Condensation energy in strongly coupled superconductors

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We consider the condensation energy E_c of strongly coupled magnetically mediated superconductors within the context of the spin-fermion model. We argue that the actual physics behind the condensation energy is much richer than in BCS theory, and that it is vital to take both the fermionic and bosonic contributions to the condensation energy into account. We argue that at strong coupling $\lambda \gg 1$, 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. In addition we argue that the same feedback effect accounts for a gain in the kinetic energy at strong coupling. We also found that the BCS relation $E_c \propto \Delta^2$, where Δ is the pairing gap, only holds for $\lambda \leqslant 1$. At larger λ, Δ keeps increasing and eventually saturates, while E_c passes through a maximum at $\lambda \sim 2$ and then exhibits a *decrease* in the strong-coupling regime.

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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 $E_c^{\rm BCS} = -VN_f\Delta^2/2$, where V is the volume, Δ is the superconducting gap, and $N_f = mp_F/(2\pi^2\hbar^3)$ 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 $C_s - C_n \approx 6.08 E_c/T_c$.

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 Δ^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 nonmonotonic 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 Δ as functions of doping clearly makes the applicability of the BCS formula to the cuprates questionable.

A large number of researchers believe that the cuprates are strongly-coupled systems. It therefore comes as no surprise that effort has already been made to explain the discrepancy between the doping dependence of Δ and $C_s - C_n$ 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, Hirsh[6] and later Norman *et al.*[5] argued 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. A somewhat different idea, related to the lowering of the Coulomb energy in the superconducting state has been proposed by Leggett.[7] [An alternative point of view, which we do not share, is that the large gap observed in, e.g., angle-resolved photoemission spectroscopy (ARPES) and tunneling experiments, is entirely distinct from the pairing gap.[8]]

In this paper we argue that these apparently disparate viewpoints regarding such non-BCS physics 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 Δ 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[9] for the normal state and extended to a superconductor by Eliashberg.[10] We first briefly review strongly coupled phonon superconductors and discuss the BCS, Bardeen-Stephen,[12] and Wada[13] expressions for the condensation energy (for a review, see Ref. 14). The BCS expression neglects both bosonic and fermionic self-energies (apart from a trivial renormalization of the dispersion). The Bardeen-Stephen and Wada expressions include the fermionic self-energy and its change between the normal and 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 the arguments of Bardeen and Stephen 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

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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 divergences are canceled out between the two terms, and the total E_c (which turns out to be the only physically meaningful quantity) is free from divergences. We furthermore demonstrate that one can avoid the divergences 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 support for the spin-fluctuation scenario for the cuprates.

A short summary of the results for the spin-fluctuation condensation energy E_c has been published in Ref. 11. In the current paper, we provide an in-depth account of how one actually calculates E_c in both the Matsubara and retarded formalisms. Such calculations are nontrivial as the electronic and spin components of the condensation energy contain ultraviolet divergences which must be canceled out in the full expression for E_c. We also compare the condensation energy for spin-fluctuation and phonon-induced superconductors.

II. CONDENSATION ENERGY

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

$$E_c = F_s - F_n. \tag{1}$$

In the Greens function technique one evaluates the grand free energy Ω. The difference $F_s - F_n$ coincides with $\Omega_s - \Omega_n$ provided that the chemical potential μ 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 Δ, and the corrections to μ due to pairing, which scale as powers of Δ/E_F, are neglected.[12]

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[15]

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

where Ω_0 is the Free energy for free fermions, Σ 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 four vector of momentum and Matsubara frequency $k = (\mathbf{k}, \omega_n)$ and the running coupling constant λ'. Note that here and below we define Σ with an extra factor of i.

Equation (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[9] who demonstrated that it is possible to reexpress Ω 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.[10] We refer the reader to Refs. 9 and 10 for the details of the derivation, and here just present the result. In the superconducting state, Ω has the form

$$\begin{aligned}\Omega = -2T\sum_k \Big\{ &\frac{1}{2}\ln[\epsilon_{\mathbf{k}}^2 + \tilde{\Sigma}^2(k) + \Phi^2(k)] - i\Sigma(k)G(k) \\ &+ i\Phi(k)F(k)\Big\} + \frac{1}{2}T\sum_q \{\ln[D^{-1}(q)] + \Pi(q)D(q)\} \\ &+ T^2\sum_{k,k'} \alpha_{k-k'}^2 \{G(k)D(k-k')G(k') \\ &+ F(k)D(k-k')F(k')\} + \cdots . \end{aligned} \tag{3}$$

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 normal and anomalous Greens functions given by

$$\begin{aligned} G(k) &= -\frac{\epsilon_{\mathbf{k}} + i\tilde{\Sigma}(k)}{\epsilon_{\mathbf{k}}^2 + \tilde{\Sigma}(k)^2 + \Phi^2(k)}, \\ F(k) &= i\frac{\Phi(k)}{\epsilon_{\mathbf{k}}^2 + \tilde{\Sigma}(k)^2 + \Phi^2(k)}, \end{aligned} \tag{4}$$

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, α_k is the electron-boson coupling and $D(q)$ is the dressed boson 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 a dimensionless quantity [see Eq. (3)], while the actual boson propagator has a dimension of inverse energy. This does not cause problems, however, as D appears only in a combination with α^2, and the extra overall energy factor can be absorbed in α^2.

Equation (3) is quite general. Its use for the calculation of E_c takes into account not just the introduction of the pairing vertex Φ but also changes in the fermionic self-energy Σ and the polarization bubble Π. Thus it calculates the contributions to E_c from both the fermions *and* bosons. We will be using Eq. (3) as the point of departure for our analysis. We first briefly review phonon superconductors and then discuss in more detail magnetically mediated superconductivity.

III. PHONON SUPERCONDUCTORS

Phonon superconductivity has been discussed in great detail in the past.[14,15,17] In order that the distinctions between

the phonon mediated and magnetically mediated superconductors may be properly appreciated, we briefly review in this section the results which will be important to us for the comparison of the two cases. We also present an interpretation of the physics behind Eliashberg theory, as well as an expression for the Free energy, valid for arbitrary $\Delta(\omega)$.

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 λ is the dimensional coupling constant which scales with $\alpha_{k-k'}$ (see below). The approximation, attributed to Migdal[16] and Eliashberg,[17] is to neglect $O(\lambda v_s/v_F)$ terms without assuming that λ is by itself small. This would imply neglecting all terms labeled as dots in Eq. (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 λ 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 ω and ϵ_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 λ 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 give 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 Ω_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 Ω_s given by Eq. (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

$$\tilde{\Sigma}(k)=\omega+iT\sum_{k'}\alpha^2_{k-k'}G(k')D(k-k'),$$

$$\Phi(k)=-iT\sum_{k'}\alpha^2_{k-k'}F(k')D(k-k'). \tag{5}$$

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 momentum transverse to the Fermi surface involves only normal and anomalous fermionic propagators, via ϵ_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 dependent 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

$$\sum_k \rightarrow N_f\int_{-\infty}^{\infty}d\epsilon, \tag{6}$$

inserting Eqs. (4) into (5), and performing the integration we obtain

$$\tilde{\Sigma}(\omega)=\omega+\pi TN_f\sum_{\omega'}\alpha^2_{\omega-\omega'}D(\omega-\omega')\times\frac{\tilde{\Sigma}(\omega')}{\sqrt{\Delta^2(\omega')+\tilde{\Sigma}^2(\omega')}},$$

$$\Phi(\omega)=\pi TN_f\sum_{\omega'}\alpha^2_{\omega-\omega'}D(\omega-\omega')\frac{\Phi(\omega')}{\sqrt{\Delta^2(\omega')+\tilde{\Sigma}^2(\omega')}}. \tag{7}$$

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 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 Eq. (5), an expression for $\Pi(k)$ can be formally obtained from the feature that Ω_s given by Eq. (3) is also stationary with respect to variations in $\Pi(k)$. The condition $\delta\Omega_s/\delta\Pi(k)=0$ yields

$$\Pi(k)=-2TD(0)\sum_{k'}\alpha^2_{k-k'}[G(k)G(k-k')+F(k)F(k-k')]. \tag{8}$$

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,

$$\Pi(k)\propto\lambda\frac{v_s}{v_F}\frac{\omega_m}{\omega_D}\frac{p_F}{|\mathbf{k}|} \tag{9}$$

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 $D(\omega_m)$. That is, for an Einstein phonon, $D_0(\omega_m)=2\omega_D^2/(\omega_D^2+\omega_m^2)$, where

ω_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 ω_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 Δ,

$$\Pi(k)\propto\lambda\frac{v_s}{v_F}\frac{\omega_m}{\Delta}\frac{\omega_m}{\omega_D}\frac{p_F}{|\mathbf{k}|}. \tag{10}$$

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[12] 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 Ω_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.,

$$\alpha_\omega=\alpha,$$

$$D(q)=D(\omega_m)=\frac{2\omega_D^2}{\omega_m^2+\omega_D^2}. \tag{11}$$

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

$$\Omega=-N_f\Bigg\{2\pi T\sum_m\frac{\omega_m\tilde{\Sigma}_{\omega_m}}{\sqrt{\tilde{\Sigma}_{\omega_m}^2+\Phi_{\omega_m}^2}}+T^2\pi^2\overline{\alpha^2}\times\sum_{m,m'}\frac{\tilde{\Sigma}_{\omega_m}\tilde{\Sigma}_{\omega_{m'}}+\Phi_{\omega_m}\Phi_{\omega_{m'}}}{\sqrt{\tilde{\Sigma}_{\omega_m}^2+\Phi_{\omega_m}^2}\sqrt{\tilde{\Sigma}_{\omega_{m'}}^2+\Phi_{\omega_{m'}}^2}}\times\frac{1}{(\omega_m-\omega_{m'})^2+\omega_D^2}\Bigg\}, \tag{12}$$

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

$$\lambda=\frac{\overline{\alpha^2}}{\omega_D^2}. \tag{13}$$

Equation (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 Eq. (12) we obtain

$$\Omega=-N_f\Bigg\{2\pi T\sum_m\frac{\omega_m^2}{\sqrt{\omega_m^2+\Delta_{\omega_m}^2}}+T^2\pi^2\overline{\alpha^2}\times\sum_{m,m'}\frac{\omega_m\omega_{m'}+\Delta_{\omega_m}\Delta_{\omega_{m'}}}{\sqrt{\omega_m^2+\Delta_{\omega_m}^2}\sqrt{\omega_{m'}{}^2+\Delta_{\omega_{m'}}^2}}\times\frac{1}{(\omega_m-\omega_{m'})^2+\omega_D^2}\Bigg\}. \tag{14}$$

Thus we see that the free energy for a phonon superconductor is dependent only upon the form of the gap Δ_{ω_m} and is not explicitly upon the self-energy Σ_{ω_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 Ω, 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 Ω_N does not explicitly depend on Σ_N. (We use the capital subscripts "S" and "N" to denote superconducting and normal states, respectively.) In the superconducting state, Eq. (14) does not imply that Ω_S is at a minimum, i.e., $\delta\Omega_S/\delta\Delta=0$. We did not 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 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 Δ^2 yields the sign change of the slope at exactly the BCS transition temperature T_c.

