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FERMI GAS WITH 4-FERMION BCS-TYPE INTERACTION

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A gas of spin 1/2 fermions with an interaction $V + W = -\sum_{\boldsymbol{k},\boldsymbol{k}'} g_{\boldsymbol{k}\boldsymbol{k}'} b_{\boldsymbol{k}}^{*} b_{-\boldsymbol{k}}^{*} b_{\boldsymbol{k}'} b_{-\boldsymbol{k}'} + \sum_{\boldsymbol{k}} \gamma_k b_{\boldsymbol{k}}^{*} b_{\boldsymbol{k}}$, where $b_{\boldsymbol{k}} = a_{\boldsymbol{k}+} a_{\boldsymbol{k}-}$ and $a_{\boldsymbol{k}\sigma}, a_{\boldsymbol{k}'\sigma'}^{*}$ satisfy Fermi anticommutation relations, is investigated. The trial ground state $|G\rangle$ is similar in form to the BCS ground state, with $b_{\boldsymbol{k}}^{*} b_{-\boldsymbol{k}}^{*}$ replacing $a_{\boldsymbol{k}+}^{*} a_{-\boldsymbol{k}-}^{*}$, but because the excitation energies are not simply additive, the trial density matrix ρ_0 differs from the BCS one. The expectation values $\langle G|H|G\rangle$and $\mathrm{Tr}(H\rho_0)$ are minimized, revealing the presence of a second-order phase transition, with $T_c > T_{c(\mathrm{BCS})}$ for appropriately adjusted γ_k. It is shown that the minimization procedure applied leads to an expression for the free energy density of H, which is asymptotically exact in the infinite-volume limit. Comparison with experimental data on high-temperature superconductors is made and for a particular choice of γ_k qualitative agreement is found with the temperature dependence of the order parameter of the BSCCO superconductor.

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1. Introduction

It is generally accepted that current carriers in high-T_c superconductors (HTSC) consist of tightly bound local pairs of spin 1/2 fermions with opposite spins, e.g. [1–4]. Hubbard-type Hamiltonians are usually proposed as theoretical models of HTSC due to the flexibility with which local pairing interactions can be modelled in these systems, e.g. [1, 2, 4, 5].

A system of strongly correlated electrons, set up in the framework of the Hubbard model, the so-called spin liquid, in which the same number of degrees of freedom, corresponding to compensated spin configurations, are removed from either k-space or real space, was proposed in Refs. [6–8]. A particular realization of the spin liquid, obtained by adding to the BCS Hamiltonian the term

$$W = \sum_{\boldsymbol{k}} \gamma_k n_{\boldsymbol{k}+} n_{\boldsymbol{k}-}, \tag{1}$$

where $n_{\boldsymbol{k}\sigma} = a^*_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma}$ and $a^*_{\boldsymbol{k}\sigma}, a_{\boldsymbol{k}\sigma}$ are fermion creation and annihilation operators corresponding to momentum $\boldsymbol{k}$ and spin σ, was investigated in Refs. [9, 10].

The interaction W in the form (1) can be viewed as a pair-binding potential of magnetic origin. However, when written in terms of $b^*_{\boldsymbol{k}} = a^*_{\boldsymbol{k}-} a^*_{\boldsymbol{k}+}$, $b_{\boldsymbol{k}} = a_{\boldsymbol{k}+} a_{\boldsymbol{k}-}$, it takes the form

$$W = \sum_{\boldsymbol{k}} \gamma_k b^*_{\boldsymbol{k}} b_{\boldsymbol{k}} \tag{2}$$

reminiscent of the kinetic energy operator of a free quantum gas. In HTSC the quasiparticles represented by the operators $b^*_{\boldsymbol{k}}, b_{\boldsymbol{k}}$, as well as fermions which are not bound by W, can be expected to interact via the phonon field, owing to the presence of a weak isotope effect in these materials [11–13]. The form of the effective BCS Hamiltonian

$$H_{\mathrm{BCS}} = T + V_{\mathrm{BCS}},$$

where

$$T = \sum_{\boldsymbol{k}\sigma} \varepsilon_k a^*_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma}, \qquad \varepsilon_k = k^2/2m - \mu,$$

$$V_{\mathrm{BCS}} = -\sum_{\boldsymbol{k},\boldsymbol{k}'} G_{\boldsymbol{k}\boldsymbol{k}'} a^*_{\boldsymbol{k}+} a^*_{-\boldsymbol{k}-} a_{-\boldsymbol{k}'-} a_{\boldsymbol{k}'+}$$

$$(G_{\boldsymbol{k}\boldsymbol{k}} = 0, \quad \mathrm{Im} G_{\boldsymbol{k}\boldsymbol{k}'} = 0, \quad G_{\boldsymbol{k}\boldsymbol{k}'} = G_{\boldsymbol{k}'\boldsymbol{k}} = G_{-\boldsymbol{k}\boldsymbol{k}'} = G_{\boldsymbol{k}-\boldsymbol{k}'} = G_{-\boldsymbol{k}-\boldsymbol{k}'})$$

and the similarity between W and T suggests therefore a 4-fermion operator of the form

$$V = -\sum_{\boldsymbol{k},\boldsymbol{k}'} g_{\boldsymbol{k}\boldsymbol{k}'} b^*_{\boldsymbol{k}} b^*_{-\boldsymbol{k}} b_{-\boldsymbol{k}'} b_{\boldsymbol{k}'} \tag{3}$$

($g_{\boldsymbol{k}\boldsymbol{k}'}$ having the same symmetry properties as $G_{\boldsymbol{k}\boldsymbol{k}'}$) as a possible phonon-mediated attraction between bound pairs in a HTSC and a full Hamiltonian of the form

$$H' = H_{\mathrm{BCS}} + W + V. \tag{4}$$

In the present paper we deal with a simplified version of H' in which $V_{\mathrm{BCS}} = 0$ and

$$H = T + W + V. \tag{5}$$

The functions $\gamma_k, g_{\boldsymbol{k}\boldsymbol{k}'}$ in H will remain unspecified, the only assumption being that their particular form should be adjusted so as to obtain the best possible agreement of the resulting theory with experiment.

In Secs. 2–4 minimization procedures for the ground-state energy of H and free energy of H are performed. The trial ground state $|G\rangle$ for H is similar in form to the BCS ground state [14], but the quasiparticle excitation energies from $|G\rangle$ are not simply additive. The structure of excited states and excitation spectrum define the structure of the trial grand canonical density matrix ρ_0 and minimization of the free energy $\mathcal{F}[\rho_0]$ determines ρ_0 uniquely. The order parameter $\Delta_{\boldsymbol{k}}$ satisfies a gap equation which has a non-zero solution below T_{c}, proving that T_{c} is the temperature at which the system undergoes a 2nd order phase transition. At $T > T_{\mathrm{c}}$ the system behaves like a gas of free fermions and free bound pairs, whereas below T_c the interaction V takes full effect and the interacting Fermi gas with the Hamiltonian H behaves like a gas of fermion quasiparticles with energies which, in general, are not additive.

If $\gamma_k = 0$, then $T_c < T_{c(\mathrm{BCS})}$ for the same values of $g_{\boldsymbol{k}\boldsymbol{k}'}$, conduction half-bandwidth δ and density of states ρ near the Fermi level $\mu_F = k_F^2/2m$ as in the one-parameter BCS model [14]. The interaction V is thus weaker than V_{BCS}, in agreement with weakness of the isotope effect in HTSC. However, $T_c > T_{c(\mathrm{BCS})}$ if $|\varepsilon_k + \gamma_k/2|$ is sufficiently small, suggesting that H could, possibly, serve as a model of HTSC.

In Sec. 5 a test on validity of this conjecture is performed by comparing experimental data on $\Delta(\beta)$ for the BSCCO superconductor with theoretical predictions for the choice $\gamma(\varepsilon_k) = -2|\varepsilon_k|$ in W. Qualitative agreement is found between predictions of the model and experiment.

In Sec. 6 it is shown by a method of Czerwonko [10] that the minimization procedures applied to H in Secs. 2–4 yield an expression for the free energy density which is asymptotically exact in the infinite-volume limit.

