Screening effects in superconductors

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Abstract

The partition function of the Hubbard model with local attraction and long-range Coulomb repulsion between electrons is written as a functional integral with an action A involving a pairing field Δ and a local potential V. After integration over V and over fluctuations in $|\Delta|^2$, the final form of A involves a Josephson coupling between the local phases of Δ and a "kinetic energy" term, representing the screened Coulomb interaction between charge fluctuations. The competition between Josephson coupling and charging energy allows to understand the relation between T_C and composition in high-T_C materials, in particular superlattices, alloys and bulk systems of low doping.

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We start with a Hamiltonian describing charge carriers (electrons or holes) on a lattice, subject to an on-site attraction, $-U$, and the long-range Coulomb repulsion, $e^2 V_C$, acting on particles on different sites:

$$H = H_0 + H_U + H_C, \tag{1a}$$

$$H_0 = \sum_{\langle l,l'\rangle} \sum_\sigma t c_{l,\sigma}^+ c_{l',\sigma} - \mu \sum_l N_l, \tag{1b}$$

$$H_U = -\frac{U}{2} \sum_{l,\sigma} c_{l,\sigma}^+ c_{l,\sigma} c_{l,-\sigma}^+ c_{l,-\sigma}, \tag{1c}$$

$$H_C = \frac{1}{2} \sum_{l \neq l'} (N_l - n_0) e^2 V_C(l,l')(N_{l'} - n_0) \tag{1d}$$

Here $c_{l,\sigma}^+ (c_{l,\sigma})$ are creation (annihilation) operators for charge carriers with spin σ at lattice site l, $\langle l, l'\rangle$ denotes pairs of nearest-neighbor sites, μ is the chemical potential, n_0 the background, neutralizing

the density of charge carriers, and $N_l = \sum_\sigma c_{l,\sigma}^+ c_{l,\sigma}$. The partition function can be written as a functional integral by means of two successive Stratonovich–Hubbard transformations [1, 2], decoupling the two interaction terms in H with the help of a complex field Δ and a real field V:

$$Z = \mathrm{Tr}\, e^{-\beta H} = \int D^2\Delta \int DV\, \mathrm{Tr}\, e^{-\beta H_0}$$

$$\times T \exp\left\{ -i \int_0^{-i\beta} d\tau\, [\tilde{H}(\Delta, V, \tau) + \varepsilon(\Delta, V, \tau)] \right\}, \tag{2}$$

$$\tilde{H}(\Delta, V, \tau) = \sum_l [\Delta^*(l,\tau) c_{l,\uparrow} c_{l,\downarrow} + \mathrm{h.c.}$$

$$+ iV(l,\tau)(N_l(\tau) - n_0)], \tag{3a}$$

$$\varepsilon(\Delta, V, \tau) = \frac{1}{U} \sum_l |\Delta(l,\tau)^2| + \frac{1}{2e^2}$$

$$\times \sum_{l \neq l'} V(l,\tau) V_C^{-1}(l,l') V(l',\tau). \tag{3b}$$

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We then evaluate the trace over the electronic degrees of freedom

$$\operatorname{Tr} e^{-\beta H_0} T \exp\left\{-i \int_0^{-i\beta} d\tau \left[\tilde{H}(\Delta, V, \tau)\right.\right.$$

$$\left.\left. + \varepsilon(\Delta, V, \tau)\right]\right\} \equiv \exp\left\{-i \int_0^{i\beta} d\tau \, F(\Delta, V, \tau)\right\} \quad (4)$$

and we expand the "free energy" F up to fourth order in Δ and to second order in V and up to leading terms in space and time gradients of the two fields:

$$F = F_0 + F_{\Delta, V} \quad (5a)$$

$$F_{\Delta, V}(\tau) = \sum_l \left[a|\Delta(l, \tau)|^2 - id\Delta^*(l, \tau) \right.$$

$$\times \left(\frac{\partial}{\partial \tau} - 2V(l, \tau)\right)\Delta(l, \tau)\right]$$