For the remainder of this paper, we will only be considering Ω evaluated at the equilibrium solution of Δ_{ω_m} when the applicability of the Luttinger-Ward formalism is rigorously justified. To this end, the Eliashberg equation for the equilibrium solution Δ_{ω_m} may be obtained by minimizing Eq. (14) with respect to Δ. This yields

$$\Delta_{\omega_m}=\pi T\overline{\alpha^2}\sum_{m'}\frac{1}{(\omega_m-\omega_{m'})^2+\omega_D^2}\frac{1}{\sqrt{\omega_{m'}^2+\Delta_{\omega_{m'}}^2}}\times\left\{\Delta_{\omega_{m'}}-\frac{\omega_{m'}}{\omega_m}\Delta_{\omega_m}\right\}. \tag{15}$$

This solution for Δ must then be substituted into Eq. (14) allowing the calculation of the free energy at its minimum, and hence $E_c=\Omega_S-\Omega_N$ where Ω_N is obtained from Ω_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 Eq. (3) should be stationary with respect to variations in Σ and Φ can be invoked even before the momentum integration is performed.[12–14] Substituting Eq. (5) into Eq. (3) and dropping the phonon piece, we obtain

$$\Omega=-T\sum_p \{\ln[\epsilon_{\mathbf{k}}^2+\tilde{\Sigma}_{\omega_m}^2+\Phi_{\omega_m}^2]-i\Sigma_{\omega_m}G(k)+i\Phi_{\omega_m}F(k)\}. \tag{16}$$

Introducing a density of states N_f, integrating over ϵ_k and subtracting the normal-state result from the superconducting result gives an expression for the condensation energy first derived by Wada:[13]

$$E_c=-N_f\pi T\sum_m \left(\sqrt{\tilde{\Sigma}_{S,\omega_m}^2+\Phi_{\omega_m}^2} - |\tilde{\Sigma}_{N,\omega_m}|+|\omega_m|\frac{|\tilde{\Sigma}_{S,\omega_m}|-\sqrt{\tilde{\Sigma}_{S,\omega_m}^2+\Phi_{\omega_m}^2}}{\sqrt{\tilde{\Sigma}_{S,\omega_m}^2+\Phi_{\omega_m}^2}}\right). \tag{17}$$

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.[12] They noticed that an integral relation between $\Sigma_{N,\omega}$ and $\Sigma_{S,\omega}$

$$N_f\pi T\sum_m \Sigma_{N,\omega}\frac{|\tilde{\Sigma}_{S,\omega_m}|}{\sqrt{\tilde{\Sigma}_{S,\omega_m}^2+\Phi_{\omega_m}^2}}-\Sigma_{S,\omega}=0 \tag{18}$$

exists 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 reexpressed 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 Eq. (18), Bardeen and Stephen obtained the following expression for $E_{c,\mathrm{el}}=E_c$:

$$E_{c,\mathrm{el}}=-N_f\pi T\sum_m (\sqrt{\tilde{\Sigma}_{S,\omega_m}^2+\Phi_{\omega_m}^2}-|\tilde{\Sigma}_{S,\omega_m}|)\times\left(1-\frac{|\tilde{\Sigma}_{N,\omega_m}|}{\sqrt{\tilde{\Sigma}_{S,\omega_m}^2+\Phi_{\omega_m}^2}}\right). \tag{21}$$

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 Eq. (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 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 Φ which is given by the BCS gap Δ ($\Phi_{\mathrm{BCS}}=\Delta$). 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

$$E_c^{\mathrm{BCS}}=-N_f\int_0^\infty \frac{2\omega^2+\Delta^2}{\sqrt{\omega^2+\Delta^2}}-2\omega=-N_f\frac{\Delta^2}{2}. \tag{22}$$

This is the result that we already cited in the Introduction. We also see that the frequency integration in Eq. (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.

IV. MAGNETICALLY MEDIATED 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

$$\Omega = -2T\sum_p \left\{\frac{1}{2}\ln[\epsilon_{\mathbf{k}}^2+\tilde{\Sigma}^2(k)+\Phi^2(k)]-i\Sigma(k)G(k) + i\Phi(k)F(k)\right\}+\frac{3}{2}T\sum_q \{\ln[D^{-1}(q)]+\Pi(q)D(q)\} + T^2\sum_{k,k'} g_{k-k'}^2\{G(k)\chi(k-k')G(k') + F(k)\chi(k-k')F(k')\}+\cdots . \quad (23)$$

The dimensionless bosonic propagator $D(q)$ is now related to the magnetic susceptibility $\chi_{ij}(q)=\chi(q)\delta_{ij}$ as $D(q)=\chi(q)/\chi(\mathbf{Q},0)$, where $\mathbf{Q}$ 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 $d_{x^2-y^2}$ pairing channel.[20] We will be studying E_c for this kind of pairing.

The spin-fermion model is described by the effective action

$$S = -\int_0^\beta d\tau\int_0^\beta d\tau'\sum_{\mathbf{k},\sigma} c_{\mathbf{k}\sigma}^\dagger(\tau)G_0^{-1}(\mathbf{k},\tau-\tau')c_{\mathbf{k}\sigma}(\tau') + \frac{1}{2}\int_0^\beta d\tau\int_0^\beta d\tau'\sum_{\mathbf{q}} \chi_0^{-1}(\mathbf{q},\tau-\tau')\mathbf{S}_{\mathbf{q}}(\tau)\cdot\mathbf{S}_{-\mathbf{q}}(\tau') + g_q\int_0^\beta d\tau\sum_{\mathbf{q}} \mathbf{s}_{\mathbf{q}}(\tau)\cdot\mathbf{S}_{-\mathbf{q}}(\tau), \quad (24)$$

where $G_0^{-1}(\mathbf{k},\tau)=\partial_\tau-\mathbf{v}_k(\mathbf{k}-\mathbf{k}_F)$ is the bare fermionic propagator, $c_{\mathbf{k},\alpha}^\dagger$ is the fermionic creation operator for an electron with crystal momentum $\mathbf{k}$ and spin projection α, $\mathbf{s}=c^\dagger\vec{\sigma}c$ is the fermionic spin (σ_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 $\mathbf{S}_\mathbf{q}$. For simplicity, below we assume $g_q=g$ to be momentum independent. The bare spin susceptibility $\chi_0^{-1}(\mathbf{q},\tau)$ is assumed to be peaked at Q and has a standard Ornstein-Zernike form, i.e., its Fourier transform over τ is

$$\chi_0(\mathbf{q},\omega)=\frac{\chi(Q)}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2-(\omega/v_s\xi^{-1})^2}, \quad (25)$$

where ξ 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

$$\lambda = 4\bar{\omega}/(3v_F\xi^{-1}), \quad (26)$$

where $\bar{\omega}=9g^2\chi(Q)/(16\pi\xi^2)$. The numerical factors are chosen for further convenience. This overall scale $\bar{\omega}$ and the coupling λ 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 ξ as $\chi(Q)$ by itself scales as ξ^2.

Near a magnetic transition, ξ is large, i.e., $\lambda\geqslant 1$, and the 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 Ref. 18 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,[19,21] $d_{x^2-y^2}$ pairing,[22] and the pseudogap.[23] We note, though, that there is still a great deal of controversy regarding the full description of these phenomena. Since, however, many researchers believe 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 anti-ferromagnetically 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, for a spin susceptibility peaked at or near $\mathbf{Q}=(\pi,\pi)$, magnetically mediated pairing yields a $d_{x^2-y^2}$ symmetry of the pairing gap.[20] At weak and moderate couplings, the momentum dependence of the pairing gap can be reasonably well approximated by a $\cos k_x-\cos k_y$ form (the first B_{1g} harmonics of the D_{4h} group[22]). 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 enu-

merate the reasoning leading to the above conclusions here. A more detailed discussion can be found in Ref. 18.

(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 a 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 λ.

(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 Π_{ω_m} dominates the frequency dependence of the spin susceptibility, 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 $\lambda \gg 1$ 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 diagrammatic 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 $\ln\lambda$ instead of powers of λ, 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 $\ln\lambda$ gives rise to vertex corrections and to the renormalization of the quasiparticle residue. There are also terms that form series in λ. 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 λ 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 insensitive to any transmutation of the bosonic dynamics.

(4) This separation of terms into perturbative series of λ and $\ln\lambda$ allows an approximation similar to that made for phonons to be made here. In the magnetic case one neglects terms $O(\ln\lambda)$ compared to terms of order λ. This is not as good of an approximation as the neglect of $\lambda v_s/v_F$ terms for phonons as $\ln\lambda$ is also large when λ is large. However, the numerical prefactors for $\ln\lambda$ series turn out to be small [a vertex correction is only $(1/8)\ln\lambda$], and in practice the neglect of logarithmic terms is well justified for all physically reasonable λ ($\lambda \sim 1-2$ at optimal doping). In addition, from a purely theoretical standpoint the $\ln\lambda$ terms can be made parametrically small by introducing a large number of fermionic flavors M [a vertex correction is then $(1/8M)\ln\lambda$]. Furthermore, a one-loop RG analysis of the logarithmic 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 λ yields a $\Sigma(k,\omega_m)$ that is predominantly dependent on frequency. More specifically, near k points on the Fermi surface connected by the antiferromagnetic wave vector $\mathbf{Q}$ (hot spots), $\Sigma(k,\omega)$ depends on ω, but not on ϵ_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 Π_{ω_m} turns out to be independent of $\Sigma(\omega)$ and is the same in the normal state as it would be for free fermions:

$$\Pi(\omega_m)=\frac{\omega_m}{\omega_{\mathrm{SF}}}=4\lambda^2\frac{\omega_m}{\overline{\omega}}. \tag{27}$$

Here we have introduced the notation $\omega_{\mathrm{SF}}=\overline{\omega}/(4\lambda^2)$. This ω_{SF} scales as ξ^{-2} and vanishes at the magnetic transition.

