VALIDITY OF SOME RESULTS IN SUPERCONDUCTIVITY THEORY

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ABSTRACT: Some of the expressions for the uncorrelated part of the two-particle propagator in terms of digamma functions, and the results obtained therefrom, contain intrinsic limitations concerning Q, the total momentum of the electron pair. We find that for such cases $Q \lesssim 2m/\beta q_F$ where m is the electron mass, $\beta = (kT)^{-1}$ and q_F is the Fermi momentum. Here we present an alternative derivation of a result previously reported that throws some light on this problem.

INTRODUCTION

In a previous publication[1] we evaluated the uncorrelated part of the two-particle propagator

*This work was begun while the author was on leave at the Department of Physics, University of Illinois.

$$L_0(\mathbf{Q}, \Omega_\nu + 2\mu) =$$

$$= i \frac{1}{-i\beta} \sum_n \int \frac{d^3\mathbf{q}}{(2\pi)^3} G(\mathbf{q}, -Z_n + \mu)\, G(\mathbf{Q}-\mathbf{q}, \Omega_\nu + Z_n + \mu)\,, \quad (1)$$

in order to obtain an explicit expression for the many-body T-matrix. In the process of obtaining such a result we performed first the integration over the momenta, and then the summation over the frequencies in a rather conventional way, since this technique simplified the work involved. However, care had to be taken to bring the mathematical results back to reproduce the physics being described. For that reason the formally divergent summation was "cured" so that the BCS result for β_c, the transition temperature, would obtain. In this manner a result was given for the T-matrix that describes the multiple scattering between pairs of particles (electrons) of total momentum Q and total energy Ω. The divergence of the T-matrix for zero Q and zero Ω was the indication that for $\beta = \beta_c$ the system was undergoing a second order phase transition to the superconducting state. This is due to the fact that ordinary (infinite) perturbation theory cannot be used for the description of the superconducting state, since the ground state energy depends on the pair potential in an exponential manner.

In Ref. 1 we mentioned that the order in which we carry out both the summation and the integration in Eq. (1) should be immaterial. The present paper shows that that is true and in so doing we discover that in order for $L_0(\mathbf{Q}, \Omega_\nu)$ to be obtainable in terms of digamma functions the total momentum Q has to be bounded, which from a physical view-point sounds reasonable since, after all, we are restricting the kinetic energy of the individual electrons of the pair to be within a shell given by

$$\frac{|q^2 - q_F^2|}{2m} \lesssim \omega_D \,.$$

Nevertheless the restriction in Q is not derivable from the expression above. We obtain, therefore, a momentum $Q_{\max}$ that consequently restricts the validity of any result that depends on the use of $L_0(\mathbf{Q}, \Omega_\nu)$ as derived in Ref. 1. In particular, our result for the T-matrix is thereby restricted and any integration performed over the total momentum has to be, by necessity of the consistency of the model, restricted to the interval $[0, Q_{\max}]$. This restriction will be extremely useful in future calculations concerning the behavior of transport coefficients in the critical region.

In the next section we perform the mathematical evaluation of Eq. (1) by carrying out first the summation over the frequencies, and then the integration over the momenta so that an expression for Q_{max} will emerge naturally if we require L_0 to be expressible in terms of digamma functions, and consequently, if we want the T-matrix derived in Ref. 1 to be valid.

EVALUATION OF THE FUNCTION

As discussed in Ref. 1 Eq. (1) may be written, after the simplifications common in the theory of metals, as follows:

$$L_0(\mathbf{Q}, \Omega_\nu + 2\mu) =$$

$$= i \frac{1}{-i\beta} \sum_n N(0) \int \frac{d\Omega_a}{4\pi} \int d\xi \, \frac{1}{-Z_n - \xi} \, \frac{1}{Z_n + \Omega_\nu - \xi + \mathbf{Q}\cdot\mathbf{v}_F - \frac{Q^2}{2m}} \, . \tag{2}$$

