Pair-breaking effects in the Pseudogap Regime: Application to High Temperature Superconductors

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Abrikosov-Gor’kov (AG) theory, the foundation for understanding pair-breaking effects in conventional superconductors, is inadequate when there is an excitation gap (pseudogap) present at the onset of superconductivity. In this paper we present an extension of AG theory within two important, and diametrically opposite approaches to the cuprate pseudogap. The effects of impurities on the pseudogap onset temperature $T^*$ and on $T_c$, along with comparisons to experiment are addressed.

Impurity effects in the high temperature superconductors have been the subject of a large body of experimental and theoretical literature concentrating on pair-breaking effects on $\Delta_{pg}$ d-wave density of states effects near $T_c \approx 65 K$, local suppressions of the order parameter $\Delta_{sc}$ transport effects, and aspects of the superconductor-insulator transition. Although there are works on the effects of a single impurity in the pseudogap models, with very few exceptions little theoretical attention has been paid to the interplay between the widely observed cuprate pseudogap and the effects of disorder on pair-breaking. This is a particularly striking omission, given that a major fraction of the superconducting phase diagram is associated with a pseudogap. The goal of the present paper is to establish a formal mean-field structure (analogous to Abrikosov-Gor’kov (AG) theory) that incorporates this pseudogap in computing both $T_c$ and gap onset temperature, $T^*$, along with other derived properties. Here we address two mean-field approaches (orthogonal in their physics, but similar in their formalism), to the incorporation of the pseudogap: one in which the pseudogap derives from superconductivity itself (“intrinsic”) and one in which it is “extrinsic”, either associated with a hidden order parameter, or with band-structure effects. This intrinsic pseudogap arises from a stronger than BCS attractive interaction which leads to finite momentum pair excitations of the normal state and condensate.

In contrast to BCS theory, in the pseudogap phase there is an excitation gap present at $T_c$, which, at low doping $x$, remains relatively $T$-independent for all $T \le T_c$. This necessarily will affect (i) fundamental characteristics of the superconducting phase as well as (ii) the nature of impurity pair-breaking. Indeed, to support (i), there are strong indications from thermodynamics and tunneling experiments that the effects of the normal state pseudogap persist below $T_c$. Evidence in support of (ii) comes from the fact that pseudogap effects appear to correlate with the degree of the $T_c$ suppression in the presence of Zn impurities. This suppression becomes progressively more rapid as the size of the pseudogap grows.

Both intrinsic and extrinsic models for the pseudogap are associated with a generic set of mean-field equations. It is reasonable to stop at a mean-field level because these materials (in some, but not all respects) do not appear to be strikingly different from BCS superconductors, and because the true critical regime appears to be rather narrow. Moreover, we believe fluctuation effects around strict BCS theory such as the phase fluctuation model of Emery and co-worker are unlikely to explain the often very large separation observed between the gap onset temperature $T^*$ and $T_c$. It seems more appropriate, thus to search for an improved mean field theory. Then additional fluctuation effects can be appended as needed.

In this generalized mean field approach, in the clean limit and for $T \le T_c$, the gap and number equations are given by

$$1 + g_{sc} T \sum_{n,k,\alpha} \frac{\varphi_{k}^2}{\omega_n^2 + E_k^2} = 0,$$  

$$n = \frac{1}{2} - T \sum_{n,k,\alpha} \frac{i \omega_n + \epsilon_k^0 - \mu}{\omega_n^2 + E_k^2},$$

where $g_{sc}$ is the coupling constant for the superconducting order parameter, $\varphi_{k} = (\cos k_x - \cos k_y)$ is the d-wave symmetry factor, $\Delta_{sc}$ represents the superconducting order parameter, and $\Delta_{pg}$ the pseudogap which persists in the $T \le T_c$ phase. Finally, $\alpha$ is a band index, which appears in some microscopic approaches to the extrinsic case. The momentum summation in the extrinsic case is over the reduced Brillouin zone. These equations depend in an important way on the electronic dispersion which differs in the two schemes. In the intrinsic school the fermionic dispersion is characterized by

$$E_k^2 = (\epsilon_k - \mu)^2 + \Delta^2(T),$$  

$$\Delta^2(T) = \Delta_{pg}^2(T) + \Delta_{sc}^2(T),$$  

$$\epsilon_k = \xi_k.$$

Here $\xi_k$ is the “bare” band structure, taken to correspond to a nearest neighbor tight-binding model. This should
be contrasted with that in the extrinsic school, 
\[
E_k^\pm = (\epsilon_k^+ - \mu)^2 + \Delta_{sc}^2(T), \quad (3a)
\]
\[
\epsilon_k^+ = \pm \sqrt{\xi_k^2 + \Delta_{pg}^2(T)}. \quad (3b)
\]