2. The ground state

Since V and V_{BCS} are similar in form, the appropriate trial ground state $|G\rangle$ for H can be expected to be similar to the BCS ground state $|\mathrm{BCS}\rangle$, with the $b^*_{\boldsymbol{k}} b^*_{-\boldsymbol{k}}$ operators replacing $a^*_{\boldsymbol{k}+} a^*_{-\boldsymbol{k}-}$:

$$|G\rangle = \prod_{\boldsymbol{k}>0} (u_{\boldsymbol{k}} + v_{\boldsymbol{k}} b^*_{\boldsymbol{k}} b^*_{-\boldsymbol{k}})|0\rangle, \tag{6}$$

where $\boldsymbol{k} : \boldsymbol{k} > 0\}$ stands for the set of vectors with one fixed, but arbitrary, component positive and $u_{\boldsymbol{k}}, v_{\boldsymbol{k}}$ are real variational parameters satisfying $u^2_{\boldsymbol{k}} + v^2_{\boldsymbol{k}} = 1$. Obviously, $u_{\boldsymbol{k}} = u_{-\boldsymbol{k}}, v_{\boldsymbol{k}} = v_{-\boldsymbol{k}}$ and $\langle G|G\rangle = 1$.

For $\langle G|H|G\rangle$ one obtains

$$\langle G|H|G\rangle = 2\sum_{\boldsymbol{k}} (\varepsilon_k + \gamma_k/2) v^2_{\boldsymbol{k}} - \sum_{\boldsymbol{k},\boldsymbol{k}'} g_{\boldsymbol{k}\boldsymbol{k}'} u_{\boldsymbol{k}} v_{\boldsymbol{k}} u_{\boldsymbol{k}'} v_{\boldsymbol{k}'}. \tag{7}$$

This expression is similar to the expectation value

$$\langle \mathrm{BCS}|H_{\mathrm{BCS}}|\mathrm{BCS}\rangle = \langle \mathrm{BCS}|T + V_{\mathrm{BCS}}|\mathrm{BCS}\rangle.$$

The only difference is that $\varepsilon_k + \gamma_k/2$ in (7) replaces ε_k in $\langle \mathrm{BCS}|H_{\mathrm{BCS}}|\mathrm{BCS}\rangle$. The $u_{\boldsymbol{k}}, v_{\boldsymbol{k}}$ which minimize $\langle G|H|G\rangle$ are therefore analogous to the BCS ones:

$$u^2_{\boldsymbol{k}} = \frac{1}{2}\left(1 + \nu_k E^{-1}_{\boldsymbol{k}}\right), \qquad v^2_{\boldsymbol{k}} = \frac{1}{2}\left(1 - \nu_k E^{-1}_{\boldsymbol{k}}\right), \tag{8}$$

where $\nu_k = \varepsilon_k + \gamma_k/2$, $E_{\boldsymbol{k}} = (\nu_k^2 + \Delta^2_{\boldsymbol{k}})^{1/2}$ and $\Delta_{\boldsymbol{k}} = \sum_{\boldsymbol{k}'} g_{\boldsymbol{k}\boldsymbol{k}'} u_{\boldsymbol{k}'} v_{\boldsymbol{k}'}$ is the solution of the zero-temperature gap equation

$$\Delta_{\boldsymbol{k}} = \frac{1}{2}\sum_{\boldsymbol{k}'} g_{\boldsymbol{k}\boldsymbol{k}'} \Delta_{\boldsymbol{k}'} E^{-1}_{\boldsymbol{k}'}. \tag{9}$$

For $g_{\boldsymbol{k}\boldsymbol{k}'} = g\chi(\boldsymbol{k})\chi(\boldsymbol{k}')$ if $\boldsymbol{k} \neq \boldsymbol{k}'$ ($\chi(\boldsymbol{k})$ denoting the characteristic function of the set $\{\boldsymbol{k} : \varepsilon_k \in [\mu - \delta, \mu + \delta]\}$) and $\gamma_k = 2\gamma\varepsilon_k, \gamma > -1$, the equation for μ, viz.,

$$\langle G|\sum_{\boldsymbol{k}\sigma} a^*_{\boldsymbol{k}\sigma} a_{\boldsymbol{k}\sigma}|G\rangle = n, \tag{10}$$

where n denotes the number of fermions, has a solution $\mu \neq \mu_{\mathrm{F}}$ and the nontrivial solution of Eq. (9) is $\Delta_{\boldsymbol{k}} = \Delta\chi(\boldsymbol{k})$, with

$$\Delta = 2\sinh\left[\frac{2(1+\gamma)}{g\rho}\right]$$

$$\times\left\{(\mu\gamma)^2 + \delta^2(1+\gamma)^2 - \left[(\mu\gamma)^2 - \delta^2(1+\gamma)^2\right]\cosh\left[\frac{2(1+\gamma)}{g\rho}\right]\right\}^{1/2}. \tag{11}$$

If $\gamma_k = 0$, then $\mu = \mu_{\mathrm{F}}$ and $\Delta_{\boldsymbol{k}} = \delta[\sinh(g\rho)^{-1}]^{-1}\chi(\boldsymbol{k})$. The proofs are given in Appendix A.

Similarly as in the BCS model,

$$E_G = \langle G|H|G\rangle = \sum_{\boldsymbol{k}}\left[\nu_k(1-\nu_k E_{\boldsymbol{k}}^{-1}) - \frac{1}{2}\Delta_{\boldsymbol{k}}^2 E_{\boldsymbol{k}}^{-1}\right]$$

suggesting that the ground-state properties of the system with the Hamiltonian H are analogous to those of H_{BCS} except for the shift of the Fermi level μ. This conjecture is proved in Sec. 6 by investigating the infinite-volume limit for H. The 3-dimensional Hubbard model in the weak-coupling limit or, equivalently, at low temperatures [4, 15, 16] and some 2-dimensional local systems [17] also exhibit BCS-type behaviour.

3. Excited states

Having found the best ground state vector $|G\rangle$ in the set of trial vectors introduced in Sec. 2, the approximate excited states can be determined by proceeding similarly as Bogolyubov and Valatin with $|\mathrm{BCS}\rangle$ [18, 19], i.e. by first solving the equation for α

$$\alpha|G\rangle = 0. \tag{12}$$

The solutions of this equation can be most conveniently written using the notation $a_{\boldsymbol{k}1} := a_{\boldsymbol{k}+}$, $a_{\boldsymbol{k}2} := a_{\boldsymbol{k}-}$, $a_{\boldsymbol{k}3} := a_{-k+}$, $a_{\boldsymbol{k}4} := a_{-\boldsymbol{k}-}$. Equation (12) is then satisfied by

$$\alpha_{\boldsymbol{k}1} = u_{\boldsymbol{k}}a_{\boldsymbol{k}1} - v_{\boldsymbol{k}}a^*_{\boldsymbol{k}2}a^*_{\boldsymbol{k}3}a^*_{\boldsymbol{k}4}, \qquad \alpha_{\boldsymbol{k}2} = u_{\boldsymbol{k}}a_{\boldsymbol{k}2} + v_{\boldsymbol{k}}a^*_{\boldsymbol{k}3}a^*_{\boldsymbol{k}4}a^*_{\boldsymbol{k}1},$$

$$\alpha_{\boldsymbol{k}3} = u_{\boldsymbol{k}}a_{\boldsymbol{k}3} - v_{\boldsymbol{k}}a^*_{\boldsymbol{k}1}a^*_{\boldsymbol{k}2}a^*_{\boldsymbol{k}4}, \qquad \alpha_{\boldsymbol{k}4} = u_{\boldsymbol{k}}a_{\boldsymbol{k}4} + v_{\boldsymbol{k}}a^*_{\boldsymbol{k}1}a^*_{\boldsymbol{k}2}a^*_{\boldsymbol{k}3}.$$

The operators $\alpha_{\boldsymbol{k}i}$ are anticommuting

$$[\alpha_{\boldsymbol{k}i}, \alpha_{\boldsymbol{k}'j}]_+ = \alpha_{\boldsymbol{k}i}\alpha_{\boldsymbol{k}'j} + \alpha_{\boldsymbol{k}'j}\alpha_{\boldsymbol{k}i} = 0, \tag{13}$$

but

$$[\alpha_{\boldsymbol{k}i}, \alpha^*_{\boldsymbol{k}j}]_+ = v^2_{\boldsymbol{k}}a^*_{\boldsymbol{k}j}a_{\boldsymbol{k}i}\left(1 - \sum_{l\neq i,j} n_{\boldsymbol{k}l}\right) \qquad \text{for } i \neq j, \tag{14}$$

$$[\alpha_{\boldsymbol{k}i}, \alpha^*_{\boldsymbol{k}i}]_+ = 1 + v^2_{\boldsymbol{k}}\left(\sum_{i\neq j<l\neq i} n_{\boldsymbol{k}j}n_{\boldsymbol{k}l} - \sum_{j\neq i} n_{\boldsymbol{k}j}\right), \tag{15}$$

where $n_{\boldsymbol{k}i} = a^*_{\boldsymbol{k}i}a_{\boldsymbol{k}i}$.

