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SUPERCONDUCTIVITY FROM CHARGED LOCAL BOSON EXCHANGE IN STRONG COUPLING APPROXIMATION

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To the Memory of Max Robert Schafroth

Abstract. A model Hamiltonian describing the charge fluctuations in the $Cu - O$ subsystem of the new high-T_c superconductors is discussed and used in a strong-coupling calculation of hole pairing. The resulting T_c has the form of a Bose-condensation temperature, which suggests that the holes form real-space Schafroth pairs instead of Cooper pairs. This conclusion is substantiated by the existence at T_c of a finite coherence length, which is obtained by identifying an appropriate correlation function. However, no indication of pairing beyond T_c is seen in the thermodynamic potential, and the gap is found to vanish as $(T_c - T)^{1/2}$.

1 - Introduction

One of the key features of the new high-T_c superconductors are the fluctuating valences on the copper and oxygen sites which result from doping by metal impurities or by oxygen. More explicitly, in the undoped "groundstate" the $Cu - O$ subsystem forms regular square lattices of Cu^{2+} ions in the $a - b$ planes with O^{2-} located midway between nearest neighbour Cu-sites. Doping then introduces holes which nominally form Cu^{3+}-ions. However, these holes may move to the neighbouring O-ions according to one of the two reactions [1]

$$Cu^{3+}O^{2-} \to Cu^{2+}O^{-} \tag{1}$$

or

$$Cu^{3+}O^{2-}Cu^{3+} \to Cu^{2+}O^{o}Cu^{2+}. \tag{2}$$

The questions whether Cu^{3+} is present and if not, which of the two reactions (1) or (2) actually takes place, are experimentally still not decided [2]. An important empirical fact in favour of the formation of neutral oxygen, that is of reaction (2), is the instability against loss of oxygen, well known in the quaternary new superconductors $La_{2-x}M_xCuO_4$ and $YBa_2Cu_3O_{6+x}$ but apparently not found in the more recent quinary compounds.

While many theoretical papers based on reaction (1), so-called "super-exchange" models, have recently been published [3,4,5], the similar reaction (2) [6] has met with less interest [7,8]. In this paper the interaction mechanism resulting from reaction (2) will be discussed in Section 2. The details of the strong coupling calculation leading to superconductivity, which were summarized in ref.8, are presented in Section 3 and 4 while in Section 5 the finer features of pair correlation, thermodynamics and gap near T_c are analysed, further details being discussed in the Appendix. For a short review of the experimental and theoretical situation see Ref.9.

The purpose of this paper is not only to propose a possible mechanism explaining the high-T_c phenomenon but also to show that in the extreme strong-coupling limit the model discussed here yields a transition temperature T_c of the form found in Bose condensation, that is, not bounded by the exponential with negative argument typical of weak-coupling theories. Because of this feature the model is of intrinsic interest, particularly in relation with the question of a continuous transition, as function of the coupling constant [10], between weakly coupled Cooper pairs, for which pairing and condensation is simultanous, and strongly bound Schafroth pairs which exist as bosons before they condense [11].

In order to see more clearly the difference between the two pairing mechanisms, a pair correlation function is defined in Section 5 by identifying appropriate diagrams. With this object, a general definition of a coherence length ξ is attempted as function both, of temperature and of coupling strength. The fact that ξ is found to be finite at T_c sheds some light on the mentioned formal similarity of T_c with the temperature of Bose condensation, although no trace of this behaviour is found in the thermodynamic potential, and the gap vanishes as $(T_c - T)^{1/2}$.

2 - Charged Local Boson Exchange Model

Reaction (2) moves two holes with opposite spin from nearest-neighbour copper sites i, j to the same oxygen site situated half-way in between (see Fig.2 of Ref.12), which is legitimate since the cost in Hund's rule energy is compensated by Jahn-Teller distortion energy [13]. In this model the two holes on the O-site also have opposite spin; moreover, these holes are approximated by a doubly charged local boson. Taking the direction i-j along the x-axis and writing the creation operators of the holes at i and j as Fourier series, this leads to an interaction Hamiltonian [14]

$$H'_x = W \sum_{\vec{k},\vec{k}'} a^+_{\vec{k}\uparrow} a^+_{\vec{k}'\downarrow} b e^{i(k_x+k'_x)d/2} + h.c., \tag{3}$$

where $a^+_{\vec{k}\sigma}$ is the creation operator of a band hole with spin σ, b is the annihilation operator of the doubly charged boson on the O-site and d the nearest-neighbour copper distance. The coupling constant W may be expressed in terms of an extended Hubbard model for the $Cu - O$ subsystem [12].

In principle, the interaction (3) should be used to calculate the self-energy [14] in a strong-coupling procedure; this calculation is sketched in the Appendix. The important point is that, since superconductivity is a condensation into the zero-momentum state, only the zero-momentum projection of Eq.(3),

$$H' = W \sum_{\vec{k}} a^+_{\vec{k}\uparrow} a^+_{-\vec{k}\downarrow} b + h.c., \tag{4}$$

is of direct physical relevance. Therefore, the Hamiltonian considered here is [8]

$$H = \sum_{\vec{k},\sigma} \varepsilon_k a^+_{\vec{k}\sigma} a_{\vec{k}\sigma} + \Omega_o b^+ b + H', \tag{5}$$

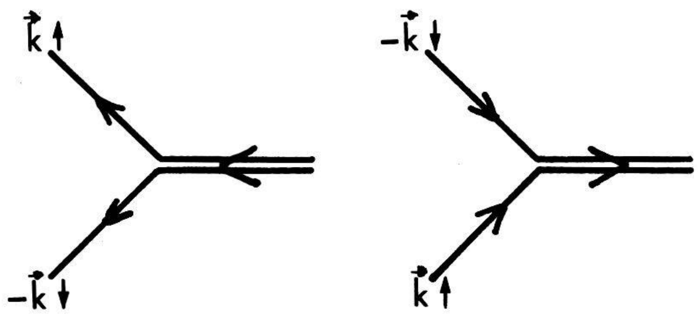

Fig.1: The vertices of interaction (4).

where ε_k and Ω_o are, respectively, the unperturbed electron and boson energies measured from the Fermi level, the filled portion of the band being $-\varepsilon_F < \varepsilon_k < 0$.

