Condensation energy in phonon and spin mediated superconductors - strong coupling approach

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Abstract

We consider the condensation energy, $E_c$ of strongly coupled, magnetically-mediated superconductors within the context of the spin-fermion model. We argue that although experimentally obtained values of $E_c$ are of the same order of magnitude as would be expected from BCS theory in optimally and overdoped cuprates, this agreement is coincidental. The actual physics behind the condensation energy is much richer. In particular, we argue that it is vital to take both the fermionic and bosonic contributions to the condensation energy into account when considering such materials, and that it is only the sum of the two contributions, $E_c$, which has physical meaning. Both the experimental and our theoretically calculated condensation energies exhibit a decrease with further underdoping past optimal doping, e.g. in the mid to strong coupling regime. Below optimal doping, the physics is qualitatively different from BCS theory as the gain in the condensation energy is a result of the feedback on spin excitations, while the fermionic contribution to $E_c$ is positive due to an “undressing” feedback on the fermions. We argue that the same feedback effect accounts for a gain in the kinetic energy at strong coupling.

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I. INTRODUCTION

Understanding the origin of the condensation energy is an important step towards identifying the mechanism of high temperature superconductivity in the cuprates. In a BCS superconductor, the condensation energy $E_c$ - the energy gain in a superconductor compared to the normal state at the same $T$, smoothly increases below $T_c$ and at $T = 0$ reaches $E_{c}^{BCS} = -VN_f\Delta^2/2$, where $V$ is the volume, $\Delta$ is the superconducting gap and $N_f = m_p F/(2\pi^2\hbar^3)$ is the fermionic density of states. [1] The decrease in the total energy upon pairing results from a fine competition between an increased kinetic energy and a decreased potential energy, both of which are much larger than $E_c$. The BCS condensation energy can be experimentally extracted from the jump of the specific heat at $T_c$ as within the BCS theory $C_s - C_n \approx 6.08E_c/T_c$.

Since the fermionic density of states is only weakly dependent on doping, the application of the BCS formula for the condensation energy to cuprate superconductors would imply that $E_c$ and $\Delta^2$ scale in the same way. However, the measured gap increases monotonically with decreasing doping [2], while the jump of the specific heat has a non-monotonic doping dependence. In the overdoped regime it initially increases with reduced doping, but below optimal doping further underdoping leads to a decrease in the specific heat jump [3]. This discrepancy between the trends in $C_s - C_n$ and in $\Delta$ as functions of doping clearly makes the applicability of the BCS formula to the cuprates questionable.

In view of this fact, and the general consensus that the cuprates are strongly coupled systems, it comes as no surprise that effort has already been made to explain the cuprate condensation energy as a result of non-BCS physics. Scalapino and White [4] conjectured that at strong coupling, the dominant contribution to the condensation energy comes from a feedback effect on the magnetic excitations of the system. On the other hand, Norman et al argued [5] that the condensation energy likely has an electronic origin, and is driven by a gain in the kinetic energy which at strong coupling is negative (in contrast to BCS theory) because of a strong “undressing” of fermions which bear a greater resemblance to free particles in the superconducting state than they do in the normal state. Similar ideas were expressed by Hirsh and Marsiglio [6]. A different idea, related to the lowering of the Coulomb energy in the superconducting state has been proposed by Leggett [7].

In this communication we argue that these apparently disparate viewpoints are in fact
consistent with each other, and describe the same strong coupling physics. We argue that at
strong coupling, the relation between $E_c$ and $\Delta$ is qualitatively different from BCS theory and
is consistent with the experimental trends in the underdoped cuprates. We show furthermore
that the strong coupling effects are in large part the result of mutual feedback between the
fermions and bosons. We make the case that the contributions to the condensation energy
from these two channels may not be considered independently from each other, and that
only the sum of the two contributions has physical meaning.

Our point of departure is the general equation for the free energy of an interacting electron
system, derived by Luttinger and Ward [8] for the normal state and extended to a super-
conductor by Eliashberg [9]. We first review strongly coupled phonon superconductors.
We discuss the validity of the Eliashberg formula and describe the BCS, Bardeen-Stephen
[10] and Wada [11] expressions for the condensation energy (for a review, see Ref. [12]).
The BCS expression neglects both bosonic and fermionic self-energies (apart from a trivial
renormalization of the dispersion). The Bardeen-Steven and Wada expressions include the
fermionic self-energy and its change between the normal and the superconducting states, but
neglect the feedback from superconductivity on phonons. The two expressions are generally
considered to be identical, however we argue that this is only true as long as the feedback
from fermions onto phonons is neglected. We review Bardeen and Steven’s arguments for
the validity of this approximation for phonon superconductors.

We next modify the Eliashberg equation for $E_c$ to the case of magnetically mediated
superconductors. We argue that in qualitative distinction to the phonon case, the feedback
effect from the superconductivity onto the bosons may not be neglected if the pairing is
magnetic. We derive the relevant equations and explicitly compute $E_c$ assuming that the
pairing is due to spin-fluctuation exchange and is described by the spin-fermion model. We
show that when the feedback on bosons is non-negligible, the calculations require care as
both electronic and spin parts of the condensation energy are ultraviolet divergent. We
explicitly show that these divergencies are cancelled out between the two terms, and the
total $E_c$ (which turns out to be the only physically meaningful quantity) is free from diver-
gencies. We furthermore demonstrate that one can avoid the divergencies by performing the
computations in real frequencies. We apply the results to the cuprates and show that our
theoretical $E_c$ agrees with the data both in magnitude and in the doping dependence. We
view this agreement as a support for the spin-fluctuation scenario for the cuprates.
II. PHONON SUPERCONDUCTORS

The condensation energy $E_c$ is the difference between the free energies in the normal and superconducting states.

$$E_c = F_s - F_n.$$  \hspace{1cm} (1)

In the Greens function technique one evaluates the grand free energy $\Omega$. The difference $F_n - F_s$ coincides with $\Omega_s - \Omega_n$ provided that the chemical potential $\mu$ does not change between the two states. In the Eliashberg theory that we will be using, this is the case as the Fermi energy is assumed to be much larger than $\Delta$, and the corrections to $\mu$ due to pairing, which scale as powers of $\Delta/E_F$, are neglected [10].

There are two ways to compute $E_c$ using Green’s functions. The first approach is to use the general formula for the ground state energy of the interacting fermionic system in terms of the integral over the running coupling constant [13]:

$$\Omega = \Omega_0 - iT \sum_k \int_0^\lambda \frac{d\lambda'}{\lambda'} G(k, \lambda') \Sigma(k, \lambda')$$  \hspace{1cm} (2)

where $\Omega_0$ is the Free energy for free fermions, $\Sigma$ is the full self-energy, and $G = (i(\omega + \Sigma(k, \lambda')) - \epsilon_k)^{-1}$ is the full Green’s function. Both are functions of a 4 vector of momentum and Matsubara frequency $k = (k, \omega_n)$ and the running coupling constant $\lambda'$. Note that here and below we define $\Sigma$ with an extra factor of $i$.

Eq. (2) is applicable to both normal and superconducting states (for the latter, $\Sigma(k, \lambda')$ has a pole), however, is not convenient for our purposes as numerical calculations then require solving the Eliashberg equations for a large set of coupling values. Still, we tried this formalism, and will discuss the results in the Appendix A. The approach which we will be using in the bulk of the paper was suggested by Luttinger and Ward [8] who demonstrated that it is possible to re-express $\Omega$ in the normal state via a series of closed linked skeleton diagrams with fully dressed fermionic and bosonic propagators. Their approach was extended to the superconducting state by Eliashberg [9]. We refer the reader to Refs.[8] and [9] for the details of the derivation, and here just present the result. In the superconducting state, $\Omega$ has the form

$$\Omega = -2T \sum_k \left\{ \frac{1}{2} \log[\epsilon_k^2 + \Sigma^2(k) + \Phi^2(k)] - i\Sigma(k)G(k) + i\Phi(k)F(k) \right\}$$

$$+ \frac{1}{2} T \sum_q \left\{ \log[D^{-1}(q)] + \Pi(q)D(q) \right\}$$
The last term in the above equation is the sum of the first two closed linked skeleton diagrams, the dots stand for higher order diagrams. The functions \( G(k) \) and \( F(k) \) are the real and anomalous Greens functions given by

\[
G(k) = -\frac{\epsilon_k + i\tilde{\Sigma}(k)}{\epsilon_k^2 + \Sigma(k)^2 + \Phi^2(k)},
\]

\[
F(k) = i\frac{\Phi(k)}{\epsilon_k^2 + \Sigma(k)^2 + \Phi^2(k)}
\]

where \( \Phi(k) \) is the pairing vertex and \( \tilde{\Sigma}(k) = \omega_n + \Sigma(k) \). The conventionally defined pairing gap \( \Delta(k) \) is the ratio of the anomalous vertex and the self-energy: \( \Delta(k) = \Phi(k)\omega_m/\tilde{\Sigma}(k) \). Finally, \( \alpha_k \) is the electron-phonon coupling, and \( D(q) \) is the dressed phonon propagator given by \( D^{-1}(q) = D_0^{-1}(q) - \Pi(q) \) where \( \Pi(q) \) is the polarization bubble, and \( D_0(q) \) is the bare propagator. A careful reader may note that we define \( D(q) \) as dimensionless quantity (see (3), while the actual phonon propagator has a dimension of inverse energy. This does not cause problems, however, as \( D \) appears only in a combination with \( \alpha^2 \), and the extra overall energy factor can be absorbed from \( \alpha^2_k \). We will be using Eq. 3 as the point of departure for our analysis.

Eq. 3 is quite general. Its use for the calculation of \( E_c \) takes into account not just the introduction of the pairing vertex \( \Phi \) but also changes in the fermionic self energy \( \Sigma \) and the polarization bubble \( \Pi \). Thus it calculates the contributions to \( E_c \) from both the fermions and bosons.

The approximations made in the phonon case are associated with the smallness of the sound velocity \( v_s \) compared to the Fermi velocity \( v_F \). It turns out that higher order closed linked diagrams form series in powers of \( \lambda v_s/v_F \), where \( \lambda \) is the dimensional coupling constant which scales with \( \alpha_{k-k'} \) (see below). The approximation, attributed to Migdal [14] and Eliashberg [15], is to neglect \( O(\lambda v_s/v_F) \) terms without assuming that \( \lambda \) is by itself small. This would imply neglecting all terms labeled as dots in (3).

The physics behind the Migdal-Eliashberg approximation is best revealed by analyzing the perturbation series for \( \Sigma(k) \) and \( \Phi(k) \). These series can be separated into terms that scale as powers of \( \lambda \) and terms that scale as powers of \( \lambda v_s/v_F \). The perturbative series in powers of \( \lambda v_s/v_F \) arises from the actual electron-phonon scattering, and the factor \( v_s/v_F \) results from the fact that in this process electrons are forced to vibrate at phonon frequencies far from...
their own resonance. This gives rise to vertex corrections (at typical pairing frequencies), and to an equal renormalization of fermionic $\omega$ and $\epsilon_k$, i.e., the quasiparticle residue is renormalized, but the quasiparticle mass remains a bare one. The vertex correction diagrams for $\Sigma(k)$ and $\Phi(k)$, embedded into the closed linked diagrams, gives rise to higher-order skeleton diagrams for the Free energy, and it is these diagrams which are dropped.

The terms that form series in $\lambda$ are different and they are not considered to be small. In the normal state, they can be understood as coming from phonon-induced interactions between electrons and their own zero-sound collective modes. These terms do not contribute to the vertex renormalization (at typical frequencies for the pairing), and gives rise to a $\Sigma(k)$ that only depends on frequency. The $O(\lambda)$ terms also contribute to the pairing problem and in the superconducting state give rise to $\Phi(k)$ that again depends only on frequency.

