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Abstract. The phase diagram of the extended Hubbard model with on-site attraction and random inter-site Coulomb energies is studied for the half-filled band case. In the strong coupling limit the problem is mapped onto the system of hard-core bosons (bipolarons) on a lattice, described by the anisotropic pseudo-spin model with infinite-range random exchange interactions—in close analogy to the Sherrington–Kirkpatrick spin-glass approach. It is found that the disorder and frustration strongly affects properties of the system leading to the appearance of the bipolaronic superconducting phase, the bipolaronic superconducting glass state as well as the bipolaronic charge glass phase, depending on the temperature range and the degree of the disorder.

1. Introduction

The effect of non-magnetic disorder on superconductivity, first addressed for metals in the pioneering works of Anderson (1959) and Abrikosov and Gorkov (1959), turns out to be of little importance for the thermodynamic properties of ordinary superconductors. Since the discovery of the new high T_c superconductors (Bednorz and Müller 1986) it has become clear that this disorder plays an important role in the attributes of the new superconductors, manifesting itself as a typical glass-type behaviour (Müller *et al* 1987).

Most subsequent work performed on glassy behaviour in high T_c superconductors has been based on phenomenological models and has argued that the glassy properties are a product of the granular nature of the samples. However, the influence of disorder at the *macroscopic* level addressed in these works has not exhausted the problem of current interest: what does the *microscopic* structural disorder do to superconductivity in strongly correlated electron systems? For example, the analogy between spin glasses and the problem of highly localised electrons interacting via the Coulomb potential is well known (Efros and Shklovski 1975, Efros 1976). In this so-called 'electron glass', on cooling from the high temperature phase, Monte Carlo simulations indicate spin-glass-like freezing (Davies *et al* 1982). From this point of view the investigation of the glassy properties with reference to a microscopic mechanism of superconductivity, with simultaneous consideration of the disorder and frustration, is an important theoretical issue.

According to the more conventional treatment, the superconducting glass model is described by a disordered array of Josephson junctions, in close analogy to that for

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granular superconductors (Morgenstern *et al* 1988). In a different approach pursued by Oppermann (1987), the possibility of a superconducting glass phase was considered in the context of the quantum theory of localisation and superconductivity in the weak-coupling regime. However, for the new high T_c superconductors it has been known for some time that the tight-binding approach with strong electron–electron correlations appears to be more appropriate than the nearly-free electron picture. Therefore, the strong-coupling theory of the superconducting glass phase is of particular interest.

2. The model

In the present paper we propose a model of superconducting glass based on the systems of strongly correlated electrons described by the Hubbard Hamiltonian with negative on-site Coulomb energy given by

$$H = \sum_{ij\sigma} t_{ij} a_{i\sigma}^{+} a_{j\sigma} - |U| \sum_{i} n_{i\uparrow} n_{i\downarrow} + \tfrac{1}{2} \sum_{\substack{ij \\ \sigma\sigma'}} V_{ij} n_{i\sigma} n_{j\sigma'} - \mu \sum_{i\sigma} n_{i\sigma} \tag{1}$$

where $a_{i\sigma}(a_{i\sigma}^{+})$ is the annihilation (creation) operator for an electron with the spin projection σ at the ith lattice site and $n_i = a_{i\sigma}^{+} a_{i\sigma}$. Furthermore, $-|U|$ is the attractive on-site potential (e.g., due to the strong electron–phonon coupling) while V_{ij} refers to the inter-site Coulomb potential (which can be either repulsive or attractive). Finally, t_{ij} is the matrix element of the electron transfer between the lattice sites, while μ represents the chemical potential.