The normalized k-excited states are therefore (cf. [18, 19]) represented by the following vectors:

$$|E_{\mathbf{k}i}\rangle := \alpha^*_{\mathbf{k}i}|G\rangle = \left(\prod_{\mathbf{k}'\neq\mathbf{k}}(u_{\mathbf{k}'} + v_{\mathbf{k}'}b^*_{\mathbf{k}'}b^*_{-\mathbf{k}'})\right) a^*_{\mathbf{k}i}|0\rangle, \tag{16a}$$

$$|E_{\mathbf{k}ij}\rangle := u_{\mathbf{k}}^{-1}\alpha^*_{\mathbf{k}i}\alpha^*_{\mathbf{k}j}|G\rangle = \left(\prod_{\mathbf{k}'\neq\mathbf{k}}(u_{\mathbf{k}'} + v_{\mathbf{k}'}b^*_{\mathbf{k}'}b^*_{-\mathbf{k}'})\right) a^*_{\mathbf{k}i}a^*_{\mathbf{k}j}|0\rangle, \tag{16b}$$

$$|E_{\mathbf{k}ijl}\rangle := u_{\mathbf{k}}^{-2}\alpha^*_{\mathbf{k}i}\alpha^*_{\mathbf{k}j}\alpha^*_{\mathbf{k}l}|G\rangle = \left(\prod_{\mathbf{k}'\neq k}(u_{\mathbf{k}'} + v_{\mathbf{k}'}b^*_{\mathbf{k}'}b^*_{-\mathbf{k}'})\right) a^*_{\mathbf{k}i}a^*_{\mathbf{k}j}a^*_{\mathbf{k}l}|0\rangle, \tag{16c}$$

$$|E_{\mathbf{k}1234}\rangle := u_{\mathbf{k}}^{-2}\alpha^*_{\mathbf{k}1}\alpha^*_{\mathbf{k}2}\alpha^*_{\mathbf{k}3}\alpha^*_{\mathbf{k}4}|G\rangle$$

$$= \left(\prod_{\mathbf{k}'\neq\mathbf{k}}(u_{\mathbf{k}'} + v_{\mathbf{k}'}b^*_{\mathbf{k}'}b^*_{-\mathbf{k}'})\right)(u_{\mathbf{k}}b^*_{\mathbf{k}}b^*_{-\mathbf{k}} - v_{\mathbf{k}})|0\rangle. \tag{16d}$$

According to Eqs. (13)–(15), the excitations represented by the operators $\alpha^*_{\mathbf{k}i}$ are neither fermions nor bosons. Nonetheless, some of their properties are the same as those of particles obeying Fermi or Bose statistics: the set of vectors (16a–d), with varying k, is an orthonormal system, the number of excitations in any state (16a–d) can be lowered by acting on it with the operators $\alpha_{\mathbf{k}i}$, e.g.,

$$\alpha_{\mathbf{k}i}|E_{\mathbf{k}ij}\rangle = u_{\mathbf{k}}|E_{\mathbf{k}j}\rangle \qquad \text{for } i\neq j, \tag{17a}$$

$$\alpha_{\mathbf{k}i}|E_{\mathbf{k}jl}\rangle = 0 \qquad \text{for } i\neq j,\ i\neq l. \tag{17b}$$

The vectors (16a–d) are eigenvectors of the operators $\alpha^*_{\mathbf{k}i}\alpha_{\mathbf{k}i}$, viz.,

$$\alpha^*_{\mathbf{k}i}\alpha_{\mathbf{k}i}|E_{\mathbf{k}i}\rangle = |E_{\mathbf{k}i}\rangle, \tag{18a}$$

$$\alpha^*_{\mathbf{k}i}\alpha_{\mathbf{k}i}|E_{\mathbf{k}ij}\rangle = u^2_{\mathbf{k}}|E_{\mathbf{k}ij}\rangle, \tag{18b}$$

$$\alpha^*_{\mathbf{k}i}\alpha_{\mathbf{k}i}|E_{\mathbf{k}ijl}\rangle = u^2_{\mathbf{k}}|E_{\mathbf{k}ijl}\rangle, \tag{18c}$$

$$\alpha^*_{\mathbf{k}i}\alpha_{\mathbf{k}i}|E_{\mathbf{k}1234}\rangle = |E_{\mathbf{k}1234}\rangle, \tag{18d}$$

but, as implied by these equations, in general, their eigenvalues are not equal to the number of excitations present in the eigenvector. The excitation energies from the ground state $|G\rangle$ are equal

$$\langle E_{\mathbf{k}i}|H|E_{\mathbf{k}i}\rangle - E_G = 2E_{\mathbf{k}} - \varepsilon_k - \gamma_k, \tag{19a}$$

$$\langle E_{\mathbf{k}ij}|H|E_{\mathbf{k}ij}\rangle - E_G = 2E_{\mathbf{k}} - \gamma_k,\ \text{if } (i,j)\in\{(1,3),(1,4),(2,3),(2,4)\}, \tag{19b}$$

$$\langle E_{\mathbf{k}ij}|H|E_{\mathbf{k}ij}\rangle - E_G = 2E_{\mathbf{k}},\ \text{if } (i,j)\in\{(1,2),(3,4)\}, \tag{19c}$$

$$\langle E_{\mathbf{k}ijl}|H|E_{\mathbf{k}ijl}\rangle - E_G = 2E_{\mathbf{k}} + \varepsilon_k, \quad i<j<l, \tag{19d}$$

$$\langle E_{\mathbf{k}1234}|H|E_{\mathbf{k}1234}\rangle - E_G = 4E_{\mathbf{k}}. \tag{19e}$$

It follows that, unlike in BCS theory, these energies are not simply additive when counted in the k-space spanned by $|G_{\mathbf{k}}\rangle = (u_{\mathbf{k}} + v_{\mathbf{k}} b^*_{\mathbf{k}} b^*_{-\mathbf{k}})|0\rangle$ and the vectors (16a–d).

The structure of the subspace $M_{\mathbf{k}} = M_{-\mathbf{k}}$ spanned by the orthonormal basis $B_{\mathbf{k}}$ consisting of $|G_{\mathbf{k}}\rangle$ and vectors (16a–d), shows that there also exist fermion operators $c_{\mathbf{k}\sigma}$ which annihilate the vector $|G_{\mathbf{k}}\rangle$. To construct these fermion operators let us introduce the unitary transformation $U_{\mathbf{k}} = U_{-\mathbf{k}}$ defined as

$$U_{\mathbf{k}} := \sum_i |E_{\mathbf{k}i}\rangle\langle E_{\mathbf{k}i}| + \sum_{i<j} |E_{\mathbf{k}ij}\rangle\langle E_{\mathbf{k}ij}| + \sum_{i<j<l} |E_{\mathbf{k}ijl}\rangle\langle E_{\mathbf{k}ijl}|$$
$$+|G_{\mathbf{k}}\rangle\langle 0| + |E_{\mathbf{k}1234}\rangle\langle 0|a_{\mathbf{k}4}a_{\mathbf{k}3}a_{\mathbf{k}2}a_{\mathbf{k}1}.$$

Obviously, $U_{\mathbf{k}}|0\rangle = |G_{\mathbf{k}}\rangle$ and

$$0 = U_{\mathbf{k}} a_{\mathbf{k}\sigma}|0\rangle = U_{\mathbf{k}} a_{\mathbf{k}\sigma} U^*_{\mathbf{k}} U_{\mathbf{k}}|0\rangle =: c_{\mathbf{k}\sigma}|G_{\mathbf{k}}\rangle,$$

$$0 = U_{\mathbf{k}} a_{-\mathbf{k}\sigma}|0\rangle = U_{\mathbf{k}} a_{-\mathbf{k}\sigma} U^*_{\mathbf{k}} U_{\mathbf{k}}|0\rangle =: c_{-\mathbf{k}\sigma}|G_{\mathbf{k}}\rangle.$$

