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THE T-MATRIX FOR PURE SUPERCONDUCTORS JUST ABOVE THE TRANSITION TEMPERATURE

Ariel A. Valladares*
Instituto de Física,
Centro de Investigación de Materiales,
Universidad Nacional de México
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RESUMEN

Se calcula la matriz T de muchos cuerpos para un sistema de fermiones que interactúan únicamente por medio de una fuerza simple de dos cuerpos y atractiva, a una temperatura apenas mayor que la temperatura de transición β_c^{-1} a la fase superconductora. Este modelo ha sido discutido por Kadanoff and Martin, quienes han mostrado que la aparición de un polo complejo en la matriz T, como función de la temperatura, para valores nulos de la energía y del impulso lineal, indican la transición a la fase superconductora. En este trabajo se evalúa la matriz T para impulso lineal total y energía diferente de cero.

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

ABSTRACT

The many-body T-matrix is calculated for a system of fermions interacting only through a simple two-body attractive interaction, just above the superconducting transition temperature β_c^{-1}. *This model has been discussed by Kadanoff and Martin who have shown that the appearance of a complex pole in the T-matrix as a function of temperature, for zero energy and momentum, signals the transition to the superconducting phase. Here the T-matrix for total momentum and energy different from zero is evaluated.*

I. INTRODUCTION

As part of a program to investigate the validity and limitations of both the non-conserving and conserving T-approximations to the two-particle Green's function[1] in the theory of superconductivity, we have calculated the many-body T-matrix for non-zero total momentum and energy, both for pure and dirty superconductors just above the transition temperature. In this paper we report the value of the T-matrix for pure superconductors using the simplified model of Kadanoff and Martin[2]. This model is such that the fermions are allowed to interact only through a two-particle constant attractive potential different from zero on a shell about the Fermi surface. The condition

$$\frac{|k^2 - k_F^2|}{2m} \leqslant \omega_D \tag{1}$$

which restricts the momentum of the incoming particles k, defines this shell. Here k_F is the Fermi momentum and ω_D is the Debye frequency*. The Debye cutoff appears here rather artificially but, as we shall see later on, its usage is connected with the appearance of some otherwise divergent integrals due to the

*We use units such that $\hbar = 1$ throughout this paper.

idealistic nature of the attractive potential proposed. Morel and Anderson[3] have shown that when a more realistic retarded potential is used, the Debye cutoff appears naturally.

The many-body T-matrix as discussed by Kadanoff and Baym[4], is characterized by the fact that multiple scattering processes of the direct and exchange types are included automatically up to an infinite order in the scattering potential. This approximation is useful for cases in which the scattering potential acting between the particles is *not* small even though its overall effect may be small because the range of this potential is short. In this discussion we are using the zero-range potential introduced in reference 2, so we expect the T-matrix to give a realistic representation of the interaction taking place in our simplified model.

The idea of considering the influence of multiple-scattering processes in the superconducting phase transition was expounded by Thouless[5], who utilized the ladder approximation to the thermodynamic potential in pure superconductors both above and below the transition temperature. Our work reproduces the results of Thouless above β_c^{-1}, but also introduces some new features due to the inclusion of impurities, and the use of the conserving T-approximation, as will be shown in a forthcoming publication[12].

In section II of this paper we define the T-matrix following the nomenclature used in reference 4, and reproduce some of the properties of this approximation which are given fully in that reference. The approximations used are clearly established in this section and the structure of the T-matrix for these approximations is also discussed. Section III presents the actual calculation of the T-matrix for our model. Some of the integrals that appear in this section are evaluated in the Appendix, where the assumptions used in obtaining the mathematical results are pointed out.

II. DEFINITIONS AND APPROXIMATIONS

The generalization of Quantum Field Theory techniques to treat condensed systems has been one of the most successful tools in the study of these systems.

