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# COMBINED BCS AND VAN HOVE SCENARIOS: A SOLVABLE THERMODYNAMICS IN HALF-FILLED SYMMETRIC BANDS

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The subcritical and low-temperature thermodynamics is obtained for half-filled symmetric bands with the logarithmic peak of DOS in the centre. The ratio of the zero temperature order parameter to the critical temperature coincides with the BCS value for $S$-pairing but is slightly different for $D$-pairing. Moreover, the relative jumps of the critical specific heat coincide with conventional BCS results for $S$- and $D$-pairing as well.

We are going to consider the $S$-, [1] and $D$-paired electrons in the band with the following DOS, per unit volume and spin

$$N(\varepsilon) = N(0)[a - \ln|\varepsilon|], \quad |\varepsilon| \le 1, \;\; a \ge 0, \tag{1}$$

with $\varepsilon$ being the particle energy in the units of the half-width of the band. Because of the bilateral symmetry, the chemical potential is equal to zero and temperature-independent in the symmetric bands at their half-filling, [2], for both normal and BCS-superconducting systems. For an appropriate choice of $N(0)$ and $a$, the DOS (1) is a quite good approximation to the real DOS in the square lattice when the tight binding overlap integrals are restricted to the nearest neighbours [3]. Similar DOS has been used in the thermodynamic calculations in HTSC [4–6], for $S$-pairing in the BCS approach [4,5] and for $S$- and $D$-pairing in the charge transfer model [6].

In the papers [4,5] the main topic was restricted to the calculation of the ratio $\Delta(0)/T_c$ and to the penetration depth [5]. Note that this problem has recently attracted a lot of attention in the context of the planar electron motion in HTSC, c.f. the review article [7].

The BCS-like gap equation [1], for our system reads

$$\frac{1}{\kappa} = \int_0^1 d\varepsilon (a - \ln\varepsilon) \left\langle d^2(\hat{\mathbf{p}}) \frac{\tanh(E_\varepsilon/2T)}{E_\varepsilon} \right\rangle_{\mathbf{p}}, \tag{2}$$

where $E_\varepsilon^2 = \varepsilon^2 + d^2(\hat{\mathbf{p}})\Delta^2$, $\Delta$ is the order parameter, $\kappa \equiv \lambda N(0)$ with $\lambda$ being $S$ or $D$ the coupling constant. The function $d^2(\hat{\mathbf{p}})$ is equal to 1 for $S$-pairing and to $\sqrt{2}(\hat{p}_x^2 - \hat{p}_y^2)$, $\hat{\mathbf{p}} = \mathbf{p}/p$, for $D$-pairing in the plane. The bracket $\langle \dots \rangle_{\mathbf{p}}$ denotes the angular average. Herein we consider only the weak coupling, $\kappa \ll 1$.

Calculating the integral (2) in the limiting cases $\Delta = 0$ or $T = 0$, with the accuracy up to the big logarithms $|\ln T_c|$ or $|\ln \Delta(0)|$, we find

$$T_c = \frac{2}{\pi} \exp\left(a + c - 1/x\right)[1 + O(x^2)], \quad (S, D), \tag{3}$$

$$\Delta(0) = 2\exp\left(a - 1/x\right)[1 + O(x^2)], \quad (S),$$

$$\Delta(0) = \frac{1}{\sqrt{2}} \exp\left(a + 1 - 1/x\right)[1 + O(x^2)], \quad (D), \tag{4}$$

where $x \equiv \sqrt{\kappa/2}$ and $c$ is the Euler constant. To accomplish the integral (2) at $T_c$ we need only the integration by parts, whereas at $T = 0$, the integration by parts after the substitution $\varepsilon = \Delta|d(\hat{\mathbf{p}})|\mathrm{sh}u$. The angular integrals for $D$-pairing are well known. As we see, the ratio $\Delta_s(0)/T_c$ attains its BCS value, [1,4,5]. On the other hand, the ratio $\Delta_D(0)/T_c$ is the product of the BCS value and $e/2\sqrt{2} \approx 0.961$. It is note worthy that this factor for $D$-pairing at energy-independent DOS, i.e., $D$-superconductors of the BCS type is $\sqrt{2/e} \approx 0.858$.