(6) Away from a hot spot, this independence from ϵ_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

$$\Sigma(k,\omega)=\lambda(k)\frac{2\omega}{1+\sqrt{1-i\dfrac{|\omega|}{\omega_{\mathrm{SF}}(k)}}}, \tag{28}$$

where

$$\lambda(k)=\lambda/[1+(\tilde{k}\xi)^2]^{1/2}, \quad \omega_{\mathrm{SF}}(k)=\omega_{\mathrm{SF}}[1+(\tilde{k}\xi)^2] \tag{29}$$

and $\tilde{k}$ is the component of $\mathbf{k}-\mathbf{k}_{\mathrm{HS}}$ 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 ξ. However, for $\omega \gg \omega_{\mathrm{SF}}(k)$, the k dependence disappears: $\Sigma(k,\omega)\approx(i\omega\overline{\omega})^{1/2}$ (we used the fact that $2\lambda(k)[\omega_{\mathrm{SF}}(k)]^{1/2}=\overline{\omega}$). Alternatively speaking, at $\omega > \omega_{\mathrm{SF}}(k)$, 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 ω and $\tilde{k}$ are. For the pairing problem, a detailed analysis shows that typical frequencies are of order $\overline{\omega}$, and typical $\tilde{k}$ are of order $\overline{\omega}/v_F$. Then typical $\omega_{\mathrm{SF}}(k)$ are of order $\overline{\omega}$, i.e., the momentum dependence along the Fermi surface introduces corrections $O(1)$. These corrections have been checked in Ref. 22 and found to be nonessential from the perspective of the basic physics. Note also that the theory assumes that $\overline{\omega} < E_F$, 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 Σ and anomalous vertex Φ 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 $\lambda \geqslant 1$, the softness of fermions compared to bosons gives rise to an effective Migdal theorem, i.e., the vertex corrections are smaller than Σ 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 Σ and Φ can be fully neglected. In the case of Φ, 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 Φ 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 Ω is stationary with respect to variations of Σ, Φ, and Π gives

$$\Sigma(k) = 3iTg^2\chi(Q)\sum_{k'} G(k')\chi(k-k'),$$

$$\Phi(k) = -3iTg^2\chi(Q)\sum_{k'} F(k')\chi(k-k'),$$

$$\Pi(k) = -2Tg^2\chi(Q)\sum_{k} [G(k)G(k-k') + F(k)F(k-k')]. \tag{30}$$

Under the assumption of the momentum independence of Σ, Φ, and Π the normal and anomalous Greens functions have the form

$$G_{\omega_m}(\mathbf{k}) = -\frac{\epsilon_{\mathbf{k}} + i\tilde{\Sigma}_{\omega_m}}{\epsilon_{\mathbf{k}}^2 + \tilde{\Sigma}_{\omega_m}^2 + \Phi_{\omega_m}^2},$$

$$F_{\omega_m}(\mathbf{k}) = i\frac{\Phi_{\omega_m}}{\epsilon_{\mathbf{k}}^2 + \tilde{\Sigma}_{\omega_m}^2 + \Phi_{\omega_m}^2} \tag{31}$$

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

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

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

$$\Pi_{\omega_m}(Q) = \frac{4\lambda^2}{\bar{\omega}}\pi T \times \sum_n \left[-1 + \frac{\tilde{\Sigma}_{\omega_n}\tilde{\Sigma}_{\omega_{n+m}} + \Phi_{\omega_n}\Phi_{\omega_{n+m}}}{\sqrt{\tilde{\Sigma}_{\omega_n}^2 + \Phi_{\omega_n}^2}\sqrt{\tilde{\Sigma}_{\omega_{n+m}}^2 + \Phi_{\omega_{n+m}}^2}} \right]. \tag{32}$$

We emphasize again that Eq. (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 λ can be represented as the ratio $(2\lambda)^2 = \bar{\omega}/\omega_{\mathrm{SF}}$ of $\bar{\omega}$ and another typical scale ω_{SF} that sets the upper boundary of the Fermi-liquid behavior in the normal state. We illustrate the form of Σ_{ω_m}, Φ_{ω_m}, and Π_{ω_m} in Fig. 1 for both the normal and superconducting state.

Substituting Eqs. (30) into (23) we obtain the equilibrium thermodynamic potential in a magnetically mediated superconductor as a sum of two parts Ω_{el} comprising the "electronic" contributions and Ω_{spin} comprising the "magnetic" part:

$$\Omega = \Omega_{\mathrm{el}} + \Omega_{\mathrm{spin}}; \quad E_c = \Omega^S - \Omega^N = E_{e,\mathrm{el}} - E_{c,\mathrm{spin}} \tag{33}$$

where

$$\Omega_{\mathrm{el}} = -T\sum_m \int \frac{d^2k}{(2\pi)^2}\{\ln[\epsilon_{\mathbf{k}}^2 + \tilde{\Sigma}_{\omega_m}^2 + \Phi_{\omega_m}^2] - i\Sigma_{\omega_m}G_{\omega_m}(k) + i\Phi_{\omega_m}F_{\omega_m}(k)\},$$

$$\Omega_{\mathrm{spin}} = \frac{3}{2}T\sum_m \int \frac{d^2k}{(2\pi)^2}\left\{\ln\left[\frac{\chi(Q,0)}{\chi(q,\omega_m)}\right] + \Pi_{\omega_m}\frac{\chi(q,\omega_m)}{\chi(Q,0)}\right\}. \tag{34}$$

The electronic term $E_{c,\mathrm{el}} = \Omega_{\mathrm{el}}^S - \Omega_{\mathrm{el}}^N$ accounts explicitly for the appearance of the anomalous pairing vertex Φ_{ω_n}, *and* for the feedback changes to the fermionic self-energy. This term by itself leads to the Wada result for the condensation energy. The term $E_{c,\mathrm{spin}} = \Omega_{\mathrm{spin}}^{sc} - \Omega_{\mathrm{spin}}^{n}$ accounts for changes to the spin propagator via the changes to the spin polarization operator Π_{ω_m}. Together these two expressions account for the feedback effects between fermions and bosons in a strong-

coupling theory. We point out that the distinction between $\Omega_{\rm el}$ and $\Omega_{\rm spin}$ 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 Σ and Φ and Π depend only on ω, the momentum integration in Eq. (34) can be performed explicitly and yields

$$E_{c,\rm el} = -N_f \pi T \sum_m \left(\sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}} - |\tilde{\Sigma}_{N,\omega_m}| + |\omega_m| \frac{|\tilde{\Sigma}_{S,\omega_m}| - \sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}}}{\sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}}} \right), \tag{35}$$

$$E_{c,\rm spin} = -\frac{3T}{8\pi\xi^2} \sum_m \Pi_{S,\omega_m} - \Pi_{N,\omega_m} + \ln \frac{1-\Pi_{S,\omega_m}}{1-\Pi_{N,\omega_m}}. \tag{36}$$

The first term $E_{c,\rm el}$ is the Wada result. The second term $E_{c,\rm spin}$ is new. Note that its expansion in $\Pi_S - \Pi_N$ 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 Π.

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 $E_{c,\rm el}$ in fact contains a divergent piece which is canceled out by the divergence in $E_{c,\rm spin}$. Indeed, consider the high frequency part of $E_{c,\rm el}$. At high frequencies, $\tilde{\Sigma}_{\omega_m}$ dominates over Φ_{ω_m}, and the electronic part of the condensation energy reduces to

$$\Omega_{\rm el} = -N_f \pi T \sum_m |\Sigma_{S,\omega_m}| - |\Sigma_{N,\omega_m}| + \cdots, \tag{37}$$

where the ellipsis stands for other terms that are all finite, as one can easily demonstrate. Examine next the equation for Σ. By making the substitution $\Delta_{\omega_m} = \Phi_{\omega_m}\omega_m / \tilde{\Sigma}_{\omega_m}$ we may write Σ_{ω_m} in the following form:

$$\Sigma_{\omega_m} = \pi\lambda T \sum_n \frac{\omega_n}{\sqrt{\omega_n^2 + \Delta_n^2}} \frac{1}{(1-\Pi_{\omega_m-\omega_n})^{1/2}}. \tag{38}$$

Were the bosonic spectrum unchanged between the superconducting and normal states ($\Pi_N = \Pi_S$) then we could expand Eq. (38) in powers of Δ_n, and would find that at large frequencies

$$\Sigma_{S,\omega_m} - \Sigma_{N,\omega_m} \propto \frac{\Delta^2_{\omega_m}}{\omega_m}. \tag{39}$$