To obtain non-trivial superconducting glass features it appears that the model must have a substantial amount of randomness *and* frustration. There have been attempts to model the superconducting glass behaviour by having the former ingredient without the latter by introducing a kind of diagonal disorder via the random site energies in the Hamiltonian (1) (Kulik and Pedan 1980, Micnas *et al* 1985), but it seems that frustration is essential for the superconducting glass properties. However, one can account for both of them in a simple and non-trivial manner by considering random inter-site Coulomb potentials V_{ij} (off-diagonal disorder). In physical terms the randomness in the variables V_{ij} is induced by structural disorder (random displacements and vacancies) which can be described by the suitable distribution $P(V_{ij})$. The standard choice is the Gaussian one and in the infinite-range case one has (Sherrington and Kirkpatrick 1975)

$$P(V_{ij}) = (N/2\pi V^2)^{1/2} \exp(-NV_{ij}^2/2V) \tag{2}$$

where V denotes the variance of the distribution and N is the number of lattice sites. In passing we note that the long-range nature of interactions originating from the Coulombic character of the inter-bond potential justifies the use of formula (2).

3. The effective pseudo-spin Hamiltonian and the order parameters

In the strong coupling regime ($t^2/U \ll 1$) the Hubbard Hamiltonian (1) can be transformed into a pseudo-spin effective Hamiltonian describing the bipolaronic system,

which can be seen as a gas of hard-core bosons on a lattice (Robaszkiewicz *et al* 1981, 1982 and references therein). The resulting Hamiltonian turns out to be

$$H = -\sum_{ij} J_{ij}(\rho_{xi}\rho_{xj} + \rho_{yi}\rho_{yj}) + \sum_{ij} K_{ij}\rho_{zi}\rho_{zj} - \mu \sum_{i} (2\rho_{zi} + 1) \tag{3}$$

where $J_{ij} = 2t_{ij}^2/|U|$, $K_{ij} = J_{ij} + 2V_{ij}$ and ρ_{ia} $(a = x, y, z)$ are the spin-$\frac{1}{2}$ matrices related to the bipolaron annihilation (b_i) and creation (b_i^+) operators by

$$\rho_{zi} = \tfrac{1}{2} - b_i^+ b_i \qquad \rho_{xi} = \tfrac{1}{2}(b_i + b_i^+) \qquad \rho_{yi} = (i/2)(b_i - b_i^+) \tag{4}$$

where $b_i^+ = a_{i\uparrow}^+ a_{i\downarrow}^+$ and $b_i = a_{i\downarrow} a_{i\uparrow}$.

It is easy to recognise that in the pseudo-spin description (4) the bipolaronic hopping term transforms into a 'ferromagnetic' coupling J_{ij} in the xy-plane, whereas K_{ij} maps onto random longitudinal interactions between pseudo-spins. The chemical potential, in turn, plays the role of an external field determined by the bipolaron number-conservation condition

$$\frac{1}{N}\sum_{i} \langle \rho_{zi} \rangle = \tfrac{1}{2} - n_b \tag{5}$$

where n_b denotes the bipolaron density. Since the V_{ij} are the same for all pairs of pseudo-spins, one obtains

$$\langle V_{ij}^2 \rangle_v - \langle V_{ij} \rangle_v^2 = V^2/N$$

and in order to ensure sensible thermodynamic limit one has also to have $J_{ij} = J/N$, i.e. $t_{ij} = t/N$ and $U = \tilde{U}/N$.

The superconducting order parameter Δ describing the off-diagonal long-range order (phase coherence between bipolarons) corresponds to the expectation value of the transverse pseudo-spin component $\Delta = \langle \rho_{xi} \rangle$. Because of disorder, in a manner analogous with the conventional spin-glass problem, we introduce the Edwards–Anderson-like ((EA) Edwards and Anderson 1975) order parameter

$$q = \lim_{t \to \infty} \langle\langle \rho_{zi}(0)\rho_{zi}(t) \rangle\rangle_v \tag{6}$$

to describe the glass phase. Here, $\rho_{zi}(t) = \frac{1}{2} - n_b(t)$ is the bipolaron occupation number operator at the time t and $\langle \ldots \rangle_v$ refers to the average of the V_{ij} interactions over the random configuration. The meaning of this quantity is that it represents the fraction of the bipolarons that get stuck in the configurations that would not change over any finite time, distinguishing between the glass $(q \neq 0)$ and non-glass $(q = 0)$ phases.

