UC Davis

UC Davis Previously Published Works

Title

High temperature superconductivity with repulsive pairing interactions

Permalink

<https://escholarship.org/uc/item/22c5g25t>

Authors

Fink, HJ

Haley, SB

Publication Date

2015-07-27

DOI

10.1016/j.physc.2015.07.003

Peer reviewed

See discussions, stats, and author profiles for this publication at: <http://www.researchgate.net/publication/280531845>

High temperature superconductivity with repulsive pairing interactions

ARTICLE · JULY 2015

DOI: 10.1016/j.physc.2015.07.003

READS

8

2 AUTHORS, INCLUDING:

[Herman J Fink](#)

University of California, Davis

109 PUBLICATIONS **845** CITATIONS

SEE PROFILE

High temperature superconductivity with repulsive pairing interactions

Herman J. Fink*, Stephen B. Haley

Department of Electrical and Computer Engineering, University of California, Davis, CA 95616, USA

ARTICLE INFO

Article history:

Received 24 June 2015

Accepted 7 July 2015

Available online 14 July 2015

Keywords:

High T_c

Non-separable pairing kernels

Repulsive electron pairing

ABSTRACT

A pairing Hamiltonian $H(\Gamma)$ with an interaction kernel Γ characterized by $[-\Gamma_0, -\alpha_0]$, where Γ_0 denotes the separable part and α_0 the degree of non-separability, produces high temperature superconductivity for both attractive $\Gamma_0 > 0$ and repulsive $\Gamma_0 < 0$ when $\alpha_0 > 0$. For $\Gamma_0 > 0$, typical HTS properties, e.g. cuprate, are produced. Repulsive $\Gamma_0 < 0$ produces a distinct difference in the kinetic energy dependence of the SC gap, significantly altering thermodynamic properties.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

High T_c superconducting (HTS) materials, particularly the cuprates [1], are a subject of extensive experimental and theoretical studies. Although it is established that Bardeen–Cooper–Schrieffer (BCS) [2] pairs $c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$ form in cuprates, the exact nature of the HTS pairing interaction remains an open question.

In Ref. [3] we presented a doping x and temperature T dependent theory that predicts many observed properties of cuprates in the SC and normal states. The non-separability of the pairing interaction kernel $\Gamma(x, T)$, and the chemical potential $\mu(x)$ are essential elements of the theory. Thermodynamic properties were studied for the case of strictly attractive pairing interactions characterized by energy scaled interaction parameters $\gamma > 0$ and $\alpha > 0$, where γ denotes the separable part of the kernel and α the degree of non-separability.

In this paper it is shown that HTS is also possible for interactions with a repulsive $\gamma < 0$. However, the SC gap, the quasi-particle energy, and the resultant thermodynamic properties are distinctly different from the attractive $\gamma > 0$ case. Changing γ from positive to negative values causes a temperature dependent reduction in the number of accessible SC states. Consequently the SC to normal state phase transition changes from second order (SOPT) to first order (FOPT), and the entropy decreases near T_c .

2. Pairing Hamiltonian: non-separable interaction kernel

It is consistent with observation that in the SC state BCS pairs $c_{-\mathbf{k}\downarrow}c_{\mathbf{k}\uparrow}$ form in HTS materials [4–7]. In the absence of transport

currents, general four fermion operator interaction Hamiltonians are reasonably reduced to include only interactions between BCS pairs [8]. Accordingly, our starting point for SC state is the “reduced” Hamiltonian,

$$\begin{aligned} H &= H_{kin} + H_{int}, \\ H_{kin} &= \sum_{\mathbf{k}} \epsilon_{\mathbf{k}} [c_{\mathbf{k}}^\dagger c_{\mathbf{k}} + c_{-\mathbf{k}}^\dagger c_{-\mathbf{k}}], \\ H_{int}(\Gamma) &= \sum_{\mathbf{k}\mathbf{k}'} \Gamma_{\mathbf{k}\mathbf{k}'} p_{\mathbf{k}}^\dagger p_{\mathbf{k}'}, \quad p_{\mathbf{k}} = c_{-\mathbf{k}} c_{\mathbf{k}}, \end{aligned} \quad (1)$$

where $p_{\mathbf{k}}$ is the pair annihilation operator. Fixed spins are implicitly indicated by $\pm \mathbf{k} \equiv \mathbf{k} \uparrow, -\mathbf{k} \downarrow$. The single particle energies, referenced to the chemical potential μ , are $\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$.