Since $c_{\mathbf{k}\sigma}$ results by transforming unitarily $a_{\mathbf{k}\sigma}$, the anticommutation relations between the operators $a_{\mathbf{k}\sigma}, a^*_{\mathbf{k}\sigma}, a_{-\mathbf{k}\sigma}, a^*_{-\mathbf{k}\sigma}$, are preserved by $c_{\mathbf{k}\sigma}, c^*_{\mathbf{k}\sigma}, c_{-\mathbf{k}\sigma}, c^*_{-\mathbf{k}\sigma}$. The structure of excited states (16a–d) is also preserved, since in $M_{\mathbf{k}}$, e.g.,

$$|E_{\mathbf{k}ij}\rangle = a^*_{\mathbf{k}i} a^*_{\mathbf{k}j}|0\rangle = U_{\mathbf{k}} a^*_{\mathbf{k}i} a^*_{\mathbf{k}j}|0\rangle = U_{\mathbf{k}} a^*_{\mathbf{k}i} U^*_{\mathbf{k}} U_{\mathbf{k}} a^*_{\mathbf{k}j} U^*_{\mathbf{k}} U_{\mathbf{k}}|0\rangle = c^*_{\mathbf{k}i} c^*_{\mathbf{k}j}|G_{\mathbf{k}}\rangle,$$

$$|E_{\mathbf{k}1234}\rangle = U_{\mathbf{k}} a^*_{\mathbf{k}1} a^*_{\mathbf{k}2} a^*_{\mathbf{k}3} a^*_{\mathbf{k}4}|0\rangle = c^*_{\mathbf{k}1} c^*_{\mathbf{k}2} c^*_{\mathbf{k}3} c^*_{\mathbf{k}4}|0\rangle.$$

4. Minimization of the free energy

The form of the trial grand canonical density matrix ρ_0 is determined by the structure of $|G\rangle$, the excited states (16a–d) and the excitation energies (19a–e). In order to write down ρ_0, let us define the projectors

$$P_{\mathbf{k}0} = |G_{\mathbf{k}}\rangle\langle G_{\mathbf{k}}|, \quad P_{\mathbf{k}i} = |E_{\mathbf{k}i}\rangle\langle E_{\mathbf{k}i}|, \quad P_{\mathbf{k}ij} = |E_{\mathbf{k}ij}\rangle\langle E_{\mathbf{k}ij}|,$$

$$P_{\mathbf{k}ijl} = |E_{\mathbf{k}ijl}\rangle\langle E_{\mathbf{k}ijl}|, \quad P_{\mathbf{k}1234} = |E_{\mathbf{k}1234}\rangle\langle E_{\mathbf{k}1234}|. \tag{20}$$

Since there exist two types of two-quasiparticle excitation energies, whereas the excitation energies of one- and three-quasiparticle excitations do not depend on the type of quasiparticles involved, therefore

$$\rho_0 = \prod_{\mathbf{k}>0} M^{-1}_{\mathbf{k}} \Bigg[P_{\mathbf{k}0} + \sum_{i=1}^{4} \exp(-\beta e_{\mathbf{k}1}) P_{\mathbf{k}i} + \exp(-\beta e'_{\mathbf{k}2})(P_{\mathbf{k}12} + P_{\mathbf{k}34})$$
$$+ \exp(-\beta e_{\mathbf{k}2})(P_{\mathbf{k}13} + P_{\mathbf{k}14} + P_{\mathbf{k}23} + P_{\mathbf{k}24})$$
$$+ \sum_{i<j<l} \exp(-\beta e_{\mathbf{k}3}) P_{\mathbf{k}ijl} + \exp(-\beta e_{\mathbf{k}4}) P_{\mathbf{k}1234} \Bigg],$$

where

$$M_{\mathbf{k}} = 1 + \sum_{i=1}^{3} 4\exp(-\beta e_{\mathbf{k}i}) + 2\exp(-\beta e'_{\mathbf{k}2}) + \exp(-\beta e_{\mathbf{k}4}).$$

In terms of

$$f_{\mathbf{k}i} = f_{-\mathbf{k}i} = 4M_{\mathbf{k}}^{-1}\exp(-\beta e_{\mathbf{k}i}), \quad i = 1, 2, 3,$$

$$f'_{\mathbf{k}2} = f'_{-\mathbf{k}2} = 2M_{\mathbf{k}}^{-1}\exp(-\beta e'_{\mathbf{k}2}), \quad f_{\mathbf{k}4} = f_{-\mathbf{k}4} = M_{\mathbf{k}}^{-1}\exp(-\beta e_{\mathbf{k}4}),$$

ρ_0 takes the form

$$\rho_0 = \prod_{\mathbf{k}>0}\left[\left(1 - \sum_{i=1}^{4} f_{\mathbf{k}i} - f'_{\mathbf{k}2}\right)P_{\mathbf{k}0} + \frac{1}{4}\sum_{i=1}^{4} f_{\mathbf{k}1}P_{\mathbf{k}i} + \frac{1}{2}f'_{\mathbf{k}2}(P_{\mathbf{k}12} + P_{\mathbf{k}34})\right.$$

$$\left. + \frac{1}{4}f_{\mathbf{k}2}(P_{\mathbf{k}13} + P_{\mathbf{k}14} + P_{\mathbf{k}23} + P_{\mathbf{k}24}) + \frac{1}{4}\sum_{i<j<l} f_{\mathbf{k}3}P_{\mathbf{k}ijl} + f_{\mathbf{k}4}P_{\mathbf{k}1234}\right]. \tag{21}$$

The entropy $\mathcal{S}[\rho_0]$ equals

$$\mathcal{S}[\rho_0] = -(T\beta)^{-1}\mathrm{Tr}(\rho_0 \ln \rho_0)$$

$$= \frac{1}{2}(T\beta)^{-1}\sum_{\mathbf{k}}\left[\left(1 - \sum_{i=1}^{4} f_{\mathbf{k}i} - f'_{\mathbf{k}2}\right)\ln\left(1 - \sum_{j=1}^{4} f_{\mathbf{k}j} - f'_{\mathbf{k}2}\right)\right.$$

$$\left. + f_{\mathbf{k}1}\ln\frac{1}{4}f_{\mathbf{k}1} + f_{\mathbf{k}2}\ln\frac{1}{4}f_{\mathbf{k}2} + f'_{\mathbf{k}2}\ln\frac{1}{2}f'_{\mathbf{k}2} + f_{\mathbf{k}3}\ln\frac{1}{4}f_{\mathbf{k}3} + f_{\mathbf{k}4}\ln f_{\mathbf{k}4}\right] \tag{22}$$

and the average energy in the state ρ_0

$$\mathcal{E}[\rho_0] = \mathrm{Tr}(H\rho_0) = 2\sum_{\mathbf{k}}\nu_k\left[\left(1 - \sum_{i=1}^{4} f_{\mathbf{k}i} - f_{\mathbf{k}4} - f'_{\mathbf{k}2}\right)v_{\mathbf{k}}^2 + \frac{1}{4}\sum_{j=1}^{4} j f_{\mathbf{k}j}\right.$$

$$\left. + \frac{1}{2}f'_{\mathbf{k}2}\right] - \sum_{\mathbf{k}'}\gamma_{k'}\left(\frac{1}{4}f_{\mathbf{k}'1} + \frac{1}{2}f_{\mathbf{k}'2} + \frac{1}{4}f_{\mathbf{k}'3}\right) - \sum_{\mathbf{k},\mathbf{k}'} g_{\mathbf{k}\mathbf{k}'}u_{\mathbf{k}}v_{\mathbf{k}}u_{\mathbf{k}'}v_{\mathbf{k}'}$$

$$\times\left(1 - \sum_{i=1}^{4} f_{\mathbf{k}i} - f_{\mathbf{k}4} - f'_{\mathbf{k}2}\right)\left(1 - \sum_{j=1}^{4} f_{\mathbf{k}'j} - f_{\mathbf{k}'4} - f'_{\mathbf{k}'2}\right). \tag{23}$$

The free energy $\mathcal{F}[\rho_0] = \mathcal{E}[\rho_0] - T\mathcal{S}[\rho_0]$ is minimized by the appropriate solutions of the equations

$$\frac{\partial \mathcal{F}}{\partial f'_{\mathbf{k}2}} = 0, \quad \frac{\partial \mathcal{F}}{\partial f_{\mathbf{k}i}} = 0, \quad i = 1, 2, 3, 4 \tag{24}$$

and

$$\frac{\partial \mathcal{F}}{\partial v_{\mathbf{k}}} = 0. \tag{25}$$

The unique solutions of Eqs. (24), expressed in terms of

$$\Delta_{\mathbf{k}} = \sum_{\mathbf{k}'} g_{\mathbf{k}\mathbf{k}'}u_{\mathbf{k}'}v_{\mathbf{k}'}\left(1 - \sum_{j=1}^{4} f_{\mathbf{k}'j} - f_{\mathbf{k}'4} - f'_{\mathbf{k}'2}\right) \tag{26}$$

and $E_{\boldsymbol{k}} = (\nu_k^2 + \Delta_{\boldsymbol{k}}^2)^{1/2}$, are

$$e_{\boldsymbol{k}1} = 2E_{\boldsymbol{k}} - \varepsilon_k - \gamma_k, \quad e_{\boldsymbol{k}2} = 2E_{\boldsymbol{k}} - \gamma_k, \quad e'_{\boldsymbol{k}2} = 2E_{\boldsymbol{k}},$$

$$e_{\boldsymbol{k}3} = 2E_{\boldsymbol{k}} + \varepsilon_k, \quad e_{\boldsymbol{k}4} = 4E_{\boldsymbol{k}}. \tag{27}$$

These excitation energies have the same form as those previously found in (19a–d).