Since $Z_n = (2n+1)(\pi/-i\beta)$ we can carry out the summation over the frequencies by means of the Poisson summation formula:

$$\frac{1}{-i\beta} \sum_n h(Z_n) = \oint_C \frac{dZ}{2\pi} f(Z)\, h(Z) \tag{3}$$

with

$$f(Z) = [e^{\beta Z} + 1]^{-1} \, , \tag{4}$$

where the contour C encircles all the poles of $h(Z)$ in the positive sense, and none of the poles of $f(Z)$. This formula is valid if we can neglect the contributions to the integral from the circle with infinite radius, which implies[2] that $h(Z)$ should vanish as $|Z| \to \infty$. Therefore we obtain

$$L_0(\mathbf{Q}, \Omega_\nu + 2\mu) =$$

$$= N(0) \int \frac{d\Omega_a}{4\pi} \int d\xi \, \frac{1 - f(\xi) - f\left[\xi - \mathbf{Q}\cdot\mathbf{v}_F + \frac{Q^2}{2m}\right]}{\Omega_\nu - 2\xi + \mathbf{Q}\cdot\mathbf{v}_F - \frac{Q^2}{2m}} \, , \tag{5}$$

where we have used the fact that $f(\Omega_\nu + \alpha) = f(\alpha)$, since

$$e^{-\beta\Omega_\nu} = e^{-2\pi n i} = 1\,,$$

and also $f(-\xi) = 1 - f(\xi)$. The term $Q^2/2m$ is smaller than the term $\mathbf{Q}\cdot\mathbf{v}_F$ by a factor $Q/2q_F$ and due to the fact that our results in terms of digamma functions will be valid only when $Q \ll q_F$, as we shall shortly show, we may neglect the term proportional to Q^2 that appears in the numerator, and expand the function $f(\xi - \mathbf{Q}\cdot\mathbf{v}_F)$ around $Q = 0$. Then keeping terms up to first order in Q, introducing the cosine between $\mathbf{Q}$ and $\mathbf{v}_F$ as the variable x, and considering that the function $f(\xi)$ is a slowly varying function, bounded $([0,1])$, and real, we obtain

$$L_0(\mathbf{Q}, \Omega_\nu + 2\mu) \cong$$

$$\cong N(0)\int\frac{d\Omega_a}{4\pi}\int d\xi\,\frac{1-2f(\xi)}{\Omega_\nu - 2\xi + \mathbf{Q}\cdot\mathbf{v}_F - \dfrac{Q^2}{2m}} + \qquad (6)$$

$$- N(0)\;Qv_F\beta\overline{f}(\xi)\int\frac{d\Omega_a}{4\pi}\,x\int d\xi\,\frac{1-f(\xi)}{\Omega_\nu - 2\xi + \mathbf{Q}\cdot\mathbf{v}_F - \dfrac{Q^2}{2m}}\;;$$

where we have used the mean value theorem for integrals.*

Now, due to the fact that the integrands of both terms are almost the same (give or take a factor of two), we see that the contribution of the second term will be negligible when $Qv_F\beta\overline{f}(\xi) < 1$, or equivalently, when

$$Q < \frac{1}{v_F\beta\overline{f}(\xi)} \approx \frac{2m}{\beta q_F}\,. \qquad (7)$$

This result is consistent with the fact that keeping terms up to first order in the Taylor expansion used in going from Eq. (5) to Eq. (6) is a valid approximation only when terms of higher order are negligible, and this happens to be true when

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*See for instance T.M. Apostol, "Mathematical Analysis", Addison Wesley, 1957, page 269.

Eq. (7) holds. If we can now prove that the first term in Eq. (6) gives rise to the result reported in Ref. 1, we will have shown that the expression quoted in that reference is valid only when the total momentum of the electron pair satisfies Eq. (7); i.e., when the second term on the r.h.s. of Eq. (6) can be neglected.

We are now going to evaluate the first term of Eq. (6). Consider then

$$I = N(0)\int \frac{d\Omega_a}{4\pi}\int d\xi \; \frac{1-2f(\xi)}{\Omega_\nu^{\cdot} + Qv_F x - \frac{Q^2}{2m} - 2\xi}$$

$$= N(0)\int \frac{d\Omega_a}{4\pi}\int_{-\omega_D}^{+\omega_D} d\xi \; \frac{\tanh\frac{\beta\xi}{2}}{t-2\xi} \quad . \qquad (8)$$

If absolute convergence of the integral when $|\xi| \to \infty$ can be assured, the limits of the ξ-integration may be relaxed to $[-\infty, +\infty]$, and the integral evaluated by contour integration techniques. To obtain this convergence we proceed as follows. We add and substract the term $(1/2\xi)\tanh(\beta\xi/2)$ to the integrand in Eq. (8), to obtain

$$I = -N(0)\left\{\int d\xi \; \frac{\tanh\frac{\beta\xi}{2}}{2\xi} + \int\frac{d\Omega_a}{4\pi}\, t\int d\xi \; \frac{\tanh\frac{\beta\xi}{2}}{2\xi(2\xi - t)}\right\} \qquad (9)$$