The mean field (MF) approximation for the Hamiltonian in Eq. (1) is

$$H_{int} = - \sum_{\mathbf{k}} [\Delta_{\mathbf{k}}^* p_{\mathbf{k}} + \Delta_{\mathbf{k}} p_{\mathbf{k}}^\dagger - \Delta_{\mathbf{k}} \langle p_{\mathbf{k}}^\dagger \rangle], \quad (2)$$

where $\Delta_{\mathbf{k}}$ is defined by

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} \Gamma_{\mathbf{k}\mathbf{k}'} \langle p_{\mathbf{k}'} \rangle. \quad (3)$$

Applying a Bogoliubov–Valatin canonical transformation, detailed in Ref. [3], diagonalizes the MF Hamiltonian in the form

$$\begin{aligned} H &= - \sum_{\mathbf{k}} E_{\mathbf{k}} (1 - n_{\mathbf{k}} - q_{\mathbf{k}}) + H_0 \\ H_0 &= \sum_{\mathbf{k}} [\epsilon_{\mathbf{k}} + \Delta_{\mathbf{k}} \langle p_{\mathbf{k}} \rangle^*] \end{aligned} \quad (4)$$

$$E_{\mathbf{k}} = \sqrt{\epsilon_{\mathbf{k}}^2 + |\Delta_{\mathbf{k}}|^2}, \quad \langle p_{\mathbf{k}} \rangle = \frac{1}{2} \frac{\Delta_{\mathbf{k}}}{E_{\mathbf{k}}} (1 - 2\langle n_{\mathbf{k}} \rangle).$$

* Corresponding author.

E-mail addresses: hjfink@ucdavis.edu (H.J. Fink), profisbh@gmail.com (S.B. Haley).

The $n_{\mathbf{k}}$ and $q_{\mathbf{k}}$ are quasi-particle number operators with corresponding energy $E_{\mathbf{k}}$. The partition function $Z = \text{Tr}[\exp(-\beta H)]$, using Eq. (4), gives the MF thermal averages $\langle n_{\mathbf{k}} \rangle = \langle q_{\mathbf{k}} \rangle = f(E_{\mathbf{k}}) = [\exp(\beta E_{\mathbf{k}}) + 1]^{-1}$, with $\beta = 1/(k_B T)$. Subsequently, non-interacting quasi-particle thermodynamic functions, e.g. thermodynamic potential Ω (free energy), average internal energy $\mathcal{U} = \langle H \rangle$, and entropy S are obtained in the forms listed in Ref. [3]. The corresponding MF expression for $\langle p_{\mathbf{k}} \rangle$ from Eq. (4) formulates Eq. (3) as a self-consistent sum equation

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \Gamma_{\mathbf{k}\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} \tanh(\beta E_{\mathbf{k}'}/2) \quad (5)$$

that determines the gap in the quasi-particle energy.

2.1. Interaction kernel

The $\mathbf{k}$ dependent symmetry of the pairing interaction kernel $\Gamma_{\mathbf{k}\mathbf{k}'}$ effects the gap symmetry which is corroborated by many experiments on cuprates, indicating a $d_{x^2-y^2}$ -wave gap $\Delta_{\mathbf{k}} \propto \cos(k_x) - \cos(k_y)$ [7,9,10]. Although a d-wave gap accounts for some $\mathbf{k}$ dependent observed HTS properties, symmetry factors do not account for the large gaps and critical temperatures in cuprate HTS [10], nor do they significantly effect thermodynamic properties that represent $\mathbf{k}$ – space averages.

Pairing interaction kernels are generally non-separable, resulting in a very complicated gap Eq. (5). A common approximation, introduced by BCS [2] is $\Gamma_{\mathbf{k}\mathbf{k}'} \approx -\Gamma_0$ [5,11]. Another approximation is separable kernel factorization, $\Gamma_{\mathbf{k}\mathbf{k}'} \approx -\Gamma_0 \psi_{\mathbf{k}} \psi_{\mathbf{k}'}$, where $\psi_{\mathbf{k}}$ characterizes the symmetry [12]. Neither of these approximations leads to HTS without assuming an unrealistically strong interaction constant Γ_0 .