It follows from (27) that the gap $\Gamma(\beta)$ in the excitation spectrum depends on the form of γ_k and is present already at $T > T_c$. In this range of temperatures

$$\Gamma(\beta) = \inf_{\boldsymbol{k}} (2|\varepsilon_k + \gamma_k/2| - \varepsilon_k - \gamma_k).$$

At $T < T_c$ the gap $\Gamma(\beta)$ widens with increasing $\Delta(\beta)$ and equals, according to (27),

$$\Gamma(\beta) = \inf_{\boldsymbol{k}} \left(2\sqrt{(\varepsilon_k + \gamma_k/2)^2 + \Delta_{\boldsymbol{k}}^2} - \varepsilon_k - \gamma_k \right).$$

The presence of a gap above and below T_c in HTSC has been observed experimentally (cf. e.g. [4]).

As for the density matrix ρ_0, with $e_{\boldsymbol{k}i}, e'_{\boldsymbol{k}2}$ given by (27), it can be written in the standard form

$$\rho_0 = [\mathrm{Tr}\exp(-\beta h_0)]^{-1} \exp(-\beta h_0),$$

but h_0 is not expressible as $E_G + \sum_{\boldsymbol{k}j} h_{\boldsymbol{k}j} \alpha^*_{\boldsymbol{k}j} \alpha_{\boldsymbol{k}j}$, or $E_G + \sum_{\boldsymbol{k}j} h_{\boldsymbol{k}j} c^*_{\boldsymbol{k}j} c_{\boldsymbol{k}j}$, as it would be in the case of noninteracting fermions or bosons.

Equation (25) takes the form

$$2\nu_k u_{\boldsymbol{k}} v_{\boldsymbol{k}} = \Delta_{\boldsymbol{k}} (u_{\boldsymbol{k}}^2 - v_{\boldsymbol{k}}^2). \tag{28}$$

The solutions $u_{\boldsymbol{k}}, v_{\boldsymbol{k}}$ are the BCS ones given by (8), with $\Delta_{\boldsymbol{k}}$ the solution of the equation

$$\Delta_{\boldsymbol{k}} = \frac{1}{2} \sum_{\boldsymbol{k}'} g_{\boldsymbol{k}\boldsymbol{k}'} \frac{\Delta_{\boldsymbol{k}'}}{(\nu_{k'}^2 + \Delta_{\boldsymbol{k}'}^2)^{1/2}} F(\beta, (\nu_{k'}^2 + \Delta_{\boldsymbol{k}'}^2)^{1/2}, \nu_{k'}, \gamma_{k'}) \tag{29}$$

resulting from (26), where

$$F(\beta, x, y, z) = \frac{\sinh 2\beta x}{\cosh 2\beta x + 4\exp(\beta z/2)\cosh \beta y + 2\exp \beta z + 1}.$$

Equation (29) is analogous in form to the gap equation of BCS theory, with $F(\beta, E_{\boldsymbol{k}}, \nu_k, \gamma_k)$ replacing $\tanh \frac{1}{2}\beta E_{\boldsymbol{k}}$. The growth and convexity properties of $F(\beta, x, y, z)$ and $\tanh \frac{1}{2}\beta x$ are similar:

(A) $F(\beta, x, y, z)$ is vanishing at $x = 0$, odd in x, increasing in x and concave in x for $x > 0$.

(B) For $x > 0, 2x > |y| + z/2 > z, F(\beta, x, y, z)$ is increasing in β.

(C) $\lim F(\beta, x, y, z) = 1$ as $\beta \to \infty$ if $x > 0, 2x > |y| + z/2 > z$.

The inequalities in (B), (C) are fulfilled if $\gamma_k = -2|\varepsilon_k| + \sigma_k$, where $|\sigma_k| \ll |\varepsilon_k|$. It follows therefore that for such γ_k Eq. (29) is satisfied at all values of $\beta \geq 0$ by the trivial solution $\Delta_{\boldsymbol{k}} = 0$ and if $g_{\boldsymbol{k}\boldsymbol{k}'} \geq 0$ is nonvanishing on a suitable subset with nonzero Lebesgue measure in $\mathcal{R}^3 \times \mathcal{R}^3$, a non-negative solution $\Delta(\beta, \boldsymbol{k})$ of this equation exists for values of β above some β_c. $\Delta(\beta, \boldsymbol{k}) > 0$ is increasing in

β in the interval (β_c, ∞) from $\Delta(\beta_c, k) = 0$ to a finite value $\Delta(\infty, k)$, because $x^{-1}F(\beta, x, y, z)$ is decreasing in x for $x > 0$. (The proof is given in Appendix B.)

The inequalities in (B), (C) are also satisfied for $\varepsilon_k > 0$ by $\gamma_k = 2|\varepsilon_k| + \sigma_k, |\sigma_k| \ll |\varepsilon_k|$. The growth in β of the right hand side of Eq. (29) can be therefore also assured by choosing $\gamma_k = 2|\varepsilon_k| + \sigma_k$ and $g_{kk'} = [g_1\chi_-(k) + g_2\chi_+(k)][g_1\chi_-(k')g_2\chi_+(k')]$, where $\chi_+(k) = \chi(k)\chi[k : \varepsilon_k > 0], \chi_-(k) = \chi(k)\chi[k : \varepsilon_k < 0], 0 < g_1 \ll g_2$.

The free energy $\mathcal{F}[\rho_0]$ expressed in terms of the solutions of Eqs. (24), (25) takes the form

$$\mathcal{F}[\rho_0] = \sum_{k} \Big[\nu_k - E_k + (2E_k)^{-1}F(\beta, E_k, \nu_k, \gamma_k)(E_k^2 - \nu_k^2) \tag{30}$$

$$-\frac{1}{2}\beta^{-1}\ln\left(1 + \sum_{i=1}^{3} 4\exp(-\beta e_{ki}) + \exp(-\beta e_{k4}) + 2\exp(-\beta e'_{k2})\right)\Big]$$

and for $\beta \in (\beta_c, \infty)$ is minimized by the nontrivial solution of Eq. (29). (The proof is given in Appendix C.) As a consequence, there is a second-order phase transition at β_c.

The equation for μ at the temperatures $T > 0$, viz.,

$$\operatorname{Tr}\left(\rho_0 \sum_{k\sigma} a^*_{k\sigma} a_{k\sigma}\right) = n \tag{31}$$

assumes the form

$$\sum_{k}\left[1 - \frac{\nu_k}{E_k}F(\beta, E_k, \nu_k, \gamma_k) - 2G(\beta, E_k, \nu_k, \gamma_k)\right] = n, \tag{32}$$

where

$$G(\beta, x, y, z) = \frac{\exp(\beta z/2)\sinh(\beta y)}{\cosh(2\beta x) + 4\exp(\beta z/2)\cosh(\beta y) + 2\exp(\beta z) + 1}.$$

5. The critical temperature in the one-parameter model

In the one-parameter model with $g_{kk'} = g\chi(k)\chi(k')$ for $k \neq k'$ the solution $\Delta_k(\beta)$ of Eq. (29) has the form $\Delta_k(\beta) = \Delta(\beta)\chi(k)$. Equation (29) for the nonzero solution $\Delta(\beta)$ simplifies to

$$2 = g\rho\int_{-\delta}^{\delta} \frac{d\varepsilon}{\left\{[\varepsilon + \gamma(\varepsilon)/2]^2 + \Delta^2\right\}^{1/2}}$$

$$\times F\left(\beta, \left\{[\varepsilon + \gamma(\varepsilon)/2]^2 + \Delta^2\right\}^{1/2}, \varepsilon + \gamma(\varepsilon)/2, \gamma(\varepsilon)\right). \tag{33}$$

The temperature β_c therefore satisfies the equation

$$2 = g\rho\int_{-\delta\beta_c}^{\delta\beta_c} \frac{dx}{|x + (1/2)\beta_c\gamma(\beta_c^{-1}x)|}$$

$$\times F\left[1, |x + (1/2)\beta_c\gamma(\beta_c^{-1}x)|, x + (1/2)\beta_c\gamma(\beta_c^{-1}x), \beta_c\gamma(\beta_c^{-1}x)\right]. \tag{34}$$