Neglecting the higher order skeleton diagrams, Eliashberg obtained the closed-form expression for $\Omega_s$ given in Eq. 3. The closed form, coupled equations for the fermionic self-energy $\Sigma(k) = \Sigma(\omega)$ and the pairing vertex $\Phi(k) = \Phi(\omega)$ then follow from the condition that $\Omega_s$ given by (3) is stationary with respect to variations in $\Sigma(k)$ and $\Phi(k)$. The conditions $\delta\Omega_s/\delta\Sigma(k) = \delta\Omega_s/\delta\Phi(k) = 0$ yield

$$\tilde{\Sigma}(k) = \omega + iT\sum_{k'} \alpha_{k-k'}^2 G(k')D(k-k')$$
$$\Phi(k) = -iT\sum_{k'} \alpha_{k-k'}^2 F(k')D(k-k')$$

(5)

The Migdal-Eliashberg approximation has two further implications. First, the fermionic dispersion may be approximated by $\epsilon_k = v_F(k - k_F)$, as typical pairing frequencies should be much smaller than $E_F$ if $\lambda v_s/v_F$ is to be small. Second, the momentum integration over $k'$ can be factorized: the integration over momenta transverse to the Fermi surface involves only normal and anomalous fermionic propagators, via $\epsilon_k$, while the integration along the Fermi surface involves only the bosonic propagator in which one can set $|k| = |k'| = k_F$, i.e., deviations from the Fermi surface are neglected leading to a bosonic propagator dependant only on frequency. Corrections to this approximation again scale as $\lambda v_s/v_F$. Finally, it is assumed (without justification) that the Fermi surface is isotropic in the sense that $v_F$ is considered to be independent of $k$. Under these approximations, the momentum integration in the equations for $\Sigma(\omega)$ and $\Phi(\omega)$ can be performed exactly. Approximating the momentum
sum by an integral over energy and an associated density of states \( N_f \) as

\[
\sum_k \rightarrow N_f \int_{-\infty}^{\infty} d\epsilon
\]

, inserting equations 4 into equation 5 and performing the integration we obtain

\[
\tilde{\Sigma}(\omega) = \omega + \pi T N_f \sum_{\omega'} \alpha_{\omega-\omega'}^2 D(\omega - \omega') \frac{\tilde{\Sigma}(\omega')}{\sqrt{\Delta^2(\omega') + \Sigma^2(\omega')}}
\]

\[
\Phi(\omega) = \pi T N_f \sum_{\omega'} \alpha_{\omega-\omega'}^2 D(\omega - \omega') \frac{\Phi(\omega')}{\sqrt{\Delta^2(\omega') + \Sigma^2(\omega')}}
\]

An essential feature of the above equations is that apart from the assumption of the smallness of \( \lambda v_s/v_F \), it is assumed assumed that the phonon polarization bubble \( \Pi(k) \), which accounts for the effects of the electrons on phonons, may be neglected. Analogously to the derivation of equation 5, an expression for \( \Pi(k) \) can be formally obtained from the feature that \( \Omega_s \) given by (3) is also stationary with respect to variations in \( \Pi(k) \). The condition \( \delta \Omega_s/\delta \Pi(k) = 0 \) yields

\[
\Pi(k) = -2TD(0) \sum_{k'} \alpha_{k-k'}^2 [G(k)G(k-k') + F(k)F(k-k')]
\]

The fact that \( \Pi(k) \) is irrelevant to the phonon problem is not immediately apparent and this issue must be considered carefully. In the normal state,

\[
\Pi(k) \propto \lambda \frac{v_s}{v_F} \frac{\omega_m}{\omega_D} \frac{p_F}{|k|}
\]

reflecting the decay of a low-energy bosonic mode into a fermionic particle-hole pair. This decay term obviously cannot be neglected at the lowest frequencies as it accounts for the leading low-frequency dependence of \( D(\omega_m) \). I.e. for an Einstein phonon, \( D_0(\omega_m) = 2\omega_D^2/(\omega_D^2 + \omega_m^2) \) where \( \omega_D \) is the Debye frequency (we recall that \( D(\omega_m) \) is dimensionless, hence \( D^{-1}(\omega_m) = D_0^{-1}(\omega_m) - \Pi(k) \approx 1 - \Pi(k) \) at the lowest frequencies. However, for \( \lambda = O(1) \), the frequencies relevant to the pairing problem are of order \( \omega_D \), typical momenta are of order \( p_F \), and hence \( \Pi(k) \) at typical frequencies is small to the same extent as \( \lambda v_s/v_F \) and other similar terms in the Eliashberg theory. In the superconducting state, the low-energy phonons are gapped, and at frequencies smaller than \( \Delta \),

\[
\Pi(k) \propto \lambda \frac{v_s}{v_F} \frac{\omega_m}{\Delta} \frac{\omega_m}{\omega_D} \frac{p_F}{|k|}.
\]
This difference between $\Pi(k)$ in the normal and superconducting states reflects a fundamental change in the bosonic dynamics at small frequencies due to the gapping of low-energy fermionic excitations. Still, however, at typical frequencies for the pairing, $\omega \sim \Delta \sim \omega_D$, $\Pi(k) \sim \lambda v_s / v_F \ll 1$, and the polarization operator can be neglected compared to the bare phonon propagator. This was shown explicitly by Bardeen and Stephen [10] who evaluated the contribution to $E_c$ from the change of the bosonic dynamics between normal and superconducting states and demonstrated that in the phonon problem the bosonic piece in $E_c$ is small compared to the electronic piece and hence can be safely neglected.

We will see below that neglecting the bosonic contribution to $E_c$ is not a justifiable approximation if one is dealing with magnetic superconductors where the bosonic mode is a collective mode of the fermions. This is the main difference between phonon and magnetic superconductors, and we will examine this issue in the next section.

For completeness, we present several useful forms for $\Omega_S$ and $E_c$ for the phonon case. For simplicity, we assume that the electron-phonon coupling is independent of frequency, and the phonon spectrum consists of a single Einstein boson with a frequency $\omega_D \sim v_s p_F$, i.e.,

$$\alpha_\omega = \alpha$$

$$D(q) = D(\omega_m) = \frac{2\omega_D^2}{\omega_m^2 + \omega_D^2}$$

Integrating over momentum in Eq. (3) as before, we obtain

$$\Omega = -N_f \{ 2\pi T \sum_m \frac{\omega_m \tilde{\Sigma}_{\omega_m}}{\sqrt{\Sigma_{\omega_m}^2 + \Phi_{\omega_m}^2}}$$

$$+ T^2 \pi^2 \alpha^2 \sum_{m,m'} \frac{\tilde{\Sigma}_{\omega_m} \tilde{\Sigma}_{\omega_{m'}} + \Phi_{\omega_m} \Phi_{\omega_{m'}}}{\sqrt{\Sigma_{\omega_m}^2 + \Phi_{\omega_m}^2} \sqrt{\Sigma_{\omega_{m'}}^2 + \Phi_{\omega_{m'}}^2}} \left( \frac{1}{(\omega_m - \omega_{m'})^2 + \omega_D^2} \right) \}$$

(12)

where we introduced $\tilde{\alpha}^2 = 2\alpha^2 N_f \omega_D^2$. The dimensionless coupling $\lambda$ introduced above is related to $\tilde{\alpha}^2$ as

$$\lambda = \frac{\tilde{\alpha}^2}{\omega_D^2}$$

(13)

Eq. (12) may be simplified by making the standard substitutions $\tilde{\Sigma}_{\omega_m} = \omega_m + \Sigma_{\omega_m} = \omega_m Z_{\omega_m}$ and $\Phi_{\omega_m} = \Delta_{\omega_m} \tilde{\Sigma}_{\omega_m} / \omega_m = \Delta_{\omega_m} Z_{\omega_m}$. Substituting these forms into (12) we obtain

$$\Omega = -N_f \{ 2\pi T \sum_m \frac{\omega_m^2}{\sqrt{\omega_m^2 + \Delta_{\omega_m}^2}}$$

$$+ T^2 \pi^2 \tilde{\alpha}^2 \sum_{m,m'} \frac{\omega_m \omega_{m'} + \Delta_{\omega_m} \Delta_{\omega_{m'}}}{\sqrt{\omega_m^2 + \Delta_{\omega_m}^2} \sqrt{\omega_{m'}^2 + \Delta_{\omega_{m'}}^2}} \left( \frac{1}{(\omega_m - \omega_{m'})^2 + \omega_D^2} \right) \}$$

(14)
Thus we see that the free energy for a phonon superconductor is dependent only upon the form of the gap $\Delta_{\omega_m}$ and is not explicitly upon the self energy $\Sigma_{\omega_m}$.

A comment is in order here. The Luttinger-Ward result for the Free energy as a series of closed linked skeleton diagrams is, strictly speaking, only valid for the minimum of $\Omega$, i.e., for the self-energy that satisfies the stationary condition. Otherwise, the Luttinger-Ward generating functional (which is what they actually calculated) does not necessarily coincide with the Free energy. In the normal state, this does not cause a problem with Eq. (14) as $\Omega_N$ does not explicitly depend on $\Sigma_N$. (We use the capital subscripts "S" and "N" to denote "superconducting state" and "normal state" respectively. Lower case "n" (and "m") refer to Matsubara frequencies.) In the superconducting state, Eq (14) does not imply that $\Omega_S$ is at a minimum, i.e., $\delta \Omega_S / \delta \Delta = 0$. We didn’t analyze in detail the corrections to Eq. (14) which would stem from the difference between the Luttinger-Ward-Eliashberg functional and the actual Free energy, but the estimates show that these corrections would be again be small in $\lambda v_s / v_F$. If this is the case, then Eq. 14 can be used for the study of the profile of the free energy, i.e. how it evolves for different solutions of the gap. In particular, we verified that for the BCS case, the expansion of Eq. 14 near $\Delta = 0$ to order $\Delta^2$ yields the sign change of the slope at exactly the BCS transition temperature $T_c$.

For the remainder of this communication, we will only be considering $\Omega$ evaluated at the equilibrium solution of $\Delta_{\omega_m}$ when the applicability of the Luttinger-Ward formalism is rigorously justified. To this end, the Eliashberg equation for the equilibrium solution $\Delta_{\omega_m}$ may be obtained by minimizing equation 14 with respect to $\Delta$. This yields

$$
\Delta_{\omega_m} = \pi T \alpha^2 \sum_{m'} \left( \frac{1}{(\omega_m - \omega_{m'})^2 + \omega_D^2 \sqrt{\omega_{m'}^2 + \Delta_{\omega_{m'}}^2}} \left\{ \Delta_{\omega_{m'}} - \frac{\omega_{m'}}{\omega_m} \Delta_{\omega_m} \right\} \right)
$$

This solution for $\Delta$ must then be substituted into equation 14 allowing the calculation of the free energy at its minimum, and hence $E_c = \Omega_S - \Omega_N$ where $\Omega_N$ is obtained from $\Omega_S$ by setting $\Delta = 0$. Performing the computations, we obtained Eq. (17) below.

There is, however, a simpler way to proceed towards $E_c$. In this approach, one specifies at the outset that one is only interested in the Free energy at equilibrium. In this case, the fact that equation 3 should be stationary with respect to variations in $\Sigma$ and $\Phi$ can be invoked even before the momentum integration is performed [10–12]. Substituting equation (5) into
equation 3 and dropping the phonon piece, we obtain
\[
\Omega = -T \sum_p \{ \log[\epsilon_k^2 + \tilde{\Sigma}_{\omega_m}^2 + \Phi_{\omega_m}^2] - i\Sigma_{\omega_m} G(k) + i\Phi_{\omega_m} F(k) \} \tag{16}
\]
Introducing a density of states \(N_f\), integrating over \(\epsilon_k\) and subtracting the normal state result from the superconducting result gives an expression for the condensation energy first derived by Wada [11].
\[
E_c = -N_f \pi T \sum_m (\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2} - |\Sigma_{N,\omega_m}| + |\omega_m| - \sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}) \tag{17}
\]
Let us clearly state what the Wada expression calculates. It is the strong coupling result for the condensation energy at thermodynamic equilibrium, under the assumption that there are no appreciable changes in the bosonic mode between the normal and superconducting states. In other words, it accounts for the appearance of the pairing vertex, as well as any changes to the fermionic self energy, but ignores any feedback effects between bosons and fermions.

An equivalent expression for \(E_c\), more advantageous for numerical calculations due to a faster convergence at high frequencies was obtained by Bardeen and Stephen [10]. They noticed that there exists an integral relation between \(\Sigma_{N,\omega}\) and \(\Sigma_{S,\omega}\)
\[
N_f \pi T \sum_m \Sigma_{N,\omega_m} \frac{|\Sigma_{S,\omega_m}|}{\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}} = 0 \tag{18}
\]
that in turn is the consequence of the fact that
\[
T \sum_m \int d^2k \Sigma_{N,\omega_m} G_{S,\omega_m}(k) = T \sum_m \int d^2k \Sigma_{S,\omega_m} G_{N,\omega_m}(k) \tag{19}
\]
as both quantities can be re-expressed as a cross-product
\[
T^2 \sum_{m,n} \int d^2k D_{\omega_n - \omega_m} G_{N,\omega_m}(k) G_{S,\omega_n}(k) \tag{20}
\]
Using equation (18), Bardeen and Stephen obtained the following expression for \(E_{c,el} = E_c\).
\[
E_{c,el} = -N_f \pi T \sum_m \left( \sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2} - |\Sigma_{S,\omega_m}| \right)^2 \left( 1 - \frac{\Sigma_{N,\omega_m}}{\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}} \right) \tag{21}
\]
The practical importance of Bardeen-Stephen result is that at high frequencies, when \( \tilde{\Sigma}_{S,\omega_m} \approx \tilde{\Sigma}_{N,\omega_m} \approx \omega_m \), the integrand in (21) behaves as \( \Phi_{\omega_m}^4 / \omega_m^3 \), and the frequency summation rapidly converges. This makes the Bardeen-Stephen expression more convenient for numerical computations than Wada’s expression.

We emphasize again that the equivalence of the two forms for \( E_c \) is the consequence of the fact that in the phonon case, the change of the bosonic self-energy \( \Pi(\omega) \) between normal and superconducting states can be neglected, and the accuracy of this approximation is governed by the same parameter \( \lambda v_s / v_F \) as the accuracy of the Eliashberg theory. In the next section we show that this is not the case for spin mediated pairing. We will see that for superconductors with an electronic pairing mechanism, the feedback on the pairing boson plays a crucial role, and the Wada’s expression for \( E_c \) would give completely erroneous results. Instead, the full expression (3) must be used.

We pause now to connect with the BCS result for the condensation energy. BCS is a weak coupling theory. It assumes that the only change between the normal and superconducting states is the introduction of the pairing vertex \( \Phi \) which is given by the BCS gap \( \Delta \). (\( \Phi_{BCS} = \Delta \)). The fermionic and bosonic self energies are both taken to be negligible. The BCS condensation energy is therefore calculated from the Wada equation with the substitution \( \tilde{\Sigma}_{\omega_m} = \omega_m + \Sigma_{\omega_m} \approx \omega_m \). Taking the zero temperature limit we obtain after some simple algebra

\[
E_{BCS}^c = -N_f \int_0^\infty \frac{2\omega^2 + \Delta^2}{\sqrt{\omega^2 + \Delta^2}} - 2\omega = -N_f \frac{\Delta^2}{2} \tag{22}
\]

This is the result that we already cited in the Introduction. We also see that the frequency integration in (22) is confined to \( \omega \sim \Delta \), i.e., the condensation energy comes from fermions in a narrow region around the Fermi surface. Although this result looks rather straightforward, the issue of which fermions contribute to the condensation energy in the BCS case is nontrivial, and we discuss it in detail in Appendix B.