In pursuit of a mechanism for HTS we consider a $\mathbf{k}$ -space root-mean-square (rms) approximation for a non-separable Γ . The rms approximation is necessary for interactions with odd symmetry, e.g. d-wave, which has a zero $\mathbf{k}$ -space average. As formulated in Ref. [3], $\Gamma = V + U$, with V separable, and U non-separable. Here we use an analogous decomposition for Γ , but denote $-V_0$ as the rms value of the matrix elements of V , and $-U_0$ and $-U_{00}$ as the rms values of the off-diagonal and diagonal elements of U , respectively. The matrix elements of the pairing interaction kernel assume the form

$$\Gamma_{\mathbf{k}\mathbf{k}'} = -\Gamma_0 - 2\alpha_0 \delta_{\mathbf{k}\mathbf{k}'}, \quad (6)$$

where

$$\Gamma_0 = V_0 + U_0, \quad 2\alpha_0 = U_{00} - U_0. \quad (7)$$

The sign convention here is that positive interaction constants are attractive and negative ones are repulsive. Note that although there are three interaction constants V_0, U_0, U_{00} , the net pairing interaction depends only on the reduced parameter set $[\Gamma_0, \alpha_0]$. Thus there is some flexibility in formulating the independent parameters Γ_0 and α_0 . For example, a repulsive $V_0 < 0$ with $|V_0| > U_0 > 0$ gives a repulsive $\Gamma_0 < 0$ with no effect on α_0 . On the other hand, a repulsive U interaction, which can give a repulsive Γ_0 , requires $|U_0| > |U_{00}|$ to maintain $\alpha_0 > 0$. Although there are other combinations of non-separable interactions resulting in the approximate two parameter $[\Gamma_0, \alpha_0]$ model, the form in Eq. (7) is sufficiently general to manifest features distinguishing repulsive from attractive pairing interactions.

Using the kernel of Eq. (6) in Eq. (5) gives

$$\left[1 - \frac{\alpha_0}{E_{\mathbf{k}}} \tanh(\beta E_{\mathbf{k}}/2)\right] \Delta(\varepsilon_{\mathbf{k}}, T) = \delta(T), \quad (8)$$

where

$$\delta(T) = \frac{\Gamma_0}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} \tanh(\beta E_{\mathbf{k}'}/2). \quad (9)$$

Noting from Eq. (8) that the only $\mathbf{k}$ -dependence of the gap is via the kinetic energy in $E_{\mathbf{k}}$, the $\Delta_{\mathbf{k}}$ will be replaced by the detailed notation $\Delta(\varepsilon_{\mathbf{k}}, T)$ where necessary for clarity. Eliminating δ by substituting $\Delta_{\mathbf{k}}$ from Eq. (8) into the summand in Eq. (9) gives

$$\sum_{\mathbf{k}} \frac{\tanh(\beta E_{\mathbf{k}}/2)}{E_{\mathbf{k}} - \alpha_0 \tanh(\beta E_{\mathbf{k}}/2)} = \frac{2}{\Gamma_0}. \quad (10)$$

In general, with $\alpha_0 \neq 0$ and $\Gamma_0 \neq 0$, the coupled Eqs. (8) and (9), or alternatively (8) and (10), must be solved self-consistently to determine the SC gap $\Delta_{\mathbf{k}}$ as a function of kinetic energy $\varepsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}} - \mu$, and the parameter $\delta(T)$ for each value of T and interaction parameter set $[\Gamma_0, \alpha_0]$. The value of $\Delta_{\mathbf{k}}$ obtained corresponds to the minimum free energy (see Appendix B in Ref. [3]).

Simplification occurs in two cases. In the separable kernel case, $\alpha_0 = 0, \Gamma_0 > 0$, it follows from Eq. (8) that $\Delta_{\mathbf{k}} = \delta(T)$ is determined by Eq. (10). This is the standard BCS gap that is an exponentially small function of Γ_0 [2,5]. In the special non-separable case $\alpha_0 > 0$ and $\Gamma_0 = \delta = 0$, Eq. (8) reduces for $\Delta_{\mathbf{k}} \neq 0$ to the form

$$\sigma(T) = \tanh\left(\frac{T_C}{T} \sigma\right), \quad \sigma = \frac{E}{\alpha_0}, \quad T_C = \frac{\alpha_0}{2k_B}. \quad (11)$$

Since $\Delta_{\mathbf{k}}$ is not explicit in Eq. (11), the quasi-particle energy $E_{\mathbf{k}} = E(T)$ is independent of $\mathbf{k}$. An exact correspondence exists between Eq. (11) and the molecular field equation for spontaneous magnetization in spin 1/2 ferromagnets, where the Brillouin function is $B_{1/2}(x) = \tanh(x)$ [11]. Setting $\sigma = M(T)/M(0)$, where $M(T)$ is the magnetization, and setting $\alpha_0 = J$, where J is the total exchange energy per unit cell, Eq. (11) is identical to the molecular field equation.