The interaction (4) is represented by the vertices of Fig.1 where oriented single and double lines stand, respectively, for the hole and the charged boson propagators. With this coupling, an effective nearest-neighbour hole-hole interaction

$$H'_{h-h} = W \sum_{\vec{k}} a^+_{\vec{k}\uparrow} a^+_{-\vec{k}\downarrow} \delta\langle b\rangle_{t=0} + h.c. \tag{6}$$

may be constructed. Making use of linear response theory [15],

$$\delta\langle b\rangle_t = i \int_{-\infty}^{t} dt' \langle [H'(t'-t), b]\rangle_{boson} e^{i\epsilon t}, \tag{7}$$

where $H'(t)$ is the interaction representation and $\epsilon = 0^+$. Evaluation of Eq.(7) and insertion into (6) leads to [1,7]

$$H'_{h-h} = |W|^2 \sum_{\vec{k},\vec{k}'} \left\{ \frac{1}{2\epsilon'_k - \Omega_o + i\epsilon} + \frac{1}{2\varepsilon_k - \Omega_o - i\epsilon} \right\} a^+_{\vec{k}\uparrow} a^+_{-\vec{k}\downarrow} a_{-\vec{k}'\downarrow} a_{\vec{k}'\uparrow}. \tag{8}$$

This expression shows that only for $\Omega_o > 0$ the effective interaction is purely attractive and, therefore, only then superconductivity is guaranteed. In a similar way we may also construct an effective nearest-neighbour boson hopping term from the original interaction (3) (see Appendix) which then may allow Bose condensation to occur. This is another possible explanation of high-T_c superconductivity [1] which, however, is distinct from the holon condensation discussed in the literature [9].

3 - Gap Equation and Renormalization Condition

We first calculate the self-energy due to the interaction (4), making use of the Nambu representation and of the Matsubara formalism [15]. The Nambu-form of Eq.(4) is

$$H' = \sum_{\vec{k}} \Psi^+_{\vec{k}} [W P_+ b + W^* P_- b^+] \Psi_{\vec{k}} , \tag{9}$$

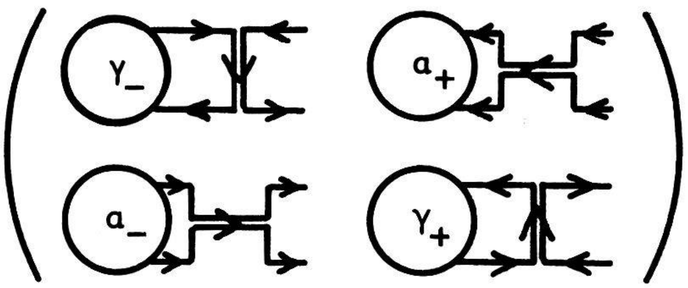

Fig.2: The self-energy matrix of Eqs.(20),(21).

where

$$\Psi_{\vec{k}} = \begin{pmatrix} a_{\vec{k}\uparrow} \\ a^{+}_{-\vec{k}\downarrow} \end{pmatrix}. \tag{10}$$

We also define the matrices

$$P_{\pm} = \frac{1}{2}(\tau_1 \pm i\tau_2); \; Q_{\pm} = \frac{1}{2}(1 \pm \tau_3), \tag{11}$$

where τ_1, τ_2, τ_3 are the Pauli matrices.

The self-energy is obtained by calculating the hole propagator matrix [15]

$$\mathcal{G}(\vec{k};\tau) = -\langle T\{\Psi_{\vec{k}}(-i\tau) \otimes \Psi^{+}_{\vec{k}}(0)\}\rangle, \tag{12}$$

where T is the time-ordering operator. To second order in H' one finds

$$\mathcal{G}(\vec{k};\tau) - \mathcal{G}^{o}(\vec{k};\tau) = \int_0^{\beta} d\tau' \int_0^{\beta} d\tau" \mathcal{G}^{o}(\vec{k};\tau')$$

$$\times \left\{\Sigma_{norm}(\vec{k};\tau' - \tau") + \Sigma_{anom}(\tau',\tau")\right\} \mathcal{G}^{o}(\vec{k};\tau"), \tag{13}$$

where the upper index o designates the free propagator and

$$\Sigma_{norm}(\vec{k};\tau) = -|W|^2 \left\{\mathcal{D}(\tau)P_{+}\mathcal{G}(\vec{k};\tau)P_{-} + \mathcal{D}(-\tau)P_{-}\mathcal{G}(\vec{k};\tau)P_{+}\right\}, \tag{14}$$

$$\Sigma_{anom}(\tau,\tau') = |W|^2 \sum_{\vec{k}} \int_0^{\beta} d\tau" \left\{\mathcal{D}(\tau - \tau")P_{+}Tr[P_{-}\mathcal{G}(\vec{k};0)]\right.$$

$$\left. +\mathcal{D}(\tau" - \tau)P_{-}Tr[P_{+}\mathcal{G}(\vec{k};0)]\right\} \delta(\tau - \tau'). \tag{15}$$

Here

$$\mathcal{D}(\tau) = -\langle T\{b(-i\tau)b^{+}(0)\}\rangle \tag{16}$$

is the charged local boson propagator. Σ_{norm} and Σ_{anom} constitute respectively the diagonal and off-diagonal elements of the self-energy matrix, as shown in Fig.2.

Fourier transformation of Eq.(13) according to the identity

$$\tilde{\phi}(i\nu_\pm) \equiv \int_0^\beta d\tau \phi(\tau) e^{i\nu_\pm \tau}, \tag{17}$$

where $\nu_\pm = (4n - 1 \pm 1)\pi/2\beta$ are bosonic/fermionic Matsubara frequencies, yields

$$\tilde{\mathcal{G}}(\vec{k}; i\nu) - \tilde{\mathcal{G}}^o(\vec{k}; i\nu) = \tilde{\mathcal{G}}(\vec{k}; \nu) \left\{ \tilde{\Sigma}_{norm}(\vec{k}; i\nu) + \tilde{\Sigma}_{anom}(i\nu) \right\} \tilde{\mathcal{G}}^o(\vec{k}; \nu), \tag{18}$$

where we have generalized the formula by replacing one of the free hole propagators to the right by a renormalized one. In this equation the Fourier-transformed self-energies are defined as