$$+ c \sum_{\langle l, l' \rangle} |\Delta(l, \tau) - \Delta(l', \tau)|^2$$

$$+ i \sum_l V(l, \tau)(\langle N_l \rangle - n_0)$$

$$+ \frac{1}{2e^2} \sum_{l, l'} V(l, \tau) V_{sc}^{-1}(l, l') V(l', \tau)$$

$$+ b \sum_l |\Delta(l, \tau)|^4. \quad (5b)$$

Here the coefficients a, b, c, d, are related to the free-electron particle–particle propagator [1–5], F_0 is the free-electron contribution, and $V_{sc}^{-1}(l, l') = V_C^{-1}(l, l') + \chi_0(l, l')$ is the screened Coulomb potential (approximated by its static limit) with $\chi_0(l, l')$ being the electronic polarizability. Integrating over the electric potential V yields

$$F_\Delta(\tau) = \sum_l \left[a|\Delta(l, \tau)|^2 + b|\Delta(l, \tau)|^4 \right.$$

$$\left. - id\Delta^*(l, \tau)\frac{\partial \Delta(l, \tau)}{\partial \tau} \right]$$

$$+ c \sum_{\langle l, l' \rangle} |\Delta(l, \tau) - \Delta(l', \tau)|^2$$

$$+ \frac{1}{2e^2} \sum_{l, l'} \rho(l, \tau) V_{sc}(l, l') \rho(l', \tau), \quad (6)$$

where $\rho(l, \tau) = 2d|\Delta(l, \tau)|^2 + \langle N_l \rangle - n_0$ represents charge density fluctuations. Next we introduce amplitude and phase of Δ. In the following, we assume to be in a relatively strong coupling regime ($t \ll U$) in which fermions bind into on-site singlet pairs at a temperature of the order of the mean field transition temperature T_{mf}, well above the superconducting phase transition, the latter being finally triggered by the onset of phase order [6–8]. Below T_{mf}, $a < 0$, so that the average amplitude has a non-vanishing mean value Δ_0 given by $a + 2b\Delta_0^2 = 0$. Charge neutrality implies $2d\Delta_0^2 + \langle N_l \rangle - n_0 = 0$ and, for $t \ll U$ [1, 3–5, 9]:

$$c = \frac{2t^2}{U^3}, \qquad d = \frac{1}{U^2}, \quad (7a)$$

$$\Delta_0^2 = \tfrac{1}{4} n_0 (2 - n_0) U^2 \approx \tfrac{1}{2} n_0 U^2 \quad \text{for } n_0 \ll 1. \quad (7b)$$

Splitting the number of pairs at a given site into $|\Delta(l, \tau)|^2 = \Delta_0^2 + \tfrac{1}{2} U^2 \delta n_p(l, \tau)$, we integrate over $\delta n_p(l, \tau)$ which (neglecting gradient terms) yields a free energy functional for phase fluctuations only:

$$F_\Theta(\tau) = J \sum_{\langle l, l' \rangle} [1 - \cos(\Theta(l, \tau) - \Theta(l', \tau))]$$

$$+ \frac{n_0}{2} \sum_l \frac{\partial \Theta(l, \tau)}{\partial \tau} - \frac{1}{2} \sum_{l, l'} \frac{\partial \Theta(l, \tau)}{\partial \tau}$$

$$\times \frac{1}{(2e)^2} W^{-1}(l, l') \frac{\partial \Theta(l', \tau)}{\partial \tau} \quad (8a)$$

with the Josephson coupling [1, 9] $J = 2c\Delta_0^2 = 2n_0(t^2/U)$, and

$$W(l, l') = \begin{cases} V_{sc}(l, l'), & l \neq l', \\ (2e)^2 b/d^2, & l = l' \end{cases}. \quad (8b)$$

Our expansion of F in powers of Δ has yielded the on-site repulsion $(2e)^2 b/d^2$ between pairs. However, due to the exclusion principle, two pairs cannot really sit on the same lattice site. Thus, in the following, we exclude $l = l'$ in the last term of (8a). By going from the "phase velocities" $(\partial \Theta(l, \tau)/\partial \tau)$ to the conjugate momenta $p(l, \tau)$ we end up with the partition function of the Hamiltonian [10]

$$H = \frac{1}{2} \sum_{l, l'} \left(p(l) - \frac{n_0}{2}\right) [(2e)^2 W(l, l')]$$

$$\times \left(p(l') - \frac{n_0}{2}\right) + J \sum_{\langle l, l' \rangle} [1 - \cos(\Theta(l) - \Theta(l'))]. \quad (9)$$