III. MAGNETIC SUPERCONDUCTORS

We now proceed to the case of magnetically mediated pairing. The bosonic mode that mediates the pairing is now the low-energy spin susceptibility. The Luttinger-Ward formalism, which deals with an arbitrary bosonic mode is still valid, i.e., the Free energy has
the same form as in Eq. 3. The only immediate modification is that now the second term of Eq. 3 has an extra factor of 3 reflecting the fact that all three components of the spin susceptibility contribute equally to the pairing. The Free energy then has the form

\[ \Omega = -2T \sum_p \{ \frac{1}{2} \log[\epsilon_k^2 + \hat{\Sigma}^2(k) + \Phi^2(k)] - i\Sigma(k)G(k) + i\Phi(k)F(k) \} + \frac{3}{2}T \sum_q \{ \log[D^{-1}(q)] + \Pi(q)D(q) \} + T^2 \sum_{k,k'} g_{k-k'}^2 \{ G(k)\chi(k - k')G(k') + F(k)\chi(k - k')F(k') \} + \ldots \]  

(23)

The dimensionless bosonic propagator \( D(q) \) is now related to the magnetic susceptibility \( \chi_{ij}(q) = \chi(q)\delta_{ij} \) as \( D(q) = \chi(q)/\chi(Q, 0) \) where \( Q \) is the momentum at which the static susceptibility is peaked. Similarly to phonons, \( \chi(q) \) is related to the bare susceptibility by \( \chi^{-1}(q) = \chi_0^{-1}(q) - \Pi(q) \). We discuss the exact form of \( \chi(q) \) below. Finally, \( g_q \) is now the coupling between the fermionic propagator and bosonic (magnetic) mode.

At this point the formalism is quite general, taking into account all changes to both the fermions and bosons. In order to proceed further, we will need to assume a specific model that will allow us to neglect higher order terms in Eq. 23. We choose the spin-fermion model in which fermions are paired via their own collective spin excitations. Several authors have demonstrated that the exchange of collective spin fluctuations peaked at or near the antiferromagnetic momentum \( Q = (\pi, \pi) \) yields an attraction in the 12 pairing channel.

We will be studing \( E_c \) for this kind of pairing.

The spin-fermion model is described by the effective action

\[ S = - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{k,\sigma} c_{k,\sigma}^\dagger(\tau)G_0^{-1}(k, \tau - \tau')c_{k,\sigma}(\tau') + \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \sum_q \chi_0^{-1}(q, \tau - \tau') S_q(\tau) \cdot S_{-q}(\tau') + g_q \int_0^\beta d\tau \sum_q s_q(\tau) \cdot S_{-q}(\tau) , \]  

(24)

where \( G_0^{-1}(k, \tau) = \partial_\tau - v_k(k - k_F) \) is the bare Fermionic propagator, \( c_{k,\sigma}^\dagger \) is the fermionic creation operator for an electron with crystal momentum \( k \) and spin projection \( \alpha \), \( s = c^\dagger \sigma c \), where \( \sigma_i \) are the Pauli matrices, and \( g \) is the coupling constant which measures the strength of the interaction between fermionic spins and the collective spin degrees of freedom described by bosonic variables \( S_q \). For simplicity, below we assume \( g_q = g \) to be momentum
independent. The bare spin susceptibility \( \chi_0^{-1}(q, \tau) \) is assumed to be peaked at \( Q \) and has a standard Ornstein-Zernike form, i.e., its Fourier transform over \( \tau \) is

\[
\chi_0(q, \omega) = \frac{\chi(Q)}{1 + \xi^2 (q - Q)^2 - (\omega/(v_s \xi^{-1}))^2}.
\]

(25)

where \( \xi \) is the magnetic correlation length. This bare susceptibility comes from fermions with energies comparable to \( E_F \) and should be considered as an input for the low-energy theory.

The dimensionless coupling constant for the model of Eq. (24) (defined such that \( \Sigma(\omega, k_F) = \lambda \omega \) in \( D = 2 \)) is,

\[
\lambda = 4\bar{\omega}/(3v_F \xi^{-1}),
\]

(26)

where \( \bar{\omega} = 9g^2 \chi(Q)/(16\pi \xi^2) \). The numerical factors are choosen for further convenience. This overall scale \( \bar{\omega} \) and the coupling \( \lambda \) are the only two parameters that matter at strong coupling. Other parameters, e.g., \( v_s \), turn out to be irrelevant (see below). Note that \( \bar{\omega} \) is in fact independent of \( \xi \) as \( \chi(Q) \) by itself scales as \( \xi^2 \).

Near a magnetic transition, \( \xi \) is large, i.e., \( \lambda \geq 1 \), and spin-fermion model is a strong coupling theory in which feedback effects between fermions and bosons are extremely important. It has been discussed in depth in [16] as a theoretical model as well as with respect to the cuprates, and provided an explanation of many unusual properties of the cuprates such as non-Fermi liquid behavior in the normal state [17], \( d_{x^2-y^2} \) pairing [18], and the pseudogap [21]. We note, though, that there is still a great deal of controversy regarding the full description of these phenomena. Since, however, it is generally believed that the cuprates are strongly coupled superconductors, it is instructive, regardless of one’s prejudices, to examine the condensation energy for the spin-fermion model in detail, so as to illustrate the importance of properly accounting for all feedback effects when dealing with a strongly coupled system. We will show that the spin-fermion model accounts for many aspects of the experimentally measured condensation energy.

A. The validity of the Eliashberg approximation

We begin by briefly discussing the validity of the Eliashberg approximation for antiferromagnetically mediated superconductivity and how the assumptions inherent in the
Luttinger-Ward condensation energy formalism are justified. For the purposes of calculating the condensation energy, there are two main issues to be discussed. First, as with phonons, it is possible in the spin-fermion model to separate the perturbative series such that the terms resulting from vertex corrections and higher order diagrams are ”small” and therefore irrelevant. Second, since the effects of pairing are greatest near ”hot spots” (points on the Fermi surface connected by $\mathbf{Q} = (\pi, \pi)$) one can invoke an effective momentum independence for the problem, while still retaining the $d_{x^2-y^2}$ pairing symmetry. We briefly enumerate the reasoning leading to the above conclusions here. A more detailed discussion can be found in Ref.[16].

1. Spin fluctuations are collective modes of fermions, hence there is no difference between the Fermi velocity and the spin velocity, i.e., $v_s \sim v_F$. Then $\lambda v_s / v_F \sim \lambda$, i.e., there is no way to separate perturbative series based on the difference between velocities. From this perspective, there is no Migdal theorem for spin fluctuations, and the perturbation theory with the bare spin propagator just holds in powers of the coupling $\lambda$.

2. The absence of small $v_s / v_F$ implies in turn that the polarization operator $\Pi(Q, \omega_m) = \Pi_{\omega_m}$ is not negligible, as it is for phonons, but is rather dominant for $\lambda \gg 1$. The consequence of this is that one must simultaneously solve for both the fermionic and bosonic self-energies.

3. In the normal state, $\Pi_{\omega_m} \propto \omega_m$ at low frequencies, i.e., when $\Pi_{\omega_m}$ dominates the frequency dependence of the spin susceptibility (strong coupling), spin fluctuations become diffusive. This transmutation of the spin dynamics from propagating with $v_s \sim v_F$ for $\lambda \ll 1$ to diffusive for $\lambda \geq 1$ implies that at strong coupling bosons become soft compared to electrons. Such softness of bosons, is precisely the physics behind the Migdal theorem. Not surprisingly then, the diagramatic series for fermionic $\Sigma(k)$ obtained with a diffusive bosonic propagator again can be separated into two different subsets of terms: one set of terms now scales as powers of $\log \lambda$ instead of powers of $\lambda$, and the reduction of the expansion parameter is a direct consequence of the softness of bosons compared to fermions. As for phonons, the series in $\log \lambda$ gives rise to vertex corrections and to the renormalization of the quasiparticle residue. There are also terms that form series in $\lambda$. As with phonons, these terms come from boson-induced interactions between electrons and their own zero-sound modes. That these series
hold in powers of the same $\lambda$ as the perturbation series with a bare boson propagator can be easily understood as at low frequencies, the interaction between fermions and their zero-sound modes is mediated by a static boson, and hence is unsensitive to any transmutation of the bosonic dynamics.

4. This separation of terms into perturbative series of $\lambda$ and $\log \lambda$ allows an approximation similar to that made for phonons to be made here. In the magnetic case one neglects terms $O(\log \lambda)$ compared to terms of order $\lambda$. This is not as good of a approximation as the neglect of $\lambda v_s/v_F$ terms for phonons as $\log \lambda$ is also large when $\lambda$ is large. However, the numerical prefactors for $\log \lambda$ series turn out to be small (a vertex correction is only $(1/8) \log \lambda$), and in practice the neglect of logarithmical terms is well justified for all physically reasonable $\lambda$ ($\lambda \sim 1 - 2$ at optimal doping). In addition, from a purely theoretical standpoint the $\log \lambda$ terms can be made parametrically small by introducing a large number of fermionic flavors $M$ (a vertex correction is then $(1/8M) \log \lambda$). Furthermore, a one-loop RG analysis of the logarithmical terms shows that they give rise to fractional exponents, but do not change the physics, and, in particular, do not affect the pairing problem.

5. As with phonons, the series in $\lambda$ yields a $\Sigma(k, \omega_m)$ that is predominantly dependant on frequency. More specifically, near $k$–points on the Fermi surface connected by the antiferromagnetic wave vector $Q$ (hot spots), $\Sigma(k, \omega)$ depends on $\omega$, but not on $\epsilon_k$. This momentum independence is crucial for the computation of the spin polarization operator: for $\Sigma(k, \omega) = \Sigma(\omega)$, the density of states is flat, and $\Pi_{\omega_m}$ turns out to be independent of $\Sigma(\omega)$ and is the same in the normal state as it would be for free fermions:

$$\Pi(\omega_m) = \frac{\omega_m}{\omega_{sf}} = 4\lambda^2 \frac{\omega_m}{\bar{\omega}}$$  \hspace{1cm} (27)

Here we have introduced the notation $\omega_{sf} = \bar{\omega}/(4\lambda^2)$. This $\omega_{sf}$ scales as $\xi^{-2}$ and vanishes at the magnetic transition.

6. Away from a hot spot, this independence from $\epsilon_k$ (i.e., on momentum perpendicular to the Fermi surface) prevails, but $\Sigma(k, \omega_m)$ still depends on the momentum along the
Fermi surface. At $T = 0$, the self-energy takes the form

$$
\Sigma(k, \omega) = \lambda(k) \frac{2\omega}{1 + \sqrt{1 - i|\omega|/\omega_{sf}(k)}},
$$

where

$$
\lambda(k) = \lambda/(1 + (\tilde{k}\xi)^2)^{1/2}, \quad \omega_{sf}(k) = \omega_{sf}(1 + (\tilde{k}\xi)^2).
$$

and $\tilde{k}$ is the component of $k - k_{hs}$ along the Fermi surface. This $k$ dependence cannot be neglected at the lowest frequencies as near the transition as $\tilde{k}$ appears in a combination with $\xi$. However, for $\omega \gg \omega_{sf}(k)$, the $k$-dependence disappears: $\Sigma(k, \omega) \approx (i\omega\bar{\omega})^{1/2}$ (we used the fact that $2\lambda(k)(\omega_{sf}(k))^{1/2} = \bar{\omega}$). Alternatively speaking, at $\omega > \omega_{sf}(k)$, the whole Fermi surface acts as one big hot spot. In this range, the Eliashberg theory becomes applicable for all momenta.

7. We see that whether or not the $k$ dependence of the self-energy can be neglected depends on what the relevant $\omega$ and $\tilde{k}$ are. For the pairing problem, a detailed analysis shows that typical frequencies are of order $\bar{\omega}$, and typical $\tilde{k}$ are of order $\bar{\omega}/v_F$. Then typical $\omega_{sf}(k)$ are of order $\bar{\omega}$, i.e., the momentum dependence along the Fermi surface introduces corrections $O(1)$. These corrections have been checked in [20] and found to be nonessential from the perspective of the basic physics. Note also that the theory assumes that $\bar{\omega} < E_F$, otherwise the linearization of the dispersion near the Fermi surface would not work. This in turn implies that the pairing is confined to fermions in the near vicinity of a hot spot.

8. In the phonon case, the momentum integration in the expressions for the Free energy, fermionic $\Sigma$ and anomalous vertex $\Phi$ can be factorized and performed exactly. Such momentum related corrections are always small to the extent of $\lambda v_s/v_F$. In the magnetic case, the corrections resulting from an analogous procedure are always smaller than 1, but whether or not they are small parametrically depends on the frequency. For frequencies relevant to the pairing, the corrections to the factorization are again $O(1)$.