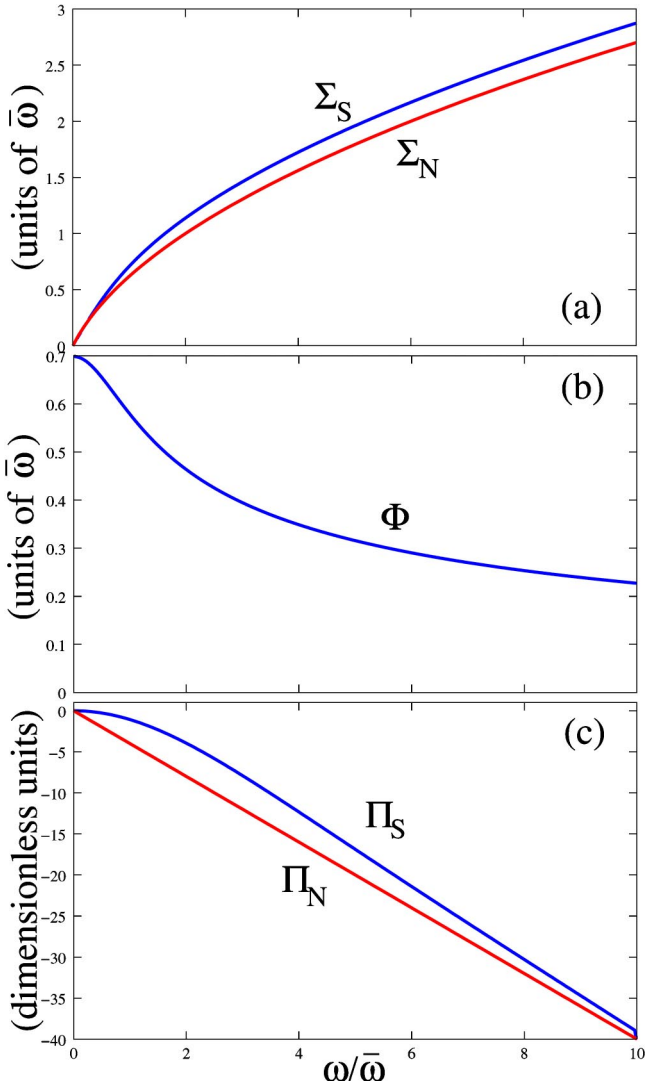

FIG. 1. Matsubara frequency solutions at $\lambda = 1$ for Σ (a), Φ (b), and Π (c) in the spin fermion model [Eq. (32)] for both the normal and superconducting states. Note that Σ is a strong function of frequency and may not be neglected. The apparent nonconvergence of Σ at high frequencies is spurious and is discussed in the text. Further note that Π changes appreciably between the normal and superconducting states. This change *must* be taken into account when calculating the condensation energy.

Since the gap Δ_{ω_m} is expected on physical grounds to vanish at the highest frequencies (and computations indeed confirm this), the frequency integral in Eq. (37) converges, i.e., the electronic part of the condensation energy would be finite. The situation is very different when changes in Π are taken into account. Although at high frequencies Π_{S,ω_n} indeed converges to Π_{N,ω_n}, the two expressions are different at frequencies comparable to typical Δ_{ω_m}. Since for arbitrary large ω_m in Eq. (38), there is a range of running ω_n where Π_S and Π_N differ, Σ_S and Σ_N do not converge at high frequencies: Σ_{S,ω_n} remains larger than Σ_{N,ω_n} by a constant. We illustrate this behavior in Fig. 1(a).

This nonconvergence of Σ_N and Σ_S seems at first glance

to imply an infinite result for the condensation energy. Indeed, this is true only under the assumption that fermonic bandwidth W is infinite, otherwise Σ_N and Σ_S converge at the scale of the bandwidth. However, even in this situation, the electronic contribution to the condensation energy turns out to be very large—of the order of W.

It turns out that this near-infinite contribution is compensated for by the *spin* part of the condensation energy, such that the total E_c remains finite even when the fermionic bandwidth is infinite. As written in Eq. (36) the spin condensation energy looks quite convergent *if* we use $\Pi_{N,\omega_m} \propto \omega_m$. However, the expression for the spin polarization operator is formally ultraviolet divergent, and extra care has to be taken in evaluating the difference between Π_{N,ω_m} and Π_{S,ω_m}.

In what follows we explicitly re-express the divergent contribution in $E_{c,\mathrm{el}}$ in terms of the spin polarization operator, and show that when we take the divergent piece from $E_{c,\mathrm{el}}$ and add it to $E_{c,\mathrm{spin}}$, the dangerous $\Pi_{N,\omega_m} - \Pi_{S,\omega_m}$ term in $E_{c,\mathrm{spin}}$ is canceled 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 Π_{N,ω_m} is absent, and $\Pi_{N,\omega_m} \propto \omega_m$. In practice, this regularization amounts to evaluating the integral over ϵ_k first, and the frequency integral later.

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

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

$$= \pi \lambda T \sum_n \mathrm{sgn}(\omega_n) \frac{1}{(1-\Pi_{S,\omega_{m-n}})^{1/2}}. \tag{40}$$

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

$$E_{c,\mathrm{el}} = -N_f \pi T \sum_m \left(\sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}} - |\tilde{\Sigma}_{\mathrm{NS},\omega_m}| \right.$$

$$\left. + |\omega_m| \frac{|\tilde{\Sigma}_{S,\omega_m}| - \sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}}}{\sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}}} \right)$$

$$+ \{ |\tilde{\Sigma}_{\mathrm{NS},\omega_m}| - |\tilde{\Sigma}_{N,\omega_m}| \}. \tag{41}$$

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

We now explicitly express this divergent piece in terms of the spin polarization operator. To accomplish this, we recall

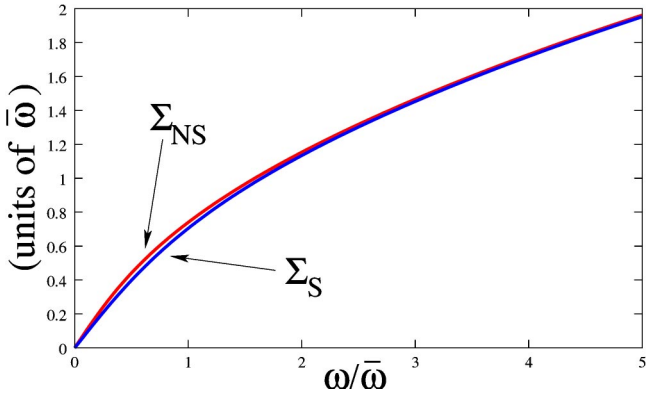

FIG. 2. Spin-fermion solutions for Σ_S and Σ_{NS} as defined by Eq. (40) in Matsubara frequencies. Note that by replacing Π_N by Π_S in the normal-state expression for Σ, we have obtained a convergent expression for the electronic part of the condensation energy as discussed in the text.

that the term $|\tilde{\Sigma}_N|$ in $E_{c,\mathrm{el}}$ arose from the integration over momentum of the ΣG term in Eq. (34). Writing this for both the normal and normal-superconducting self-energies, we have

$$N_f \pi T \sum_m |\Sigma_{N,\mathrm{NS},\omega_m}| = T \sum_m \int \frac{d^2k}{(2\pi)^2} i\Sigma_{N,\mathrm{NS},\omega_m} G_{N,\omega_m}. \tag{42}$$

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

$$+ T \sum_m \int \frac{d^2k}{(2\pi)^2} i\Sigma_{N,\mathrm{NS},\omega_m} G_{N,\omega_m}$$

$$= T \sum_m \int \frac{d^2k}{(2\pi)^2} \left\{ -3g^2 \pi T \sum_n \int \frac{d^2q}{(2\pi)^2} \chi_{N,\mathrm{NS},\omega_n}(q) \right.$$

$$\left. \times G_{N,\omega_{n+m}}(k+q) \right\} G_{N,\omega_n}(k)$$

$$= -\frac{3}{2} T \sum_n \int \frac{d^2q}{(2\pi)^2} \frac{\chi_{N,\mathrm{NS},\omega_n}(q)}{\chi(0)}$$

$$\times \left\{ 2g^2 \chi(0) \pi T \sum_m \int \frac{d^2k}{(2\pi)^2} \right.$$

$$\left. \times G_{N,\omega_{n+m}}(k+q) G_{N,\omega_n}(k) \right\}$$

$$= -\frac{3}{2\chi_0} T \sum_n \int \frac{d^2q}{(2\pi)^2} \chi_{N,\mathrm{NS},\omega_n}(q) \Pi_{N,\omega_n}. \tag{43}$$

Performing the integration over q we find that

$$-\pi T N_f \sum_m \left(|\Sigma_{\mathrm{NS},\omega_m}| - |\Sigma_{N,\omega_m}|\right)$$

$$= -T\frac{3}{8\pi\xi^2}\sum_m \Pi_{N,\omega_m} \ln\frac{1-\Pi_{S,\omega_m}}{1-\Pi_{N,\omega_m}}. \quad (44)$$

We now move the divergent piece from Ω_{el} to Ω_{spin} and write the condensation energy as $E_c = \delta\tilde{\Omega}_{\mathrm{el}} + \delta\tilde{\Omega}_{\mathrm{spin}}$ with

$$\delta\tilde{\Omega}_{\mathrm{el}} = -N_f \pi T \sum_m \left(\sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}} - |\tilde{\Sigma}_{\mathrm{NS},\omega_m}| + |\omega_m| \frac{|\tilde{\Sigma}_{S,\omega_m}| - \sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}}}{\sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}}} \right), \quad (45)$$

$$\delta\tilde{\Omega}_{\mathrm{spin}} = -\frac{3T}{8\pi\xi^2}\sum_m \Pi_{S,\omega_m} - \Pi_{N,\omega_m} + (1+\Pi_{N,\omega_n}) \times \ln\frac{1-\Pi_{S,\omega_m}}{1-\Pi_{N,\omega_m}}. \quad (46)$$

The electronic part is now fully convergent. For the spin part, one can easily check that at large frequencies, when Π_{N,ω_m} and Π_{S,ω_m} are both large, the expansion of the logarithm in $E_{c,\mathrm{spin}}$ 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 Π_{N,ω_m}. This implies that the condensation energy is actually free from divergencies, as it indeed should be based on physical reasoning.