In all further calculations, we will apply the conventional methods of the theory, cf., e.g., [8,9], substituting the DOS (1) into the appropriate integrals determining thermodynamic functions. Let us discuss the subcritical properties first. For the order parameter we have

$$\Delta(T) = \Delta_{\mathrm{BCS}}(T)(1 - 0.121x) + O(\tau^{3/2}), \quad (S),$$

$$\Delta(T) = \sqrt{\frac{2}{3}}\Delta_{\mathrm{BCS}}(T)(1 - 0.121x) + O(\tau^{3/2}), \quad (D), \tag{5}$$

where $\tau \equiv 1 - T/T_c$. The sub or supercritical specific heat, per unit volume, is given by

$$C = 2\pi^2 N(0)\left\{\left[\frac{4T_c}{7\zeta(3)x}(1 + O(\tau)) + O(1)\right]\Theta(\tau) - \frac{1}{3}T(\ln T + O(1))\right\}, \tag{6}$$

for the $S$-pairing, where $\Theta$ is the Heaviside step function. For the $D$-pairing, the term proportional to $\Theta$ should be multiplied by $4/9$. Hence, the critical jump of the specific heat in the main term coincides with the BCS value divided by $x$ or $9/4\,x$, for $S$ or $D$ pairing, respectively. On the other hand, the relative jump coincides with the BCS results because of the term $O(T\ln T)$ for $S$ pairing and with $4/9$ of the BCS value for $D$ pairing.

Let us pass to the compressibility, $(\partial\varrho/\partial\mu)_{V,T}\varrho^{-2}$, where $\varrho$ is the density of the system. We have the general formula, valid for half-filled symmetric bands

$$\left(\frac{\partial\varrho}{\partial\mu}\right)_{V,T} = 2N(0)\left\langle \frac{a}{E_1} + \int_0^1 d\varepsilon \frac{\tanh(E_\xi/2T)}{E_\varepsilon} \right\rangle_{\mathbf{p}} . \tag{7}$$

For the normal system, from (7) we get

$$\left(\frac{\partial\varrho}{\partial\mu}\right)_{V,T} = 2N(0)[a + c + \ln(2/\pi T)], \tag{8}$$

and the compressibility is logarithmically divergent if $T \to 0$. Note that in the normal systems, the spin susceptibility $\chi$ equals $\mu_B^2(\partial\varrho/\partial\mu)_{V,T}$, with $\mu_B$ being Bohr's magneton. For $S$ and $D$ paired systems we have

$$\left(\frac{\partial\varrho}{\partial\mu}\right)_{V,T} = 2N(0)\left[\frac{1}{x} + \tau - \tau\left(1 + \frac{4\pi^2 T_c^2}{7\zeta(3)}\right)\Theta(\tau)\right], \tag{9}$$

with the accuracy $O(\tau^2)$. Note that the difference between $S$ and $D$ paired systems is of the same order. Let us add that the difference between the normal and superconducting phases is equal to the term proportional to $\Theta$. The spin susceptibility is equal to, cf. [10]

$$\begin{aligned} \chi &= \frac{2}{x}\mu_B^2 N(0)[1 - 2\tau + O(\tau x)], \quad (S), \\ \chi &= \frac{2}{x}\mu_B^2 N(0)\left[1 - \frac{4}{3}\tau + O(\tau x)\right], \quad (D). \end{aligned} \tag{10}$$

Note that the simplicity of the coefficients at $\tau$ in Eqs. (10) are the result of analytic calculation of some integral not appearing in usual sources [11].

