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Superconducting glass properties in the random infinite-range interaction Hubbard model: stability analysis and phase diagrams

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Abstract. The extended Hubbard model with on-site attraction and random infinite-range inter-site Coulomb interaction is studied for arbitrary band filling. In the strong-coupling limit the problem is mapped onto a system of hard-core bosons (local electron pairs) on a lattice described by the anisotropic pseudo-spin model with infinite-range random interactions—in close analogy to the standard Sherrington–Kirkpatrick spin-glass approach. With the use of thermofield dynamics as a substitute for the 'n-replica trick', and a one-loop approximation for the dynamic self-interaction, the stability of the mean-field-type solution with respect to the action of fluctuations is investigated in the parameter space including the temperature, degree of disorder and band-filling parameter.

1. Introduction

In a classical picture, superconducting glass phases can occur in granular superconductors when the phase of the superconducting order parameter is frustrated in loops of Josephson-coupled grains (Shih *et al* 1984, Ebner and Stroud 1985) where the frustration appears as a result of an applied magnetic field. Phase diagrams which include the glass phase were obtained either by Monte Carlo simulation (Shih *et al* 1984, Ebner and Stroud 1985) or by the field theoretic approach via the 'n-replica trick' to the model of disordered arrays of Josephson-coupled grains (Sajeev and Lubensky 1986). This model assumes the existence of a gap energy inside the grains.

The need for a quantum theory, when grains are smaller than 100 Å was stressed by Deutscher (1984) and by Sajeev and Lubensky (1986) and an appropriate theory based on the weak-coupling regime was then constructed to describe the superconducting glass features (Oppermann 1987) in the context of a quantum theory of localisation and superconductivity. Here, the possibility of superconducting glass phases appeared as a result of the destruction of conventional superconductivity at strong disorder near the metal–insulator transition. Under the increasing disorder, first the gap disappears and, after an interval of gapless superconductivity, a transition into a glass state with vanishing BCS order parameter occurs (Oppermann 1987). Because of this, no global supercurrent and no Meissner effect exists below the glass transition temperature. However, for the high-T_c superconductors exhibiting glass features in the Meissner state (Müller *et al* 1987) it has been known for some time that the tight-binding approach with strong

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electron–electron correlations appears to be more appropriate than the nearly-free-electron picture.

The analogy between spin glasses and the problem of highly localised electrons interacting via the Coulomb potential is well known (Efros and Shklovskii 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 glassy properties with simultaneous reference to the microscopic mechanism of superconductivity has been pursued recently by considering the strong-coupling regime and analysing the extended Hubbard model with on-site attraction and random inter-site Coulomb energies (Kopeć and Wróbel 1990). Within the mean-field theory a multiplicity of phases has been found including the normal (N) or non-glass phase, the superconducting (SC) phase, the superconducting glass (SCG) phase (which is non-ergodic and predicted to be in the Meissner state) and the charge glass (CG) phase (which is non-ergodic and non-superconducting). However, the results presented were confined to the half-filled band only. In the present paper we extend the above analysis to the arbitrary band-filling case and calculate phase diagrams for the model by considering the parameter space which includes the temperature, degree of disorder and band-filling parameter.

2. The model Hamiltonian and order parameters

The system of strongly correlated electrons under study is described by the Hubbard Hamiltonian with negative on-site Coulomb energies given by

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

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

To account for disorder and frustration in the model Hamiltonian (1), randomness in the variables V_{ij} is introduced (off-diagonal disorder). In physical terms this would mean for example a structural disorder (random vacancies and displacements) which can be described by a suitable distribution of random variables $P(V_{ij})$. The most convenient choice is Gaussian and referring to the work of Sherrington and Kirkpatrick (1975) one writes

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

where V denotes the variance of the distribution and N is the number of lattice sites. The meaning of expression (2) is that we are considering the case of infinite-range interactions between the lattice sites (the number of nearest neighbours for a given lattice site is equal to the number N of lattice sites) which is justified by the long-range nature of interactions originating from the Coulombic character of the inter-bond potential.