From the definition of $E_{\mathbf{k}}$ the gap is given by

$$\Delta(\varepsilon_{\mathbf{k}}, T) = \sqrt{E^2(T) - \varepsilon_{\mathbf{k}}^2}, \quad (12)$$

where $E(T)$ is obtained from the solution of Eq. (11). Its value varies from $E(0) = \alpha_0$ to $E(T_C) = 0$. At $T = 0$ the gap $\Delta(\varepsilon_{\mathbf{k}}, T)$ has a maximum value α_0 on the Fermi surface, and zero value on the surfaces $\varepsilon_{\mathbf{k}} = \mu \pm \alpha_0$. As T increases $E(T)$ decreases, shrinking the range of $\varepsilon_{\mathbf{k}}$. At T_C only electrons on the Fermi surface contribute to the SC state.

In the general case, $\alpha_0 \neq 0, \Gamma_0 \neq 0$, determination of $\Delta_{\mathbf{k}}$ requires extensive numerical computation. Nevertheless, considerable information can be extracted analytically. From Eq. (8)

$$\Delta(\varepsilon_{\mathbf{k}} = 0, 0) = \alpha_0 + \delta(0). \quad (13)$$

Below it is proven that $\Delta(\varepsilon_{\mathbf{k}} = 0, 0)$ given by Eq. (13) is the maximum gap for both positive and negative δ ; whereas the corresponding quasi-particle energy $E_{\mathbf{k}}$ at the Fermi surface is minimum for $\delta > 0$ and maximum for $\delta < 0$. Noting from Eq. (9) that $\text{sign}(\delta) = \text{sign}(\Gamma_0)$, it follows that a positive(negative) δ corresponds to an attractive(repulsive) Γ_0 , respectively.

From Eq. (8) one obtains the following derivatives for $\Delta_{\mathbf{k}} \equiv \Delta(\varepsilon_{\mathbf{k}}, T)$ and $E(\varepsilon_{\mathbf{k}}, T)$ at $T = 0$:

$$\begin{aligned} \frac{d\Delta_{\mathbf{k}}}{d\varepsilon_{\mathbf{k}}} &= -\frac{\alpha_0 \varepsilon_{\mathbf{k}} \Delta_{\mathbf{k}}}{E_{\mathbf{k}}^3 - \alpha_0 \varepsilon_{\mathbf{k}}^2}, & \frac{d^2 \Delta_{\mathbf{k}}}{d^2 \varepsilon_{\mathbf{k}}} &= -\frac{\alpha_0}{|\Delta_{\mathbf{k}}|^2}, \\ \frac{dE_{\mathbf{k}}}{d\varepsilon_{\mathbf{k}}} &= \frac{\varepsilon_{\mathbf{k}} E_{\mathbf{k}} (E_{\mathbf{k}} - \alpha_0)}{E_{\mathbf{k}}^3 - \alpha_0 \varepsilon_{\mathbf{k}}^2}, & \frac{d^2 E_{\mathbf{k}}}{d^2 \varepsilon_{\mathbf{k}}} &= \frac{\delta}{|\Delta_{\mathbf{k}}|^2}, \end{aligned} \quad (14)$$

where the second derivatives are evaluated at $\varepsilon_{\mathbf{k}} = 0$, for $|\Delta_{\mathbf{k}}| \neq 0$. The distinct difference in the gap solutions for attractive $\Gamma_0 > 0$ and repulsive $\Gamma < 0$ are manifest in Eq. (14).

For $\delta > 0$, it follows from Eq. (8) and the definition of $E_{\mathbf{k}}$ that $E_{\mathbf{k}} > \alpha_0$ and the denominator $E_{\mathbf{k}}^3 - \alpha_0 \varepsilon_{\mathbf{k}}^2 > 0$ for all values of $\varepsilon_{\mathbf{k}}$. It

follows from Eq. (14) that the solutions $\Delta(\varepsilon_{\mathbf{k}}, 0)$ form unrestricted open contours, with a maximum on the Fermi surface $\varepsilon_{\mathbf{k}} = \varepsilon_{\mathbf{k}} - \mu = 0$. The asymptotic value $\Delta(\varepsilon_{\mathbf{k}} \rightarrow \infty, 0) = \delta$. For $\delta > 0$, Eq. (14) shows that the quasi-particle energy $E(\varepsilon_{\mathbf{k}} = 0, 0)$ is minimum for $\Gamma_0 > 0$. Hence, the kinetic energy increases faster than the gap decreases.