Considering low-temperature properties, let us start from the energy difference between $S$ or $D$ and the normal system. Almost repeating the calculations of Ref. 1 (cf. also the comments after the formula (4)) we find

$$\frac{1}{V}(E_{\rm sup} - E_n) = -\frac{1}{2}N(0)\Delta^2(0)\begin{cases} 1/x + 1/2, & (S), \\ 1/x + 1 - 3/2\,\ln 2, & (D). \end{cases} \tag{11}$$

For the low-temperature order parameter we find

$$\frac{\Delta(T)}{\Delta(0)} = 1 - \begin{cases} (\pi T/\Delta)^{1/2}\ \exp(-\Delta/T)\,(1 - x\ln T + O(x)), & (S), \\ \sqrt{2}\,x\,(\ln T + O(1))(T/\Delta)^3 \sum\limits_{n=1}^{\infty}(-1)^n n^{-3}, & (D). \end{cases} \tag{12}$$

Note that $\sqrt{2}\sum_{n=1}^{\infty}(-1)^n n^{-3} \approx -1.2750$. The specific heat, per unit volume, is given by

$$C = N(0)T \begin{cases} (2\pi\Delta^5/T^5)^{1/2}\ \exp(-\Delta/T)\ (1/x - \ln T + O(1)), & (S), \\ 12\sqrt{2}(T/\Delta)(\ln T + O(1)) \sum_{n=1}^{\infty}(-1)^n\, n^{-3}, & (D). \end{cases} \tag{13}$$

Determining the compressibility, one can write

$$\left(\frac{\partial \varrho}{\partial \mu}\right)_{V,T} = 2N(0)\left(\frac{1}{x} - \frac{\Delta(T)-\Delta(0)}{\Delta(0)}\right) + 2N(0)\begin{cases} 0, & (S), \\ 1 - 1/2\,\ln 2, & (D). \end{cases} \tag{14}$$

As we see, the infinite limit value of $(\partial\varrho/\partial\mu)_{V,T}$ in the normal state is replaced here by the large value $2N(0)/x + O(1)$, as a result of a quasiparticle distribution functions smeared out in the superconducting state. For the spin susceptibility we have

$$\chi = \mu_B^2 N(0)\begin{cases} (2\pi\Delta/T)^{1/2}\ \exp(-\Delta/T)\ (1/x + a + c - \ln T + O(x)),\ (S), \\ -2\sqrt{2}\ \ln 2\ (T/\Delta)\ (\ln T + O(1)),\ (D). \end{cases} \tag{15}$$

It is interesting to note that the temperature derivative of $\chi$ is logarithmically divergent for the $D$-pairing.

In calculations of subcritical thermodynamic functions we applied their series expansions with respect to $\Delta^2$ and used the typical integral of the BCS theory [1,8,9]. In the low-temperature limit, the asymptotic form of the integral was obtained, according to the ideas of Ref. 12. For $D$-pairing, it was done in a more sophisticated way. The validity of these results for this model is firm through the general theorem proved by Bogoliubov [13].

Note that for the chemical potential, $\mu$, such that $0 < |\mu| \ll 1$, even for the normal systems we have two low-temperature regimes, $|\mu| \ll T \ll 1$ and $T \ll |\mu| \ll 1$. For the superconductivity systems we have 3! regimes obtained by the permutations of $\Delta(T)$, $|\mu|$ and $T$. Moreover, because the particle-hole symmetry is broken and, hence, $\mu_s - \mu_n = O(\Delta^2)$ we deal with the first-order phase transition, because the subcritical $\Omega_s - \Omega_n$ is $O(\Delta^4)$ and the character of $\Delta$ still remains unchanged [2].

Note that treating our system as a gas we find that the relative jump of the critical specific heat is equal to

$$1.43\ \varrho^2/p\left.\left(\frac{\partial\varrho}{\partial\mu}\right)\right|_{T_c} = 1.43\ x\ \frac{(a+1)^2}{(a+\frac{3}{4})} + O(x^2(1+a^2)), \tag{16}$$

for $S$-pairing and $\frac{2}{3}$ of this value for $D$-pairing.

The details of calculations and some formulae calculated to higher orders will be published elsewhere. In addition, the normal system will be considered also at filling close to the particle-hole symmetric case.

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