Martin and Schwinger[6] have developed a very elegant theory for this purpose. Very succintly we can say that the bases of their method are:

i) The equations of motion that the Green's functions, or time-dependent field correlation functions, should obey. These equations of motion are obtained directly from the Heisenberg equations of motion that the field operators satisfy, and therefore are a consequence of the Quantum-Mechanical treatment of the problem.

ii) The boundary condition, which permits first, to characterize fully the solutions to the equations of motion, since these equations are first-order differential equations in the time variables, and the boundary condition is a time-boundary condition; and second, to introduce directly in the formalism the thermodynamical characterization of the averages in terms of which the correlation functions are defined.

iii) The analytic continuations necessary to pass from the complex-frequency Fourier analysis (which takes into account the boundary condition), to the real-frequency Fourier coefficients. Baym and Mermin[7] have shown that, given a Fourier coefficient $G(z_\nu)$ defined for a set of discrete points in the complex z-plane, a unique analytic continuation $G(z)$ may be achieved, if and only if, a) $G(z)$ is analytic for z off the real axis, and b) $G(z) \to 0$ when $z \to \infty$ along any straight line in the upper or lower half-plane.

The Green's functions or time-dependent field correlation functions are grand-canonical averages of diagonal matrix elements of certain products of field operators. For our purposes, we shall be interested in the one-electron Green's function $G_1(1,1')$, in terms of which the T-matrix is defined. This function G_1 is defined as

$$G_1(1,1') = -i \frac{TR\left[e^{-\beta(H-\mu N)} T(\psi(1)\psi^+(1')\right]}{TR\, e^{-\beta(H-\mu N)}} \qquad (2)$$

where T is the chronological operator that orders from right to left in order of increasing distance from the origin towards $(-i\beta)$, along the negative part of the

imaginary axis in the complex t-plane. T also introduces a change in sign according to the number of permutations of the operators in passing from the standard ordering in Eq. (2) to the ordering required by the operator T. This change in sign is represented by $(-1)^P$, where P is the number of permutations. Therefore we may symbolically write

$$T(\quad) = (-1)^P (\quad)_+ \tag{3}$$

where $(\quad)_+$ indicates only the time-ordering operation. The field operators in Eq. (2) satisfy the anticommutation relations

$$\{\psi(1), \psi(1')\} = \{\psi^+(1), \psi^+(1')\} = 0 \ ,$$

$$\{\psi(1), \psi^+(1')_{t_1 = t_1'}\} = \delta(r_1 - r_1') \ , \tag{4}$$

where the number in the arguments represent both space and time variables. The reason for the appearance of complex-time arguments in this formalism is due to the fact that, in this manner, the boundary condition takes an especially simple form[4, 6],

$$G_1(1,1')\big|_{t_1 = 0} = -e^{\beta\mu} G_1(1,1')\big|_{t_1 = -i\beta} \ , \tag{5}$$

and therefore it can be included directly in the formalism by expanding the function $G_1(1,1')$ in a Fourier series along the interval $[0, -i\beta]$ in the complex t-plane. Then

$$G_1(1,1') = \frac{1}{-i\beta} \sum_\nu e^{-i\omega_\nu (t_1 - t_1')} G_1(r_1, r_1'; \omega_\nu) \ , \tag{6}$$

where we have assumed that the system is "homogeneous" in time. Clearly, if we want condition (5) to be satisfied by the representation (6), we should have

$$\omega_\nu = \mu + z_\nu \equiv \mu + \frac{(2\nu+1)}{-i\beta}\pi \quad , \qquad \nu = \text{integer}, \tag{7}$$

which defines the set of discrete points for which the coefficient $G_1(r_1, r_1', \omega_\nu)$ has been calculated.

The function $G_1(1,1')$ is obtained from the equation of motion

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right) G_1(1,1') = \delta(1-1') - i\int dr_2\, v(r_1 - r_2)\, G_2(12;1'2^+)\Big|_{t_1 = t_2} \tag{8}$$

where $v(r_1 - r_2)$ is a two-body potential acting between the particles. G_2 is the two-electron Green's function defined as

$$G_2(12;1'2') = (-i)^2\, \frac{TR\left[e^{-\beta(H-\mu N)}\, T(\psi(1)\psi(2)\psi^+(2')\psi^+(1')\right]}{TR\, e^{-\beta(H-\mu N)}} \tag{9}$$

and

$$2^+ \equiv (r_2, t_2 + \epsilon), \text{ when } \epsilon \to 0^+ \tag{10}$$

Since we are assuming that the particles are free between the scatterings due to the two-body attractive potential that produces the condensation in momentum space of the Fermi liquid, typical of the superconducting phase, the equation that would describe this free propagation can be obtained from Eq. (8) by setting the potential equal to zero; that is,

$$\left(i\frac{\partial}{\partial t_1} + \frac{\nabla_1^2}{2m}\right) G_1^0(1,1') = \delta(1-1') \tag{11a}$$