The first integral in the equation above is nothing but the BCS equation for β_c and its solution is well known[3]. The second term is now convergent as $|\xi|^{-2}$ when $|\xi| \to \infty$ and therefore we may relax the limits of integration. Care should be taken with the zero of the denominator for $\xi = 0$; however, since $\tanh\beta\xi/2 \to 0$ when $\xi \to 0$ also, it can be shown that the origin is not a singular point and does not have to be considered when discussing the poles of the analytic continuation of the integrand. Then

$$I = -N(0)\left\{\ln\frac{2\beta\omega_D\gamma}{\pi} + \int\frac{d\Omega_a}{4\pi}\,\mathcal{J}\right\}$$

with

$$\mathcal{I} = t\int_{-\infty}^{+\infty} d\xi \, \frac{\tanh \frac{\beta\xi}{2}}{2\xi\,(2\xi - t)} = \frac{\beta t}{2} \oint_C \frac{\tanh y}{2y\left(2y - \frac{\beta t}{2}\right)}\, dy \tag{10}$$

where C encircles all the poles $y_n = (2n+1)(\pi i/2)$(with n a whole number) of the function tanh y, in the positive sense. Therefore

$$\mathcal{I} = \sum_{n>0} \left\{ \frac{2}{2n+1+i\beta t/2\pi} - \frac{2}{2n+1} \right\} .$$

The summation can be written in terms of digamma functions as[4]:

$$\mathcal{I} = \psi(\tfrac{1}{2}) - \psi(\tfrac{1}{2} + \tfrac{i\beta}{2\pi}\,\tfrac{t}{2}) \tag{11}$$

from which we finally obtain

$$I = - N(0)\int \frac{d\Omega_a}{4\pi} \left\{ \ln \frac{2\beta\omega_D\gamma}{\pi} + \right.$$
$$\left. + \psi(\tfrac{1}{2}) - \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\,\frac{\Omega_\nu + Qv_F x - \frac{Q^2}{2m}}{2}\right)\right\} \tag{12}$$

a result identical to the one derived in the Appendix to Ref. 1.

CONCLUSIONS

We have just shown that the result obtained in Ref. 1 for the uncorrelated part of the two-particle Green's function and consequently, the T-matrix calculated therein is valid only if the total momentum of the electron pair is restricted as in Eq. (7):

$$Q < \frac{2m}{\beta q_F} \equiv Q_{\max} \quad ,$$

for if we neglect the second term in Eq. (6) we have that $L_0(\mathbf{Q}, \Omega_\nu + 2\mu) \equiv I$, with I given by Eq. (12). Moreover we have shown that the order in which the summation and integration are performed is immaterial, as it should be.

That the restriction (7) is important can be seen by giving an order-of-magnitude calculation of Q_{max}. We know that q_F is related to the interparticle spacing a_0 by $q_F \sim (a_0)^{-1}$. Since $a_0 \sim 1\,\text{Å}$, we get $q_F \sim 10^8\ \text{cm}^{-1}$. On the other hand, for temperatures of the order of 10 kelvins we obtain a $Q_{max} \sim 10^4$. Therefore the assumption utilized in the paragraph above Eq. (6) is seen to be justified *a posteriori*, since $Q/q_F \lesssim (Q_{max}/q_F) \sim 10^{-4} \ll 1$ and consequently the term $Q^2/2m$ is much smaller than $\mathbf{Q} \cdot \mathbf{v}_F$. Moreover, $Q \lesssim Q_{max}$ represents a restriction additional to the better known[5,6] constraint on the *total* energy $\omega \leqslant \omega_D$ characteristic of the BCS model.

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RESUMEN

Algunas de las expresiones obtenidas para la parte no correlacionada del propagador de dos partículas en términos de funciones digama, y resultados que la contengan, tienen limitaciones intrínsecas en relación al valor del momento Q de los pares electrónicos. Se encuentra que en tales casos $Q \lesssim 2m/\beta q_F$, donde m es la masa, $\beta = (kT)^{-1}$ y q_F es el momento de Fermi del sistema de consideración. Aquí se presenta otra manera de derivar un resultado publicado previamente que aclara estas limitaciones.