In the strong-coupling regime that we are interested in, the Hubbard Hamiltonian (1) can be mapped onto a pseudo-spin effective Hamiltonian describing the system of local electron pairs (bipolarons in the case of strong electron–phonon coupling) which can be seen as a gas of hard-core bosons on a lattice (Robaszkiewicz *et al* 1981, 1982, and references therein). The resulting effective pseudo-spin Hamiltonian takes the form

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

where $J_{ij} = 2t_{ij}/|U|$, $K_{ij} = J_{ij} + 2V_{ij}$ while S_{ai} ($a = x, y, z$; $i = 1, \ldots, N$) are the $\frac{1}{2}$-spin matrices related to the local pair annihilation operators b_i and creation operators b_i^+ in the following way:

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

where $b_i^+ = a_{i\uparrow}^+ a_{i\downarrow}^+$ and $b_i = a_{i\uparrow} a_{i\downarrow}$. The pseudo-spin Hamiltonian (3) is supplemented by the local pair number conservation condition

$$\frac{1}{N}\sum_{i} \langle\langle S_{zi}\rangle\rangle_{\mathrm{av}} = \tfrac{1}{2} - n_b \tag{5}$$

where n_b denotes the number of local pairs, $\langle \ldots \rangle$ is the thermal average while $\langle \ldots \rangle_{\mathrm{av}}$ refers to the configurational averaging

$$\langle \ldots \rangle_{\mathrm{av}} = \int \prod_{ij} \mathrm{d}V_{ij}\, P(V_{ij}) \ldots . \tag{6}$$

Since V_{ij} are the same for all pairs of pseudo-spins, one has

$$\langle V_{ij}^2 \rangle_{\mathrm{av}} - \langle V_{ij} \rangle_{\mathrm{av}}^2 = V^2/N \tag{7}$$

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

The superconducting order parameter Δ describes the off-diagonal long-range order (phase coherence between local pairs) and corresponds to the expectation value of the transverse pseudo-spin component

$$\Delta = \langle\langle S_{xi}\rangle\rangle_{\mathrm{av}}. \tag{8}$$

Because of the disorder present, in a manner similar to the conventional spin-glass problem, one introduces the Edwards–Anderson (1975) order parameter

$$q = \lim_{t \to \infty} \langle\langle S_{zi}(0) S_{zi}(t)\rangle\rangle_{\mathrm{av}} \tag{9}$$

in order to single out the glassy phase. By definition, $S_{zi}(t) = \frac{1}{2} - n_{bi}(t)$ ($n_{bi}(t) = b_i^+(t) b_i(t)$) is the pair occupation number at the time t and the meaning of the quantity (9) is that it represent the fraction of local pairs that get stuck in configurations in phase space that would not change over any finite time, distinguishing between the glass ($q \neq 0$) and non-glass ($q = 0$) phases. However, as has been pointed out earlier (Kopeć and Wróbel 1990), the definition (9) is able to single out the glassy phase only in the half-filled band case ($n_b = \frac{1}{2}$). In pseudo-spin language (3) this is the case of zero external field ($\mu = 0$). For an arbitrary band filling, it follows that, for any temperature, $q \neq 0$ since a longitudinal field is present. In such a situation the parameter q alone is ineffective in characterising the glassy phase. In this case the glass transition would be

analogous to the transition according to de Almeida and Thouless (AT) (1978) rather than to the zero-field spin-glass transition.

3. Stability analysis

In the following, we report on the stability analysis of the mean-field theory of the infinite-range interaction system described by the Hamiltonian (3) and the distribution (2) which will be performed in the space of parameters including the temperature, degree of disorder and band-filling number (i.e. k_BT, V and n_b, respectively).

The method that we use to handle both the disorder and the quantum features of the problem has been described earlier (Kopeć and Wróbel 1990). It relies on thermofield dynamics (TFD) Umezawa *et al* 1982), a real-time finite-temperature quantum field theory. The best merit of this method is that, while avoiding the use of the 'n-replica trick' to perform the quenched average, it deals directly with the physical observables such as response and correlation functions.