By Fourier-transforming the above equation both in time and space we obtain

$$G_1^0(k, z_\nu + \mu) = \frac{1}{z_\nu - \epsilon(k) + \mu} \quad , \tag{11b}$$

where we show explicitly the dependence on μ, the chemical potential. $\epsilon(k)$ is given by the free-particle expression $k^2/(2m)$.

When the scattering potential is taken into account Eq. (8) may be solved in terms of Eqs. (11) to give

$$G_1(1,1') = G_1^0(1,1') + \int G_1^0(1,\bar{2})\, \Sigma(\bar{2},\bar{2}')\, G_1(\bar{2}',1') \quad , \tag{12}$$

$$\Sigma(2,2') = -i \int V(2-\bar{3})\, G_2(2\bar{3}; \bar{4}\bar{3}^+)\, G_1^{-1}(\bar{4},2') \quad , \tag{13}$$

the self-energy or mass operator. The bars over the arguments, e.g. $\bar{2}$, indicate both space and time integrations with the time argument varying in the interval $[0, -i\beta]$, and $V(1-2) = \delta(t_1 - t_2)\, v(r_1 - r_2)$. Since our system is homogeneous in space and time, we can find the Fourier transform of Eq. (12) and solve for G_1, obtaining

$$G_1(k, z_\nu + \mu) = \frac{1}{z_\nu - \epsilon(k) + \mu - \Sigma(k, z_\nu + \mu)} \quad . \tag{14}$$

It is clear, from the equation above, that the real part of the mass operator Σ, gives rise to a correction to the electron energy. The imaginary part will give us information about the life-time of the particle in the state of momentum k. The contribution of the real part of Σ may be taken into account by redefining the electron energies $\epsilon(k)$ to include this term. Since we are not interested in renormalization effects in this paper, we are going to neglect altogether the corrections due to the mass operator in Eq. (14), and, as far as the T-approximation to the *two-particle* Green's function is concerned, we will assume that the propagation of an electron is going to be represented by Eqs. (11). This is our first approximation.

The second approximation we shall make refers to the structure of the attractive potential that shall be used. We propose it to be of the form

$$V(1-2) = -\lambda V \delta(1-2)\, \delta_{\alpha+\beta,\,0} \quad , \tag{15a}$$

with

$$V = \begin{cases} |V| \text{ , for } \dfrac{|k^2 - k_F^2|}{2m} \leqslant \omega_D \\ \\ 0 \text{ , for } \dfrac{|k^2 - k_F^2|}{2m} > \omega_D \end{cases} . \tag{15b}$$

Since the potential proposed is a zero-range attractive potential of strength λV, the only kind of particles that would interact through it are particles with opposite spins, due to the Pauli exclusion principle. This fact is shown explicitly in Eqs. (15) by means of the function $\delta_{\alpha+\beta,\,0}$. Here α and β refer to the projection of the spins of the particles along the axis of quantization. The dimensionless constant λ is assumed to vary between zero and one, and it will become useful in future calculations. The Debye cutoff ω_D that appears in Eqs. (15), has already been discussed in the introduction. So, the second-quantized Hamiltonian for our system may be written as

$$H(t) = \sum_{\alpha} \int dr \psi_{\alpha}^{+}(r,t) \left(-\frac{\nabla^2}{2m} \right) \psi_{\alpha}(r,t) +$$

$$- \frac{\lambda V}{2} \sum_{\alpha} \int dr \psi_{\alpha}^{+}(r,t) \psi_{-\alpha}^{+}(r,t) \psi_{-\alpha}(r,t) \psi_{\alpha}(r,t) \quad . \tag{16}$$