$$\tilde{\Sigma}_{\dots}(i\nu)\delta_{\nu,\nu'} = \beta^{-1} \int_0^\beta d\tau \int_0^\beta d\tau' e^{i\nu\tau} \Sigma_{\dots}(\tau, \tau') e^{-i\nu'\tau'} \tag{19}$$

and are found to be

$$\tilde{\Sigma}_{norm}(\vec{k}; i\nu) = -\beta^{-1}|W|^2 \sum_{\nu_+} \tilde{\mathcal{D}}(i\nu_+) \left\{ P_+ \tilde{\mathcal{G}}(\vec{k}; i\nu - i\nu_+) P_- + P_- \tilde{\mathcal{G}}(\vec{k}; i\nu + i\nu_+) P_+ \right\} \tag{20}$$

and

$$\tilde{\Sigma}_{anom} = \beta^{-1}|W|^2 \tilde{\mathcal{D}}(0) \sum_{\vec{k}} \sum_{\nu_-} \left\{ P_+ Tr[P_- \tilde{\mathcal{G}}(\vec{k}; i\nu_-)] + P_- Tr[P_+ \tilde{\mathcal{G}}(\vec{k}; i\nu_-)] \right\}. \tag{21}$$

Writing now

$$\tilde{\mathcal{G}}(\vec{k}; i\nu) = \alpha_+ P_+ + \alpha_- P_- + \gamma_+ Q_+ + \gamma_- Q_- \tag{22}$$

and

$$\tilde{\mathcal{G}}^{-1}(\vec{k}; i\nu) = \Delta_+ P_+ + \Delta_- P_- + Z_+ Q_+ + Z_- Q_- \tag{23}$$

where $P_\pm$ and $Q_\pm$ are defined in Eq.(11), the relations

$$\alpha_\pm = \frac{\Delta_\pm}{K} \; ; \; \gamma_\pm = -\frac{Z_\mp}{K} \tag{24}$$

hold with

$$K \equiv \Delta_+ \Delta_- - Z_+ Z_-. \tag{25}$$

Making use of Eqs.(10),(12) and (22) one easily finds for the free hole propagator (upper index o)

$$\alpha^o_\pm = 0 \; ; \; \gamma^o_\pm = \frac{1}{i\nu \mp \varepsilon_k} \tag{26}$$

and with Eqs.(24),(25)

$$\Delta^o_\pm = 0 \; ; \; Z^o_\pm = i\nu \mp \varepsilon_k. \tag{27}$$

Multiplying Eq.(18) from the left by $\tilde{\mathcal{G}}^{-1}$ and from the right by $(\tilde{\mathcal{G}}^o)^{-1}$, inserting the self-energies from Eqs.(20),(21) and the expressions (22) and (23) one obtains an equation in which both sides are expressed in terms of the matrices $P_\pm$ and $Q_\pm$. Making use of the algebra of these matrices defined in Eq.(11) and of relation (24), comparison of the coefficients of these matrices finally yields four equations, namely the gap equations

$$\Delta_\pm(\vec{k}; i\nu) = -\beta^{-1}|W|^2\tilde{\mathcal{D}}(0)\sum_{\vec{k}'}\sum_{\nu_-}\frac{\Delta_\pm(\vec{k}'; i\nu_-)}{K(\vec{k}'; i\nu_-)} \tag{28}$$

and the renormalization conditions

$$Z_\pm(\vec{k}; i\nu) - Z^o_\pm(\vec{k}; i\nu) = -\beta^{-1}|W|^2\sum_{\nu_+}\tilde{\mathcal{D}}(i\nu_+)\frac{Z_\pm(\vec{k}; i\nu \mp i\nu_+)}{K(\vec{k}; i\nu \mp i\nu_+)}. \tag{29}$$

These are Eqs.(5) and (6) of Ref.8 where, however, the obvious solution

$$\Delta_\pm(\vec{k}; i\nu) = \Delta = const. \tag{30}$$

of Eqs.(28) had been inserted. Note also that our definitions (12) and (16) of the propagators have the opposite sign of those used in Ref.8.

4 - Solutions of Gap and Renormalization Equations

In the approximation of an unrenormalized charged local boson propagator (16),

$$\tilde{\mathcal{D}}(i\nu) = \frac{1}{i\nu - \Omega_o}, \tag{31}$$

and with Eq.(30) the gap equation (28) becomes

$$\Lambda^{-1} = \sum_{\vec{k}} F(\varepsilon_k) = \int_{-\varepsilon_F}^{+\varepsilon_F} d\varepsilon N(\varepsilon)F(\varepsilon), \tag{32}$$

where $N(\varepsilon)$ is the density of states and the integral extends over the whole band (which is assumed to be half filled),

$$F(\varepsilon_k) \equiv \beta^{-1}\sum_{\nu_-} K^{-1}(\vec{k}; i\nu_-) \tag{33}$$

and

$$\Lambda \equiv \frac{|W|^2}{\Omega_o}. \tag{34}$$

In weak-coupling approximation, $\Lambda \ll \varepsilon_F$, the solution of Eqs.(29),(32) is obtained with the values (27),(30) so that, according to the definition (25),

$$K_{weak} = E_k^2 + \nu^2 \ ; E_k^2 \equiv \varepsilon_k^2 + \Delta^2. \tag{35}$$

The renormalization conditions then are fulfilled to zeroth order in W while Eq.(33) takes the form

$$F_{weak}(\varepsilon_k) = \frac{1}{2E_k} tanh \frac{\beta E_k}{2}, \tag{36}$$

which is obtained by the usual contour integration around the imaginary frequency axis and deformation of this path around the poles at $\pm E_k$. Note that with (36) the gap equation (32) requires Λ to be positive or $\Omega_o > 0$, in agreement with the comment after Eq.(8). The zero-temperature gap now becomes [1]

$$\Delta_{weak} \simeq 2\varepsilon_K e^{-1/\Lambda N(0)}, \tag{37}$$

where $N(0)$ is the density of states at the Fermi level.