In order to incorporate thermal effects in TFD, one is forced to double the degrees of freedom of the system under study by associating with any operator A ($=A^1$) a tilde conjugate operator $\tilde{A}$ ($=A^2$). In particular the dynamics are generated by the so-called thermal Hamiltonian $\hat{H}$:

$$\hat{H} = H - \tilde{H} = H[S^1] - H[S^2] \tag{10}$$

where H is the original Hamiltonian of the system while $\tilde{H}$ refers to the tilde conjugate counterpart. The basic concept of TFD is the notion of the thermal vacuum $|0(\beta)\rangle$ constructed in such a way that the quantum expectation value between the bra and ket thermal vacua corresponds to the statistical average (Umezawa *et al* 1982)

$$\langle 0(\beta)|\ldots|0(\beta)\rangle = \mathrm{Tr}[\exp(-\beta H)]\ldots/\mathrm{Tr}[\exp(-\beta H)] \tag{11}$$

where $\beta = 1/k_BT$.

To proceed, one starts from the disorder-averaged generating functional for TFD causal Green functions in a form of the functional integral (Kopeć and Wróbel 1990)

$$\langle Z[\eta]\rangle_{\mathrm{av}} = \int \prod_{a\alpha} D\varphi_a^\alpha \prod_{\alpha\beta} DQ^{\alpha\beta} \exp(-N\mathcal{L}[\boldsymbol{\varphi}, \mathbf{Q}] + \Omega[\eta]) \tag{12}$$

where the single-site dynamic Lagrangian reads

$$\mathcal{L}[\boldsymbol{\varphi}, \boldsymbol{Q}] = \tfrac{1}{2}[(\varphi_x, \varphi_x) + (\varphi_y, \varphi_y) - (\varphi_z, \varphi_z)] + \mathrm{Tr}(Q^2) - \ln(\Phi[\boldsymbol{\varphi}, \mathbf{Q}]). \tag{13}$$

Here, $\Omega[\eta]$ denotes the source term the precise form of which depends on the kinds of correlation that we are interested in. Furthermore,

$$(\varphi_a, \varphi_a) = \int_{-\infty}^{+\infty} \mathrm{d}t \sum_\alpha \varphi_a^\alpha(t)\varphi_a^\alpha(t)$$

$$\mathrm{Tr}(Q^2) = \int_{-\infty}^{+\infty} \mathrm{d}t \int_{-\infty}^{+\infty} \mathrm{d}t' \sum_{\alpha\beta} Q^{\alpha\beta}(t, t')Q^{\beta\alpha}(t', t) \tag{14}$$

where $Q^{\alpha\beta}(t, t')$ represents a 2×2 symmetric matrix field. Subsequently,

$$\Phi[\boldsymbol{\varphi}, \mathbf{Q}] = \langle 0, \beta | U_{\varphi,Q}(-\infty, +\infty) | 0, \beta\rangle \tag{15}$$

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

$$U_{\varphi,Q}(-\infty,+\infty) = T\exp\left(-\mathrm{i}\int_{-\infty}^{+\infty}\mathrm{d}t\int_{-\infty}^{+\infty}\mathrm{d}t'\,\hat{H}_{\varphi,Q}(t,t')\right) \tag{16}$$

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

$$\hat{H}_{\varphi,Q}(t,t') = \sum_{\alpha\beta}\{(2\varepsilon_\alpha J)^{1/2}[\varphi_x^\alpha(t)S_x^\alpha(t) + \varphi_y^\alpha(t)S_y^\alpha(t) - \varphi_z^\alpha(t)S_z^\alpha(t)]\delta(t-t')\delta_{\alpha\beta} + 4(\varepsilon_\alpha\varepsilon_\beta)^{1/2}VQ^{\alpha\beta}(t,t')S_z^\alpha(t)S_z^\beta(t')\} \tag{17}$$

where $\varepsilon_1 = 1$, $\varepsilon_2 = -1$ and the pseudo-spin operators appearing in (17) are defined in the interaction picture as

$$S_a^\alpha(t) = \exp(\mathrm{i}\hat{H}_0 t)\,S_a^\alpha(0)\exp(-\mathrm{i}\hat{H}_0 t). \tag{18}$$