For $\delta < 0$, the quasi-particle energy $E_{\mathbf{k}} < \alpha_0$. This gives a pole in the derivatives of both $\Delta_{\mathbf{k}}$ and $E_{\mathbf{k}}$ for some value $|\varepsilon_{\mathbf{k}}|_0 = w_0$. These solutions form closed contours, with no solution for energies $|\varepsilon_{\mathbf{k}}| > w_0$. Using the pole equation, $E_{\mathbf{k}}^3 = \alpha_0 \varepsilon_{\mathbf{k}}^2$, Eq. (8) at $T = 0$ leads to

$$w_0 = [\alpha_0^{2/3} - |\delta|^{2/3}]^{3/2}, \quad (15)$$

$$\Delta_{\mathbf{k}|_0} = [|\delta| w_0^2]^{1/3}, \quad E_{\mathbf{k}|_0} = [\alpha_0 w_0^2]^{1/3}.$$

Eq. (15) gives the boundary values for the solutions with $\delta < 0$ corresponding to repulsive $\Gamma_0 < 0$. Solutions exist between the surfaces $\varepsilon_{\mathbf{k}0} = \mu \pm w_0(\alpha_0, \Gamma_0)$. Thus w_0 is the half-width of the SC region at $T = 0$. At the Fermi surface the maximum gap is given by Eq. (13). For $T > 0$, it is expected from the $\delta = 0$ solution given above, and from inspection of Eq. (8), that the bounding surfaces move toward the Fermi surface as T increases, i.e. the accessible SC $\mathbf{k}$ -space volume decreases from its $T = 0$ value.

For $\delta < 0$, Eq. (14) shows that the quasi-particle energy $E(\varepsilon_{\mathbf{k}}, 0)$ is maximum on the Fermi surface, given by $E(\varepsilon_{\mathbf{k}} = 0, 0) = \Delta_{\max} = \alpha_0 - |\delta|$. Thus, in the repulsive case the gap decreases faster than the kinetic energy increases.

For $\delta < 0$ there is also a small gap solution of the form $|\Delta_{\mathbf{k}}| \approx |\varepsilon_{\mathbf{k}}| |\delta| / \alpha_0$ near the Fermi surface. Since the free energy corresponding to the small gap is much higher than that of the large gap solution, the small gap solution has no physical consequence.

Detailed analysis of the gap $|\Delta_{\mathbf{k}}|$ depends on the form of the kinetic energy $\varepsilon_{\mathbf{k}}$, e.g. isotropic $\varepsilon_{\mathbf{k}} = \varepsilon_0 k^2$, tight binding $\varepsilon_{\mathbf{k}} = \varepsilon_0 [\cos(k_x) + \cos(k_y)]$, etc. Such functions determine the shape of the Fermi surface and the $\Gamma_0 < 0$ solution boundary surfaces. In the next section the distinct effects of $\Gamma_0 > 0$ versus $\Gamma_0 < 0$ are clearly illustrated using an isotropic approximation.

3. Isotropic approximation

Integrals are formulated from the $\mathbf{k}$ space sums using an isotropic approximation, replacing $\varepsilon_{\mathbf{k}}$ by its $\mathbf{k}$ -space angular average $\varepsilon = \langle \varepsilon_{\mathbf{k}} \rangle$. The density of states $N(\varepsilon)$ is approximated by its mean value N_0 over the integration range, defined below. It is convenient to introduce the following scaling of the physical functions:

$$\phi = \frac{\delta}{\varepsilon_m}, \quad \Phi = \frac{\langle \Delta(\varepsilon_{\mathbf{k}}) \rangle}{\varepsilon_m}, \quad Y = \sqrt{y^2 + \Phi^2}, \quad (16)$$

$$y = \frac{\varepsilon}{\varepsilon_m}, \quad t = \frac{T}{T_m}, \quad \varepsilon_m \equiv k_B T_m.$$

The scaled kinetic energy, relative to the Fermi level is the integration variable y and the scaled quasi-particle energy is Y .

Using the scaling in Eq. (16) the coupled Eqs. (8) and (9) assume the form

$$\left[1 - \frac{\alpha}{Y} \tanh(Y/2t)\right] \Phi(y, t) = \phi(t), \quad (17)$$

$$\frac{\gamma}{2} \int dy \frac{\Phi(y, t)}{Y(y, t)} \tanh(Y/2t) = \phi(t). \quad (18)$$

The constraint Eq. (10), in which the δ has been eliminated, has the scaled form

$$\int dy \frac{\tanh(Y/2t)}{Y - \alpha \tanh(Y/2t)} = \frac{2}{\gamma}. \quad (19)$$

The scaled material parameters, using Eq. (7), are

$$\gamma = \eta + v, \quad 2\alpha = (U_{00} - U_0)/\varepsilon_m, \quad (20)$$

$$\eta = N_0 V_0, \quad v = N_0 U_0.$$

The pairing interaction constants that ultimately determine all functions in the SC state are $[\gamma, \alpha]$. The value of γ is constrained in cuprates by the relatively small density of states N_0 ; whereas the parameter α can be relatively large for small ε_m [3].