We see from the above considerations that at strong coupling, $\lambda \geq 1$, the softness of fermions compared to bosons gives rise to an effective Migdal theorem, i.e., the vertex corrections are smaller than $\Sigma$ which in turn predominantly depends on frequency. Contrary
to the phonon case, there is no single parameter governing the validity of the Eliashberg approximation. There are logarithmically divergent corrections, but they do not affect the physics of the pairing, at least in the one-loop approximation. There are also physically irrelevant $O(1)$ corrections stemming from the momentum dependence of the fermionic self-energy and the pairing vertex along the Fermi surface. An Eliashberg-type theory is valid when both corrections are neglected. As we stated previously, this is quite reasonable from a physical perspective, and we now proceed under the assumption that the momentum dependence of $\Sigma$ and $\Phi$ can be fully neglected. In the case of $\Phi$, this implies that we approximate the $d_{x^2-y^2}$ pairing vertex (and, hence the gap $\Delta = \Phi_\omega/(\omega + \Sigma_\omega)$) by its value at a hot spot, taking into account the fact that the $d-$wave symmetry of $\Phi$ implies that it has a different sign between hot spots separated by $Q$.

B. Thermodynamic potential at equilibrium

We now proceed by calculating the thermodynamic potential at its equilibrium value. As in the phonon case, the condition that $\Omega$ is stationary with respect to variations of $\Sigma$, $\Phi$ and $\Pi$ gives

$$\Sigma(k) = 3i T g^2 \chi(Q) \sum_{k'} G(k') \chi(k - k')$$
$$\Phi(k) = -3i T g^2 \chi(Q) \sum_{k'} F(k') \chi(k - k')$$
$$\Pi(k) = -2 T g^2 \chi(Q) \sum_k [G(k) G(k - k') + F(k) F(k - k')]$$

(30)

Under the assumption of the momentum independence of $\Sigma$, $\Phi$ and $\Pi$ the real and anomalous Greens functions have the form

$$G_{\omega_m}(k) = -\frac{\epsilon_k + i\bar{\Sigma}_{\omega_m}}{\epsilon_k^2 + \Sigma_{\omega_m}^2 + \Phi_{\omega_m}^2},$$
$$F_{\omega_m}(k) = \frac{i\Phi_{\omega_m}}{\epsilon_k^2 + \Sigma_{\omega_m}^2 + \Phi_{\omega_m}^2}$$

(31)

and the $d_{x^2-y^2}$-pairing implies $F_\omega(k + Q) = -F_\omega(k)$. Furthermore, as we discussed, the momentum integration in Eqs. 30 can be factorized and performed exactly. This yields

$$\Sigma_{\omega_m} = \lambda \pi T \sum_n \frac{\bar{\Sigma}_{\omega_n}}{\sqrt{\Sigma_{\omega_n}^2 + \Phi_{\omega_n}^2}} \frac{1}{(1 - \Pi_{\omega_{m-n}})^{1/2}},$$

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\[
\Phi_{\omega_m} = \lambda \pi T \sum_n \frac{\Phi_{\omega_n}}{\sqrt{\sum_{\omega_n}^2 + \Phi_{\omega_n}^2}} \frac{1}{(1 - \Pi_{\omega_{m-n}})^{1/2}},
\]
\[
\Pi_{\omega_m}(Q) = \frac{4\lambda^2}{\bar{\omega}} \pi T \sum_n \left[-1 + \frac{\sum_{\omega_n}^2 \sum_{\omega_{n+m}} + \Phi_{\omega_n} \Phi_{\omega_{n+m}}}{\sqrt{\sum_{\omega_n}^2 + \Phi_{\omega_n}^2} \sqrt{\sum_{\omega_{n+m}}^2 + \Phi_{\omega_{n+m}}^2}} \right].
\]

We emphasize again that Eqs. (32) contain only two inputs: the overall energy scale \(\bar{\omega}\) that is set by the spin-fermion interaction, and the dimensionless spin-fermion coupling \(\lambda \propto \xi\) that diverges as the system approaches the antiferromagnetic instability. We also recall that the energy scale \(\bar{\omega}\) is the ultimate upper cutoff for the strong coupling behavior (\(\Sigma_{\omega_m} < \omega_m\) for \(\omega_m > \bar{\omega}_m\)), while dimensionless \(\lambda\) can be represented as the ratio \((2\lambda)^2 = \bar{\omega}/\omega_{sf}\) of \(\bar{\omega}\) and another typical scale \(\omega_{sf}\) that sets the upper boundary of the Fermi-liquid behavior in the normal state. We illustrate the form of \(\Sigma_{\omega_m}, \Phi_{\omega_m}\) and \(\Pi_{\omega_m}\) in figure 1 for both the normal and superconducting state.

Substituting equations 30 into 23 we obtain the equilibrium thermodynamic potential in a magnetically mediated superconductor:

\[
\Omega = -T \sum_m \int \frac{d^2 k}{(2\pi)^2} \left\{ \log[\epsilon_k^2 + \Sigma_{\omega_m}^2 + \Phi_{\omega_m}^2] - i \Sigma_{\omega_m} G_{\omega_m}(k) + i \Phi_{\omega_m} F_{\omega_m}(k) \right\}
+ \frac{3}{2} T \sum_m \int \frac{d^2 k}{(2\pi)^2} \left\{ \log[\chi(Q,0)\chi(q,\omega_m)] + \Pi_{\omega_m} \frac{\chi(q,\omega_m)}{\chi(Q,0)} \right\}
\]

The difference between the above equation and equation 12 (apart from the extra factor of 3) is that we have retained the bosonic part of the free energy as it is by no means small. In light of this, it is convenient to represent \(\Omega\) as the the sum of two parts \(\Omega_{el}\) comprising the "electronic" contributions and \(\Omega_{spin}\) comprising the "magnetic" part. Accordingly,

\[
E_c = E_{c,el} + E_{c,spin}
\]

where

\[
\Omega_{el} = -T \sum_m \int \frac{d^2 k}{(2\pi)^2} \left\{ \log[\epsilon_k^2 + \Sigma_{\omega_m}^2 + \Phi_{\omega_m}^2] - i \Sigma_{\omega_m} G_{\omega_m}(k) + i \Phi_{\omega_m} F_{\omega_m}(k) \right\}
\]
\[
\Omega_{spin} = \frac{3}{2} T \sum_m \int \frac{d^2 k}{(2\pi)^2} \left\{ \log[\chi(Q,0)\chi(q,\omega_m)] + \Pi_{\omega_m} \frac{\chi(q,\omega_m)}{\chi(Q,0)} \right\}
\]

The electronic term \(E_{c,el} = \Omega_{el}^S - \Omega_{el}^N\) accounts explicitly for the appearance of the anomalous pairing vertex \(\Phi_{\omega_n}\), and for the feedback changes to the fermionic self-energy. This term by
FIG. 1: Matsubara frequency solutions at $\lambda = 1$ for $\Sigma$ (a), $\Phi$ (b) and $\Pi$ (c) in the spin fermion model (eqs 32) for both the normal and superconducting states. Note that $\Sigma$ is a strong function of frequency and may not be neglected. The apparent non-convergence of $\Sigma$ at high frequencies is spurious and is discussed in the text. Further note that $\Pi$ changes appreciably between the normal and superconducting states. This change must be taken into account when calculating the condensation energy.

itself leads to the Wada result for the condensation energy. The term $E_{c,\text{spin}} = \Omega_{\text{spin}}^{sc} - \Omega_{\text{spin}}^{n}$ accounts for changes to the spin propagator via the changes to the spin polarization operator $\Pi_{\omega_m}$. Together these two expressions account the feedback effects between fermions and bosons in a strong coupling theory. We point out that the distinction between $\Omega_{\text{el}}$ and $\Omega_{\text{spin}}$ is quite artificial, as the two are intimately connected by mutual feedback. It is the sum of the two which is physically relevant, and the two parts of $E_c$ may not be considered
separately unless, as in the phonon case, one of them is negligible.

As $\Sigma$ and $\Phi$ and $\Pi$ depend only on $\omega$, the momentum integration in Eqs.35 can be performed explicitly and yields

$$E_{c,el} = -N_f \pi T \sum_m (\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2} - |\Sigma_{N,\omega_m}|)$$

$$+ |\omega_m| \left(\frac{|\Sigma_{S,\omega_m}| - \sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}}{\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}}\right)$$

$$E_{c,spin} = -\frac{3T}{8\pi\xi^2} \sum_m \Pi_{S,\omega_m} - \Pi_{N,\omega_m} + \log \frac{1 - \Pi_{S,\omega_m}}{1 - \Pi_{N,\omega_m}}$$

The first term $E_{c,el}$ is the Wada result. The second term $E_{c,spin}$ is new. Note that its expansion in $\Omega$ begins with the quadratic term. This is the obvious consequence of the fact that the Free energy is stationary with respect to a variation of $\Pi$.

C. A cancellation of divergencies

At a first glance, the electronic part of the condensation energy is qualitatively the same as the phonon result. This turns out, however, not to be the case as $E_{c,el}$ in fact contains a divergent piece which is cancelled out by the divergence in $E_{c,spin}$. Indeed, consider the high frequency part of $E_{c,el}$. At high frequencies, $\sum_{\omega_m}$ dominates over $\Phi_{\omega_m}$, and the electronic part of the condensation energy reduces to

$$\Omega_{el} = -N_f \pi T \sum_m |\Sigma_{S,\omega_m}| - |\Sigma_{N,\omega_m}| + ...$$

where dots stand for other terms that are all finite, as one can easily demonstrate. Examine next the equation for $\Sigma$. By making the substitution $\Delta_{\omega_m} = \Phi_{\omega_m} \omega_m / \Sigma_{\omega_m}$ we may write $\Sigma_{\omega_m}$ in the following form.

$$\Sigma_{\omega_m} = \pi \lambda T \sum_n \frac{\omega_n}{\sqrt{\omega_n^2 + \Delta_n^2}} \frac{1}{(1 - \Pi_{\omega_m - \omega_n})^{1/2}}$$

Were the bosonic spectrum unchanged between the superconducting and normal states ($\Pi_N = \Pi_S$) then we could expand equation (39) in powers of $\Delta_n$, and would find that at large frequencies

$$\Sigma_{S,\omega_m} - \Sigma_{N,\omega_m} \propto \frac{\Delta_{\omega_m}^2}{\omega_m}$$

Since the gap $\Delta_{\omega_m}$ is expected on physical grounds to vanish at the highest frequencies (and computations indeed confirm this), the frequency integral in (38) converges, i.e., the
electronic part of the condensation energy would be finite. The situation is very different when changes in $\Pi$ are taken into account. Although at high frequencies $\Pi_{S,\omega_n}$ indeed converges to $\Pi_{N,\omega_n}$, the two expressions are different at frequencies comparable to typical $\Delta_{\omega_n}$. Since for arbitrary large $\omega_m$ in equation (39), there is a range of running $\omega_n$ where $\Pi_S$ and $\Pi_N$ differ, $\Sigma_S$ and $\Sigma_N$ do not converge at high frequencies: $\Sigma_{S,\omega_n}$ remains larger than $\Sigma_{N,\omega_n}$ by a constant. We illustrate this behavior in figure 1 (a).

This non-convergence of $\Sigma_N$ and $\Sigma_S$ seems at first glance to imply an infinite result for the condensation energy! It turns out that this apparent infinity is compensated for by the spin part of the condensation energy. As written in equation (37) the spin condensation energy looks quite convergent if we use $\Pi_{N,\omega_n} \propto \omega_m$. However, the expression for the spin polarization operator is formally ultraviolet divergent, and extra care has to be taken in evaluating the difference between $\Pi_{N,\omega_m}$ and $\Pi_{S,\omega_m}$.

In what follows we explicitly re-express the divergent contribution in $E_{c,el}$ in terms of the spin polarization operator, and show that when we take the divergent piece from $E_{c,el}$ and add it to $E_{c,spin}$, the dangerous $\Pi_{N,\omega_m} - \Pi_{S,\omega_m}$ term in $E_{c,spin}$ is cancelled out, and the remaining terms are all convergent, and in evaluating them we can safely use the regularization in which the ultraviolet divergent piece in $\Pi_{N,\omega_m}$ is absent, and $\Pi_{N,\omega_m} \propto \omega_m$. In practice, this regularization amounts to evaluating the integral over $\epsilon_k$ first, and the frequency integral later.

In order to accurately single out the divergent piece in $E_{c,el}$ and relate it to the spin polarization operator, we use a trick originally suggested by Bardeen and Stephen and define a mixed self energy $\Sigma_{NS}$ ($NS$ stands for normal-superconducting). This is the normal state Eliashberg equation for $\Sigma$ but with the superconducting polarization bubble.

$$i \Sigma_{NS,\omega_m} = -\alpha^2 \pi T \sum_n \int \frac{d^2q}{(2\pi)^2} \chi_{S,\omega_n}(q) G_{N,\omega_{n+m}}(k + q)$$
$$= \pi \lambda^2 T \sum_n \frac{1}{(1 - \Pi_{S,\omega_{m-n}})^{1/2}} \text{sgn}(\omega_n) $$ (41)

We plot $\Sigma_{NS}$ given by the above equation along with $\Sigma_S$ in figure 2 and show that they converge at high frequencies. We then add and subtract $\Sigma_{NS}$ from $E_{c,el}$.

$$E_{c,el} = -N_f \pi T \sum_{m} \left( \sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2} - |\Sigma_{NS,\omega_m}| \right)$$
$$+ |\omega_m| \frac{|\Sigma_{S,\omega_m}| - \sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}}{\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}}$$

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FIG. 2: Spin-fermion solutions for $\Sigma_S$ and $\Sigma_{NS}$ as defined by equation 41 in Matsubara frequencies.