4. The results

A common theoretical approach to the spin-glass problem is to map the physical disordered system onto an effective pure one by use of the familiar 'n-replica trick' (Edwards and Anderson 1975). Unfortunately, a straightforward application of this technique to the present problem is obstructed by the non-commuting nature of the operators appearing in (3). Recently, however, an alternative approach has been implemented for the case of the quantum spin glass (Kopeć 1988) based on thermo-field dynamics (TFD) (Umezawa *et al* 1982). This method allows one to circumvent the use of replicas and incorporates in a natural way the dynamic definition of the glass-order parameter (6).

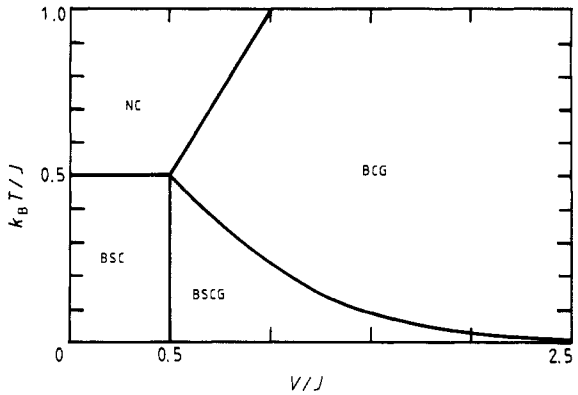

Figure 1. Phase diagram of the system resulting from equations (7).

However, before we give the highlights of the calculation we quote the main results of this work expressed in terms of the self-consistent equations for the superconducting and glass-order parameter that read

$$\Delta = J\Delta \int_{-\infty}^{+\infty} \frac{dz}{(2\pi)^{1/2}} e^{-z^2/2} \tanh[\beta\Theta(z)/2]/\Theta(z) \tag{7a}$$

$$q = \frac{1}{4}\int_{-\infty}^{+\infty} \frac{dz}{(2\pi)^{1/2}} e^{-z^2/2}[\mu + 4Vzq^{1/2}/\Theta(z)]^2 \tanh^2[\beta\Theta(z)/2] \tag{7b}$$

where $\Theta(z) = [(2J\Delta)^2 + (\mu + 4Vzq^{1/2})^2]^{1/2}$, $\beta = 1/k_B T$ and $J = 2t^2/|\tilde{U}|$. Equations (7*a*) and (7*b*) are subject to the conditions that fix the chemical potential μ for a given bipolaron density n_b:

$$\tfrac{1}{2} - n_b = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{dz}{(2\pi)^{1/2}} e^{-z^2/2}[\mu + 4Vzq^{1/2}/\Theta(z)] \tanh[\beta\Theta(z)/2]. \tag{7c}$$

Although equations (7) are valid for the arbitrary value of n_b, in the rest of this work we will consider only the half-filled band case ($n_b = \frac{1}{2}$). In the pseudo-spin language this is the case of the zero external field ($\mu = 0$). For arbitrary band-filling it follows from equation (7*b*) that for any temperature $q \neq 0$ since the longitudinal field is present. In this case, the glass transition would be analogous to the transition on the de Almeida–Thouless line (de Almeida and Thouless 1978) rather than the zero field spin-glass transition. Therefore in the general case ($n_b \neq \frac{1}{2}$) equations (7) have to be supplemented by the corresponding stability condition in order to determine the glass transition boundary in the parameter space ($k_B T$, V, n_b). For the $n_b = \frac{1}{2}$ case it is straightforward to solve (7*a*) and (7*b*) numerically for Δ and q and also to obtain analytic results in limiting cases. The resulting phase diagram is shown in figure 1, where the following phases emerge.