In accordance with the analysis in the previous section, the gap solutions $\Phi \propto \langle |\Delta| \rangle$ form unbounded open contours for $\gamma \propto \Gamma_0 > 0$, and closed contours for $\gamma < 0$. Thus the integration range $[y_1, y_2]$ is restricted. For $\gamma > 0$ we invoke a bandwidth limited kinetic energy cutoff $\pm \varepsilon_m$, with concomitant scaled integration range $[-1, 1]$ [3]. For $\gamma \leq 0$ the situation is more complicated. The scaled integration range $[-y_0(t), y_0(t)]$ is a function of temperature and the parameters $[\gamma, \alpha]$. The boundary value y_0 is obtained by considering the derivative of Eq. (17), which leads to

$$\frac{d\Phi}{dy} = \frac{-\alpha y \Phi^2 A(y, t)}{\phi(t) y^2 + B(y, t) \Phi(y, t)^3}, \quad (21)$$

$$A(y, t) = \frac{1}{Y} \tanh(Y/2t) - \frac{1}{2t} \cosh^{-2}(Y/2t),$$

$$B(y, t) = 1 - \frac{\alpha}{2t} \cosh^{-2}(Y/2t) \geq 0.$$

Noting from Eq. (18) that $\text{sign}(\phi) = \text{sign}(\gamma)$, Eq. (21) has a pole at $\phi(t) y_0^2 + B(y_0, t) \Phi(y_0, t)^3 = 0$ for repulsive $\gamma < 0$. The pole equation is an internally imposed boundary condition that a self-consistent solution set $[\Phi(y, t), \phi(t), y_0(t)]$ must satisfy.

The maximum gap occurs on the Fermi surface at $y = 0$. From Eq. (17) for $t = 0$ it is

$$\Phi(0, 0) = \alpha + \phi(0). \quad (22)$$

Eq. (22) is valid for values of the interaction parameters such that $\alpha + \phi(0) \geq 0$. It is evident that having all interactions attractive gives the largest gap $\Phi(0, 0) > \alpha > 0$; whereas a repulsive $\gamma < 0$ gives $\Phi(0, 0) < \alpha$. An important feature of Eq. (22) is the linear dependence of the gap on the interaction parameter α . This linearity is instrumental in explaining cuprate HTS for $\gamma > 0$ and $\alpha \gtrsim 0.1$ [3].

Below, numerical results based on solutions of the coupled Eqs. (17), (18) or (19), and the pole of Eq. (21) are illustrated, with the focus on the difference between the attractive and repulsive γ solutions. In all figures the non-separability parameter $\alpha = 0.25$.

The SC gap $\Phi(y, t = 0)$ is plotted in Fig. 1. The open contours correspond to attractive $\gamma > 0$ and the closed contours to repulsive

Fig. 1. The SC gap $\Phi(y, t = 0)$ is shown as a function of the scaled kinetic energy y , relative to the Fermi surface, for several values of $\phi(0)$ in the range $[-0.1, 0.1]$, corresponding to the interaction parameter γ in the much larger range $[-1.4, 0.2]$ shown in Fig. 2. The interaction parameter $\alpha = 0.25$ in all figures.

$\gamma < 0$. In the closed contours, only the upper parts, $\Phi(y) > \Phi(y_0)$, are physically relevant. The curve for $\gamma = \phi = 0$, given by

$$\Phi(y, 0) = \sqrt{\alpha^2 - y^2}, \quad (23)$$

separates the open from closed contour regions.

The relationship between the interaction parameter γ and the parameter $\phi(t=0)$ is shown in Fig. 2. For positive γ the figure shows that $\gamma > \phi > 0$. In accordance with Eq. (22) the SC gap at the Fermi surface is $\Phi(0,0) > \alpha$. It is also shown that relatively large negative values of γ produce only small negative ϕ . Consequently, the SC gap at the Fermi surface is smaller than α , but remains close to α even for relatively strong repulsive γ .

The quasi-particle energy $Y(y, t=0)$ is shown in Fig. 3. The open contours correspond to attractive $\gamma > 0$ and the closed contours to repulsive $\gamma < 0$. For $\gamma > 0$ the kinetic energy increases more rapidly than the SC gap decreases; whereas, for $\gamma < 0$ the upper gap solution in $Y(y)$ decreases more rapidly than the kinetic energy increases.