Note that by replacing $\Pi_N$ by $\Pi_S$ in the normal state expression for $\Sigma$, we have obtained a convergent expression for the electronic part of the condensation energy as discussed in the text.

\[
+ \left\{ |\tilde{\Sigma}_{NS,\omega_m}| - |\tilde{\Sigma}_N,\omega_m| \right\}
\]

One can easily make sure that $E_{c,el}$ now consists of a convergent piece plus the divergent $|\tilde{\Sigma}_{NS}| - |\tilde{\Sigma}_N|$. The above is actually $|\Sigma_{NS}| - |\Sigma_N|$ as the $\omega_m$’s cancel.

We now explicitly express this divergent piece in terms of the spin polarization operator. To accomplish this, we recall that the term $|\tilde{\Sigma}_N|$ in $E_{c,el}$ arose from the integration over momentum of the $\Sigma G$ term in Eq. 35. Writing this for both the normal and normal-superconducting self energies, we have:

\[
N_f \pi T \sum_m |\Sigma_{N,NS,\omega_m}| = T \sum_m \int \frac{d^2k}{(2\pi)^2} i\Sigma_{N,NS,\omega_m} G_{N,\omega_m}
\]

By using the expressions for $\Sigma$ and $\Pi$ the above may be written as a term in $E_{c,spin}$ as follows:

\[
+ T \sum_m \int \frac{d^2k}{(2\pi)^2} i\Sigma_{N,NS,\omega_m} G_{N,\omega_m} \\
= T \sum_m \int \frac{d^2k}{(2\pi)^2} \left\{ -3g^2\pi T \sum_n \int \frac{d^2q}{(2\pi)^2} \chi_{N,NS,\omega_n}(q) G_{N,\omega_n+m}(k+q) \right\} G_{N,\omega_n}(k) \\
= -\frac{3}{2} T \sum_n \int \frac{d^2q}{(2\pi)^2} \chi_{N,NS,\omega_n}(q) \left\{ 2g^2\chi(0)\pi T \sum_m \int \frac{d^2k}{(2\pi)^2} G_{N,\omega_n+m}(k+q) G_{N,\omega_n}(k) \right\} \\
= -\frac{3}{2\chi_0} T \sum_n \int \frac{d^2q}{(2\pi)^2} \chi_{N,NS,\omega_n}(q) \Pi_{N,\omega_n}
\]

Performing the integration over $q$ we find that

\[-\pi T N_f \sum_m \left| |\Sigma_{NS,\omega_m}| - |\Sigma_{N,\omega_m}| \right| = -T \frac{3}{8\pi \xi^2} \sum_m \Pi_{N,\omega_m} \log \frac{1 - \Pi_{S,\omega_m}}{1 - \Pi_{N,\omega_m}}
\]
We now move the divergent piece from $\Omega_{el}$ to $\Omega_{spin}$ and write the condensation energy as

$$E_c = \delta \tilde{\Omega}_{el} + \delta \tilde{\Omega}_{spin}$$

with

$$\delta \tilde{\Omega}_{el} = -N_f \pi T \sum_m \left( \sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2} - |\Sigma_{NS,\omega_m}| \right) + |\omega_m| \left| \frac{\Sigma_{S,\omega_m}}{\sqrt{\Sigma_{S,\omega_m}^2 + \Phi_{\omega_m}^2}} \right|$$

$$\delta \tilde{\Omega}_{spin} = -\frac{3T}{8\pi \xi^2} \sum_m \Pi_{S,\omega_m} - \Pi_{N,\omega_m} + (1 + \Pi_{N,\omega_n}) \log \frac{1}{1 - \Pi_{S,\omega_m}}$$

The electronic part is now fully convergent. For the spin part, one can easily check that at large frequencies, when $\Pi_{N,\omega_m}$ and $\Pi_{S,\omega_m}$ are both large, the expansion of the logarithm in $E_{c,spin}$ cancels the dangerous $\Pi_{S,\omega_m} - \Pi_{N,\omega_m}$ term. The remaining terms are all ultraviolet convergent, i.e., are insensitive to the regularization procedure used to evaluate $\Pi_{N,\omega_m}$. This implies that the condensation energy is actually free from divergencies, as it indeed should be based on physical reasoning.

D. The relation between $\delta \tilde{\Omega}_{el}$ and $\delta \tilde{\Omega}_{spin}$.

At this point, the electronic and spin contributions to the condensation energy seem to be rather different as the electronic part contains $N_f$, while the spin part doesn’t. However, $\delta \tilde{\Omega}_{el}$ and $\delta \tilde{\Omega}_{spin}$ are in fact of the same order as we now demonstrate. Indeed, as we already said, typical frequencies for the pairing are of order $\bar{\omega}$, and at these frequencies

$$\Pi_{S,\omega_m} \sim \Pi_{N,\omega_n} \sim \frac{\bar{\omega}}{\omega_{sf}}$$

Similarly,

$$\Sigma_{S,\omega_n} \sim \Sigma_{N,\omega_n} \sim \bar{\omega}$$

Then using equation 47 for $\delta \tilde{\Omega}_{spin}$:

$$\delta \tilde{\Omega}_{spin} \sim \frac{\bar{\omega}^2}{\omega_{sf} \xi^2} \sim \frac{\bar{\omega}^3}{v_F^2}$$

where the last step uses the definition of $\omega_{sf}$ given previously. At the same time

$$\delta \tilde{\Omega}_{el} \sim N_f \omega^2$$
The Fermionic density of states \( N_f \) is a product of \( 1/v_F \) (the leftover of the integration over \( \varepsilon_k \), and a typical \( \tilde{k} \) along the Fermi surface). As typical \( \tilde{k} \sim \bar{\omega}/v_F \),

\[
N_f \sim \frac{\bar{\omega}}{v_F^2} \tag{52}
\]

Substituting this result into (51), we find

\[
\delta \tilde{\Omega}_{el} \sim \frac{\bar{\omega}^3}{v_F^2}, \tag{53}
\]

i.e., \( \delta \tilde{\Omega}_{el} \) and \( \delta \tilde{\Omega}_{spin} \) are indeed of the same order.

In the above discussion \( N_f \) appears as an extra parameter in \( \delta \tilde{\Omega}_{el} \). This is because in the calculations we neglected the momentum dependence along the Fermi surface (the actual momentum integral over \( d\tilde{k} \) is replaced by a typical \( \tilde{k} \)). If this momentum dependence was included (i.e., by using the self-energy from Eq. (28) with \( k \)-dependent \( \lambda(k) \) and \( \omega_{sf}(k) \)), then the electronic part would be free from uncertainties. Unfortunately, this computation also requires the knowledge of the \( k \)-dependence of \( \Phi(k) \) along the Fermi surface, which is technically difficult to obtain. In contrast, \( \delta \tilde{\Omega}_{spin} \) is the result of a full two-dimensional integration over bosonic momenta, and the result for \( \delta \tilde{\Omega}_{spin} \) is free from uncertainties.

Fortunately, it turns out that within the (approximate) computational scheme that we are using, \( N_f \) and \( 1/(\omega_{sf}\xi^2) \) can be related. Their relation follows from Eq. (45), as both the fermionic self-energy and the spin polarization operator are fully expressed in terms of \( \bar{\omega} \) and \( \lambda \). By evaluating the constant pieces in \( \Sigma_{NS,\omega_m} - \Sigma_{N,\omega_m} \) and in \( \Pi_{S,\omega_m} - \Pi_{N,\omega_m} \) at high frequencies and comparing the two sides of Eq. (45), one can express \( N_f \) in terms of \( 1/(\omega_{sf}\xi^2) \). Once this is done, there is no further uncertainty in the condensation energy - it is given by the universal function of \( \lambda \) times \( \bar{\omega}^2/(\omega_{sf}\xi^2) \propto \bar{\omega}^3/v_F^2 \).

At the risk of belaboring this point, we note that the fact that \( E_{c,el} \) and \( E_{c,spin} \) are of the same order implies that one cannot replace Wada’s expression for for electronic part of the condensation energy by a Bardeen-Steven formula. Indeed, the ability to do this in a phonon superconductors was based on the integral relation between \( \Sigma_{N,\omega} \) and \( \Sigma_{S,\omega} \), Eq. 18. For our case, the r.h.s. of this relation is finite and is given by

\[
K = \frac{3}{8\omega_{sf}\xi^2} \int_0^{\infty} d\omega_m \log \frac{\omega_{sf} + \omega_m}{\omega_{sf} + \omega_m f_{\omega_m}} S(\omega_m) \tag{54}
\]

where \( f_{\omega_m} = \Pi_{s,\omega_m}/\Pi_{n,\omega_m} \), and

\[
S(\omega_m) = \int_0^{\infty} d\omega_n \frac{\phi_n^2}{\sqrt{\Sigma_{s,\omega_n}^2 + \phi_n^2 + \Sigma_{s,\omega_n}}} + \int_0^{\omega_m} d\omega_n \frac{\Sigma_{s,\omega_n}}{\sqrt{\Sigma_{s,\omega_n}^2 + \phi_n^2}} \tag{55}
\]
A simple order of magnitude estimate shows that $K$ is of the same order as $\Sigma_{s,\omega_m}$, i.e., for magnetic superconductors, the transformation from Wada’s to Bardeen and Steven’s formula for the electronic condensation energy introduces a correction of the same order as $E_{c,el}$.

One final remark. The electronic and spin parts of $E_c$ are only of the same order of magnitude as long as $\bar{\omega} < E_F$. When the effective coupling exceeds $E_F$, typical $\tilde{k} = O(1)$, i.e., the whole Fermi surface is involved in the pairing. In this limit, the spin-fermion calculations are not controllable. Estimates show, however, that typical frequencies for the pairing now scale as $\omega_{sf}\xi^2 \sim v_F^2/\bar{\omega} \sim J$ where $J$ is the exchange integral for the corresponding Heisenberg model. (Recall that $\bar{\omega} \sim g^2\chi(Q)/\xi^2$ where the RPA approximation, $g$ is equivalent to Hubbard $U$. In the same approximation, near a magnetic transition $\chi(Q) \sim \xi^2/U$, i.e., $\bar{\omega} \sim U$.) Estimating $\delta\tilde{\Omega}_{spin}$ at typical frequencies, we indeed find $\delta\tilde{\Omega}_{spin} \sim J$ in agreement with the result by Scalapino and White [4]. The same reasoning yields $\delta\tilde{\Omega}_{el} \sim N_f J^2 \sim J^2/v_F \ll J$. We see therefore that at very large couplings, the spin part of the condensation energy clearly prevails over the electronic part, i.e., the condensation energy comes entirely from the spin part. This again agrees with Scalapino and White [4].

IV. THE COMPUTATIONS

In this section we present our results for the electronic and spin contributions to the condensation energy for various $\lambda$. In practice, we found it advantageous to perform the calculations of $\delta\tilde{\Omega}_{spin}$ and $\delta\tilde{\Omega}_{el}$ in real frequencies rather than in Matsubara frequencies. The main reason for this was simply that we had previously evaluated $\Sigma(\omega)$, $\Phi(\omega)$ and $\Pi(\omega)$ at real frequencies and various couplings and could use these results in the present computations. A more subtle reason is that in retarded formalism, the problem of divergencies in $E_{c,el}$ and $E_{c,spin}$ can be avoided in a straightforward manner. (see below)

A. Condensation energy in real frequencies

We first derive the expression for the condensation energy in real frequencies, in terms of retarded $\Sigma(\omega)$, $\Phi(\omega)$ and $\Pi(\omega)$. The Matsubara equations for $E_{c,el}$ and $E_{c,spin}$ given in equation 35 have the following form.

$$E_{c,el} = -\pi T \sum_m f(i\omega_m)$$
\[ E_{c,\text{spin}} = -\pi T \sum_n g(i\omega_n) \]  
(56)

where the \( E_{c,el} \) has a sum over fermionic frequencies and \( E_{c,\text{spin}} \) has a sum over bosonic frequencies. The retarded form of these equations, assuming no branch cuts except on the real axis are

\[ E_{c,el} = -\int_0^\infty f''_{\text{ret}}(\omega) \tanh(\frac{\omega}{2T}) d\omega \]
\[ E_{c,\text{spin}} = -\int_0^\infty g''_{\text{ret}}(\omega) \coth(\frac{\omega}{2T}) d\omega \]  
(57)

where \( f'' \) is the imaginary part of \( f \) (\( f' \) is the real part) and \( g \) is similar. It remains to analytically continue \( f(\omega_m) \) and \( g(\omega_n) \) to the real axis. With the Matsubara definitions used in section 2, the analytic continuations are as follows.

\[ \Sigma(\omega_m) \to -i\Sigma_{\text{ret}}(\omega) \]
\[ \Phi(\omega_m) \to \Phi_{\text{ret}}(\omega) \]
\[ \Pi(\omega_m) \to \Pi_{\text{ret}}(\omega) \]  
(58)

The retarded formulas for the condensation energy are then

\[ E_{c,el} = -N_f \int_0^\infty \{[\beta + \text{Re} \Sigma_N(\omega)] \]
\[ + \omega[1 - \frac{\text{Im} \Sigma_S(\omega) \alpha - \text{Re} \Sigma_S(\omega) \beta}{|\alpha|^2 + |\beta|^2}]\} \tanh(\frac{\omega}{2T}) d\omega \]
\[ E_{c,\text{spin}} = -\frac{3}{8\pi^2\xi^2} \int_0^\infty \{\text{Im} \Pi_S - \text{Im} \Pi_N \]
\[ + \text{Im} \log \frac{1 - \Pi_S(\omega)}{1 - \Pi_N(\omega)}\} \coth(\frac{\omega}{2T}) d\omega \]  
(59)

Where \( \sqrt{\Phi^2(\omega) - \Sigma_S^2(\omega)} = \alpha + i\beta \). We point out that extreme care must be taken with these equations in order to get the correct sign of the imaginary parts of both the square root and the logarithm.