We now analyse Eq.(29) in the strong-coupling limit $\Lambda \gg \varepsilon_F$. Inserting the boson propagator (31) and replacing the bosonic summation variable ν_+ by the fermionic one, $\nu_- = \nu \mp \nu_+$, the renormalization coefficients

$$r_\pm = Z_\pm - Z_\pm^o \tag{38}$$

satisfy the conditions

$$r_\pm(\vec{k}; i\nu) = \pm\beta^{-1}|W|^2 \sum_{\nu_-} \frac{1}{i\nu_- - i\nu \pm \Omega_o} \frac{Z_\pm(\vec{k}; i\nu_-)}{K(\vec{k}; i\nu_-)}$$

$$= \mp|W|^2 \frac{1}{2\pi i} \int_\Gamma dz f(z) \frac{1}{z - i\nu \pm \Omega_o} \frac{Z_\pm(\vec{k}; z)}{K(\vec{k}; z)}, \tag{39}$$

where Γ surrounds the imaginary z-axis in the positive sense and $f(\varepsilon) = (e^{\beta\varepsilon} + 1)^{-1}$ is the Fermi distribution function.

Inserting (27),(38) into Eq.(25) one finds the expression

$$-K = z^2 + (r_+ + r_-)z - E_k^2 + \varepsilon_k(r_+ - r_-) + r_+r_-$$

$$= [z - \zeta_+(\vec{k}; z)][z - \zeta_-(\vec{k}; z)], \tag{40}$$

where the second equality defines the zeros of the denominator K formally as

$$\xi_+ = \zeta_+(\vec{k}; \xi_+) \ ; \ \xi_- = \zeta_-(\vec{k}; \xi_-) \tag{41}$$

and where it is understood that these zeros may be multiple. With this notation, deformation of the path Γ in Eq.(39) formally yields

$$r_\pm(\vec{k}; i\nu) = \pm|W|^2 \left\{ \frac{[i\nu \mp \Omega_o \mp \varepsilon_k + r_\pm(\vec{k}; i\nu \mp \Omega_o)]n(\mp\Omega_o)}{[i\nu \mp \Omega_o - \zeta_+(\vec{k}; i\nu \mp \Omega_o)][i\nu \mp \Omega_o - \zeta_-(\vec{k}; i\nu \mp \Omega_o)]} \right.$$

$$-\sum\left(\frac{[\xi_+ \mp \varepsilon_k + r_{\pm,+}]f(\xi_+)}{[\xi_+ - i\nu \pm \Omega_o][\xi_+ - \eta_+)]} + \frac{[\xi_- \mp \varepsilon_k + r_{\pm,-}]f(\xi_-)}{[\xi_- - i\nu \pm \Omega_o][\xi_- - \eta_+]}\right)\Bigg\}. \tag{42}$$

Here $n(\omega) = -f(i\nu_- + \omega)$ is the Bose distribution function, the sum runs over all zeros $\xi_\pm$, and $\eta_\pm \equiv \zeta_\mp(\vec{k};\xi_\pm)$, $r_{\pm,\pm} \equiv r_\pm(\vec{k};\xi_\pm)$.

Since large Matsubara frequencies ν_- are essential for the convergence of the sum in the gap equation (32), Eq.(42) must first be solved asymptotically for $\beta|\nu| \gg 1$. One finds with Eq.(40)

$$r_\pm \equiv r_\pm(\vec{k};i\nu) = O(\nu^{-1})\ ; K \equiv K(\vec{k};i\nu) = \nu^2 + O(\nu^0). \tag{43}$$

Even with these estimates Eq.(42) is not of much use, except in the extreme strong-coupling limit where $\beta_c\Omega_o \ll 1$, $\beta_c^{-1} \equiv T_c$ being the transition temperature. In this case the first term in the outer bracket of Eq.(42) dominates and $|\nu| \geq \pi\beta_c^{-1} \gg \Omega_o$. Hence, for $T \simeq T_c$, Ω_o may be neglected and Eq.(42) becomes

$$Z_\pm - Z_\pm^o \simeq \beta^{-1}\Lambda\frac{Z_\pm}{K}, \tag{44}$$

where Eqs.(27),(33),(38) and (40) have been used. Solving for $Z_\pm$ and inserting into Eq.(25) this yields a cubic equation for K,

$$(K - \Delta^2)(K - D^2)^2 - (\nu^2 + \varepsilon_k^2)K^2 = 0, \tag{45}$$

where

$$D^2 = \beta^{-1}\Lambda. \tag{46}$$

Near T_c where $\Delta \simeq 0$, the solution of Eq.(45) with the asymptotic behaviour (43) then is

$$K_o \simeq \frac{1}{4}\left(\sqrt{\nu^2 + \varepsilon_k^2} + \sqrt{\nu^2 + \varepsilon_k^2 + 4D^2}\right)^2. \tag{47}$$

An extension of this formula to second order in Δ is given in the Appendix.

Insertion of the expression (47) into the function (33) yields, after transforming the Matsubara sum into the contour integral over the path Γ,

$$F_o(\varepsilon_k) = -\frac{1}{2\pi i}\int_\Gamma \frac{4f(z)dz}{\left(\sqrt{\varepsilon_k^2 - z^2} + \sqrt{4D^2 + \varepsilon_k^2 - z^2}\right)^2}. \tag{48}$$

Multiplying numerator and denominator by $(\sqrt{\varepsilon_k^2 - z^2} - \sqrt{4D^2 + \varepsilon_k^2 - z^2})^2$, Eq.(48) becomes

$$F_o(\varepsilon_k) = -\frac{1}{4\pi i D^4}\int_\Gamma dz f(z)$$
$$\times\left(2D^2 + \varepsilon_k^2 - z^2 + \sqrt{z^2 - \varepsilon_k^2}\sqrt{z^2 - 4D^2 - \varepsilon_k^2}\right). \tag{49}$$

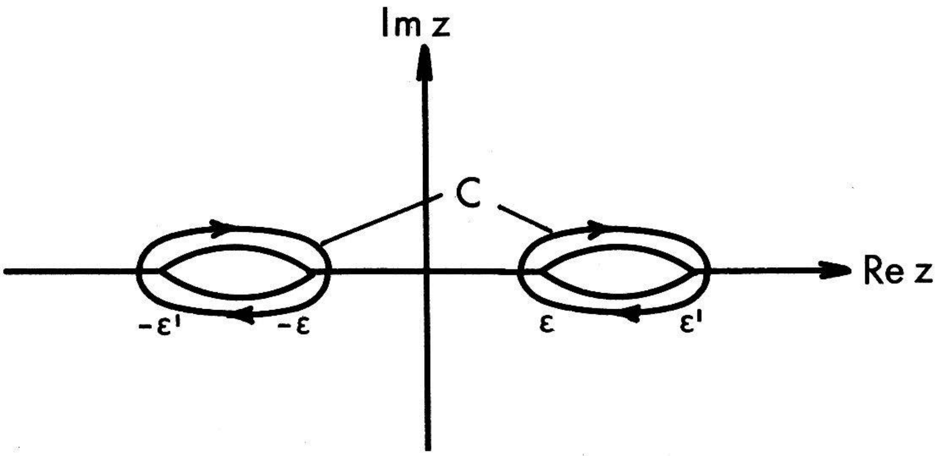

Fig.3: Cuts and integration path C in Eq.(50).