(i) The normal (NC) and non-glass phase: $\Delta = q = 0$.

(ii) The bipolaronic superconducting phase (BSC): $\Delta \neq 0$, $q = 0$.

(iii) The bipolaronic superconducting glass phase (BSCG): $\Delta \neq 0$, $q \neq 0$. In this case both off-diagonal long-range superconducting order and diagonal glass order are predicted to coexist. Due to the non-vanishing of q, the system of bipolarons is stuck into a

particular configuration in the phase space and cannot easily relax into another one, implying hysteresis and a non-ergodic behaviour typical of glasses. Because Δ is finite the BSCG is predicted to be in the Meissner state.

(iv) The bipolaronic charge glass (BCG) phase: $\Delta = 0, q \neq 0$. In this phase the superconducting long-range order is suppressed, whereas the glass order persists, indicating non-ergodic behaviour.

5. The method

Now we present the logic that leads to equations (7). Because the highlights of the TFD method in the context of the quantum spin-glass problem have already appeared in the literature (Kopeć 1988), we can be brief. In order to incorporate thermal effects in TFD one requires the doubling of degrees of freedom (Umezawa *et al* 1982) by associating with any operator $A(\equiv A^1)$ a tilde-conjugate one $\tilde{A}^+(\equiv A^2)$. Specifically, the dynamics are generated by the thermal Hamiltonian $\hat{H}$

$$\hat{H} = H - \tilde{H} \equiv H[\rho^1] - H[\rho^2] \tag{8}$$

where H is the Hamiltonian of the bipolaronic system (3). The temperature enters the theory through the thermal vacuum $|0(\beta)\rangle$ which is constructed in such a way that the quantum-mechanical expectation value between the thermal vacua corresponds to the thermal average (Umezawa *et al* 1982)

$$\langle 0(\beta)| \ldots |0(\beta)\rangle = \mathrm{Tr} \ldots \exp(-\beta H)/\mathrm{Tr} \exp(-\beta H). \tag{9}$$

Because of the thermal vacuum amplitude normalisation condition (Matsumoto *et al* 1984), it is possible to perform a disorder average with $P(V_{ij})$ On the generating functional for the real-time TFD causal Green function without resorting to replicas. Proceeding in an analogous way to the case of a quantum Ising spin glass (Kopeć 1988), we arrive at the disorder averaged generating functional written in the form of the functional integral

$$\langle Z[\eta]\rangle_v = \int \left[\prod_{a\alpha} D\varphi_a^\alpha\right]\left[\prod_{\alpha\beta} DQ^{\alpha\beta}\right] \exp(-N\mathcal{L}[\varphi, Q] + \Omega[\eta]) \tag{10}$$

where the single-site dynamic Lagrangian reads

$$\mathcal{L}[\varphi, Q] = \frac{\mathrm{i}}{2}[(\varphi_x, \varphi_x) + (\varphi_y, \varphi_y) - (\varphi_z, \varphi_z)] + \mathrm{Tr}\, Q^2 - \ln \Phi[\varphi, Q] \tag{11}$$

while $\Omega[\eta]$ refers to the source term, the precise form of which depends on the kind of correlations we are interested in. Furthermore,

$$\begin{aligned} (\varphi_a, \varphi_a) &\equiv \int_{-\infty}^{+\infty} \mathrm{d}t \sum_\alpha \varphi_a^\alpha(t)\varphi_a^\alpha(t) \\ \mathrm{Tr}\, Q^2 &\equiv \int_{-\infty}^{+\infty} \mathrm{d}t \int_{-\infty}^{+\infty} \mathrm{d}t' \sum_{\alpha\beta} Q^{\alpha\beta}(t, t')Q^{\beta\alpha}(t', t) \end{aligned} \tag{12}$$

where $Q^{\alpha\beta}(t, t')$ represents a 2×2 symmetric matrix field, $a = x, y, z$, and $\alpha, \beta = 1, 2$. Subsequently