The SC gap $\Phi(y, t)$ is shown in Fig. 4 for several values of t , with fixed $\gamma = -0.4$. As t increases both the gap $\Phi(y, t)$ and $y_0(t)$ decrease to non-zero values near t_c . Since $\Phi(y, t_c) \neq 0$, a first order phase transition occurs. For decreasing temperatures supercooling is a possibility similar to that observed in low κ LT superconductors [13]. The FOPT is evident in Fig. 5 where the gap $\Phi(y=0, t)$ on the Fermi surface is shown. The dashed curve is the corresponding gap for $\gamma = 0$. In this special case $\Phi(y=0, t) = Y(t)$ is determined by

Fig. 2. The interaction parameter γ is plotted versus $\phi(t=0)$. Note that large negative γ values produces relatively small negative ϕ values.

Fig. 3. The scaled quasi-particle energy $Y(y, t=0)$ is shown as a function of y for several values of $\phi(0)$ from -0.1 to 0.1 .

$$\sigma(t) = \tanh\left(\frac{t_c}{t}\sigma\right), \quad \sigma = \frac{Y(t)}{\alpha}, \quad t_c = \frac{\alpha}{2}. \quad (24)$$

The solution of Eq. (24) gives a second order phase transition (SOPT) similar to the $\gamma > 0$ results [3].

The entropy $S(t)$, a measure of the number of accessible states, is calculated from Eq. (A.3) and shown in Fig. 6 as a function of t . For $t \ll t_c$ the entropy exhibits the usual increase as the increase in thermal energy increases the number of accessible states. Near t_c an unusual decrease in $S(t)$ occurs due to the strong decrease in the range $2y_0(t)$ of the scaled kinetic energy y when $\gamma \leq 0$, resulting in a net decrease in the number of accessible energy states. This behavior is also evident in the analytic expression for $S(t)$ for the case $\gamma = 0$. Since Y is independent of y and the kinetic energy limit is $y_0(t) = Y(t)$, Eqs. (A.3) and (24) yield the scaled entropy $\tilde{S} = S(t)/k_B^2 N_0 T_m$ as

$$\tilde{S} = 4t_c \sigma(t) \ln[g_+(\sigma)g_-(\sigma)] \quad (25)$$

$$g_{\pm} = 2(1 \pm \sigma)^{-(1 \pm \sigma)},$$

where $\sigma(t)$ is the solution of Eq. (24). The dashed curve in Fig. 6 is from Eq. (25).

The specific heat $C = T\partial S/\partial T = t\partial S/\partial t$. Thus the SC state specific heat becomes negative as t approaches t_c . For $\gamma = 0$, Eq. (25) gives

Fig. 4. The scaled SC gap $\Phi(y, t)$ is shown for $\gamma = -0.4$ as a function of y for several values of the scaled temperature from $t = 0.01$ to the smallest contour at $t = 0.122 \approx t_c$.

Fig. 5. The maximum scaled SC gap at the Fermi surface $\Phi(y=0, t)$ is shown for $\gamma = -0.4$ and $\gamma = 0$ (dashed curve) as a function of t . For $\gamma < 0$ a FOPT occurs at $t = t_c$, with $\Phi(t_c) \neq 0$. Results for $\gamma = -0.4$ were calculated with intervals $\Delta t = 0.001$ between $t = 0$ and $t = \alpha/2 = 0.125$. No solution was found for $t > 0.122$.

Fig. 6. Scaled HTS entropy $S(t)$, calculated from Eq. (A.3), is plotted as a function of temperature for repulsive $\gamma = -0.4$, and $\gamma = 0$ (dashed curve). See the text for an explanation of the unusual temperature dependence.

the scaled $\tilde{C} = C/k_B^2 N_0 T_m$ as

$$\tilde{C}(t) = 4t_c t \frac{\partial \sigma}{\partial t} \ln \left[4 \frac{(1-\sigma)^{2\sigma-1}}{(1+\sigma)^{2\sigma+1}} \right]. \quad (26)$$

Since $\partial \sigma / \partial t < 0$ for all $0 < t \leq t_c$, the specific heat becomes negative for $\sigma(t) < \sigma(t_0) = 0.6346$, at which point the argument of the logarithm in Eq. (26) is unity. Using $\sigma(t_0)$ in Eq. (24) gives the universal ratio $t_0/t_c = 0.8472$, independent of α . In general for $\gamma \leq 0$, the SC state specific heat becomes negative as t approaches t_c . This unusual behavior near t_c is due to the strong reduction in the range of accessible energy states when γ is repulsive.