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

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 does not. However, $\delta\tilde{\Omega}_{\mathrm{el}}$ and $\delta\tilde{\Omega}_{\mathrm{spin}}$ are in fact of the same order as we now demonstrate. Indeed, as we already said, typical frequencies for the pairing are of order $\overline{\omega}$, and at these frequencies

$$\Pi_{S,\omega_n} \sim \Pi_{N,\omega_n} \sim \frac{\overline{\omega}}{\omega_{\mathrm{SF}}}. \quad (47)$$

Similarly,

$$\Sigma_{S,\omega_n} \sim \Sigma_{N,\omega_n} \sim \overline{\omega}. \quad (48)$$

Then using Eq. (46) for $\delta\tilde{\Omega}_{\mathrm{spin}}$:

$$\delta\tilde{\Omega}_{\mathrm{spin}} \sim \frac{\overline{\omega}^2}{\omega_{\mathrm{SF}}\xi^2} \sim \frac{\overline{\omega}^3}{v_F^2}, \quad (49)$$

where the last step uses the definition of ω_{SF} given previously. At the same time

$$\delta\tilde{\Omega}_{\mathrm{el}} \sim N_f \overline{\omega}^2. \quad (50)$$

The fermionic density of states N_f is a product of $1/v_F$ (the leftover of the integration over ϵ_k, and a typical $\tilde{k}$ along the Fermi surface). As typical $\tilde{k} \sim \overline{\omega}/v_F$,

$$N_f \sim \frac{\overline{\omega}}{v_F^2}. \quad (51)$$

Substituting this result into Eq. (50), we find

$$\delta\tilde{\Omega}_{\mathrm{el}} \sim \frac{\overline{\omega}^3}{v_F^2}, \quad (52)$$

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

In the above discussion N_f appears as an *extra* parameter in $\delta\tilde{\Omega}_{\mathrm{el}}$. 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 $\omega_{\mathrm{SF}}(k)$] 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, $\delta\tilde{\Omega}_{\mathrm{spin}}$ is the result of a full two-dimensional integration over bosonic momenta, and the result for $\delta\tilde{\Omega}_{\mathrm{spin}}$ is free from uncertainties.

Fortunately, it turns out that within the (approximate) computational scheme that we are using, N_f and $1/(\omega_{\mathrm{SF}}\xi^2)$ can be related. Their relation follows from Eq. (44), as both the fermionic self-energy and the spin polarization operator are fully expressed in terms of $\overline{\omega}$ and λ. By evaluating the constant pieces in $\Sigma_{\mathrm{NS},\omega_m} - \Sigma_{N,\omega_m}$ and in $\Pi_{S,\omega_m} - \Pi_{N,\omega_m}$ at high frequencies and comparing the two sides of Eq. (44), one can express N_f in terms of $1/(\omega_{\mathrm{SF}}\xi^2)$. Once this is done, there is no further uncertainty in the condensation energy—it is given by the universal function of λ times $\overline{\omega}^2/(\omega_{\mathrm{SF}}\xi^2) \propto \overline{\omega}^3/v_F^2$.

A remark is in order here. The electronic and spin parts of E_c are only of the same order of magnitude as long as $\overline{\omega} < E_F$. 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 $\omega_{\mathrm{SF}}\xi^2 \sim v_F^2/\overline{\omega} \sim J$ where J is the exchange integral for the corresponding Heisenberg model. [Recall that $\overline{\omega} \sim g^2\chi(Q)/\xi^2$ 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., $\overline{\omega} \sim U$.] Estimating $\delta\tilde{\Omega}_{\mathrm{spin}}$ at typical frequencies, we indeed find $\delta\tilde{\Omega}_{\mathrm{spin}} \sim J$ in agreement with the result by Scalapino and White.[4] The same reasoning yields $\delta\tilde{\Omega}_{\mathrm{el}} \sim N_f J^2 \sim J^2/v_F \ll J$. 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]

V. THE COMPUTATIONS

In this section we present our results for the electronic and spin contributions to the condensation energy for various λ. In practice, we found it advantageous to perform the calculations of $\delta\tilde{\Omega}_{\rm spin}$ and $\delta\tilde{\Omega}_{\rm el}$ 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 $E_{c,\rm el}$ and $E_{c,\rm spin}$ 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 $E_{c,\rm el}$ and $E_{c,\rm spin}$ given in Eq. (34) have the following form.

$$E_{c,\rm el} = -\pi T \sum_m f(i\omega_m),$$

$$E_{c,\rm spin} = -\pi T \sum_n g(i\omega_n), \tag{53}$$

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

$$E_{c,\rm el} = -\int_0^\infty f''_{\rm ret}(\omega)\tanh\left(\frac{\omega}{2T}\right)d\omega,$$

$$E_{c,\rm spin} = -\int_0^\infty g''_{\rm ret}(\omega)\coth\left(\frac{\omega}{2T}\right)d\omega, \tag{54}$$

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 Sec. II, the analytic continuations are as follows:

$$\Sigma(\omega_m) \to -i\Sigma_{\rm ret}(\omega),$$

$$\Phi(\omega_m) \to \Phi_{\rm ret}(\omega),$$

$$\Pi(\omega_m) \to \Pi_{\rm ret}(\omega). \tag{55}$$

The retarded formulas for the condensation energy are then

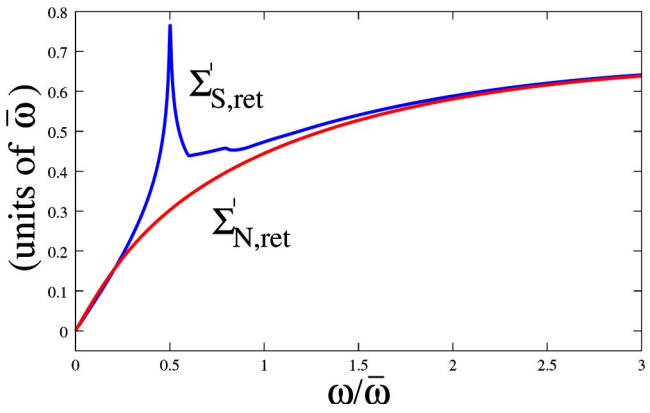

FIG. 3. The real part of the retarded self-energy for both the normal and superconducting states. Observe that $\Sigma'_{S,\rm ret}$ and $\Sigma'_{N,\rm ret}$ converge at high frequencies in contrast to the constant offset in Matsubara frequencies. The constant offset goes into the imaginary part of $\Sigma_{\rm ret}$ which does not affect E_c in the retarded formalism.

$$E_{c,\rm el} = -N_f \int_0^\infty \left\{ [\beta + \mathrm{Re}\,\tilde{\Sigma}_N(\omega)] + \omega\left[1 - \frac{\mathrm{Im}\,\Sigma_S(\omega)\alpha - \mathrm{Re}\,\Sigma_S(\omega)\beta}{|\alpha|^2 + |\beta|^2}\right]\right\} \tanh\frac{\omega}{2T}d\omega,$$

$$E_{c,\rm spin} = -\frac{3}{8\pi^2\xi^2}\int_0^\infty \left\{ \mathrm{Im}\,\Pi_S - \mathrm{Im}\,\Pi_N + \mathrm{Im}\ln\frac{1-\Pi_S(\omega)}{1-\Pi_N(\omega)}\right\}\coth\frac{\omega}{2T}d\omega, \tag{56}$$

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 $E_{c,\rm el}$. 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 Σ with an extra i, this constant is *imaginary*. On the other hand, the first two terms in the retarded formula for $E_{c,\rm el}$ at high frequencies where $\Phi \to 0$ can be written as

$$\mathrm{Im}\,\sqrt{-\Sigma_S^2(\omega)} + \mathrm{Re}\,\Sigma_N(\omega) = \mathrm{Re}\,\Sigma_N(\omega) - \mathrm{Re}\,\Sigma_S(\omega). \tag{57}$$

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 $E_{c,\rm el}$ only depends on the difference of $\mathrm{Re}\,\Sigma$ between the normal and superconducting states, and the integral of this difference is fully convergent. We illustrate this in Fig. 3. Analogous reasoning also shows that $E_{c,\rm spin}$ is also free from divergencies.

Indeed, the absence of divergencies in the retarded formalism is just the consequence of using the Kramers-Krönig transform which misses the divergent pieces in $E_{c,\rm spin}$ and $E_{c,\rm el}$. However, since we already demonstrated that the full

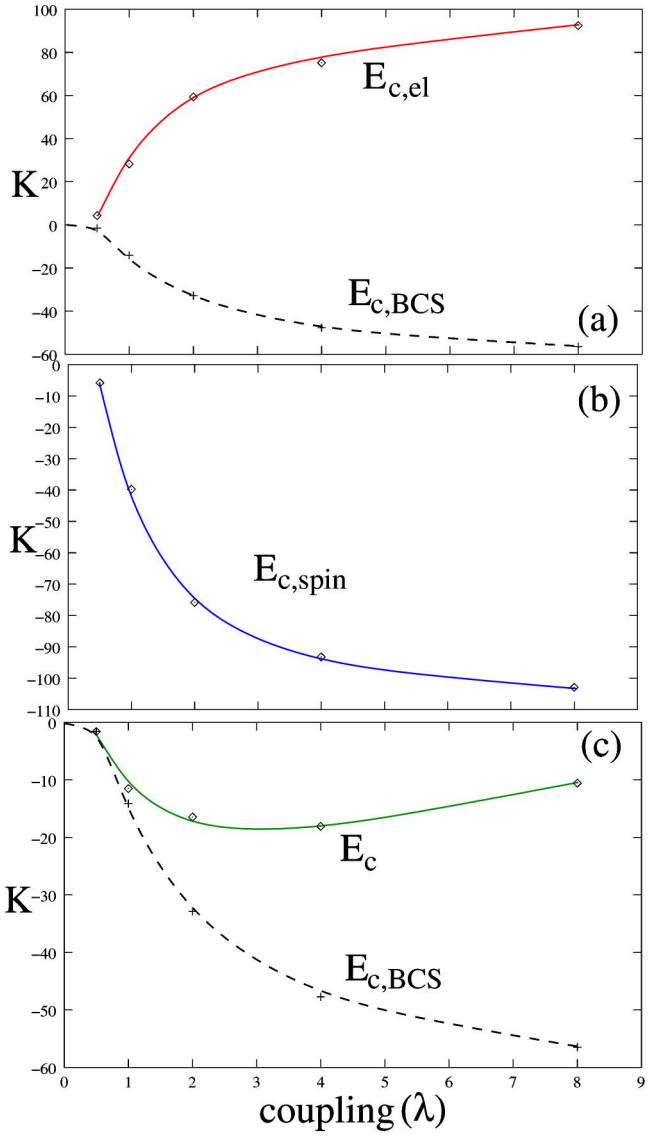

FIG. 4. The condensation energy for various couplings λ. (a) and (b) are the electronic ($E_{c,\mathrm{el}}$) and spin ($E_{c,\mathrm{spin}}$) contributions to the condensation energy, respectively. (c) is the total condensation energy per unit cell at $T=0$ for various couplings λ. The lines are a guide for the eye. We used $N_f=1$ st/eV and $N_s\sim 0.17$ st/eV as explained in the text. For comparison, we also plotted the condensation energy given by the BCS formula using the $\Delta(\omega=0)$ given by the spin-fermion model. 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. The change in curvature of the BCS result at small couplings reflects the fact that the spin-fermion model becomes BCS-like for $\lambda\leqslant 0.5$ changing the functional dependence of $\Delta(\omega=0)$ on λ.