Here the sign of the square-root term is determined by the cuts which are chosen as indicated in Fig.3. Convergence of the integral in Eq.(49) being guaranteed by the asymptotic form (43) of K, the contour Γ may be deformed into the path C encircling these cuts in the negative sense, as shown in Fig.3. It is then evident that only the square-root term in Eq.(49) contributes to the integral along C so that

$$F_o(\varepsilon) = -\frac{1}{4\pi i D^4}\int_C dz f(z)\sqrt{z^2-\varepsilon^2}\sqrt{z^2-\varepsilon'^2}, \tag{50}$$

where $\varepsilon' \equiv \sqrt{\varepsilon^2+4D^2}$. A careful examination of the cuts of Fig.3 yields for the last integral

$$F_o(\varepsilon) = \frac{1}{2\pi D^4}\int_{|\varepsilon|}^{\varepsilon'} dx\sqrt{x^2-\varepsilon^2}\sqrt{\varepsilon'^2-x^2}\tanh\frac{\beta x}{2}. \tag{51}$$

We are not interested in an exact evaluation of the integral (51) but rather give the following estimates, valid when $tanh(\beta x/2)$ may be approximated, respectively, by $\beta x/2$ and by 1: $0 < F(\varepsilon) < 2/\pi D$ and

$$F_o(\varepsilon) \simeq \frac{\beta}{4}\ ; \beta D < 1\ ;$$

$$F_o(0) \simeq \frac{4}{3\pi D}\ ; \beta D \gg 1\ . \tag{52}$$

Insertion of the last two expressions with $\beta^{-1} = T_c$ into the gap equation (32) finally yields

$$T_c \simeq \Lambda \times \begin{cases} n/2\ ; n > 2\ ; \\ (8n/3\pi)^2\ ; n \ll 1\ , \end{cases} \tag{53}$$

where $n \equiv \int_{-\varepsilon_F}^{0} N(\varepsilon)d\varepsilon$ is the number of holes per unit cell. This result, which up to minor factors is that of Ref.8, has the form of a Bose-condensation temperature for a boson mass proportional to Λ^{-1} but with an n-dependence different from the well-known $n^{2/3}$-law. Remarkably, T_c is not exponentially bounded for large Λ-values.

5 - Pair Correlation, Thermodynamics and Gap near T_c

An analogous but much simpler calculation as the one leading to Eqs.(20),(21) yields for the boson self-energy

$$\Pi(i\nu_+) = \beta^{-1}|W|^2 \sum_{\vec{k}} \sum_{\nu_-} Tr\left(\tilde{\mathcal{G}}(\vec{k}; i\nu_-)P_+\tilde{\mathcal{G}}(\vec{k}; i\nu_- - i\nu_+)P_-\right), \tag{54}$$

where, in view of Eqs.(11) and (22) the trace is simply $\gamma_+(\vec{k}; i\nu_-)\gamma_-(\vec{k}; i\nu_- - i\nu_+)$. Since according to Eqs.(10),(12) and (22), $\gamma_\pm(\vec{k}; i\nu)$ is the hole propagator of momentum $\pm\vec{k}$ and spin $\pm$, Π is a sum of zero-momentum singlet hole pairs as shown in Fig.4. Using Eqs.(24),(25),(30) and (33) one finds

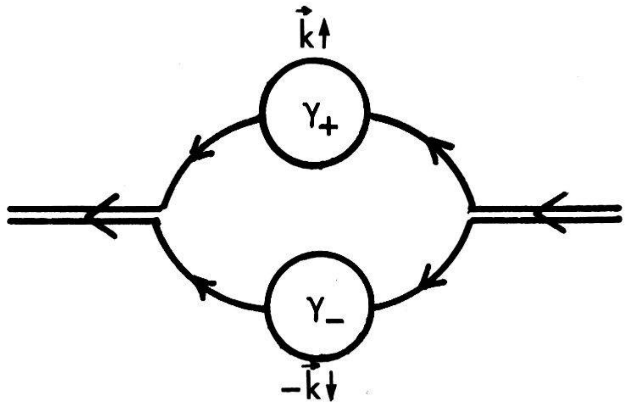

Fig.4: Boson self-energy of Eq.(54).

$$\Pi(0) = -|W|^2 \sum_{\vec{k}} \left(F(\varepsilon_k) - \Delta^2\Phi(\varepsilon_k)\right), \tag{55}$$

where

$$\Phi(\varepsilon_k) \equiv \beta^{-1} \sum_{\nu_-} \frac{1}{K^2(\vec{k}; i\nu_-)}. \tag{56}$$

Now, the term $\Delta^2\Phi(\varepsilon_k)$ in Eq.(55) vanishes both, at T_c and also in the weak-coupling approximation (35) where it is easy to see by transforming the ν-sum into an integral around the poles at $\pm E_k$ that $\Phi = 0$. Therefore, in both situations examined in this paper, $\Pi(0)$ is given as $\vec{k}$-sum of the function $F(\varepsilon_k)$, so that this function may be interpreted as the Fourier transform of the correlation function of zero-momentum singlet pairs,

$$\tilde{F}(\vec{r}) = \sum_{\vec{k}} F(\varepsilon_k) e^{i(\vec{k}-\vec{k}_F)\cdot\vec{r}} \tag{57}$$

(we neglect the dependence on the direction of $\vec{k}_F$). This correlation function may thus also be considered as a generalisation of the square modulus of Cooper's ground-state wave function $\chi_o(r,0)$ [16].