$$\Phi[\varphi, Q] = \langle 0, \beta | U_{\varphi,Q}\ (-\infty, +\infty)|0, \beta\rangle \tag{13}$$

where $|0, \beta\rangle$ denotes the thermal vacuum corresponding to the single-site Hamiltonian $H_0 = -\mu \Sigma\, (2\rho_z + 1)$, while

$$U_{\varphi,Q}(+\infty,-\infty) = T\exp\left(-\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\int_{-\infty}^{+\infty}\mathrm{d}t'\hat{H}_{\varphi,Q}(t,t')\right) \tag{14}$$

is the time-ordered exponential resulting from the interaction picture. The effective time-dependent single-site thermal Hamiltonian then reads

$$\hat{H}_{\varphi,Q}(t,t') = \sum_{\alpha\beta}\{(2\varepsilon_\alpha J)^{1/2}[\varphi_x^\alpha(t)\rho_x^\alpha(t) + \varphi_y^\alpha(t)\rho_y^\alpha(t) - \varphi_z^\alpha(t)\rho_z^\alpha(t)] \times \delta(t-t')\delta_{\alpha\beta} + 2(\varepsilon_\alpha\varepsilon_\beta)^{1/2}VQ^{\alpha\beta}(t,t')\rho_z^\alpha(t)\rho_z^\beta(t')\} \tag{15}$$

where $\varepsilon_1 = 1$ and $\varepsilon_2 = -1$. Finally, the pseudo-spin operators appearing in (14) are defined in the interaction picture in the standard way as

$$\rho_a^\alpha(t) = \exp(\mathrm{i}\hat{H}_0 t)\rho_a^\alpha(0)\exp(-\mathrm{i}\,\hat{H}_0 t) \qquad (a = x, y, z;\ \alpha = 1, 2). \tag{16}$$

The effective dynamic Hamiltonian (15) contains the fluctuating local field φ_a^α and the dynamic pseudo-spin self-interaction $Q^{\alpha\beta}(t,t')$, which have to be calculated self-consistently. In the $N\to\infty$ limit the saddle point method can be used, which amounts to finding for φ and Q fields their stationary point values φ_0 and Q_0 from equations

$$\delta\mathcal{L}[\varphi, Q]/\delta\varphi_a^\alpha = 0 \qquad \delta\mathcal{L}[\varphi, Q]/\delta Q^{\alpha\beta} = 0. \tag{17}$$

Consequently one obtains

$$\begin{aligned} &\varphi_{0a}^\alpha = (2\varepsilon_\alpha J)^{1/2}\langle\rho_a^\alpha\rangle_\beta \qquad Q_0^{\alpha\beta} = \tfrac{1}{2}(\varepsilon_\alpha\varepsilon_\beta)^{1/2}VG^{\alpha\beta}(t,t') \\ &G_{\alpha\beta}(t,t') = -\mathrm{i}\langle T\rho_z^\alpha(t)\rho_z^\beta(t')\rangle_\beta \end{aligned} \tag{18}$$

where

$$\langle\ldots\rangle_\beta \equiv \langle 0,\beta|\ldots U_{\varphi_0,Q_0}(-\infty,+\infty)|0,\beta\rangle. \tag{19}$$

In the glass phase the dynamic self-interaction, acquires a time-persistent contribution. Therefore we factorise the causal TFD matrix Green function into the finite ($G_{\mathrm{reg}}^{\alpha\beta}$) and time-persistent ($G_{\mathrm{sing}}^{\alpha\beta}$) parts:

$$G^{\alpha\beta}(t,t') = G_{\mathrm{reg}}^{\alpha\beta}(t,t') + G_{\mathrm{sing}}^{\alpha\beta}(t,t'). \tag{20}$$