The effective dynamic thermal Hamiltonian (17) contains the fluctuating local field $\varphi_a^\alpha(t)$ which is related to the superconducting order parameter (8) and the pseudo-spin self-interaction $Q^{\alpha\beta}(t,t')$ connected with the glass order parameter (9) (cf Kopeć and Wróbel 1990). Both quantities have to be calculated self-consistently via the saddle-point method (formally exact in the $N\to\infty$ limit). The resulting equations are then (Kopeć and Wróbel 1990)

$$\Delta = J\Delta\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{(2\pi)^{1/2}}\exp\left(-\frac{z^2}{2}\right)\frac{\tanh[\beta\theta(z)/2]}{\theta(z)}$$

$$q = \frac{1}{2}\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{(2\pi)^{1/2}}\exp\left(-\frac{z^2}{2}\right)\left(\frac{\mu+4Vzq^{1/2}}{\theta(z)}\right)^2\tanh^2\left(\frac{\beta\theta(z)}{2}\right) \tag{19}$$

where $\theta(z) = [(2J\Delta)^2 + (\mu + 4Vzq^{1/2})^2]^{1/2}$ and $J = 2t^2/|\tilde{U}|$. The constraint (5) fixing the number of local pairs takes the following form:

$$\frac{1}{2} - n_b = \frac{1}{2}\int_{-\infty}^{+\infty}\frac{\mathrm{d}z}{(2\pi)^{1/2}}\exp\left(-\frac{z^2}{2}\right)\frac{\mu+4Vzq^{1/2}}{\theta(z)}\tanh[\beta\theta(z)]. \tag{20}$$

As emphasised earlier for any band filling different from $n_b = \frac{1}{2}$ it follows from equations (19) and (20) that, for arbitrary temperature, $q \neq 0$ because the non-vanishing chemical potential μ plays the role of an external field in our pseudo-spin description. Therefore the glass transition in this case would be analogous to the AT (1978) transition rather than to the zero-field glass transition. This implies that, in the general case ($n_b \neq \frac{1}{2}$), equations (19) and (20) have to be supplemented by the stability condition in order to determine the glass transition boundaries in the space of parameters k_BT, V and n_b. It should also be pointed out that the stability condition determines the limits of the applicability of the single-glass-order-parameter (9) description. In the instability regions, one expects the precise characterisation of the glassy phase to be obstructed with similar difficulties as in the case of the low-temperature phase in magnetic spin glasses where, in order to resolve these difficulties, an infinite number of glass order parameters have to be introduced (Parisi 1979).

A physically sensible solution must be stable, i.e. has no negative eigenvalues of the matrix of the quadratic form R_{XY} resulting from the expansion of the effective action (13) in terms of fluctuations about the saddle-point value. Specifically,

$$R_{XY} = \delta^2\mathcal{L}[\boldsymbol{\varphi},\mathbf{Q}]/(\delta X\,\delta Y)|_{X=X_0,Y=Y_0} \tag{21}$$

where X, $Y = \varphi_a(t)$, $Q^{\alpha\beta}(t,t')$ and $\alpha,\beta = 1,2$; $a = x,y,z$. Owing to the symmetry

involved in determining the glass phase stability boundary, one has to consider the fluctuations in the Q-field sector of the matrix (21). Furthermore, since

$$\mathcal{L}[\boldsymbol{\varphi}_0, \mathbf{Q}_0 + \delta\mathbf{Q}] - \mathcal{L}[\boldsymbol{\varphi}_0, \mathbf{Q}_0]$$
$$= \mathrm{Tr}[\delta\mathbf{Q}\delta\mathbf{Q} - (4V)^2\, \delta\mathbf{Q}\mathbf{G}_\tau(z)\, \delta\mathbf{Q}\mathbf{G}_\tau(z)]_2 + \mathrm{O}((\delta\mathbf{Q})^3) \tag{22}$$

where $G_\tau^{\alpha\beta}(z) = \varepsilon_\alpha \varepsilon_\beta G^{\alpha\beta}(z)$ is the thermofield causal Green function with the Gaussian noise component which acts as a random longitudinal static field to generate time-persistent autocorrelations (cf Kopeć *et al* 1989) and

$$[\ldots]_z = \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{(2\pi)^{1/2}} \exp\left(-\frac{z^2}{2}\right) \ldots . \tag{23}$$