Now that we have established the approximations to be used in this paper, we are going to analyze the structure of the T-matrix using these approximations. As given in reference 4 the many-body T-matrix is defined by the equation

$$<12|T|1'2'> = V(1-2)\,\delta(1-1')\,\delta(2-2') + \\ + iV(1'-2')\int <12|T|\bar{1}\bar{2}>\, G(\bar{1},1')\,G(\bar{2},2') \,. \tag{17}$$

It is clear from the equation above that T has the following structure,

$$<12|T|1'2'> = \delta(t_1-t_2)\,\delta(t_1'-t_2')\,<r_1, r_2|T(t_1-t_1')|r_1', r_2'> \tag{18}$$

for instantaneous two-body potentials. In particular, if the potential has the form given by Eq. (15) the structure simplifies even more and we have

$$<1\alpha, 2\beta|T|1'\alpha, 2'\beta> = <1|T_\lambda^{\alpha\beta}|1'>\,\delta(1-2)\,\delta(1'-2')\,\delta_{\alpha+\beta,\,0} \tag{19}$$

Using this result and Eq. (15), we find that Eq. (17) becomes

$$<1|T_\lambda^{\alpha,-\alpha}|1'> = -\lambda V\delta(1-1') - i\lambda V\int <1|T_\lambda^{\alpha,-\alpha}|\bar{1}>\, G_\alpha(\bar{1},1')\,G_{-\alpha}(\bar{1},1') . \tag{20}$$

The subscript λ in T is meant to remind us of the presence of the "strength" parameter that appears in the scattering potential. The superscripts in T clearly show that the potential we are using acts between particles of opposite spin as was discussed previously. If we now suppress the spin indices, and introduce the definition

$$L_0(1,2) = iG(1,2)\,G(1,2) \tag{21}$$

where $(-i)\,L_0(1,2)$ is clearly the uncorrelated part of the two-particle Green's function, we may write Eq. (20) as

$$<1|T_\lambda|1'> = -\lambda V\delta(1-1') - \lambda V\int <1|T_\lambda|\bar{1}>\, L_0(\bar{1},1') \,. \tag{22}$$

This is the equation that we shall solve approximately in the next section, in order to find an explicit expression for the T-matrix for non-zero total momentum and energy of the pair.

III. CALCULATION OF THE T-MATRIX

By looking at Eq. (22) and taking into account the boundary condition of Eq. (5), we find that the T-matrix satisfies the following boundary condition[4],

$$< 1 \mid T \mid 1' > \mid_{t_1 = 0} = e^{2\beta\mu} < 1 \mid T \mid 1' > \mid_{t_1 = -i\beta} \quad . \tag{23}$$

Therefore, we can Fourier-analyze the time structure of the T-matrix as

$$< 1 \mid T \mid 1' > = \frac{1}{-i\beta} \sum_{\nu} e^{-i\omega_\nu (t_1 - t_1')} < r_1 \mid T(\omega_\nu) \mid r_1' > \tag{24}$$

with

$$\omega_\nu = 2\mu + \frac{2\pi\nu}{-i\beta} = 2\mu + \Omega_\nu \quad , \tag{25}$$

where ν is an integer. The Fourier coefficients are then given by

$$< \mid T(2\mu + \Omega_\nu) \mid > = \int_0^{-i\beta} d(t_1 - t_1')\, e^{i(2\mu + \Omega_\nu)(t_1 - t_1')} < \mid T(t_1 - t_1') \mid > \quad .$$

Using these results we can Fourier-transform Eq. (22) to obtain

$$T_\lambda(\mathbf{Q}, \Omega_\nu + 2\mu) = \frac{-\lambda V}{1 + \lambda V L_0(\mathbf{Q}, \Omega_\nu + 2\mu)} \tag{26}$$

with

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

$$= i \frac{1}{-i\beta} \sum_n \int \frac{dq}{(2\pi)^3} G(q, -z_n + \mu)\, G(\mathbf{Q} - q, \Omega_\nu + z_n + \mu) \ , \qquad (27)$$

where the G's are given by Eq. (11). In the equations above, $\mathbf{Q}$ and $(\Omega_\nu + 2\mu)$ are the total momentum and energy of the pair.