4. Conclusions

Using a pairing Hamiltonian, the role of the interaction kernel in HTS is studied via a parameter α that measures the deviation from a separable kernel, and a parameter γ , a measure of separability. The parameters γ and α are the scaled interaction constants Γ_0 and α_0 . It was shown that even weak interactions with $\alpha > 0$ produce an effective pairing glue, with concomitant large values of the SC gap at $T = 0$ and the transition temperature T_c . The case $\alpha = 0$ is the well known pairing kernel that produces small SC gaps of LTS. The case $\alpha > 0$ with attractive $\gamma > 0$ produces HTS, with a second order SC to normal state phase transition. An important consequence of $\alpha > 0$ is that the gap at the Fermi surface and the critical temperature T_c are quasi-linear functions of α , and relatively weak non-linear functions of γ , which is instrumental in explaining many features of cuprate HTS [3].

In this paper, the effects of $\gamma \leq 0$ on the SC state were examined. For $\gamma = 0$ the quasi-particle energy satisfies the molecular field equation for the reduced magnetization of a spin 1/2 ferromagnet, which has a SOPT. In the general case, $\alpha > 0, \gamma \neq 0$, the SC gap and quasi-particle energies exhibit significantly different behavior as a

function of the kinetic energy for attractive versus repulsive γ . Repulsive $\gamma < 0$ quenches superconductivity, somewhat analogous to the quenching by a magnetic field. The result is a first order phase transition in zero magnetic field, and unconventional temperature dependence of the entropy and specific heat. Although the SC state is not as robust as it is for attractive $\gamma > 0$, it was shown that $T_c(\gamma < 0)$ is a very weak function of $\gamma < 0$, i.e. the SC state exists at temperatures slightly below $T_c(\gamma = 0)$ even for relatively strong repulsive $\gamma < 0$. We interpret this static result as an indication that the SC state arising from a non-separable interaction kernel is quite stable against large repulsive fluctuations in the separable part of the kernel. Whether any materials exhibit the unusual SC state behavior for static $\gamma < 0$ is not known, but the theory presented points out the possibility and explains the phenomenon.

Appendix A. Thermodynamic functions

The integral forms of the thermodynamic potential Ω , internal energy $\mathcal{U}$, and entropy S , as formulated in Ref. [3], are

$$a\Omega(t) = -4tI_0(t) + I_1(t), \quad (A.1)$$

$$a\mathcal{U}(t) = -2I_2(t) + I_1(t), \quad (A.2)$$

$$S(t) = 2k_B N_0 \epsilon_m [2I_0(t) - (1/t)I_2(t)], \quad (A.3)$$

where $a = 1/(N_0 \epsilon_m^2)$.

The integrals $I_n(t)$ in Eqs. (A.1)–(A.3) are

$$\begin{aligned} I_0(t) &= \frac{1}{2} \int dy \ln \left[2 \cosh \left(\frac{Y}{2t} \right) \right], \quad t = \frac{T}{T_m} \\ I_1(t) &= \frac{1}{2} \int dy \frac{\Phi^2}{Y} \tanh \left(\frac{Y}{2t} \right) \\ I_2(t) &= \frac{1}{2} \int dy Y \tanh \left(\frac{Y}{2t} \right). \end{aligned} \quad (A.4)$$

The limits of integration are in general functions of $[\gamma, \alpha, t]$, as explained after Eq. (19).

References

- [1] J.G. Bednorz, K.A. Müller, Z. Phys. B64 (1986) 189.
- [2] J. Bardeen, L.N. Cooper, J.R. Schrieffer, Phys. Rev. 108 (1957) 1175.
- [3] S.B. Haley, H.J. Fink, Physica C 500 (2014) 44.
- [4] C.E. Gough et al., Nature 326 (1987) 855.
- [5] M. Tinkham, Introduction to Superconductivity, 2nd e. edition., McGraw-Hill, 1996.
- [6] H.R. Ott et al., Superconductivity in New Materials, Elsevier, 2011. pp. 81.
- [7] E.W. Carlson et al., Superconductivity, Novel Superconductors, Springer, 2008. pp. 1225.
- [8] J.B. Ketterson, S.N. Song, Superconductivity, 1st ed., Cambridge University Press, 1999.
- [9] P.A. Lee, N. Nagosa, X-Gang Wen, Rev. Mod. Phys. 78 (2006) 17.
- [10] C.C. Tsuei, J.R. Kirtley, Superconductivity, Novel Superconductors, Springer, 2008.
- [11] J. Callaway, Quantum Theory of the Solid State, 2nd ed., Academic Press, 1991.
- [12] A. Bussmann-Holder, R. Micnas, A. Bishop, Eur. Phys. J. B 37 (2003) 345.
- [13] H. Parr, Phys. Rev. B 14 (1976) 2842.