If $\delta\beta_{\rm c} \gg 1$ and the integrand on the rhs of Eq. (34) vanishes sufficiently fast as $x \to \pm\infty$, then

$$(\beta_{\rm c}\delta)^{-1} \exp\left(\int_{-\delta\beta_{\rm c}}^{\delta\beta_{\rm c}} \frac{dx'}{|x' + (1/2)\beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x')|}\right.$$
$$\left.\times F\left[1, |x' + (1/2)\beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x')|, x' + (1/2)\beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x'), \beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x')\right]\right)$$
$$= \lim_{x\to\infty} x^{-1} \exp\left(\int_{-x}^{x} \frac{dx'}{|x' + (1/2)\beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x')|}\right.$$
$$\left.\times F\left[1, |x' + (1/2)\beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x')|, x' + (1/2)\beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x'), \beta_{\rm c}\gamma(\beta_{\rm c}^{-1}x')\right]\right) = c_\gamma .$$

Thus

$$\frac{2}{g\rho} = \ln(\beta_{\rm c}\delta c_\gamma)$$

and

$$\beta_{\rm c}^{-1} = \delta c_\gamma \exp\left(-\frac{2}{g\rho}\right).$$

$T_{\rm c}$ can be therefore increased to exceed $T_{\rm c(BCS)}$ by allowing $|x + \gamma(x)/2|$, where $\gamma(x) = -2|x| + \sigma(x)$, to assume values sufficiently small on a sufficiently large interval above zero. Similarly, if $\gamma(x) = 2|x| + \sigma(x)$ with $|\sigma(x)| \ll |x|$ and $g_{\boldsymbol{k}\boldsymbol{k}'} = [g_1\chi_-(\boldsymbol{k}) + g_2\chi_+(\boldsymbol{k})][g_1\chi_-(\boldsymbol{k}') + g_2\chi_+(\boldsymbol{k}')]$, then $T_{\rm c}$ can be raised by allowing $|x + \gamma(x)/2|$ to assume sufficiently small values on a sufficiently large interval below zero.

If $\gamma(x) = 0$, then $T_{\rm c} < T_{\rm c(BCS)}$, because for such γ

$$\beta_{\rm c}^{-1} = c_0\delta \exp\left[-(g\rho)^{-1}\right] \tag{35}$$

with

$$c_0 = \lim_{x\to\infty} x^{-1} \exp\left(\int_0^x dx' x'^{-1} \frac{\sinh x' \cosh x'}{(\cosh x' + 1)^2}\right)$$
$$< \lim_{x\to\infty} x^{-1} \exp\left(\int_0^x dx' x'^{-1} \tanh(x'/2)\right) = c_{\rm BCS} = 1.14. \tag{36}$$

The inequality $T_{\rm c} < T_{\rm c(BCS)}$ for $\gamma = 0$ shows that interaction V is weaker than $V_{\rm BCS}$, which agrees with the weakness of the isotope effect in HTSC and confirms the, generally accepted, decisive role of the pair-binding potential W in raising $T_{\rm c}$ in these materials, e.g. [20–22].

Consider now Eq. (32) for μ if $g_{\boldsymbol{k}\boldsymbol{k}'} = g\chi(\boldsymbol{k})\chi(\boldsymbol{k}')$ for $\boldsymbol{k} \neq \boldsymbol{k}'$.In the range of low temperatures (large β) the term $\sum_{\boldsymbol{k}} 2G(\beta, E_{\boldsymbol{k}}, \nu_k, \gamma_k)$ on the left hand side of Eq. (32) is negligible compared to the first two summands. The resulting simplified equation is not solvable in general. For $\gamma_k = 0$ the solution is $\mu = \mu_{\rm F}$.

Another difference between the thermodynamics of H and $H_{\rm BCS}$ is in the dependence of the ratio $\Delta(\beta)\Delta(\infty)^{-1}$ on the temperature. In BCS theory this ratio depends exclusively on $TT_{\rm c}^{-1}$. This is not the case in the present model due to the fact that β enters into F through $\beta E_{\mathbf{k}}, \beta\nu_k, \beta\gamma_k$ and not exclusively through $\beta E_{\mathbf{k}}$. We have examined to what extent the plot of $\Delta(\beta)\Delta(\infty)^{-1}$ resulting from Eq. (33) for $\gamma(\varepsilon) = -2|\varepsilon|$ (in which case conditions (B), (C) are fulfilled and the gap in the excitation spectrum equals $\Gamma(\beta) = 2\Delta(\beta)$) can be adjusted to fit the experimental data on $\Delta(\beta)\Delta(\infty)^{-1}$ determined on two types of junctions for the BSCCO superconductor and depicted in Refs. [23, 24]. For $\gamma(\beta) = -2|\varepsilon|$, Eq. (9) for $\Delta(\infty)$ takes the form

$$g\rho = \frac{4}{4\delta\beta_c a^{-1} + \operatorname{arcsinh}(4\delta\beta_c a^{-1})}, \tag{37}$$

where $a = 2\Delta(\infty)\beta_c$ and Eq. (34) reduces to

$$2 = g\rho \left(\int_{-\delta\beta_c}^{0} \frac{\sinh(4x)}{2x[\cosh(4x) + 4\exp(x)\cosh(2x) + 2\exp(2x) + 1)]} \mathrm{d}x \right.$$
$$\left. + \int_{0}^{\delta\beta_c} \frac{\mathrm{d}x}{[1+\exp(-x)]^2} \right). \tag{38}$$

Given a, Eqs. (37), (38) allow us to determine $g\rho$ and $\delta\beta_c$. For the choice $a = 2.5$, similar as in other fitting methods (e.g. Ref. [24]), one obtains $\delta\beta_c = 7.17$, $g\rho = 0.2738$. The resulting graph of $\Delta(\beta)\Delta(\infty)^{-1}$, with $2\Delta(\infty) = 1.81 \times 10^{-2}$ eV for $T_c = 84$ K [24], is depicted in Fig. 1 and compared with experimental data on BSCCO of Ref. [24]. Another comparison with the $\Delta(\beta)\Delta(\infty)^{-1}$ data of Refs. [23, 24] for BSCCO and $T_c = 85$ K, with $a = 2.025$, $\delta\beta_c = 124.783$,

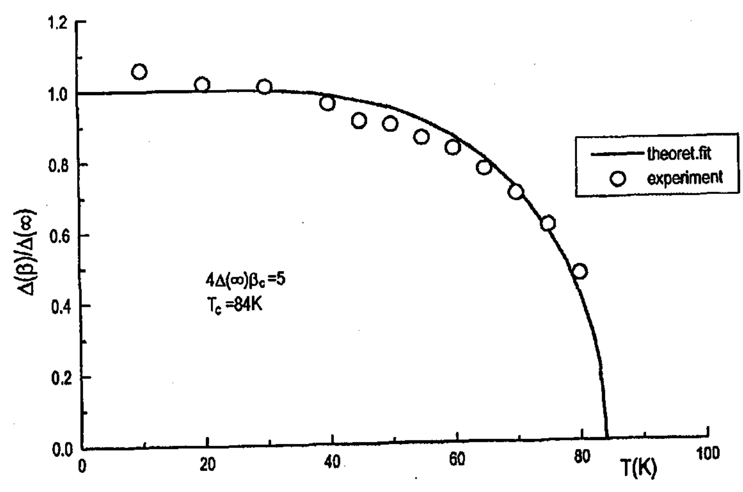

Fig. 1. Temperature dependence of $\Delta(\beta)/\Delta(\infty)$ for a BSCCO/BSCO/Au tunnel junction. The solid line is the $\Delta(\beta)/\Delta(\infty)$ function resulting from Eq. (33) fitted to $a = 2.5$, $T_c = 84$ K. Experimental data (o) after Ref. [24].

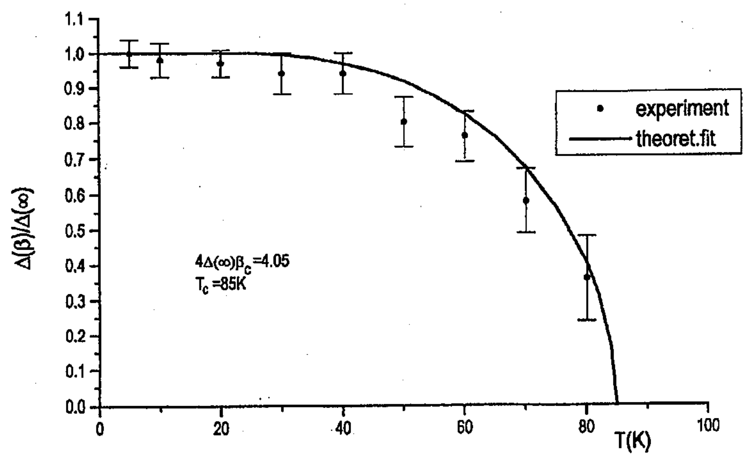

Fig. 2. Temperature dependence of $\Delta(\beta)/\Delta(\infty)$ for a BSCCO/Nb junction. The solid line is the $\Delta(\beta)/\Delta(\infty)$ function resulting from Eq. (33) fitted to $a = 2.025$, $T_c = 85$ K. Experimental data (•) after Refs. [23, 24].