The evaluation of Eq. (27) is given in the Appendix, where the result

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

$$= -N(0) \int \frac{d\Omega_a}{2\pi} \left\{ ln \frac{2\beta\omega_D \gamma}{\pi} + \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{x}{2}\right) \right\} \qquad (28)$$

is obtained, and the assumptions involved are discussed. In Eq. (28) the ψ's are the di-gamma functions[8,11] and the integration is performed over the solid angle Ω_a. Moreover, $ln\gamma = C = 0.577$ and

$$x = \frac{-i\beta}{2\pi} \left\{ \Omega_\nu + \frac{\mathbf{Q} \cdot \mathbf{q}_F}{m} - \frac{Q^2}{2m} \right\} . \qquad (29)$$

Now let us go back to Eq. (26). As discussed in several places[2,4,5,9], a phase transition will occur whenever the denominator vanishes for pairs such that $\mathbf{Q} = 0$, and $\Omega_\nu = 0$. If we know V, this would give us the critical temperature for the superconducting phase transition, β_c^{-1}, as the solution to the equation

$$1 + \lambda V L_0^c(0, 2\mu) = 0 \qquad (30)$$

From this condition the BCS result for the transition temperature[10] follows. To see this, let us write out Eq. (30).

$$L_0^c(0,2\mu) = -N(0)\ ln\ \frac{2\beta_c\omega_D\gamma}{\pi} = -\frac{1}{\lambda V} \tag{31}$$

or

$$ln\ \frac{\pi}{2\beta_c\omega_D\gamma} = -\frac{1}{\lambda N(0)\,V}$$

from which we obtain the BCS equation

$$\beta_c^{-1} = \frac{2\gamma}{\pi}\,\omega_D\, e^{-\frac{1}{\lambda N(0)V}} \tag{32}$$

in the weak-coupling limit.

Instead of writing Eq. (26) as a function of the parameter λV we choose to write it as a function of the parameter β_c (experimentally, more easily determined) given above. Doing this Eq. (26) becomes

$$T_\lambda(\mathbf{Q}, \Omega_\nu + 2\mu) = \{L_0^c(0,2\mu) - L_0(\mathbf{Q}, \Omega_\nu + 2\mu)\}^{-1} \tag{33}$$

from which the following is obtained:

$$T_\lambda^{-1}(\mathbf{Q}, \Omega_\nu) =$$

$$= N(0)\left\{ ln\ \frac{\beta}{\beta_c} + \psi\left(\frac{1}{2}\right) - \int \frac{d\Omega_a}{4\pi}\ \psi\left(\frac{1}{2} + \frac{-i\beta}{2\pi}\ \frac{\Omega_\nu + \dfrac{\mathbf{Q}\cdot\mathbf{q}_F}{m} - \dfrac{Q^2}{2m}}{2}\right)\right\} \tag{34}$$

Now, as stated at the beginning of section II, the analytic continuation of $T(\mathbf{Q}, \Omega_\nu)$ in this case is obtained simply by letting $\Omega_\nu \to \Omega$, with Ω a complex variable, since all the requirements listed then are satisfied here. The real-frequency response functions, $T^{>}(\omega)$ and $T^{<}(\omega)$, are obtained by means of the

optical theorem derived in reference 4 (in particular Eq. 13-22) from the equation for $T(\mathbf{Q}, \Omega)$.

Finally, the complex-frequency result that we shall utilize in our evaluation of both the conserving and non-conserving T-approximation to the two-particle Green's function for pure superconductors, is given by

$$T_{\lambda}^{-1}(\mathbf{Q}, \Omega) =$$

$$= N(0)\left\{ \ln\frac{\beta}{\beta_c} + \psi\left(\frac{1}{2}\right) - \int\frac{d\Omega_a}{2\pi}\,\psi\left(\frac{1}{2} + \frac{-i\beta}{2\pi}\,\frac{\Omega + \frac{\mathbf{Q}\cdot\mathbf{q}_F}{m} - \frac{Q^2}{2m}}{2}\right)\right\}. \tag{35}$$

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APPENDIX

As stated, our purpose now is to evaluate the product of two one-particle propagators given by