$\delta\Omega$ is free from divergencies, we can safely use the Kramers-Krönig transformation separately for $E_{c,\mathrm{spin}}$ and $E_{c,\mathrm{el}}$.

The fact that no divergence exists for the retarded formulas also allows us to relate the prefactors in front of $E_{c,\mathrm{el}}$ and $E_{c,\mathrm{spin}}$ in a straightforward manner. In real frequencies, Eq. (44) takes the form

$$-N_f\int_0^\infty \{\mathrm{Re}\,\Sigma_{\mathrm{NS}}(\omega)-\mathrm{Re}\,\Sigma_N(\omega)\}\tanh\frac{\omega}{2T}d\omega$$
$$=\frac{3}{8\pi^2\xi^2}\int_0^\infty\Big\{\mathrm{Re}\,\Pi_N(\omega)\mathrm{Im}\ln\frac{1-\Pi_S(\omega)}{1-\Pi_N(\omega)}$$
$$+\mathrm{Im}\,\Pi_N(\omega)\mathrm{Re}\ln\frac{1-\Pi_S(\omega)}{1-\Pi_N(\omega)}\Big\}\coth\frac{\omega}{2T}d\omega. \quad (58)$$

Since in the retarded formalism, $\int_{-\infty}^{\infty}\mathrm{Re}\,\Sigma_{\mathrm{NS}}(\omega)-\mathrm{Re}\,\Sigma_N(\omega)d\omega$ is a convergent quantity, and the right-hand side (RHS) of Eq. (58) is also convergent, we can explicitly evaluate (numerically) both sides of Eq. (58) and relate N_f and $3/8\pi^2\omega_{\mathrm{SF}}\xi^2$, which we label as the spin density of states N_s [$N_s=(8/3\pi^2)\overline{\omega}/v_F^2$].

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, (58) and evaluated the ratio N_f/N_s for various λ. We found that with very small variations $N_f/N_s\approx 5.9$.

In Figs. 4(a),4(b) we present the results for the electronic and spin contributions to the condensation energy for different values of the coupling λ. To set the overall scale, we adopt a commonly used estimate $N_f=1$ st/eV.[21] 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(c) 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., $\overline{\omega}<\omega_{\mathrm{SF}}$, 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 $\lambda\geqslant 1$, i.e., in the strongly coupled regime, the electronic contribution to the condensation energy is *positive* and quite large. From Fig. 4(a) it appears that the electronic contribution changes sign at $\lambda\sim 0.4$. $E_{c,\mathrm{el}}$ is negative below this coupling strength and is positive for all $\lambda\geqslant 1/2$ presented in the figure. Second, for all λ shown, the spin part $E_{c,\mathrm{spin}}$ is negative [see Fig. 4(b)]. It can be shown that $E_{c,\mathrm{spin}}$ continues to be negative at $\lambda\to 0$ where $\Pi\to 0$ as λ^2 [see Eq. (32)]. Indeed, by expanding the logarithm in Eq. (58) we obtain

$$E_{c,\mathrm{spin}}(\lambda\to 0)=-N_s\frac{\omega_{\mathrm{SF}}}{2}\int_0^\infty \mathrm{Im}\{\Pi_S^2-\Pi_N^2\}$$
$$=-N_s\omega_{\mathrm{SF}}\int_0^\infty\{\mathrm{Re}\,\Pi_S\mathrm{Im}\,\Pi_S$$
$$-\mathrm{Re}\,\Pi_N\mathrm{Im}\,\Pi_N\}<0. \quad (59)$$

The above equation is negative, as in the retarded formalism, $\mathrm{Re}\,\Pi_N=0$ and both $\mathrm{Re}\,\Pi_S\leqslant 0$ and $\mathrm{Im}\,\Pi_S<0$, and scale as λ^4 as $\lambda\to 0$.

We also see from Figs. 4(a),4(b) that at large λ, both the spin and the electronic parts of the condensation energy nearly saturate: to a large positive value for $E_{c,\mathrm{el}}$ and a large negative value for $E_{c,\mathrm{spin}}$. The total condensation energy E_c is negative and much smaller than either $E_{c,\mathrm{el}}$ or $E_{c,\mathrm{spin}}$ due to a substantial cancellation between these two components of E_c. Although this cancellation seems quite delicate, it is actually robust since $E_{c,\mathrm{el}}$ and $E_{c,\mathrm{spin}}$ are intimately linked via mutual feedback, and cannot 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 λ. We see that the condensation energy flattens at $\lambda \sim 2$, and its magnitude decreases at large couplings despite the fact that the pairing gap increases monotonically with λ.[22] This behavior is very counterintuitive from a BCS perspective, where the condensation energy scales with Δ^2. It clearly indicates that for $\lambda \geqslant 1$, the physics is qualitatively different from BCS theory. To emphasize this strong deviation from BCS theory we plot in Fig. 4(c) the strong coupling result of E_c along with the BCS condensation energy $-N_f\Delta^2/2$ using the same Δ and N_f. We clearly see that for $\lambda \geqslant 1$, corresponding to optimally doped and underdoped cuprates, BCS theory yields qualitatively different results for E_c.

Our results are in line with earlier work which demonstrated that for $\lambda \geqslant 1$, 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''-$\overline{\omega}$ and ''lower'' ω_{SF} scales of spin-fermion theory. As $\overline{\omega} = 4\lambda^2 \omega_{\mathrm{SF}}$ this ratio grows quickly, and already $\overline{\omega}/\omega_{\mathrm{SF}} = 4$ 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[23] 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 λ increases, the 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 cannot lead to a gain in E_c. Such behavior is very counter intuitive from a BCS perspective, where the pairing emerges due to an exchange of virtual, off-shell bosons, and the condensation energy scales with Δ^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 nonmagnetic impurities.[22] However, in a dirty superconductor with nonmagnetic impurities, the condensation energy retains its BCS form despite the fact that the superfluid stiffness is renormalized down.[24] Obviously, this is not what we found.

VI. 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

$$E_{\mathrm{kin}} = 2T\sum_m \int \frac{d^2k}{(2\pi)^2}\epsilon_k G_{\omega_m}(k), \tag{60}$$

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_{kin} in a superconductor we obtain

$$\delta E_{\mathrm{kin}} = 2N_f \pi T \sum_m \sqrt{\tilde{\Sigma}^2_{S,\omega_m} + \Phi^2_{\omega_m}} - |\tilde{\Sigma}_{N,\omega_m}|. \tag{61}$$

In the BCS limit, $\lambda \ll 1$, $\Phi_{\omega_n} = \Delta$, $\Sigma = 0$, $\tilde{\Sigma}_{\omega_n} = \omega_n$, and

$$\delta E^{\mathrm{BCS}}_{\mathrm{kin}} = 2N_f \pi T \sum_m \sqrt{\omega_m^2 + \Delta^2} - |\omega_m| \tag{62}$$

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

$$\delta E^{\mathrm{BCS}}_{\mathrm{kin}} = N_f \Delta^2 \ln \frac{\omega_{\max}}{\Delta}. \tag{63}$$

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

We now consider finite λ. As before, we perform the computations in real frequencies. The analytic continuation of Eq. (61) gives

$$\delta E_{\mathrm{kin}} = +2N_f \int_0^\infty \{\mathrm{Im}\sqrt{\Phi^2(\omega) - \tilde{\Sigma}^2_S(\omega)} + \mathrm{Re}\,\tilde{\Sigma}_N(\omega)\}\tanh\frac{\omega}{2T} d\omega. \tag{64}$$

The result of this calculation at finite λ is presented in Fig. 5. For comparison, we also present in this figure the BCS result for E_{kin} obtained with the same $\Delta(\omega=0)$ and a cutoff frequency $\omega_{\max} = 1$ eV (recall that the BCS result for

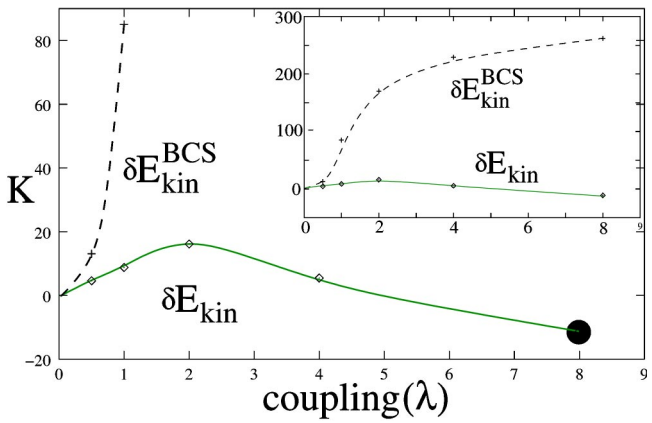

FIG. 5. Kinetic energy $\delta E_{\rm kin}$ compared to the BCS result $T=0$ for various couplings λ. The parameters are the same as in Fig. 4. The kinetic energy change is positive at low couplings, but negative at high coupling. This is in sharp contrast to the positive and quite large BCS kinetic energy. For the BCS result we used the exact $\Delta(\omega=0)$ and set the upper cutoff of frequency integration at $\omega_{\rm max}=1$ eV. The inset shows the kinetic energy at a larger scale. The dot at $\lambda=8$ indicates the value of the total condensation energy E_c which for this λ almost coincides with $\delta E_{\rm kin}$.

$E_{\rm kin}$ depends logarithmically on the upper cutoff of the frequency integration). At low couplings the kinetic energy is positive, as one naively expects. At larger λ, however, the kinetic energy passes through a maximum at $\lambda\sim 2$ and then becomes negative at large λ.