We first point out that there is no divergent term in \( E_{c,el} \). Indeed, in the Matsubara formalism, the divergent term comes from the fact that at high frequencies, \( \Sigma_S(\omega_n) \) and \( \Sigma_N(\omega_n) \) are separated by a constant. Since we defined \( \Sigma \) with an extra \( i \), this constant is imaginary. On the other hand, the the first two terms in the retarded formula for \( E_{c,el} \) at high frequencies where \( \Phi \to 0 \) can be written as

\[ \text{Im} \sqrt{-\Sigma_S^2(\omega)} + \text{Re} \Sigma_N(\omega) = \text{Re} \Sigma_N(\omega) - \text{Re} \Sigma_S(\omega) \]  
(60)
Observe that $\Sigma'_{S,\text{ret}}$ and $\Sigma'_{N,\text{ret}}$ converge at high frequencies in contrast to the constant offset in Matsubara frequencies. The constant offset goes into the imaginary part of $\Sigma_{\text{ret}}$ which does not affect $E_c$ in the retarded formulism. This follows from the fact that $\Sigma_S(\omega) = \Sigma'(\omega) + i|\Sigma''(\omega)|$ and the branch cut is on the negative real axis. We see that $E_{c,\text{el}}$ only depends on the difference of $\text{Re}\Sigma$ between the normal and superconducting states, and the integral of this difference is fully convergent. We illustrate this in figure 3 Analogous reasoning also shows that $E_{c,\text{spin}}$ is also free from divergencies.

Indeed, the absence of divergencies in the retarded formalism is just the consequence of using the Kramers-Kronig transform which misses the divergent pieces in $E_{c,\text{spin}}$ and $E_{c,\text{el}}$. However, since we already demonstrated that the full $\delta \Omega$ is free from divergencies, we can safely use the Kramers-Kronig transformation separately for $E_{c,\text{spin}}$ and $E_{c,\text{el}}$.

The fact that no divergence exists for the retarded formulas also allows us to relate the prefactors in front of $E_{c,\text{el}}$ and $E_{c,\text{spin}}$ in a straightforward manner. In real frequencies, Eq. 45 takes the form

$$-N_f \int_0^\infty \{ \text{Re}\Sigma_{NS}(\omega) - \text{Re}\Sigma_N(\omega) \} \tanh \frac{\omega}{2T} d\omega$$

$$= \frac{3}{8\pi^2\xi^2} \int_0^\infty \{ \text{Re}\Pi_N(\omega) \text{Im} \log \frac{1 - \Pi_S(\omega)}{1 - \Pi_N(\omega)} + \text{Im}\Pi_N(\omega) \text{Re} \log \frac{1 - \Pi_S(\omega)}{1 - \Pi_N(\omega)} \} \coth \frac{\omega}{2T} d\omega$$

(61)

Since in the retarded formalism, $\int_{-\infty}^\infty \text{Re}\Sigma_{NS}(\omega) - \text{Re}\Sigma_N(\omega)d\omega$ is a convergent quantity, and the r.h.s. of (61) is also convergent, we can explicitly evaluate (numerically) both sides of (61) and relate $N_f$ and $3/8\pi^2\omega_s\xi^2$ which we label as spin density of states $N_s$ ($N_s = (8/3\pi^2)\bar{\omega}/v_F^2$).
FIG. 4: Electronic ($E_{c,el}$), spin ($E_{c,spin}$), and total ($E_c$) condensation energy per unit cell at $T = 0$ for various couplings $\lambda$. The lines are a guide for the eye. The sum of $E_{c,el}$ and $E_{c,spin}$ produces a total condensation energy which is negative. We used $N_f = 1\,\text{st/eV}$, and $N_s \sim 0.17\,\text{st/eV}$ as explained in the text.

**B. Results**

As we have already stated, we use previously obtained results for $\Sigma(\omega)$, $\Phi(\omega)$ and $\Pi(\omega)$. First, we computed both sides of Eq. (61) and evaluated the ratio $N_f/N_s$ for various $\lambda$. We found that with very small variations, $N_f/N_s \approx 5.9$.

In Fig. 4 we present the results for the electronic and spin contributions to the condensation energy for different values of the coupling $\lambda$. To set the overall scale, we adopt a commonly used estimate $N_f = 1\,\text{st/eV}$ [19]. We emphasize that changing $N_f$ will only change the overall scale and not the functional form of $E_c(\lambda)$.

We see from Fig. 4 that the total condensation energy is negative, as it indeed should be in a superconductor, but that this negativity is of a very different origin than in BCS theory. In BCS theory, which corresponds to $\lambda \ll 1$, i.e., $\bar{\omega} < \omega_{sf}$, the system behaves as a conventional Fermi liquid. In this limit, the pairing potential is static, i.e., the spin part of $E_c$ is negligible, and condensation energy is entirely electronic and negative. We see however for $\lambda \geq 1$, i.e the strongly coupled regime, the the electronic contribution to the condensation energy is positive and quite large. From the figure it appears that the electronic contribution changes sign at $\lambda \sim 0.4$. $E_{c,el}$ is negative below this coupling strength and is positive for all $\lambda \geq 1/2$ presented in the figure. Second, for all $\lambda$ shown, the spin part $E_{c,spin}$ is negative. It can be shown that $E_{c,spin}$ continues to be negative at $\lambda \to 0$ where $\Pi \to 0$ as $\lambda^2$. (see Eq. 28)
Indeed, by expanding the logarithm in Eq. 61 we obtain

\[
E_{c,\text{spin}}(\lambda \to 0) = -N_s \frac{\omega_{sf}}{2} \int_0^\infty \text{Im}\{\Pi_S^2 - \Pi_N^2\}
\]

\[
= -N_s \omega_{sf} \int_0^\infty \{\text{Re}\Pi_S \text{Im}\Pi_S - \text{Re}\Pi_N \text{Im}\Pi_N\} < 0
\] (62)

The above equation is negative, as in the retarded formalism, \(\text{Re}\Pi_N = 0\) and both \(\text{Re}\Pi_S \leq 0\) and \(\text{Im}\Pi_S < 0\), and scale as \(\lambda^4\) as \(\lambda \to 0\).

We also see from the figure that at large \(\lambda\), both the spin and the electronic parts of the condensation energy nearly saturate: to a large positive value for \(E_{c,\text{el}}\) and a large negative value for \(E_{c,\text{spin}}\). The total condensation energy \(E_c\) is negative and much smaller than either \(E_{c,\text{el}}\) or \(E_{c,\text{spin}}\) due to a substantial cancellation between these two components of \(E_c\). Although this cancellation seems quite delicate, it is actually robust since \(E_{c,\text{el}}\) and \(E_{c,\text{spin}}\) are intimately linked via mutual feedback, and can not be considered separately. It is the sum of the two which has physical meaning. Any estimate of the total condensation energy based merely upon either the electronic or spin part will give a highly erroneous result.

We now consider the functional dependence of \(E_c\) on \(\lambda\). In figure 5, we see that the condensation energy flattens at \(\lambda \sim 2\), and decreases at large couplings despite the fact that the pairing gap increases monotonically with \(\lambda\) [20]. This behavior is very counterintuitive from a BCS perspective, where the condensation energy scales with \(\Delta^2\). It clearly indicates that for \(\lambda \geq 1\), the physics is qualitatively different from BCS theory. To emphasize this strong deviation from BCS theory we plot in Fig.5 the strong coupling result of \(E_c\) along with the BCS condensation energy \(-N_f \Delta^2/2\) using the same \(\Delta\) and \(N_f\). We clearly see that for \(\lambda \geq 1\), corresponding to optimally doped and underdoped cuprates, BCS theory yields qualitatively incorrect results for \(E_c\).

Our results are in line with earlier work which demonstrated that for \(\lambda \geq 1\), the pairing predominantly involves fermions located in the non-Fermi liquid frequency range. For these fermions, retardation effects not included in BCS theory become dominant. Such retardation effects take place between the “upper” - \(\bar{\omega}\) and “lower” \(\omega_{sf}\) scales of spin-fermion theory. As \(\bar{\omega} = 4\lambda^2 \omega_{sf}\) this ratio grows quickly, and already \(\bar{\omega}/\omega_{sf} = 4\) at \(\lambda = 1\). This explains why the deviations from BCS behavior are already strong at this coupling. Understanding in detail the strong coupling physics behind the decrease in \(E_c\) is currently the subject of a separate study [21] and a complete theory of this phenomenon does not exist at the moment. Most likely, however, this decrease is a reflection of the fact that as \(\lambda\) increases, the
FIG. 5: Total condensation energy $E_c$ compared with the BCS result $E_{c}^{BCS}$ at $T = 0$ for various couplings $\lambda$. We used $N_s \sim 0.17st/eV$ and $N_f/N_s \sim 5.9$ as explained in the text. Observe that the BCS condensation energy monotonically increases as the coupling gets larger, while the actual condensation energy flattens at $\lambda \sim 2$ and slightly decreases at large couplings.

actual attraction between fermions goes down, retardation of the spin-mediated interaction becomes the major factor, and the pairing process increasingly involves incoherent (diffusive) fermions and on-shell bosons. As the exchange of on-shell bosons is an energy conserving process, it can not lead to a gain in $E_c$. Such behavior is very counterintuitive from a BCS perspective, where the pairing emerges due to an exchange of virtual, off-shell bosons, and the condensation energy scales with $\Delta^2$.

One final comment. Although magnetically mediated superconductors are often compared to dirty superconductors, we point out that at $T = 0$, the physics of the two is already qualitatively different. Analogies between the two are often made due to the fact that thermal spin fluctuations scatter at finite momentum transfer but zero energy transfer and act in the same way as non-magnetic impurities [20]. However, in a dirty superconductor with non-magnetic impurities, the condensation energy retains its BCS form despite of the fact that the superfluid stiffness is renormalized down [22]. Obviously, this is not what we found.

V. KINETIC ENERGY

As we stated in the introduction, several groups have argued [5, 6] that the condensation energy is driven by a gain in the kinetic energy which at strong coupling is negative (in
contrast to BCS theory) because of a strong “undressing” of fermions which bear a greater resemblance to free particles in the superconducting state than they do in the normal state.

In this section we consider, within our model, the change in the kinetic energy when the system enters the superconducting state. The conventionally defined kinetic-energy for an interacting fermionic system is

$$E_{\text{kin}} = 2T \sum_m \int \frac{d^2k}{(2\pi)^2} \varepsilon_k \, G_{\omega_m}(k)$$  \hspace{1cm} (63)$$

where $G_{\omega_m}(k)$ is the full fermionic Green’s function that contains the self-energy. Integrating over momentum and subtracting the normal state result from $E_{\text{kin}}$ in a superconductor we obtain

$$\delta E_{\text{kin}} = 2N_f \pi T \sum_m \sqrt{\Sigma^2_{S,\omega_m} + \Phi^2_{\omega_m}} - |\Sigma_{N,\omega_m}|$$  \hspace{1cm} (64)$$

In the BCS limit, $\lambda \ll 1$, $\Phi_{\omega_m} = \Delta$, $\Sigma = 0$, $\Sigma_{\omega_m} = \omega_m$ and

$$\delta E_{\text{kin}}^{\text{BCS}} = 2N_f \pi T \sum_m \sqrt{\omega_m^2 + \Delta^2} - |\omega_m|$$  \hspace{1cm} (65)$$

which is obviously positive and furthermore depends logarithmically on the upper limit of the frequency integration, which is $\omega_{sf}$ in our case (we recall that in the BCS limit, $\omega_{sf} \gg \bar{\omega}$). At $T = 0$, we have

$$\delta E_{\text{kin}}^{\text{BCS}} = N_f \Delta^2 \log \frac{\omega_{\text{max}}}{\Delta}$$  \hspace{1cm} (66)$$

In the same BCS limit, the potential part of the condensation energy $\delta E_{\text{pot}}^{\text{BCS}}$ is also logarithmically divergent, and to a logarithmical accuracy cancels out $\delta E_{\text{kin}}^{\text{BCS}}$. The subleading terms do not cancel and yield $E_c^{\text{BCS}} = -N_f \Delta^2/2$.

We now consider finite $\lambda$. As before, we perform the computations in real frequencies. The analytic continuation of equation 64 gives

$$\delta E_{\text{kin}} = +2N_f \int_0^\infty \{ \text{Im} \sqrt{\Phi^2(\omega) - \Sigma^2_N(\omega)} + \text{Re} \Sigma_N(\omega) \} \tanh \frac{\omega}{2T} d\omega$$  \hspace{1cm} (67)$$

The result of this calculation at finite $\lambda$ are presented in Fig 6. At low couplings the kinetic energy is positive, as one naively expects. At larger $\lambda$, however, the kinetic energy passes through a maximum at $\lambda \sim 2$ and then becomes negative at large $\lambda$.