$\tilde{F}$ may now be used to define the coherence length ξ quite generally as

$$\xi^2 \equiv \langle \vec{r}^{\,2} \rangle \equiv \frac{\int \vec{r}^{\,2} \tilde{F}(\vec{r}) d^3 r}{\int \tilde{F}(\vec{r}) d^3 r}. \tag{58}$$

Inserting Eq.(57), expressing $\vec{r}^{\,2}$ as $(\partial/i\partial\vec{k})^2$ acting on the exponential in (57) and transferring the derivatives to $F(\varepsilon_k)$ by partial summation (integration) one finds

$$\xi^2 = \frac{\sum_{\vec{k}} (\partial\varepsilon_k/\partial\vec{k})^2 F''(\varepsilon_k) \delta_{\vec{k},\vec{k}_F}}{\sum_{\vec{k}} F(\varepsilon_k) \delta_{\vec{k},\vec{k}_F}} = -v_F^2 \frac{F''(0)}{F(0)}, \tag{59}$$

where v_F is the Fermi velocity. Applied to the weak-coupling expression (36) this gives

$$\xi^2{}_{weak} = \frac{v_F^2}{\Delta^2{}_{weak}} \left(1 - \frac{\beta\Delta_{weak}}{\sinh\beta\Delta_{weak}}\right), \tag{60}$$

which in the limit $T \to 0$ yields correctly $\xi = v_F/\Delta_{weak}$. The limit $T \to T_c$, however, becomes $\xi = v_F/\sqrt{6}T_c$ instead of ∞. But the cancellation of the infinity in Eq.(60) is very subtle; it suffices in fact to modify slightly the definition (58) which, anyhow, is not well adapted to finite temperatures.

The obvious modification is to substitute in Eq.(59) $\delta_{\vec{k},\vec{k}_F}$ by $-f'(\varepsilon_k)$, neglecting anisotropy effects. Introducing the density of states $N(\varepsilon)$ and using a Taylor expansion for $F(\varepsilon)$, $F''(\varepsilon)$ and $N(\varepsilon)$ one obtains the modified expression

$$\xi^2 = -v_F^2 \frac{F''(0) + \frac{\pi^2}{6}T^2 \left[F^{IV}(0) + \mu F''\right]}{F(0) + \frac{\pi^2}{6}T^2 \left[F''(0) + \mu F(0)\right]}, \tag{61}$$

where $\mu \equiv N''(0)/N(0)$. With this modified definition, ξ is found to diverge as $\Delta_{weak}^{-2} \propto (T_c - T)^{-1}$.

The point of interest now is a comparison with the result obtained with the strong-coupling expression (51). The derivatives needed in Eq.(61) are obtained by observing that the integration limits in (51) do not contribute and that the integrand depends on ε in the form $\varepsilon^2 - x^2$. Therefore $\partial/\partial\varepsilon = -(\varepsilon/x)\partial/\partial x$ and one obtains

$$\xi^2 = -\frac{v_F^2}{4T_c^2} \frac{\int_0^\lambda dyy\sqrt{\lambda^2 - y^2}\, \frac{\partial}{\partial y}\frac{1}{y} \left[1 + \frac{\pi^2}{6}T_c^2\mu + \frac{\pi^2}{8}\frac{\partial}{\partial y}\frac{1}{y}\right] \tanh y}{\int_o^\lambda dyy\sqrt{\lambda^2 - y^2} \left[1 + \frac{\pi^2}{6}T_c^2\mu + \frac{\pi^2}{24}\frac{\partial}{\partial y}\frac{1}{y}\right] \tanh y}, \tag{62}$$

where $\lambda \equiv \beta D$ and $y \equiv \beta x/2$. It is easy to verify that all integrals in Eq.(62) are finite (except for particular values of μ for which the denominator vanishes). Therefore ξ is finite at T_c, indicating that the pairs are of the Schafroth-type [11].

In view of this rather surprising result it is of interest to see how the thermodynamic potential behaves at T_c. The contribution of the interaction (4) to the grand-canonical potential is given, to second order, by the Hartree- and exchange-type contributions [15] of Fig.5,

$$\Delta\Omega_H = \beta^{-1}|W|^2 \sum_{\vec{k},\vec{k}'} \int_0^\beta d\tau \int_0^\beta d\tau' \mathcal{D}(\tau-\tau') Tr[\mathcal{G}(\vec{k};0)P_+] Tr[\mathcal{G}(\vec{k}';0)P_-]$$

$$= -\Lambda\beta^{-2} \sum_{\vec{k},\vec{k}'} \sum_{\nu,\nu'} \alpha_-(\vec{k};i\nu)\alpha_+(\vec{k}';i\nu') \tag{(63}$$

and

$$\Delta\Omega_{ex} = -\beta^{-1}|W|^2 \sum_{\vec{k}} \int_0^\beta d\tau \int_0^\beta d\tau' \mathcal{D}(\tau-\tau') Tr\left(\mathcal{G}(\vec{k};\tau-\tau')P_-\mathcal{G}(\vec{k};\tau'-\tau)P_+\right)$$

$$= -|W|^2\beta^{-2} \sum_{\vec{k}} \sum_{\nu,\nu'} \tilde{\mathcal{D}}(i\nu'-i\nu)\gamma_-(\vec{k};i\nu)\gamma_+(\vec{k};i\nu'), \tag{64}$$

respectively. Comparison of Figs.4 and 5 shows that Eq.(64) may be obtained from the boson self-energy (54) while (63) has no counterpart because the corresponding diagram would be disconnected.

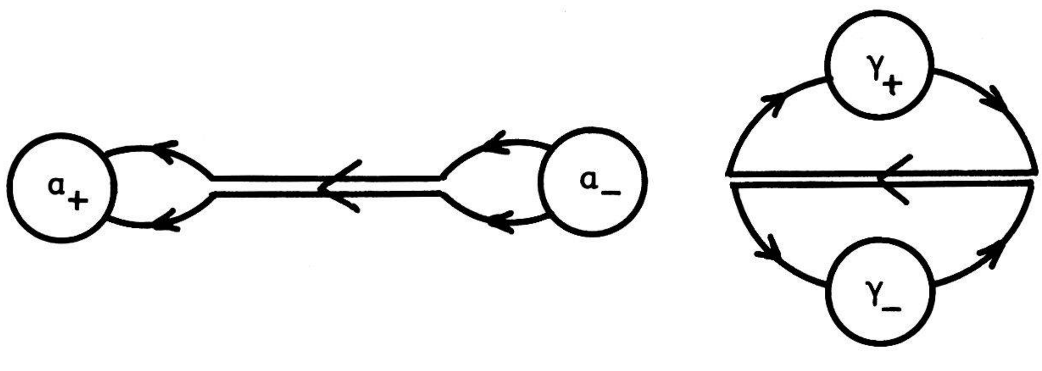

Fig.5: The Hartree- and exchange-type diagrams of Eqs.(63) and (64), respectively.