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 $E_{\rm kin}$, and the change in the self-energy due to the ''undressing'' of fermions that lowers $E_{\rm kin}$. At weak coupling, the particle-hole mixing obviously dominates. The sign change between small and large λ implies that at strong coupling the situation is reversed, and the lowering of $E_{\rm kin}$ via the change in the self-energy due to the ''undressing'' of fermions overcomes the effect of particle-hole mixing This behavior is very similar to that obtained by Norman *et al.*[5] As the first term in $E_{c,\rm el}$ is equal to $-\delta E_{\rm kin}/2$ [see Eqs. (36) and (61)], 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 5 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 2Δ. This *simultaneously* gives rise to two effects. First, the spin propagator develops the excitonic (resonance) peak at $\omega_{\rm res}<2\Delta$. 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 $\Delta+\omega_{\rm res}$ (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.

VII. 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 $\overline{\omega}^3/v_F^2$ and both depend only on the dimensionless coupling λ. 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 λ. We found that at large λ, 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 λ.[22] This behavior is very counter intuitive from a BCS perspective, where the condensation energy scales with Δ^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 nonconserving 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 Δ 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 $E_{\rm kin}$ overcomes the effect of particle-hole mixing which tends to increase $E_{\rm kin}$. This behavior has no analog for phonon superconductors. We argued that a negative $E_{\rm kin}$ is fully consistent with a positive $E_{c,{\rm el}}$, 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 lowering of the kinetic energy *or* the interplay between the lowering of $\delta\Omega_{\rm spin}$ and the increase of $E_{c,{\rm el}}$. 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 $N_f \sim 1$ st/eV as typical for near optimally doped cuprates, we obtained a small value for E_c of ~ 15 K at optimal doping (which in our model corresponds to $\lambda \sim 1.5-2$,[18] larger λ 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.[18] 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 $N_f \sim 1$ st/eV that we were using is fully consistent with $\bar{\omega} \sim 2.5-3\times 10^3$ K. Indeed, using Fermi surface averaged $v_F \sim 0.6$ meV (Ref. 22) we obtain $N_s = (8/3\pi^2)\bar{\omega}/v_F^2 \sim 0.15-0.19$ st/eV. Using then $N_f/N_s \sim 5.9$ obtained in the paper, we find $N_f \sim 1$ st/eV, i.e., precisely the same value as we used.

Our $E_c \sim 15$ K is in good agreement with experiment. Loram *et al.*[3] extracted $E_c \approx 0.12 k_B T_c \sim 10$ K 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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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:[9,15,25,26]

$$E - E_0 = -i \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} \int \frac{d^2k d\omega}{(2\pi)^3} G_{\omega_m}(k) \Sigma^*_{\omega_m}, \qquad \text{(A1)}$$

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 λ_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 $G^{-1}_{\omega_m}(k) = i(\omega_m + \Sigma^*_{\omega_m}) - \epsilon_k$. In the normal state, $\Sigma^*_{n,\omega_m} = \Sigma_{n,\omega_m}$, where Σ is a conventional self-energy, while in the superconducting state,

$$\Sigma^*_{s,\omega_m} = \Sigma_{s,\omega_m} + \frac{i\Phi^2_{\omega_m}}{\epsilon_k + i\tilde{\Sigma}_{s,\omega_m}}. \qquad \text{(A2)}$$

Equation (A1) is particularly suitable for the strong coupling computations in the normal state. Here we can use

$$\int \frac{d^2k}{4\pi^2} G_{\omega_m}(k) = -i\pi N_f \,\mathrm{sgn}\,\omega_m. \qquad \text{(A3)}$$

Substituting this result into Eq. (A1) we reduce $E - E_0$ to a single frequency integral. Using the $T = 0$ normal state result for the spin-fermion model $\Sigma_{n,\omega_m} = 2\lambda\omega_m/[1 + (1 + |\omega_m|/\omega_{\rm SF})^{1/2}]$, and introducing the sharp upper cutoff for the low-energy theory at $\omega_{\max} \sim E_F$, we obtain

$$E - E_0 = -N_f (\omega^3_{\max}\bar{\omega})^{1/2} \int_0^{2\lambda(\omega_{\max}/\bar{\omega})^{1/2}} \frac{dx}{(\sqrt{1+x^2}+1)^2}. \qquad \text{(A4)}$$

This expression is convenient for the analysis of the variation of the ground-state energy with λ.

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

$$E_c = -i \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} \int \frac{d^2k d\omega}{(2\pi)^3} [G_{s,\omega_m}(k)\Sigma^*_{s\omega_m} - G_{n,\omega_m}(k)\Sigma^*_{n\omega_m}]. \qquad \text{(A5)}$$

Using $G\Sigma^* = -i(1 - G_0^{-1}G)$, we can rewrite Eq. (A5) as

$$E_c = N_0 \int \frac{d\epsilon_k d\omega_m}{2\pi} \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} [G_{s,\omega_m}(k) - G_{n,\omega_m}(k)] \times (i\omega_m - \epsilon_k). \qquad \text{(A6)}$$

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

$$E_c = -N_f \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} \int_0^{\infty} d\omega_m \left(\sqrt{\tilde{\Sigma}_{s,\omega_m}^2 + \Phi_{\omega_m}^2} - \tilde{\Sigma}_{n,\omega_m} - \omega_m \frac{\tilde{\Sigma}_{s,\omega_m} - \sqrt{\tilde{\Sigma}_{s,\omega_m}^2 + \Phi_{\omega_m}^2}}{\sqrt{\tilde{\Sigma}_{s,\omega_m}^2 + \Phi_{\omega_m}^2}} \right). \quad \text{(A7)}$$

This looks very similar to the Wada result [Eq. (36)] but note the minus sign in front of the ω_m. This extra minus sign results in a negative total E_c for all couplings. The condensation energy, Eq. (A6), 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.

1. BCS limit

In the BCS limit, E_c reduces to

$$E_c = -N_f \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} \Delta_{\lambda_1}^2 \int_0^{\infty} \frac{d\omega_m}{\sqrt{\Delta_{\lambda_1}^2 + \omega_m^2}} \quad \text{(A8)}$$

where Δ is the gap value for the running coupling λ_1. Using the BCS relation between Δ and the coupling constant

$$1 = \lambda_1 N_f \int_0^{\infty} \frac{d\omega_m}{\sqrt{\Delta^2 + \omega_m^2}} \quad \text{(A9)}$$

one can rewrite (A8) as

$$E_c = -\int_0^{\lambda} \frac{d\lambda_1}{\lambda_1^2} \Delta_{\lambda_1}^2 . \quad \text{(A10)}$$

From (A9),

$$\Delta_{\lambda_1} = \Delta_{\lambda} e^{1/N_f \lambda - 1/N_f \lambda_1}. \quad \text{(A11)}$$

Integrating over λ_1 we obtain

$$E_c = -\frac{1}{2} N_f \Delta^2. \quad \text{(A12)}$$

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 $\delta E_{\rm kin}$ in the Luttinger-Ward formalism and found that in the BCS limit, the kinetic energy scales as $\Delta^2 \ln \omega_{\rm max}/\Delta$ [see Eq. (63)]. In the running coupling constant formalism, the kinetic energy difference $\delta \tilde{E}_{\rm kin}$ extracted from Eq. (A6) in the BCS limit reduces to

$$\delta \tilde{E}_{\rm kin}^{\rm BCS} = 2N_0 \int_0^{\lambda} \frac{d\lambda_1}{\lambda_1} \int_0^{\infty} \frac{\Delta_{\lambda_1}^2 d\omega_m}{\omega_m + \sqrt{\Delta_{\lambda_1}^2 + \omega_m^2}}. \quad \text{(A13)}$$

Using Eq. (A9) and performing the computations with the logarithmic accuracy we find $\delta \tilde{E}_{\rm kin}^{\rm BCS} = N_0 \Delta^2/2$, i.e., contrary to Eq. (63) the newly defined kinetic energy does not depend logarithmically on the upper limit of frequency integration. Similarly, $\delta \tilde{E}_{\rm pot}^{\rm BCS} = -N_0 \Delta^2$ such that the sum of the two yields the correct total condensation energy, Eq. (A12). This once again demonstrates that only total E_c is a physically meaningful quantity.

2. $\lambda = 1$

We numerically computed E_c for $\lambda = 1$ by calculating the integrand of Eq. (A7) for $\lambda_1 = 0$, 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 $E_c = -15.8$ K compared to the -11.5 K calculated via the Eliashberg approach. This agreement is quite reasonable as our implementation of the running coupling constant formalism was highly approximate: it used only three numerically calculated values of the integrand, fitting the rest with a phenomenological function. For a more accurate estimate, the integrand must be calculated at many more values of the running coupling constant. This is, however, extremely computationally intensive, as at each value of the running coupling constant the self-energies, pairing vertex, etc., must be numerically calculated over their whole frequency range. The running coupling constant formalism is therefore very difficult to implement accurately for a nontrivial self-energy or pairing vertex.

APPENDIX B: ULTRAVIOLET CONVERGENCE OF THE CONDENSATION ENERGY

In this appendix, we explore the consequences of assuming infinite energy bands in calculations of the condensation energy. Although in reality, energy bands are of finite extent, for theoretical purposes, one often extends the integration of both energy and frequency to infinity. In this case the order of the integrations, i.e., energy versus frequency matters and it is this issue that we examine here. Specifically we will show that the integration order depends upon whether the ultraviolet convergence of the integral arises from an effective energy or frequency ''cutoff.''

1. BCS limit

We begin with the calculation of the condensation energy in the BCS limit. The integral for the condensation energy in BCS theory with *infinite bandwidths* is formally ultraviolet divergent as Δ does not vanish at large momentum and frequency [see Eq. (B3) below]. The ordering of the integration is thus highly relevant, and the correct way is to perform the frequency integration first as the ultraviolet divergence is artificial, caused by the infinite limits of the momentum integral. We will show explicitly that if the momentum integral is restricted to a finite bandwidth, the order of the integration does not matter, and one obtains the correct result $E_c = -N_f \Delta^2/2$ integrating in either order and then setting the fermionic bandwidth to infinity at the end of the calculations.