As we already mentioned in the Introduction, the sign of $E_c$ depends on the interplay between two competing effects: the effect of particle-hole mixing that increases $E_{\text{kin}}$, and the change in the self-energy due to the “undressing” of fermions that lowers $E_{\text{kin}}$. At weak
FIG. 6: Kinetic energy $\delta E_{\text{kin}}$ compared with total condensation energy $E_c$ at $T = 0$ for various couplings $\lambda$. The parameters are the same as in Fig. 2. The kinetic energy change is positive at low couplings, but negative at high coupling.

coupling, the particle-hole mixing obviously dominates. The sign change between small and large $\lambda$ implies that at strong coupling the situation is reversed, and the lowering of $E_{\text{kin}}$ via the change in the self-energy due to the “undressing” of fermions overcomes the effect of particle-hole mixing. This behaviour is very similar to that obtained by Norman et. al. [5].

As the first term in $E_{c,\text{el}}$ is equal to $-\delta E_{\text{kin}}/2$ (see Eqs. (37 and 64), one can indeed argue that the condensation energy at large couplings is at least partly driven by the lowering of the kinetic energy. However, a comparison of Figs. 4 and 6 shows that this is just another way to interpret strong coupling effects that affect both the fermionic and bosonic propagators via mutual feedback.

A simple explanation of why this is so is the following. In the superconducting state, the spin decay into fermions is forbidden at energies smaller than $2\Delta$. This simultaneously gives rise to two effects. First, the spin propagator develops the excitonic (resonance) peak at $\omega_{\text{res}} < 2\Delta$. The energy released by the creation of an exciton results in a gain in the magnetic part of the condensation energy. Secondly, the fermions cannot decay until their frequency exceeds $\Delta + \omega_{\text{res}}$ (this is the magnetic analog of the Holstein effect). The elimination of fermionic scattering at low frequencies implies that the fermionic self-energy $\Sigma(\omega)$ in the superconducting state is reduced compared to that in the normal state. This lowers the kinetic energy. Obviously, the two effects (the gain in the magnetic part and the lowering of the kinetic energy) come from the same physics.
VI. CONCLUSIONS

Our goal in this paper was to emphasize the importance of taking all contributions to the condensation energy into account when considering a strongly coupled superconductor. Specifically, we considered the case of $d_{x^2-y^2}$ pairing mediated by the exchange of near-critical overdamped antiferromagnetic spin fluctuations. We demonstrated that although Eliashberg theory is valid for a strongly coupled magnetic superconductor, the reason for its validity is qualitatively different from that for phonon superconductors as the spin velocity and Fermi velocity are of the same order. Due to this fact, approximations appropriate for phonon superconductors are generally not valid in magnetic superconductors. Specifically, we demonstrated that the assumption that the bosonic polarization bubble can be neglected, which was rigorously justified by Bardeen and Stephen for phonon superconductors, breaks down for magnetically-mediated superconductors and makes the Wada and Bardeen-Stephen formalisms invalid.

We obtained the full expression for the condensation energy within the spin-fermion model and showed that the spin and electronic parts of the condensation energy are of the same order $\bar{\omega}^3/v_F^2$ and both depend only on the dimensionless coupling $\lambda$. The BCS behavior is restored at $\lambda \ll 1$. Even at moderate couplings, the condensation energy is highly non-BCS. The electronic contribution to the condensation energy is positive, while the spin part is negative and larger in magnitude than the electronic part which makes the full $E_c$ negative. As in the BCS limit the electronic condensation energy is negative and equal to $-N_f \Delta^2 / 2$, this implies that the electronic condensation energy changes sign at a rather small $\lambda$. We found that at large $\lambda$, both the spin and the electronic parts of the condensation energy nearly saturate. As a result, the full condensation energy flattens at $\lambda \sim 2$, and decreases at large couplings despite the fact that the pairing gap increases monotonically with $\lambda$ [20]. This behavior is very counterintuitive from a BCS perspective, where the condensation energy scales with $\Delta^2$ and is also inconsistent with the behavior of $E_c$ in dirty superconductors. This behavior results from the fact that there is a substantial cancellation between the spin and electronic parts of the condensation energy and the total $E_c$ is thus substantially smaller than either the spin or electronic parts.

We argued that the reduction of $E_c$ at large coupling is likely the result of the fact that at strong coupling the pairing is predominantly due to an energy conserving exchange of
on-shell (real) bosons as opposed to the BCS theory in which the pairing is caused by the energy non-conserving exchange of virtual bosons. The reduction of $E_c$ at strong coupling also indicates that in this limit coherent superconductivity becomes fragile, and a large $\Delta$ only indicates that the system needs a finite energy to destroy spin singlets.

Finally, we computed the kinetic energy and found that at strong coupling it is negative which indicates that at high couplings the change in the self-energy due to the “undressing” of fermions, which lowers $E_{kin}$ overcomes the effect of particle-hole mixing which tends to increase $E_{kin}$. This behavior has no analog for phonon superconductors. We argued that a negative $E_{kin}$ is fully consistent with a positive $E_{c,el}$, and that, in principle, it is correct to argue that the condensation energy at large couplings is at least partly driven by the lowering of the kinetic energy. However, our results show that the lowering of $E_c$ may be thought of as being due to either the the lowering of the kinetic energy, or the interplay between the lowering of $\Delta \Omega_{spin}$ and the increase of $E_{c,el}$. Both explanations are valid interpretations of the strong coupling effects which affect the fermionic and bosonic propagators via mutual feedback.

By taking into account all contributions to the self energy, and taking $N_f \sim 1st/eV$ as typical for near optimally doped cuprates, we obtained a small value for $E_c$ of $\sim 15K$ at optimal doping, (which in our model corresponds to $\lambda \sim 1.5 - 2$ [16], larger $\lambda$ describe underdoped cuprates). This is rather remarkable as all typical energies in the problem are much higher, i.e $\bar{\omega} \sim 2.5 - 3 \times 10^3 K$ [16]. This small value of $E_c$ is partly due to small prefactors, but is also the result of substantial cancellation between the spin and electronic contributions to $E_c$. Note also that $N_f \sim 1st/eV$ that we were using is fully consistent with $\bar{\omega} \sim 2.5 - 3 \times 10^3 K$. Indeed, using Fermi surface averaged $v_F \sim 0.6meV$ [20] we obtain $N_s = (8/3\pi^2)\bar{\omega}/v_F^2 \sim 0.15 - 0.19st/eV$. Using then $N_f/N_s \sim 5.9$ obtained in the paper, we find $N_f \sim 1st/eV$, i.e., precisely the same value as we used.

Our $E_c \sim 15K$ is in good agreement with experiment. Loram et al [3] extracted $E_c \approx 0.12k_BT_c \sim 10K$ from the jump of the specific heat at $T_c$. The change of the functional form of $E_c$ around $\lambda = 2$ is also consistent with the experimental fact that $E_c$ changes its behavior from BCS-like to non-BCS around optimal doping. A decrease of $E_c$ at strong couplings (i.e., for underdoped cuprates) is also consistent with what Loram et al found in the specific heat experiments in the underdoped regime [3]. We caution, however, that the relation between $E_c$ and the amount of the jump in the specific heat at $T_c$, from which the
experimental $E_c$ was extracted may be more complex than in the BCS theory which was used to extract $E_c$ from the data. This analysis is clearly called for.

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VII. APPENDIX A - A RUNNING COUPLING CONSTANT APPROACH

The condensation energy may also be computed using a general formula for the ground state energy of the interacting electron system [8, 13, 23]:

$$E - E_0 = -i \int_0^\lambda \frac{d\lambda_1}{\lambda_1} \int \frac{d^2k d\omega}{(2\pi)^3} G_{\omega_m}(k) \Sigma^*_{\omega_m}$$  \hspace{1cm} (68)

where $E_0$ is the ground state energy of free electrons, and the Green’s function and the self-energy are evaluated for the running coupling constant $\lambda_1$. This formula is valid both in the normal and superconducting state. The “effective” self-energy $\Sigma^*_{\omega_m}$ is related to $G_{\omega_m}(k)$ in the same way as a conventional self-energy, i.e., as $G_{\omega_m}^{-1}(k) = i(\omega_m + \Sigma^*_{\omega_m}) - \epsilon_k$. In the normal state, $\Sigma^*_{\omega_m} = \Sigma_{n,\omega_m}$, where $\Sigma$ is a conventional self-energy, while in the superconducting state,

$$\Sigma^*_{s,\omega_m} = \Sigma_{s,\omega_m} + \frac{i\Phi^2_{\omega_m}}{\epsilon_k + i\Sigma_{s,\omega_m}}$$  \hspace{1cm} (69)

Eq. (68) is particularly suitable for the strong coupling computations in the normal state. Here we can use

$$\int \frac{d^2k}{4\pi^2} G_{\omega_m}(k) = -i\pi N_f \text{sign}\omega_m$$  \hspace{1cm} (70)

Subsituting this result into (68) we reduce $E - E_0$ to a single frequency integral. Using the $T = 0$ normal state result for the spin-fermion model $\Sigma_{n,\omega_m} = 2\lambda\omega_m/(1 + (1 + |\omega_m|/\omega_{sf})^{1/2})$, and and introducing the sharp upper cutoff for the low-energy theory at $\omega_{max} \sim E_F$, we obtain

$$E - E_0 = -N_f(\omega_{max}^3\overline{\omega})^{1/2} \int_0^{2\lambda(\omega_{max}^3\overline{\omega})^{1/2}} \frac{dx}{(\sqrt{1 + x^2} + 1)^2}$$  \hspace{1cm} (71)

This expression is convenient for the analysis of the variation of the ground state energy with $\lambda$. 

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The condensation energy, i.e., the energy difference between normal and superconducting state, is given by

$$E_c = -i \int_0^\lambda \frac{d\lambda_1}{\lambda_1} \int \frac{d^2k d\omega}{(2\pi)^3} \left( G_{s,\omega_m}(k)\Sigma^*_s - G_{n,\omega_m}(k)\Sigma^*_n \right)$$  \hspace{1cm} (72)

Using $G\Sigma^* = -i(1 - G^{-1})G$, we can rewrite (72) as

$$E_c = N_0 \int \frac{d\epsilon d\omega_m}{2\pi} \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} \left( G_{s,\omega_m}(k) - G_{n,\omega_m}(k) \right)(i\omega_m - \epsilon_k)$$  \hspace{1cm} (73)

Performing the momentum integration in the Green’s functions, we obtain

$$E_c = -N_f \int_0^\lambda \frac{d\lambda_1}{\lambda_1} \int_0^\infty d\omega_m \left( \sqrt{\Sigma^2_{s,\omega_m} + \Phi^2_{\omega_m}} - \Sigma_{n,\omega_m} - \omega_m \right)$$

$$\left( \frac{\Sigma^2_{s,\omega_m} + \Phi^2_{\omega_m}}{\sqrt{\Sigma^2_{s,\omega_m} + \Phi^2_{\omega_m}}} \right)$$  \hspace{1cm} (74)

This looks very similar to the Wada result (Eq. 37) but note the minus sign in front of the $\omega_m$. This extra minus sign results in a negative total $E_c$ for all couplings.

The condensation energy, Eqn. (73) can also be formally divided into kinetic and potential energy terms, but this division is subjective for interacting systems, and we will not discuss this.

A. BCS limit

In the BCS limit, $E_c$ reduces to

$$E_c = -N_f \int_0^\lambda \frac{d\lambda_1}{\lambda_1} \Delta^2 \int_0^\infty d\omega_m \frac{d\omega_m}{\sqrt{\Delta^2 + \omega_m^2}}$$  \hspace{1cm} (75)

where $\Delta$ is the gap value for the running coupling $\lambda_1$. Using the BCS relation between $\Delta$ and the coupling constant

$$1 = \lambda_1 N_f \int_0^\infty \frac{d\omega_m}{\sqrt{\Delta^2 + \omega_m^2}}$$  \hspace{1cm} (76)

one can rewrite (75) as

$$E_c = -\int_0^\lambda \frac{d\lambda_1}{\lambda_1^2} \Delta^2$$  \hspace{1cm} (77)

From (76),

$$\Delta_{\lambda_1} = \Delta e^{\frac{1}{N_f \lambda_1}} e^{\frac{1}{\pi_f \lambda_1}}$$  \hspace{1cm} (78)

Integrating over $\lambda_1$ we obtain

$$E_c = -\frac{1}{2} N_f \Delta^2$$  \hspace{1cm} (79)
This is indeed the same result as we obtained using the Eliashberg formula.

Note in passing that our previous assertion that the separation of \( E_c \) into a kinetic and potential energy is subjective is true even in the BCS limit, as the interaction is the source of the pairing. Indeed, earlier we computed \( \delta E_{\text{kin}} \) in the Luttinger-Ward formalism and found that in the BCS limit, the kinetic energy scales as \( \Delta^2 \log \omega_{\text{max}}/\Delta \) (see Eq. (66)). In the running coupling constant formalism, the kinetic energy difference \( \delta \tilde{E}_{\text{kin}} \) extracted from (73) in the BCS limit reduces to

\[
\delta \tilde{E}_{\text{kin}}^{\text{BCS}} = 2N_0 \int_0^\lambda \frac{d\lambda_1}{\lambda_1} \int_0^\infty \frac{\Delta^2 \lambda_1 d\omega_m}{\omega_m + \sqrt{\Delta^2 \lambda_1 + \omega_m^2}}
\]

Using (76) and performing the computations with the logarithmical accuracy we find \( \delta \tilde{E}_{\text{kin}}^{\text{BCS}} = N_0 \Delta^2 / 2 \), i.e., contrary to Eq. (66) the newly defined kinetic energy does not depend logarithmically on the upper limit of frequency integration. Similarly, \( \delta \tilde{E}_{\text{pot}}^{\text{BCS}} = -N_0 \Delta^2 \) such that the sum of the two yields the correct total condensation energy, Eq. (79). This once again demonstrates that only total \( E_c \) is a physically meaningful quantity.