It is clear that $\Delta\Omega_H$ vanishes in the normal phase; applying Eqs. (24),(30),(32) and (33) one finds in the superconducting phase

$$\Delta\Omega_H^S = -\frac{\Delta^2}{\Lambda}. \tag{65}$$

On the other hand, the renormalization conditions (29) may be used to simplify Eq.(64), the result being

$$\Delta\Omega_{ex} = \beta^{-1}\sum_{\vec{k}}\sum_{\nu}\frac{Z_+(Z_- - Z_-^o)}{K}, \tag{66}$$

which vanishes in the weak coupling limit. We are interested, however, in the strong coupling limit near T_c where we may insert the approximate expression (44) and obtain

$$\Delta\Omega_{ex} \simeq D^2\beta^{-1}\sum_{\vec{k}}\sum_{\nu}\frac{Z_+Z_-}{K^2}. \tag{67}$$

So far the gap equation (32) has not been used in the evaluation of $\Delta\Omega_{ex}$ so that Eq.(67) is valid both, in the normal and the superconducting phases. In the normal phase where $K = -Z_+Z_-$ we obtain in view of definition (33)

$$\Delta\Omega_{ex}^N \simeq -D^2\sum_{\vec{k}}F_o(\varepsilon_k), \tag{68}$$

where F_o is the zero-gap approximation (51). In the superconducting phase, use of Eqs.(25),(32),(33) and of definition (56) allows to evaluate Eq.(67) as follows:

$$\Delta\Omega_{ex}^S \simeq -\beta^{-1} + \Delta^2D^2\sum_{\vec{k}}\Phi(\varepsilon_k). \tag{69}$$

Thus the total potential difference between the superconducting and normal phases near T_c obtained from Eqs.(65),(68) and (69) is

$$\Omega^S - \Omega^N \simeq D^2\sum_{\vec{k}}F_o(\varepsilon_k) - \beta^{-1} - \Delta^2\left(\frac{1}{\Lambda} - D^2\sum_{\vec{k}}\Phi_o(\varepsilon_k)\right), \tag{70}$$

where Φ_o is the function (56) obtained with K_o from Eq.(47). In close analogy with the procedure leading to Eq.(51) one finds the expression

$$\Phi_o(\varepsilon) = \frac{1}{2\pi D^8}\int_{|\varepsilon|}^{\varepsilon'} dx\left(\frac{\varepsilon^2+\varepsilon'^2}{2} - x^2\right)\sqrt{x^2-\varepsilon^2}\sqrt{\varepsilon'^2-x^2}\tanh\frac{\beta x}{2}, \tag{71}$$

for which the following estimates are found under the same conditions as those used to derive Eqs.(52):

$$\Phi_o(\varepsilon) \simeq 0\ ; \beta D < 1\ ;$$

$$\Phi_o(0) \simeq \frac{8}{15\pi D^3}\ ; \beta D \gg 1\ . \tag{72}$$

Inserted into Eq.(70), making use of (53), this leads to

$$\Omega^S - \Omega^N \simeq \begin{cases} -(\Delta^2/\Lambda) + T_c(1 - T/T_c) \; ; n > 2 \; ; \\ -(3\Delta^2/5\Lambda) + (T_c/2)(1 - T/T_c) \; ; n \ll 1 \; . \end{cases} \tag{73}$$

In order for the last expressions to have a definite sign, we must know the temperature dependence of the gap Δ near T_c. This may be obtained from the result (A15) derived for the denominator function K in the Appendix where $t^2 = \varepsilon^2 - x^2$ has to be used here; one finds

$$F(\varepsilon) = F_o(\varepsilon) + \Delta^2 F_1(\varepsilon) + O(\Delta^4) \tag{74}$$

with

$$F_1(\varepsilon) \equiv \frac{1}{4\pi D^4} \int_{|\varepsilon|}^{\varepsilon'} dx \sqrt{x^2 - \varepsilon^2} \sqrt{\varepsilon'^2 - x^2} \left(\frac{\varepsilon^2 - x^2}{D^4} + \frac{2}{\varepsilon'^2 - x^2} \right) \tanh \frac{\beta x}{2}. \tag{75}$$

Estimates analogous to those made for obtaining Eqs.(52) and (72) yield

$$F_1(\varepsilon) \simeq -\frac{\beta^3}{96} \; ; \beta D < 1 \; ;$$

$$F_1(0) \simeq -\frac{1}{15\pi D^3} \; ; \beta D \gg 1 \; , \tag{76}$$

where in the first expression only the second term in the development $\tanh(\beta x/2) = (\beta x/2) - (\beta^3 x^3/24) + \ldots$ contributes. Inserting the estimates (52),(76) with (74) into the gap equation (32) one finds

$$\Delta^2 \simeq \begin{cases} 96 T_c^2 (1 - T/T_c) \; ; n > 2 \; ; \\ 10(3\pi/8n)^2 T_c^2 (1 - T/T_c) \; ; n \ll 1 \; , \end{cases} \tag{77}$$

where use was made of Eq.(53).

Finally, inserting the last result into Eq.(73) we obtain

$$\Omega^S - \Omega^N \simeq \begin{cases} -(48n - 1) T_c (1 - T/T_c) \; ; n > 2 \; ; \\ -(11/2) T_c (1 - T/T_c) \; ; n \ll 1 \; . \end{cases} \tag{78}$$

This result shows that below T_c the superconducting phase is indeed stable. However, there is no sign of a possible persistence of the pairing to $T > T_c$, as could have been suspected from the finite expression (62) for the coherence length ξ. Comparison of Eq.(53) with Fig.8 of Ref.10 would suggest that our coupling is still too weak to form bound pairs. However, in Ref.10 the pair mass is constant whereas Eq.(53) suggests a pair mass proportional to $|W|^{-2}$, from which one might conclude that our pairs still keep together above T_c. This conclusion is physically not unreasonable since our basic interaction (3) is a lattice model, in which case Ref.10 is totally unreliable at and above T_c.