In the BCS theory, the pairing problem may be described by an effective quadratic Hamiltonian

$$H=H_0+\sum_{k,\alpha}\epsilon_k a^\dagger_{k,\alpha}a_{k,\alpha}+\frac{\Delta}{2}g_{\alpha,\beta}(a^\dagger_{k,\alpha}a^\dagger_{-k,\beta}+a_{k,\beta}a_{-k,\alpha}), \tag{B1}$$

where $g_{\alpha\beta}$ is the antisymmetric matrix.[25] The condensation energy can then be straightforwardly obtained by simply averaging both the normal and anomalous terms in Eq. (B1). Expressing the average products of the pairs of operators in terms of frequency integrals of normal and anomalous Green's functions, linearizing the fermionic dispersion, and taking care to avoid double counting of the anomalous term, we obtain at $T=0$

$$E_c=-\frac{N_f\Delta^2}{2}I, \tag{B2}$$

where

$$I=\int\frac{d\epsilon d\omega}{\pi}\frac{\omega^2-\epsilon^2}{(\epsilon^2+\omega^2)(\epsilon^2+\omega^2+\Delta^2)}. \tag{B3}$$

We see that a naive integration treating both ω_m and ϵ in Eq. (B3) 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.

Indeed, integrating first over ω_m in infinite limits, and then integrating over ϵ_k we obtain

$$I=2\int_0^\infty\left(\sqrt{x^2+1}-2x+\frac{x^2}{\sqrt{x^2+1}}\right)dx, \tag{B4}$$

where $x=\epsilon_k/\Delta$. One can easily make sure that the integral converges at large x. Performing elementary integration, we easily obtain $I=1$. On the other hand, integrating first over ϵ_k in infinite limits, and then integrating over ω we obtain

$$I=-\int_0^\infty dx\left(\frac{1+2x^2}{\sqrt{x^2+1}}-2x\right), \tag{B5}$$

where now $x=\omega/\Delta$. The integral again converges at the upper limit, and performing the integration we obtain $I=-1$, i.e., the result opposite to Eq. (B4).

As we argued above, the correct way to proceed in the BCS limit is to perform the integration over ω 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, extends only up to $\Lambda\sim W$ where W is the fermionic bandwidth. Integrating first over ω_m in infinite limits, and then integrating over $|\epsilon_k|<\Lambda$ we obtain Eq. (B4) with the upper limit Λ/Δ. As the integrand in Eq. (B4) is convergent, $I=1$ up to corrections which vanish as $\Lambda\to\infty$. This yields $E_c=-N_f\Delta^2/2$ as it indeed should be.

It is instructive to show that once the integral over ϵ_k is restricted to a finite range, one also obtains the correct E_c by performing the ϵ integration first. Indeed, integrating in Eq. (B3) first over ϵ_k between $-\Lambda$ and Λ, and then over ω, we obtain

$$I=-\frac{2}{\pi}\int_0^\infty dx\left(\frac{1+2x^2}{\sqrt{x^2+1}}\tan^{-1}\frac{\Lambda^*}{\sqrt{x^2+1}}-2x\tan^{-1}\frac{\Lambda^*}{x}\right), \tag{B6}$$

where $\Lambda^*=\Lambda/\Delta$ and $x=\omega/\Delta$. If we formally set $\Lambda^*=\infty$ at this stage, we obtain a convergent integral over x which yields $I=-1$ which, we know, is incorrect. Keeping Λ^* large but finite we find that there is an extra contribution to the integral from large $x\sim\Lambda^*$. This extra contribution overshadows the contribution from $x=O(1)$ and changes the sign of I To see this, we change variables to $y=x/\Lambda^*$ and rewrite Eq. (B5) as

$$I=-1+\frac{8}{\pi}(\Lambda^*)^2\int_0^\infty dyy\left(\tan^{-1}\frac{1}{y}-\tan^{-1}\frac{1-[2y^2(\Lambda^*)^2]^{-1}}{y}\right). \tag{B7}$$

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

$$I=-1+\frac{4}{\pi}\int_0^\infty\frac{dy}{y^2+1}=-1+2=1 \tag{B8}$$

as it indeed should be. Note that the integral in Eq. (B8) is confined to $y=O(1)$, i.e., to $\omega\sim\Lambda$.

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. (B4) 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 implied in Eq. (B7). This peculiarity, however, is only present in the BCS limit, where the gap remains finite even at the largest frequencies. Away from the BCS limit, 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.

By considering the BCS limit we have learned the following important lesson. If the ultraviolet convergence is due to a finite bandwidth (or to a vanishing of the pairing gap at large momenta due to self-energy corrections which depend on ϵ_k), the correct way to proceed is to perform the frequency integration first. In this situation, one readily reproduces the BCS condensation energy by keeping the bandwidth finite and setting it to infinity at the very end of calculations. In Eliashberg-type theories however, one approaches the BCS limit *assuming* that even for very small couplings the convergence of the integral for E_c is imposed by the frequency dependence of the pairing gap (i.e., the typical frequency beyond which E_c converges is smaller than W). In this situation, the momentum integration must be performed first. The fact that the results for E_c in the BCS limit differ by a factor of (-1) depending on whether the

frequency or momentum integration is performed first implies that in Eliashberg theory the integrand for the condensation energy at vanishing coupling should have the opposite sign compared to the first case. Alternatively speaking, the BCS limit of the integrands of E_c in Eliashberg-type theories and theories where ϵ_k integration is bound should have opposite signs.

2. A relation between E_c in Refs. 5 and 14

The above reasoning explains the apparent sign difference between the expressions for the condensation energy in Refs. 5 and 14. In Ref. 14, Scalapino derived the condensation energy for phonon superconductors by averaging the electron-phonon Hamiltonian

$$\langle H\rangle = -i\int \frac{d^d k d\omega}{(2\pi)^{d+1}}(\omega+\epsilon_k)G(k,\omega) - \left\langle \sum_\nu \frac{P_\nu^2}{M}\right\rangle, \tag{B9}$$

where the last term is twice the expectation value of the ion kinetic energy. He then used Chester's result[27] 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 (B9) in a superconductor and the normal state:[28]

$$E_c = \langle H_{sc}\rangle - \langle H_n\rangle = -i\int \frac{d^d k d\omega}{(2\pi)^{d+1}}(\omega+\epsilon_k)[G_n(k,\omega)-G_s(k,\omega)]. \tag{B10}$$

He further assumed that $\Sigma=\Sigma(\omega)$, performed the integration over momentum first (with infinite limits), and reproduced Wada's formula, Eq. (17). In the BCS limit of vanishing $\Sigma(\omega)$ and a constant Δ, 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 α is nearly zero. They argued that in this situation, the condensation energy should be given solely by the first term in (B9), i.e.,

$$E_c = -i\int \frac{d^d k d\omega}{(2\pi)^{d+1}}(\omega+\epsilon_k)[G_s(k,\omega)-G_n(k,\omega)]. \tag{B11}$$

This expression has opposite sign compared to Eq. (B10). Still, the authors of Ref. 5 argued that their expression also reproduces the BCS result $E_c=-N_0\Delta^2/2$.

The analysis of the BCS limit shows that both authors are indeed right. Indeed, the Wada expression for the condensation energy implies that $\Delta(\omega)$ decreases above $\omega_{\max}\ll\Lambda$, i.e., the momentum integral comes first, and the frequency integration comes second. The frequency dependence of the pairing gap comes 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, even in the BCS limit.

Reference 5 on the other hand, implies that the frequency dependence imposed by the kinetic energy of ions is irrelevant, and ultraviolet convergence is imposed by the fact that the momentum integration has to be performed over a finite range. As we said, in this situation one has to integrate first over frequency and then over momentum. 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 opposite results for E_c actually yield the same BCS condensation energy.

Which expression is correct away from the BCS limit? This obviously depends on whether the ultraviolet convergence is imposed by either momentum or frequency. At the risk of belaboring the point we note here that the correct way to proceed in a general case when the self-energy depends on both the momentum and frequency 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. The only approximation in the Eliashberg formula is the neglect of vertex corrections [which account for higher-order terms labeled by dots in Eq. (3)].

Suppose now that for one reason or another, vertex corrections can be neglected. For the case when $\Sigma(k,\omega)\approx\Sigma(\omega)$, and $\Delta=\Delta(\omega)$ decreases above $\omega_{\max}\ll\Lambda$, the physically motivated ordering of the integrations should be integration over ϵ_k first (in infinite limits), and the integration over frequency afterward. Imposing this ordering on the Eliashberg Free energy yields the Wada formula which also follows from Eq. (B10). If instead we had incorrectly used Eq. (B11) [with $\Sigma\approx\Sigma(\omega)$], we would have obtained a rapid variation of E_c once $\omega_{\max}$ becomes smaller than Λ, and eventually Eq. (B11) would have yielded the result opposite in sign to Eq. (52).

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, Eq. (B11) should be used. This can be explicitly verified by comparing the Luttinger-Ward-Eliashberg formula with the bosonic term dropped, Eq. (16), with Eq. (B11). Setting $\Sigma(k,\omega)=\Sigma(\epsilon_k)$ and $\Phi(k,\omega)=\Phi(\epsilon_k)$ in Eq. (16) and integrating over frequency we obtain from Eq. (16)

$$E_c = -N_f\int_0^\infty d\epsilon\left(\sqrt{\tilde{\Sigma}_{S,\epsilon}^2+\Phi_\epsilon^2} - |\tilde{\Sigma}_{N,\epsilon}| + \epsilon\frac{|\tilde{\Sigma}_{S,\epsilon}|-\sqrt{\tilde{\Sigma}_{S,\epsilon}^2+\Phi_\epsilon^2}}{\sqrt{\tilde{\Sigma}_{S,\epsilon}^2+\Phi_\epsilon^2}}\right), \tag{B12}$$

where $\tilde{\Sigma}_\epsilon=\epsilon-\Sigma(\epsilon)$. This expression is the analog of the

Wada formula for $\Sigma=\Sigma(k)$. If one does the same with Eq. (B11), the frequency integration is straightforward and by proper evaluation of the arguments of the logarithms we obtain *exactly the same expression as* Eq. (B12). 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. (B10) or (B11) are valid when $\Sigma(k,\omega)\approx\Sigma(\omega)$ and $\Sigma(k,\omega)\approx\Sigma(k)$, respectively.

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