Furthermore, the Fourier-transformed Green function reads

$$G^{\alpha\beta}(\omega, z) = [\![\boldsymbol{\Sigma}(\omega, z)\{1/[1 - VQ_\tau(\omega, z)\boldsymbol{\Sigma}(\omega, z)]\}]\!]^{\alpha\beta} \tag{24}$$

where $Q_\tau^{\alpha\beta} = \varepsilon_\alpha \varepsilon_\beta Q^{\alpha\beta}$. Working out terms quadratic in fluctuations in equation (22), one finally obtains the stability condition in the form

$$1 - (4V)^2 \int_{-\infty}^{+\infty} \frac{\mathrm{d}z}{(2\pi)^{1/2}} \exp\left(-\frac{z^2}{2}\right) K_{zz}^2(z) \geqslant 0 \tag{25}$$

where

$$K_{zz}(z) = \tfrac{1}{2}[(2J\Delta)^2/\theta^3(z)] \tanh[\beta\theta(z)/2]$$
$$+ \tfrac{1}{4}[(\mu + 4Vzq^{1/2})/\theta(z)]^2 \operatorname{sech}^2[\beta\theta(z)/2]. \tag{26}$$

Equations (25) and (26) constitute an analogue of the AT stability condition. For $n_b = \frac{1}{2}$ ($\mu = 0$), approaching from the high-temperature phase, one obtains $q = 0$ as the solution of equation (19). Above the glass freezing temperature this solution is stable but below this temperature the solution is unstable and so must be rejected. In fact, below the glass freezing temperature the solution with $q \neq 0$, as happens for $n_b \neq \frac{1}{2}$, also shows regions of instability as follows from the inequality (25). In order to single out these regions, one has to solve equations (19) and (20) self-consistently by observing equation (25) as a constraint superimposed on the solution for the order parameters.

For arbitrary band filling n_b the numerical solution of equations (19), (20) and (25) for the order parameters Δ and q gives the phase diagrams depicted in figures 1–4, where the following phases emerge.

(i) Normal conducting (N) phase. This does not exhibit glassy behaviour (stable in the sense of the criterion (25)).

(ii) Superconducting (SC) phase. The local electron pairs exhibit phase coherence (long-range order characterised by the non-vanishing parameter Δ).

(iii) Superconducting glass (SCG) phase. In this case, both the off-diagonal long-range superconducting order parameter and the diagonal glass order parameter q are predicted to coexist. In the case of non-half-filled band the glassy phase has to be determined via the stability condition (25) where the glassy phase occurs in the regions of instability of the solution for Δ and q. Here, the system possesses global phase coherence; however, owing to the inherent instability the system of local pairs is stuck in a particular configuration in phase space and cannot easily relax into another configuration, implying hysteresis and as is typical for glasses non-ergodic behaviour.

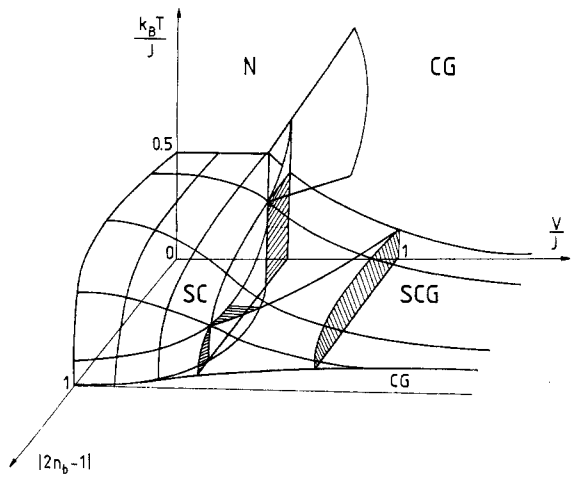

Figure 1. Phase diagram of the system in parameter space: the temperature k_BT, band-filling number n_b and degree of V disorder.