$g\rho = 0.016$, $2\Delta(\infty) = 1.48 \times 10^{-2}$ eV is given in Fig. 2. For the crude choice $\gamma(\varepsilon) = -2|\varepsilon|$, agreement with experiment appears to be satisfactory in both cases.

Another confrontation with HTSC experimental data can be obtained by comparing the values of $2a = 2\Gamma(\infty)/k_{\rm B}T_{\rm c}$. In HTSC this ratio assumes values between 2.4 and 11 [24]. In the present model, for $\gamma(\varepsilon) = -2|\varepsilon|, 2a = 5$ and 4.05 in the two cases discussed above. In general, for this choice of $\gamma(\varepsilon)$, $2a$ depends on the value of $g\rho$ according to Eq. (37) and

$$\lim 2a = 0 \text{ as } g\rho \to 0, \qquad \lim 2a = \infty \text{ as } g\rho \to \infty.$$

Thus, all non-negative values of $2a$ are admissible and the range [2.4, 11] observed in HTSC is covered by the present model. Further properties of the system described by H are under investigation.

6. Asymptotic exactness of the variational procedure for H

In Ref. [10] Czerwonko developed a method of evaluating the infinite-volume limit of free energy density for a Fermi gas with BCS attraction and repulsion between fermions with equal momenta and opposite spins (described by W with $\gamma_k > 0$). His method is applicable to the Hamiltonian H defined in Eq. (5) with $g_{\boldsymbol{k}\boldsymbol{k}'}$ of the form $g_{\boldsymbol{k}\boldsymbol{k}'} = \lambda L^{-3} g_{\boldsymbol{k}} g_{\boldsymbol{k}'}$, L^3 denoting the volume of the system, and allows us to prove the asymptotic equality

$$\lim_{L\to\infty} (-\beta L^3)^{-1} \ln \operatorname{Tr} \exp(-\beta H) = \lim_{L\to\infty} \min_{\rho_0} L^{-3} \mathcal{F}[\rho_0], \tag{39}$$

where $\mathcal{F}[\rho_0]$ is given by the expression (30). In order to carry out this proof, let us first note that the sum of diagonal terms in the potential V with $g_{\boldsymbol{k}\boldsymbol{k}'} = \lambda L^{-3} g_{\boldsymbol{k}} g_{\boldsymbol{k}'}$, viz.,

$$\lambda L^{-3} \sum_{\boldsymbol{k}} g_{\boldsymbol{k}} g_{\boldsymbol{k}} b^*_{\boldsymbol{k}} b^*_{-\boldsymbol{k}} b_{-\boldsymbol{k}} b_{\boldsymbol{k}}$$

is uniformly bounded in L if $g_{\boldsymbol{k}}$ is square-integrable on $\mathcal{R}^3$:

$$L^{-3} \| \lambda \sum_{\boldsymbol{k}} g_{\boldsymbol{k}} g_{\boldsymbol{k}} b^*_{\boldsymbol{k}} b^*_{-\boldsymbol{k}} b_{-\boldsymbol{k}} b_{\boldsymbol{k}} \| \leq |\lambda| L^{-3} \sum_{\boldsymbol{k}} g^2_{\boldsymbol{k}} \leq (2\pi)^{-3} |\lambda| \int_{\mathcal{R}^3} g^2_{\boldsymbol{k}} \mathrm{d}^3 k$$

and therefore does not contribute to $L^{-3} \ln \mathrm{Tr} \exp(-\beta H)$ in the limit $L \to \infty$, $n \to \infty, nL^{-3} = d$. This form of $g_{\boldsymbol{k}\boldsymbol{k}'}$ thus fulfils asymptotically the requirements imposed in the Introduction.

Let us write H, with $g_{\boldsymbol{k}\boldsymbol{k}'} = \lambda L^{-3} g_{\boldsymbol{k}} g_{\boldsymbol{k}'}$, in the form

$$H = \sum_{\boldsymbol{p}\sigma} \varepsilon_p n_{\boldsymbol{p}\sigma} - \lambda L^{-3} B^* B + \sum_{\boldsymbol{p}} \gamma_p n_{\boldsymbol{p}+} n_{\boldsymbol{p}-},$$

where $B = \sum_{\boldsymbol{k}} g_{\boldsymbol{k}} b_{-\boldsymbol{k}} b_{\boldsymbol{k}}$. H can be rewritten as

$$H = \sum_{\boldsymbol{p}\sigma} \varepsilon_p n_{\boldsymbol{p}\sigma} - \lambda L^{-3} (B^* + B) \langle B \rangle + \sum_{\boldsymbol{p}} \gamma_p n_{\boldsymbol{p}+} n_{\boldsymbol{p}-} + \lambda L^{-3} \langle B \rangle^2$$

$$-\lambda L^{-3} (B^* - \langle B \rangle)(B - \langle B \rangle) \equiv H' - \lambda L^{-3} (\Delta B^*)(\Delta B), \tag{40}$$

where

$$\langle B^* \rangle = \langle B \rangle = [\mathrm{Tr} \exp(-\beta H')]^{-1} \, \mathrm{Tr}[B \exp(-\beta H')], \tag{41}$$

$\Delta B = B - \langle B \rangle$. The gauge invariance of H admits the choice $\langle B \rangle = \mathrm{Re} \langle B \rangle = \langle B^* \rangle$. The thermodynamical perturbation method [10, 25–29] for the statistical sum $Z_H = \mathrm{Tr} \exp(-\beta H)$ then yields

$$Z_H = A \mathrm{Tr} \exp(-\beta H'), \quad \text{where} \quad \lim_{L \to \infty} L^{-3} \ln A = 0. \tag{42}$$

Thus in order to evaluate $\lim L^{-3} \ln Z_H$, as $L \to \infty$, it suffices to diagonalize H'. This Hamiltonian can be written as

$$H' = \sum_{\boldsymbol{p} > 0} H_{\boldsymbol{p}} + \lambda L^{-3} \langle B \rangle^2$$

with

$$H_{\boldsymbol{p}} = \varepsilon_p \sum_{\sigma} (n_{\boldsymbol{p}\sigma} + n_{-\boldsymbol{p}\sigma}) - 2\lambda g_{\boldsymbol{p}} L^{-3} \langle B \rangle (b^*_{\boldsymbol{p}} b^*_{-\boldsymbol{p}} + b_{\boldsymbol{p}} b_{-\boldsymbol{p}})$$

$$+\gamma_p (n_{\boldsymbol{p}+} n_{\boldsymbol{p}-} + n_{-\boldsymbol{p}+} n_{-\boldsymbol{p}-}). \tag{43}$$

$H_{\boldsymbol{p}}$ acts in the 16-dimensional space of states

$$(a^*_{\boldsymbol{p}+})^{n_1} (a^*_{\boldsymbol{p}-})^{n_2} (a^*_{-\boldsymbol{p}+})^{n_3} (a^*_{-\boldsymbol{p}-})^{n_4} |0\rangle, \tag{44}$$

where $n_i = 0, 1, i = 1, 2, 3, 4$. All the states (44), except for the two with $n_1 = n_2 = n_3 = n_4 = 0$ and $n_1 = n_2 = n_3 = n_4 = 1$, prove to be eigenstates of $H_{\boldsymbol{p}}$. Due to the commutation relations fulfilled by $H_{\boldsymbol{p}}$, viz.,

$$[H_{\boldsymbol{p}}, 2S] = 0, \quad [H_{\boldsymbol{p}}, \Lambda_\alpha] = 0,$$

where

$$2S = \sum_{\alpha = \pm 1} \sum_{\sigma = \pm 1} \sigma n_{\alpha \boldsymbol{p}, \sigma}, \quad \Lambda_\sigma = n_{\boldsymbol{p}, \sigma} - n_{-\boldsymbol{p}, -\sigma}, \tag{45}$$

denote the spin projection and two seniorities Λ_+, Λ_-, the diagonalization of $H_{\boldsymbol{p}}$ can be carried out independently in the invariant subspaces of $H_{\boldsymbol{p}}$ with fixed eigenvalues of $2S$ and Λ_+, Λ_-. This procedure reveals the following eigenstructure of $H_{\boldsymbol{p}}$:

		Eigenvalue of			
	Eigenvector	$H_{\boldsymbol{p}}$	$2S$	Λ_+	Λ_-
1.	$\|1000\rangle$	ε_p	1	1	0
2.	$\|0100\rangle$	ε_p	−1	0	1
3.	$\|0010\rangle$	ε_p	1	0	−1
4.	$\|0001\rangle$	ε_p	−1	−1	0
5.	$\|1010\rangle$	$2\varepsilon_p$	2	1	−1
6.	$\|0101\rangle$	$2\varepsilon_p$	−2	−1	1
7.	$\|1001\rangle$	$2\varepsilon_p$	0	0	0
8.	$\|0110\rangle$	$2\varepsilon_p$	0	0	0
9.	$\|1100\rangle$	$2\varepsilon_p + \gamma_p$	0	1	1
10.	$\|0011\rangle$	$2\varepsilon_p + \gamma_p$	0	−1	−1
11.	$\|1110\rangle$	$3\varepsilon_p + \gamma_p$	1	1	0
12.	$\|0111\rangle$	$3\varepsilon_p + \gamma_p$	−1	−1	0
13.	$\|1101\rangle$	$3\varepsilon_p + \gamma_p$	−1	0	1
14.	$\|1011\rangle$	$3\varepsilon_p + \gamma_p$	1	0	−1
15.	$u_{\boldsymbol{p}}\|0000\rangle + v_{\boldsymbol{p}}\|1111\rangle$	$2\varepsilon_p + \gamma_p - 2E_{\boldsymbol{p}}$	0	0	0
16.	$u_{\boldsymbol{p}}\|1111\rangle - v_{\boldsymbol{p}}\|0000\rangle$	$2\varepsilon_p + \gamma_p + 2E_{\boldsymbol{p}}$	0	0	0

where $u_{\boldsymbol{p}}^2, v_{\boldsymbol{p}}^2$ are given by Eq. (8) with

$$\Delta_{\boldsymbol{p}} = \lambda L^{-3} g_{\boldsymbol{p}} \langle B \rangle . \tag{46}$$

Evaluation of $Z_{H'} = \mathrm{Tr}\exp(-\beta H')$ is now a matter of some simple algebra. One obtains

$$Z_{H'} = \exp(-\lambda\beta L^{-3}\langle B\rangle^2) \prod_{\boldsymbol{p}>0} 2\exp(-2\beta\nu_p)$$

$$\times [\cosh(2\beta E_{\boldsymbol{p}}) + 4\exp(\beta\gamma_p/2)\cosh\beta\nu_p + 2\exp(\beta\gamma_p) + 1] \tag{47}$$

and Eq. (41) for $\langle B\rangle$, written as

$$\frac{\partial}{\partial\lambda}\beta^{-1}\ln Z_{H'} = L^{-3}\langle B\rangle^2$$

takes the form

$$\frac{1}{2}L^{-3}\sum_{\boldsymbol{p}} \lambda g_{\boldsymbol{p}}^2 \langle B\rangle^2 E_{\boldsymbol{p}}^{-1} F(\beta, E_{\boldsymbol{p}}, \nu_p, \gamma_p) = \langle B\rangle^2 \tag{48}$$

and reduces to Eq. (29) with $g_{\boldsymbol{p}\boldsymbol{p}'} = \lambda L^{-3} g_{\boldsymbol{p}} g_{\boldsymbol{p}'}$, for $\Delta_{\boldsymbol{p}}$ defined by Eq. (46). Using Eq. (48), one finds that the free energy $\mathcal{F} = -\beta^{-1}\ln Z_{H'}$ is equal to $\mathcal{F}[\rho_0]$ given by the expression (30). This proves, together with Eq. (42), the equality (39) and establishes asymptotic exactness of the minimization procedure carried out in Secs. 2–4.

7. Conclusions

We have demonstrated that the Fermi gas with the Hamiltonian H is asymptotically solvable in the infinite-volume limit. The ground state (6) is a BCS-type product state of bound quadruples, the excitations are fermions but excitation energies are not simply additive. The system exhibits a 2nd order phase transition: at $T > T_c$ only free fermions and free bound pairs are present, at $T < T_c$ the system behaves like a gas of fermion quasiparticles with energies which are not additive. A gap is present in the spectrum which depends on the form of the pair-binding potential W. The transition temperature T_c also strongly depends on W and exceeds $T_{c(BCS)}$ if $|\varepsilon + \gamma(\varepsilon)/2|$ is sufficiently small in a sufficiently large range. The experimentally measured temperature dependences of the gap parameter of the BSCCO superconductor have been compared with the theoretical dependences resulting from H with $W = -\sum_{\boldsymbol{k}} 2|\varepsilon_k| n_{\boldsymbol{k}+} n_{\boldsymbol{k}-}$, adjusted bandwidth δ and zero-temperature gap parameter $2\Delta(\infty) = 2a\beta_c^{-1}$ for two values of $2a$, viz., $2a = 5,\ 4.05$. The theoretical curves agree qualitatively with the experimental ones. Further questions relating to the Hamiltonians H and H', in particular quantitative agreement with experiment for other choices of $\gamma(\varepsilon)$, are under investigation.

Appendix A

For the 1-parameter model with $\gamma_k = 2\gamma\lambda_k, \gamma > -1$, Eq. (10) assumes the form

$$\sum_{\lambda_k < \mu - \delta} 2 + \rho \int_{\mu-\delta}^{\mu+\delta} \left(1 - \frac{\varepsilon(1+\gamma) - \mu}{\{[\varepsilon(1+\gamma) - \mu]^2 + \Delta^2\}^{1/2}}\right) \mathrm{d}\varepsilon = n$$

and after performing integration simplifies to

$$\sum_{\lambda_k < \mu} 2 = n + \rho(1+\gamma)^{-1}$$
$$\times \left(\left\{[\mu\gamma + \delta(1+\gamma)]^2 + \Delta^2\right\}^{1/2} - \left\{[\mu\gamma - \delta(1+\gamma)]^2 + \Delta^2\right\}^{1/2}\right)$$

with the solution $\mu < \mu_F$ if $-1 < \gamma < 0$ and $\mu > \mu_F$ if $\gamma > 0$. For $\gamma = 0$ the solution is $\mu = \mu_F$.

The gap equation (9), for the same form of γ_k as assumed above, is

$$2 = g\rho \int_{\mu-\delta}^{\mu+\delta} \mathrm{d}\varepsilon \left\{[\varepsilon(1+\gamma) - \mu]^2 + \Delta^2\right\}^{-1/2}.$$

On performing integration

$$\int (x^2+1)^{-1/2} \mathrm{d}x = \mathrm{arcsinh} x$$

and solving for Δ, one obtains the solution (11).

Appendix B

In order to prove that $x^{-1}F(\beta, x, y, z)$ is decreasing in x for $x > 0$, let us first note that F has the form

$$F(\beta, x, y, z) = \frac{\sinh(2\beta x)}{\cosh(2\beta x) + g_0(\beta, y, z)}$$

and therefore, as a function of x, has the same growth and convexity properties as $\tanh \beta x$. For any function $F(x)$ with these properties, $(x^{-1}F(x))' < 0$, as can be seen from the Taylor expansion

$$F(x) = F(0) + xF'(x'), \qquad x' \in (0,x), \qquad F(0) = 0$$

and concavity of F for $x > 0 : F'(x) < F'(x')$.

Appendix C

For $\mathcal{F}[\rho_0]$ given by Eq. (30)

$$\frac{\partial \mathcal{F}}{\partial E_{\boldsymbol{k}}} = \frac{1}{2}\left[E_{\boldsymbol{k}}\beta\frac{\partial F(\beta, E_{\boldsymbol{k}}, \nu_k, \gamma_k)}{\partial \beta E_{\boldsymbol{k}}} - F(\beta, E_{\boldsymbol{k}}, \nu_k, \gamma_k)\right]\left(1 - \frac{\nu_k^2}{E_{\boldsymbol{k}}^2}\right). \tag{C.1}$$

Since $\nu_k^2 E_{\boldsymbol{k}}^{-2} \le 1$, the proof of the inequality

$$\mathcal{F}[\Delta_{\boldsymbol{k}} \neq 0] < \mathcal{F}[\Delta_{\boldsymbol{k}} = 0]$$

can be carried out by demonstrating that

$$\frac{\partial}{\partial \beta E_{\boldsymbol{k}}}(\beta E_{\boldsymbol{k}})^{-1} F(\beta, E_{\boldsymbol{k}}, \nu_k, \gamma_k) < 0. \tag{C.2}$$

This has been done in Appendix B.

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