Hamiltonian (9) describes the relevant physics of short coherence length superconductors in terms of Josephson coupled spatial phase variations and "charge fluctuations" coupled by the screened Coulomb interaction. It is also the "phase-only" representation of the Hamiltonian of interacting bosons [10–12]. Its critical behavior, in particular the influence of the "background", $-\frac{1}{2}n_0$, has been studied in these references. Here, we apply expression (9) to calculate the transition temperature of strongly anisotropic superconductors, such as superlattices and bulk systems in the underdoped regime [13]. We make the following approximations: (i) H is restricted to one superconducting layer; (ii) the screened Coulomb interaction, which takes into account the electric coupling between layers, is modelled by a Yukawa-form, with a Thomas–Fermi screening length λ_{TF}, depending on the density n_0 of charge carriers according to the well-known formula

$$\lambda_{TF}^{-1} = \frac{1}{2\pi}\frac{2.95}{\sqrt{r_s/a_0}}\ [\mathring{A}^{-1}],$$

where $r_s = (3/(4\pi n_0))^{1/3}$ and a_0 is the Bohr radius; (iii) considering only $n_0 \ll 1$, the "background shift", $-\frac{1}{2}n_0$, in the first term of (9) is neglected. We make connection with previous work [14, 15] by mapping (9) onto a "capacity model":

$$\frac{1}{2}\sum_{l,l'} p(l)[(2e)^2 W(l, l')]p(l') \approx \frac{(2e)^2}{2C}\sum_l p(l)^2, \qquad (10)$$

with

$$\frac{1}{2C} = \frac{1}{e^2}\sum_{l=0} W(l, 0) = \frac{2\pi\lambda_{TF}}{\varepsilon a_L^2}\,e^{-a_L/\lambda_{TF}}.$$

This is the XY-model with kinetic energy [14, 15], ε being the dielectric constant of the interlayer material and a_L the lattice constant. In Ref. [14] the critical temperature in two dimensions was evaluated in the "self-consistent harmonic approximation" (SCHA) which gives results in good agreement with Monte Carlo simulations [16]. A good overall fit of the numerical SCHA result is [17] $T_C(\alpha) \approx T_C(0)\sqrt{1 - \alpha/\alpha_C}$ where $\alpha = (2e)^2/(2CJ)$ is the ratio between charging and Josephson energy. When α approches $\alpha_C = 6.2$, T_C goes to zero. This approach has been successfully applied [14, 15] to

calculating the superconducting transition temperature for superlattices and for alloys by determining the appropriate effective capacity through electrostatic considerations.

We finally use Hamiltonian (9) to find T_C as a function of doping for high-T_C superconductors in the underdoped regime. For $YBa_2Cu_3O_7$, our "capacity model" has allowed to fit the T_C variation of both, superlattices and alloys, in a coherent way, using SCHA [14, 15] for $J = 120$ K at optimal doping ($n_0 \approx 0.16$ of holes per cell [13]). Below optimal doping, the ratio α increases when the number n_0 of charge carriers is reduced: the n_0 dependence of J is given following Eq. (8a) and C varies with n_0 through the screening length λ_{TF}. Using the above expression for $T_C(\alpha)$, with doping-dependent J and C, we then find that T_C should be zero for $n_0 \approx 0.07$, in good agreement with the measured phase diagram [13]. This shows that the phase boundary in the underdoped regime can be understood in terms of Bose–Einstein condensation of preformed pairs, T_C being suppressed by phase fluctuations when the minimum doping is approached.

In summary, starting from the attractive Hubbard model with long-range Coulomb repulsion, we have given a microscopic derivation of a description of short coherence length superconductors in terms of the superconducting phase, the Hamiltonian for which includes a "charging energy" and a Josephson coupling. This is a microscopic justification of such a Hamiltonian, which has been used previously [14, 15] in calculating T_C for superlattices and alloys and also allows understanding the phase boundary of bulk oxides in the underdoped regime.

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