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

$$= i \frac{1}{-i\beta} \sum_n \int \frac{d\mathbf{q}}{(2\pi)^3} G(\mathbf{q}, -z_n + \mu)\, G(\mathbf{Q}-\mathbf{q}, \Omega_\nu + z_n + \mu)\,, \tag{A1}$$

with

$$G(\mathbf{q}, -z_n + \mu) = \frac{1}{-z_n + \mu - \epsilon(\mathbf{q})} \tag{A2}$$

$$G(\mathbf{Q}-\mathbf{q}, \Omega_\nu + z_n + \mu) = \frac{1}{z_n + \Omega_\nu + \mu - \epsilon(\mathbf{q}) - \frac{Q^2}{2m} + \frac{\mathbf{Q}\cdot\mathbf{q}}{m}} \tag{A3}$$

We now make the usual simplifications in the theory of metals,

$$\int \frac{d\mathbf{q}}{(2\pi)^3} \longrightarrow N(0) \int \frac{d\Omega_a}{4\pi} \int d\xi\,, \tag{A4}$$

with $N(0)$ the density of states at the Fermi level, and

$$\xi = \epsilon(\mathbf{q}) - \mu \tilde{=} \epsilon(\mathbf{q}_F) - \mu + v_F \cdot (\mathbf{q}-\mathbf{q}_F) \tilde{=} v_F \cdot (\mathbf{q}-\mathbf{q}_F)\,. \tag{A5}$$

When Eqs. (A2) to (A5) are substituted into Eq. (A1), we obtain:

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

$$= i \frac{1}{-i\beta} \sum_n N(0) \int \frac{d\Omega_a}{4\pi} \int_{-\omega_D}^{+\omega_D} d\xi \; \frac{1}{-z_n - \xi} \; \frac{1}{z_n + \Omega_\nu - \xi - \dfrac{Q^2}{2m} + \dfrac{\mathbf{Q}\cdot\mathbf{q}_F}{m}} \; . \tag{A6}$$

We now have two possible ways of evaluating Eq. (A6) which must be equivalent. We can either integrate over ξ first and then sum over n, or vice versa. We propose to do it the first way, since in this manner we can obtain $\int d\xi$ by means of complex-integration techniques. Since the integrand is convergent as ξ^{-2} when $\xi \to \infty$, we may relax the limits of integration to $[-\infty, +\infty]$. (Were we to sum over n first, and then integrate over ξ, we would have to be more careful with the limits of integration). Then, using contour integration techniques we obtain

$$L_0(\mathbf{Q}, \Omega_\nu + 2\mu) = -N(0) \int \frac{d\Omega_a}{4\pi} \sum_{n \geq 0} \frac{1}{(2n+1) + \dfrac{-i\beta}{2\pi}\left(\Omega_\nu + \dfrac{\mathbf{Q}\cdot\mathbf{q}_F}{m} - \dfrac{Q^2}{2m}\right)} \tag{A7}$$

where we have used the explicit form for z_n; that is,

$$z_n = \frac{(2n+1)\pi}{-i\beta}$$

Now, as discussed in reference 11, the formally divergent summation in (A7) can be "cured" in several different ways. Such divergency is due to the simplified model that we are using for the interaction, and disappears when a more realistic retarded electron-electron interaction is considered. If we use the "usual" method of curing the divergence we obtain (see reference 11):

$$\sum_{n \geq 0} \frac{1}{2n+1+x} = \ln \frac{2\gamma}{\pi} \beta\omega_D + \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{x}{2}\right) , \tag{A8}$$

from which we derive

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

$$= - N(0) \int \frac{d\Omega_a}{4\pi} \left\{ \ln \frac{2\gamma}{\pi} \beta\omega_D + \psi\left(\frac{1}{2}\right) - \psi\left(\frac{1}{2} + \frac{-i\beta}{2\pi} \frac{\Omega_\nu + \frac{\mathbf{Q}\cdot\mathbf{q}_F}{m} - \frac{Q^2}{2m}}{2} \right) \right\} \tag{A9}$$

that is, Eq. (28). It is important to point out that the "usual" method of curing the divergence agrees with results obtained in the weak-coupling limit, $\omega_D >> \beta_c^{-1}$, for the transition temperature. (See Section III).