In the thermal equilibrium case one has, for the Fourier-transformed finite-time part (Kopeć 1988),

$$G_{\mathrm{reg}}^{\alpha\beta}(t,t') = \begin{pmatrix} G^{\mathrm{R}}(\omega) & 0 \\ 0 & -G^{\mathrm{A}}(\omega) \end{pmatrix}^{\alpha\beta} - \frac{2\mathrm{i}\,C_{\mathrm{reg}}(\omega)}{\mathrm{e}^{\beta\omega}+1}\begin{pmatrix} 1 & \mathrm{e}^{\beta\omega/2} \\ \mathrm{e}^{\beta\omega/2} & 1 \end{pmatrix}^{\alpha\beta} \tag{21}$$

with $G^{\mathrm{R(A)}}(\omega)$ being the retarded (advanced) Green function. Correspondingly, $C_{\mathrm{reg}}(\omega)$ is the thermodynamic correlation function, which is related to $G^{\mathrm{R}}(\omega)$ by means of the fluctuation–dissipation theorem

$$C_{\mathrm{reg}}(\omega) = \coth(\beta\omega/2)\,\mathrm{Im}\,G^{\mathrm{R}}(\omega). \tag{22}$$

Furthermore, it turns out that the time-persistent part has the form

$$G_{\mathrm{sing}}^{\alpha\beta}(\omega) = -2\pi\,\mathrm{i}q\delta(\omega)\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}^{\alpha\beta} \tag{23}$$

where q is the EA type glass-order parameter (6). Indeed, by substituting equation (23) into (20) and using relation (21), one obtains for the fall correlation function

$$C(\omega) = C_{\mathrm{reg}}(\omega) + 2\pi q\delta(\omega) \tag{24}$$

according to the dynamic EA definition of the glass-order parameter. Moreover, the

time-persistent contribution to the effective thermal Hamiltonian (15) can be written in the form of a static random component, which acts as random longitudinal field to generate the time-persistent autocorrelation. Accordingly, the effective thermal average (19) becomes

$$\langle \ldots \rangle_\beta = \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{(2\pi)^{1/2}} \mathrm{e}^{-z^2/2} \langle 0(\beta, z) | \ldots U^{\mathrm{reg}}_{\varphi_0, Q_0}(-\infty, +\infty) | 0(\beta, z) \rangle \tag{25}$$

where $|0(\beta, z)\rangle$ is the thermal vacuum associated with the single-site Hamiltonian $H_0' = H_0 + 2Vzq^{1/2}\rho_z$ with static noise, while the time-ordered exponential (14) now contains only the finite-time part of the dynamic self-interaction. It turns out, however, that the finite part of the dynamic pseudo-spin self-interaction also persists in the non-glass phase, making the explicit solution of the self-consistent equations (18) a highly non-trivial task. This is the special feature of the quantum problem, where the dynamic effects contribute even to the static quantities. Nevertheless, one can resort to the static approximation (Kopeć 1988), which effectively replaces the dynamic quantities (like the response functions) by their zero-frequency counterparts, thus approximating the dynamic pseudo-spin self-interaction by the static quantity. Proceeding in this way one finally arrives at equations (7).

6. Final remarks

Closing, we should point out that the result (7), involving a single glass-order parameter description, seems to correspond to the replica-symmetric solution, which turns out to be unstable in the glass phase. Thus, the precise characterisation of the superconducting glass phase is obstructed, with similar difficulties to those arising in the case of the low temperature phase in the magnetic spin glasses. The investigation of the stability of the solution (7) is of great interest, since it would enable one to extend the analysis presented to the case of non-half-filled band, where the glass parameter q alone is ineffective in singling out the glassy phase. Also of interest are other distributions of random variables V_{ij} (e.g. the Gaussian distribution with a non-vanishing mean, opening the possibility for the bipolaronic charge disproportionation phase), as well as the inclusion of the electromagnetic vector potential in order to study the superconducting glass phase boundary as a function of the external magnetic field. We hope to return to these questions in future work.

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