Appendix

i - Self-energy due to interaction (3)

Formally, the self-energy due to interaction (3) is again given by Eqs.(20), (21), the difference being contained in the hole propagator $\mathcal{G}$. In a site representation, Eq.(12) is replaced by

$$\mathcal{G}_{ij}(\tau) = -\langle T\Phi_{ij}(-i\tau) \otimes \Phi^{+}{}_{ij}(0)\rangle, \tag{A1}$$

where i and j are nearest-neighbour copper sites,

$$\Phi_{ij} = \begin{pmatrix} c_{i\uparrow} \\ c^{+}_{j\downarrow} \end{pmatrix} \tag{A2}$$

and $c_{i\sigma}$ is the Fourier-transform of $a_{\vec{k}\sigma}$ in Eq.(10). The question now is, how to determine the time dependence. In a strongly localized narrow-band situation the dominant term in the Hamiltonian is an on-site Hubbard term

$$H_o = U \sum_i n_{i\uparrow} n_{i\downarrow}, \tag{A3}$$

which was also the assumption used for the determination of the coupling constant W in Ref.12. With this H_o,

$$\dot{c}_{i\sigma} = i[H_o, c_{i\sigma}] = -iU n_{i-\sigma} c_{i\sigma}, \tag{A4}$$

so that the free propagator becomes

$$\mathcal{G}^{o}{}_{ij}(\tau) = \delta_{ij} \begin{pmatrix} G^{o}{}_{i\uparrow}(\tau) & ,0 \\ 0 & ,G^{o}_{j\downarrow}(\tau) \end{pmatrix}, \tag{A5}$$

where

$$G^{o}_{i\uparrow}(\tau) = -\langle e^{-Un_{i\downarrow}\tau} c_{i\uparrow} c^{+}_{i\uparrow}\rangle = -\frac{1+e^{-U\tau}}{3+e^{-\beta U}}\ ;$$

$$G^{o}_{j\downarrow}(\tau) = -\langle e^{+Un_{j\uparrow}\tau} c^{+}_{j\downarrow} c_{j\downarrow}\rangle = -\frac{1+e^{U(\tau-\beta)}}{3+e^{-\beta U}}\ . \tag{A6}$$

Fourier transformation according to the identity (17) then yields

$$\tilde{G}^{o}_{s\sigma}(i\nu) = -\left(\frac{2}{i\nu} + \frac{1+e^{-\beta U}}{i\nu - \sigma U}\right)\left(3+e^{-\beta U}\right)^{-1} ; s = i, j\ ; \sigma = \pm. \tag{A7}$$

Making use of Eqs.(22)-(25) a strong-coupling formalism based on the purely repulsive free Hamiltonian (A3) may be developed, from which it is not unreasonable to expect superconductivity to emerge [17].

ii - Boson hopping term due to interaction (3)

The boson hopping term due to interaction (3) may be obtained with the method used to derive Eq.(8) [15]: Labelling the oxygen site of the boson operator by an index l, we may write

$$H'_{b-b} = W \sum_{\vec{k},\vec{k}'} b_l e^{i(k_x+k'_x)d/2} \delta\langle a^+_{\vec{k}\uparrow} a^+_{\vec{k}'\downarrow}\rangle_{t=0} + h.c., \tag{A8}$$

where from linear response theory

$$\delta\langle a^+_{\vec{k}\uparrow} a^+_{\vec{k}'\downarrow}\rangle_t = i \int_{-\infty}^{t} dt' \langle [H'_y(t'-t), a^+_{\vec{k}\uparrow} a^+_{\vec{k}'\downarrow}]\rangle_{holes} e^{i\epsilon t}. \tag{A9}$$

Here H'_y is the interaction (3) with the boson operator on a nearest-neighbour site l' of l, which is only possible if l' is nearest to one of the copper sites i or j and hence, if the line $l'-i$ or $l'-j$ is along the y-direction. Evaluation of Eq.(A9) and insertion into (A8) leads to the hopping term

$$H'_{b-b} = |W|^2 b^+_{l'} b_l \sum_{\vec{k},\vec{k}'} e^{i(k_x+k'_x-k_y-k'_y)d/2} \frac{1-f(\varepsilon_k)-f(\varepsilon_{k'})}{\varepsilon_k+\varepsilon_{k'}} + h.c., \tag{A10}$$

which in the case of the interaction (4), where $\vec{k}' = -\vec{k}$, simplifies to

$$H'_{b-b} = |W|^2 b^+_{l'} b_l \sum_{\vec{k}} \frac{1-2f(\varepsilon_k)}{2\varepsilon_k} + h.c.. \tag{A11}$$

iii - Denominator function K to second order in Δ

In powers of Δ^2 the solution of Eq.(45) is

$$K = K_o + \Delta^2 \frac{K_o - D^2}{K_o + D^2} + O(\Delta^4). \tag{A12}$$

Inserting K_o from Eq.(47) one obtains

$$\begin{aligned} 2(K_o + D^2)K &= t^4 + t^2(5D^2+\Delta^2) + 4D^4 \\ &+(t^2+3D^2+\Delta^2)t\sqrt{t^2+4D^2} + O(\Delta^4), \end{aligned} \tag{A13}$$

where the abbreviation $t^2 \equiv \nu^2 + \varepsilon_k^2$ is used. Multiplying numerator and denominator of Eq.(A13) by the right-hand side of this equation but with the opposite sign of the square-root term, one arrives after some algebra at the following expression:

$$\frac{1}{K} = \frac{t^2+2D^2 - t\sqrt{t^2+4D^2}[1+2\Delta^2(t^2+4D^2)^{-1}] + O(\Delta^4)}{2D^4 - 2\Delta^2 t^2 + O(\Delta^4)}, \tag{A14}$$

which may finally be written in the form

$$\begin{aligned} \frac{2D^4}{K} &= (t^2+2D^2)\left(1+\frac{\Delta^2 t^2}{D^4}\right) \\ &-t\sqrt{t^2+4D^2}\left(1+\frac{\Delta^2 t^2}{D^4}+\frac{2\Delta^2}{t^2+4D^2}\right) + O(\Delta^4). \end{aligned} \tag{A15}$$

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