B. \( \lambda = 1 \)

We numerically computed \( E_c \) for \( \lambda = 1 \) by calculating the integrand of eqn 74 for \( \lambda = 0, 0.5 \) and 1, numerically fitting these three data points and then integrating the resultant function over the coupling constant. This resulted in a condensation energy of \( E_c = -15.8K \) compared to the \(-11.5K\) calculated via the Eliashberg approach. This agreement is very impressive given the highly approximate nature of the calculation. Unfortunately, the running coupling constant formalism is very computationally intensive, hence our motivation for using the Eliashberg approach in this paper.

VIII. APPENDIX B - A PECULIARITY OF THE BCS APPROXIMATION

In this Appendix, we elaborate on our earlier discussions of the result for the condensation energy in the BCS limit. In BCS theory, the pairing problem may be described by an effective quadratic Hamiltonian

\[
H = H_0 + \sum_{k,\alpha} \epsilon_k a^\dagger_{k,\alpha} a_{k,\alpha} + \Delta \frac{g_{\alpha,\beta}}{2} (a^\dagger_{k,\alpha} a^\dagger_{-k,\beta} + a_{k,\beta} a_{-k,\alpha})
\]
where $g_{\alpha\beta}$ is the antisymmetric matrix [23]. The condensation energy can then be straightforwardly obtained by simply averaging both the normal and anomalous terms in (81). Expressing the average products of the pairs of operators in terms of frequency integrals of normal and anomalous Green functions, and taking care to avoid double counting of the anomalous term, we obtain the zero temperature result

$$E_c = -\frac{N_f \Delta^2}{2} I$$  \hspace{1cm} (82)

where

$$I = \int \frac{d\epsilon d\omega}{\pi} \frac{\omega^2 - \epsilon^2}{(\epsilon^2 + \omega^2)(\epsilon^2 + \omega^2 + \Delta^2)}$$  \hspace{1cm} (83)

We know that the correct result is $I = 1$. However, a naive integration treating both $\omega_m$ and $\epsilon$ in (83) on an equal footing, results in a vanishing integral. This vanishing is surely artificial, as the 2D integral over $d\epsilon d\omega$ is logarithmically divergent and therefore the result does depend on the order of limits of the integration. This situation is a typical example of an anomaly.

The correct way is to perform the integration over $\omega$ first as in the Hamiltonian approach to the pairing, the interaction is independent of frequency, and hence there is no cutoff in the frequency integration. The integration over energy, on the other hand, is obtained by simplifying the original integral over momenta and is only valid as long as the density of states is a constant which is true up to an upper cutoff $\Lambda \sim \epsilon_F$. Integrating first over $\omega_m$ in infinite limits, and then integrating over $\epsilon_k$ we obtain

$$I = 2 \int_0^{\Lambda/\Delta} \left( \sqrt{x^2 + 1} - 2x + \frac{x^2}{\sqrt{x^2 + 1}} \right)$$  \hspace{1cm} (84)

One can easily make sure that the integral converges at large $x$ and therefore does not depend on the upper limit as long as $\Delta \ll \Lambda$. Setting the upper limit to infinity we easily obtain $I = 1$ as it indeed should be.

It is also instructive to reproduce the correct result by integrating over $\epsilon_k$ first. A formal integration in the infinite limit yields an incorrect $I = -1$. However, integrating in (83) first over $\epsilon_k$ between $-\Lambda$ and $\Lambda$, and then over $\omega$, we obtain

$$I = -\frac{2}{\pi} \int_0^{\infty} dx \left( \frac{1 + 2x^2}{\sqrt{x^2 + 1}} \tan^{-1} \frac{\Lambda^*}{\sqrt{x^2 + 1}} - 2x \tan^{-1} \frac{\Lambda^*}{x} \right)$$  \hspace{1cm} (85)

where $\Lambda^* = \Lambda/\Delta$. If we formally set $\Lambda^* = \infty$, the integral will be convergent and yield an incorrect result, $I = -1$. However, keeping $\Lambda^*$ large but finite we find after changing
variables to \( y = \frac{x}{\Lambda^*} \)

\[
I = -1 + \frac{8}{\pi}(\Lambda^*)^2 \int_0^\infty dy \left( \tan^{-1} \frac{1}{y} - \frac{1}{y} - \frac{\tan^{-1} \frac{1}{y} - \frac{1}{y}}{y} \right)
\]

(86)

Expanding under \( \tan^{-1} \) in \( 1/(\Lambda^*)^2 \) and evaluating the remaining integral we find

\[
I = -1 + \frac{4}{\pi} \int_0^\infty \frac{dy}{y^2 + 1} = -1 + 2 = 1
\]

(87)

as it indeed should be.

The physical implication of this result is that in the BCS theory, the condensation energy can be equally viewed as coming from the energy levels near the Fermi surface, as implied in Eq. (84) where the integral is confined to \( x = O(1) \), i.e., to \( \omega \sim \Delta \), or as coming from very deep levels below the Fermi surface, as implicated in Eq. (86) where the integral is confined to \( y = O(1) \), or to \( \omega \sim \Lambda \sim E_F \). Such an uncertainty is typical for an anomaly which can be equivalently viewed as coming from either low energies or high energies [24].

This peculiarity, however, is only present in the BCS limit, where the gap remains finite even at the largest frequencies (this is what causes logarithmical divergencies in the integrals). In the Eliashberg theory, the gap vanishes at infinite frequency, the integrals are convergent, and the condensation energy can only be viewed as coming from the levels near the Fermi surface.

A. A relation between \( E_c \) in Refs. [5] and [12]

The peculiar nature of the BCS limit also explains the apparent sign difference between the expressions for the condensation energy in Refs. [5] and [12]. In Ref. [12], Scalapino derived the condensation energy by averaging the interaction electron-phonon Hamiltonian:

\[
< H > = -i \int \frac{d^dkd\omega}{(2\pi)^{d+1}} (\omega + \epsilon_k)G(k, \omega) - \left< \sum_\nu \frac{P_\nu^2}{M} \right>
\]

(88)

where the last term is twice the expectation value of the ion kinetic energy. He then used Chester’s result [25] for the relation between the isotopic dependence of the upper critical field and the change in the ion kinetic energy between normal and superconducting states, and found that for the isotope exponent \( \alpha = 1/2 \), the change in the ion kinetic energy is precisely minus twice the change in the electronic propagator. As a result, the condensation
energy turns out to be minus the difference between the first terms in (88) in a superconductor and the normal state:

\[ E_c = \langle H_{sc} \rangle - \langle H_n \rangle = -i \int \frac{d^d k d\omega}{(2\pi)^{d+1}} (\omega + \epsilon_k) \left( G_n(k, \omega) - G_s(k, \omega) \right) \]  
(89)

[Note that we define \( E_c \) with the opposite sign compared to Refs. [5] and [12] - our \( E_c \) is negative, while their \( E_c \) is positive].

For a nonzero self-energy \( \Sigma = \Sigma(\omega) \), the momentum and frequency integral in (89) is ultraviolet convergent because the pairing gap \( \Delta = \Delta(\omega) \) vanishes at \( \omega \to \infty \), and the ordering of the momentum and frequency integration does not matter. Performing integration over frequency first, one obtains, after simple manipulations, Wada’s formula, Eqn. (17). In the BCS limit of vanishing \( \Sigma(\omega) \) and a constant \( \Delta \), this yields \( E_c = -N_0 \Delta^2 / 2 \), as we discussed earlier.

The authors of Ref [5], on the other hand, assumed that the condensation energy is not due to phonons, and that \( \alpha \) is nearly zero, as in the near optimally doped cuprates. They argued that in this situation, the condensation energy should be given solely by the first term in (88), i.e.,

\[ E_c = -i \int \frac{d^d k d\omega}{(2\pi)^d} (\omega + \epsilon_k) \left( G_s(k, \omega) - G_n(k, \omega) \right) = \int \frac{d^d k}{(2\pi)^d} \int_0^\infty (\omega + \epsilon_k) \left( A_s(k, \omega) - A_n(k, \omega) \right) \]  
(90)

where \( A(k, \omega) = (1/\pi) ImG(k, \omega) \) is the quasiparticle spectral function. This expression has opposite sign compared to Eqn (89). Still, the authors of Ref [5] argued that their expression also reproduces the BCS result \( E_c = -N_0 \Delta^2 / 2 \).

The consideration in the previous subsection of this appendix shows that both expressions are correct in the BCS limit (despite the fact that the one is minus the other!). The way in which the condensation energy was obtained in ref [5] implies that the momentum and frequency integral must be physically motivated, i.e., if the momentum integral over \( d^d k \approx N_0 d\epsilon_k \) is extended to infinite limits, one has to integrate first over momentum and then over frequency. On the contrary, the Wada expression for the condensation energy implies that the momentum integral comes first, and the frequency integration comes second. As we already know, in the BCS limit, interchanging the order of the integration changes the result by a factor \(-1\). This explains why the two apparently opposite results for \( E_c \) actually yield the same condensation energy.
A comparison of the two results shows that that in the BCS limit, the change in the ion kinetic energy merely sets the proper regularization of the ultraviolet divergent integral for $E_c$. If one regularizes the integral by restricting the momentum integration to $|\epsilon_k| \leq \Lambda \sim E_F$ (this is what we called the physically motivated regularization), the ion kinetic energy may be completely neglected. Reversing the ordering of the integration is equivalent to imposing a constraint on the frequency integral. This constraint can only come from the frequency dependence of the phonon propagator, i.e., from the kinetic energy of ions. Obviously in this situation, the ion kinetic energy cannot be neglected.

Away from the BCS limit, the correct way to proceed in the general case is to use the Luttinger-Ward-Eliashberg expression for Free energy, Eq. (3). This expression is valid for arbitrary $\Sigma(k, \omega)$ and it also includes the full feedback on bosons. Note that the expression for $\Omega$ is more general than the Eliashberg theory for phonon superconductivity as Eqn (3) actually doesn’t assume that $\Sigma$ depends only on frequency, and that one can factorize the momentum integration in the expressions for the self-energy and the pairing vertex, Eqs (5). The only approximation in the Eliashberg formula is the neglect of vertex corrections (which account for higher-order terms labeled by dots in (3)). Still, it is of interest to understand which of the two expressions for $E_c$, Eqn 89 or 90, one should use for the situation where the feedback effect on the bosonic propagator can, for one reason or another, be neglected. We argue that the answer depends on whether the self-energy predominantly depends on $k$ or on $\omega$.

Indeed, in the BCS limit, the physical motivation for the ordering of the momentum and frequency integrations (first over frequency and then over $\epsilon_k$) was associated with the fact that, for a constant gap, the ultraviolet divergence of the momentum and frequency integral for $E_c$ was cut by that the integration over $\epsilon_k$ cannot extend to $|\epsilon_k| > \Lambda \sim E_F$. Suppose now that the Eliashberg theory is valid, i.e., $\Sigma \approx \Sigma(\omega)$, and $\Delta = \Delta(\omega)$. As we already said, this $\Delta(\omega)$ vanishes above some characteristic frequency $\omega_0$ which decreases when fermion-boson coupling increases. Once this frequency becomes smaller than $\Lambda$, the cutoff of the ultraviolet divergence is provided by the frequency integral, rather than momentum integral. In this situation, the physically motivated ordering of the integrations should be integration over $\epsilon_k$ first (in infinite limits), and the integration over frequency afterwards. This ordering is implicit in Eq. 89. Not surprisingly, this expression yields Wada formula which in turn follows from the Eliashberg Free energy provided that $\Sigma = \Sigma(\omega)$. If instead we used Eqn.
we would obtain a rapid variation of $E_c$ once $\bar{\omega}$ becomes smaller than $\Lambda$, and eventually Eqn (90) would yield the result opposite in sign to Eq (53).

On the other hand, when the self-energy predominantly depends on $k$, the cut of the ultraviolet divergence is still provided by the momentum integral. In this situation, the ionic kinetic energy can be neglected, and Eqn. 90 should be used. This can be explicitly verified by comparing the Luttinger-Ward-Eliashberg formula with the bosonic term dropped, Eqn. (16), with Eqn. (90). Setting $\Sigma(k, \omega) = \Sigma(\epsilon_k)$ and $\Phi(k, \omega) = \Phi(\epsilon_k)$ in (16) and integrating over frequency we obtain

$$E_c = -N_f \int_0^\infty \, d\epsilon (\sqrt{\Sigma_{S,\epsilon}^2 + \Phi_{\epsilon}^2} - |\tilde{\Sigma}_{N,\epsilon}|$$

$$+ \frac{|\Sigma_{S,\epsilon}| - \sqrt{\Sigma_{S,\epsilon}^2 + \Phi_{\epsilon}^2}}{\sqrt{\Sigma_{S,\epsilon}^2 + \Phi_{\epsilon}^2}} \right)$$

where $\tilde{\Sigma}_\epsilon = \epsilon + \Sigma(\epsilon)$. This expression is the analog of the Wada formula for the condensation energy (17). We now do the same in Eqn. (90). The frequency integration is straightforward and by proper evaluation of the arguments of the logarithms we obtain *exactly the same expression as Eqn. (91)*. This proves our point that in theories where the feedback from the pairing on bosonic propagator can be neglected, Eq. (16) is valid for any $\Sigma(k, \omega)$, while Eqs. (89) or (90) are valid when $\Sigma(k, \omega) \approx \Sigma(\omega)$ and $\Sigma(k, \omega) \approx \Sigma(k)$, respectively.

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