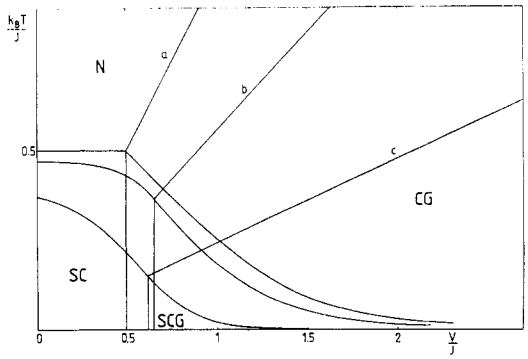

Figure 2. V–T phase diagram for several values of band-filling parameter n_b: line a, 0.5; line b, 0.7; line c, 0.9.

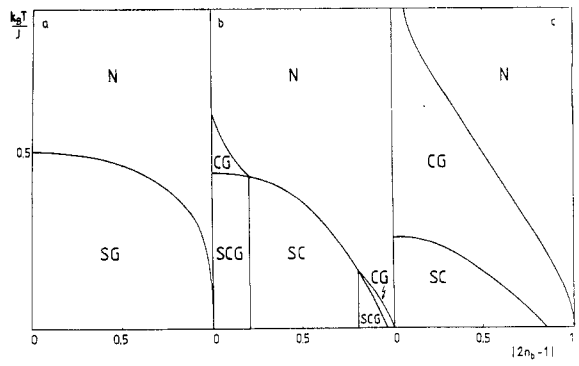

Figure 3. T–n_b phase diagram for different values of the reduced variance of the Gaussian distribution V/J: (*a*) 0; (*b*) 0.6; (*c*) 1.

Because of the non-vanishing superconducting order parameter Δ the SCG phase is predicted to be in the Meissner state.

(iv) Charge glass (CG) phase. Here, $\Delta = 0$ but the system exhibits instabilities as in (iii). In this state the global phase coherence is suppressed but glassy features are present.

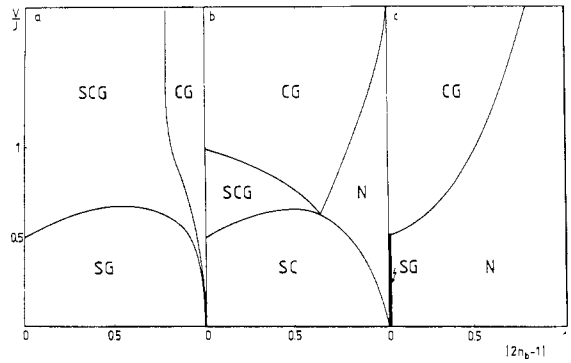

Figure 4. V–n_b phase diagram for different values of the reduced temperature k_BT/J: (*a*) 0; (*b*) 0.25; (*c*) 0.5.

The presented phase diagrams were obtained for a Gaussian distribution of random inter-site Coulomb energies. Of interest are other distributions of V_{ij} such as the Gaussian distribution with a non-vanishing mean which opens the possibility, in addition to the phases presented in (i)–(iv), that the charge disproportionation phase is a kind of state with modulated charge density.

4. Concluding remarks

In this paper we have attempted to understand the problem of disorder and glassy behaviour in a system of strongly correlated electrons described by the extended Hubbard model with negative on-site Coulomb energy—from knowledge of the conventional spin-glass problem. In particular, the system under study maps onto a pseudo-spin Heisenberg model with random interactions with conserved longitudinal 'magnetisation' as a consequence of fixed band filling. The transverse 'magnetisation', in turn, refers to the long-range off-diagonal superconducting order parameter due to the negative Coulomb energy. In close analogy to the magnetic systems the glass order parameter can be introduced and by using the analogy between the chemical potential and longitudinal 'magnetic field' the stability criteria follows in a similar way to the well known AT analysis. However, to include the effect of the real magnetic field in the system, one has to couple the electromagnetic vector potential to the kinetic term in the Hamiltonian (1) in a gauge-invariant manner which would enable one to single out the superconducting glass phase boundary as a function of the external applied magnetic field. We hope to return to this question in future work.

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