The fermionic dispersions of the two schools differ as a direct consequence of the mechanisms that generate the respective pseudogaps. At the mean field level, a pseudogap due to pairing correlations forms as particles and holes mix to form the fermionic quasiparticles. Those of a spin- or charge-ordered state, though, are particle-hole mix to form the fermionic quasiparticles. Those gap due to pairing correlations forms as particles and respective pseudogaps. At the mean field level, a pseudogap or-der and the momentum summation is over half of the Brillouin zone. Here we consider the pseudogap with the counterpart equation is

\[
\chi^{pp}(q, i\omega_n) = T \sum_{k,m} \frac{\nu_m + \epsilon_k}{\nu_m^2 + E_k^2} \frac{\varphi_{k-q/2}^2}{i(\nu_n - \omega_n + \epsilon_{k-q})}.
\]
\[
\Delta_{pg}^2 = -T \sum_n \sum_{q\neq 0} g_{sc} \chi^{pp}(q, i\omega_n, \Delta). \quad (4)
\]

Note that \(\chi^{pp}\) depends on the full excitation gap \(\Delta\). Here \(\Delta_{pg}(T)\) is associated with the number of finite momentum pair excitations of the condensate. These occur when the strength of the attractive interaction \(g_{sc}\) is progressively increased, so that it is larger than that associated with the BCS regime. For the intrinsic school, the counterpart equation is

\[
\chi^{ph}(0, 0, \Delta_{sc}, \Delta_{pg}) = T \sum_{n,k,\alpha} \frac{\varphi_k^2 (\epsilon_k^\alpha - \mu)}{(\omega_n + E_k^2)^2} \xi_k^2
\]
\[
= -g_{pp}^{-1}, \quad (5)
\]

where \(g_{pp}\) is the coupling constant for the pseudogap order and the momentum summation is over half of the Brillouin zone. Here we consider the pseudogap with the same \(d\)-wave structure as the superconducting order.

Figure 1 shows the temperature dependencies of the different energy gaps obtained by solving the complete set of equations in the two pseudogap schools within the underdoped regime. In the intrinsic case \(T^*\) marks the gradual onset of the pseudogap, which is associated with bosonic or pair excitations formed in the presence of a stronger-than-BCS attractive interaction. Only at and below \(T_c\) does the identification of \(\Delta\) become precise, so that for this (intrinsic) case we plot an extrapolation of Eqs. 1a, 1b, and 4 to \(T \geq T_c\). Figure 1a shows that below \(T_c\) the fraction of the bosonic population joining the condensate of zero-momentum pairs (\(\Delta_{pg}^2\)) increases at the expense of the finite-momentum bosonic fraction (\(\Delta_{sc}^2\)) until the fully condensed ground state is reached. By contrast, for the extrinsic case (Fig. 1b) superconductivity forms on top of a pre-existing excitation gap in the effective band structure which first appears at \(T^*\), the phase transition temperature marking the onset of the extrinsic order.

One can capture the key physics of these two schemes in a reasonably accurate phenomenological approach. The bosonic excitations associated with the mean-field theory Eqs. 1a, 1b and 4 lead to the temperature dependence of the pseudogap below the clean limit critical temperature \(T_{c0}\)

\[
\Delta_{pg}^2(T) \approx \Delta_{c0}^2 \left( \frac{T}{T_{c0}} \right)^{3/2}, \quad T \leq T_{c0}. \quad (6)
\]

These bosons are, thus, associated with a quasi-ideal Bose gas. By contrast for the extrinsic case, in the well-established pseudogap regime, below \(T_{c0}\), the pseudogap
appear around the Fermi energy. Van Hove singularities centered around the Fermi energy. Van Hove singularities are also apparent here as relatively sharp structures. In contrast, there exist two distinct features for the extrinsic model. Here we define $\Delta(T = 0) = \Delta_{pg}(T = 0)$. In both Eqs. (6) and (7) above, we may view $\Delta(T = 0)$ as a phenomenological parameter taken from experiment. We will adopt this approach here in large part because it provides a more readily accessible theoretical framework for the community, and because it connects more directly with experiment.

The pronounced differences between the fermionic dispersion in these two theoretical schools can be seen from the associated densities of states (DOS) plotted in Fig. 3, which compares the intrinsic and extrinsic models at $T = 0$. In the intrinsic model one sees only one excitation gap feature $\Delta = \sqrt{\Delta_{sc}^2 + \Delta_{pg}^2}$ in Fig. 2 centered around the Fermi energy. Van Hove singularities are also apparent here as relatively sharp structures. In contrast, there exist two distinct features for the extrinsic theory. The more prominent pseudogap peaks is centered around $-\mu$, while the superconducting peaks appear around the Fermi energy. Indeed, for this extrinsic case, only in the limit $\mu = 0$ can one readily define an excitation gap $\Delta$ as in a conventional superconducting phase, satisfying Eq. (7). That the superconducting order parameter and pseudogap contribute to separate features in the density of states represents a rather clear signature of this extrinsic pseudogap school. To date, the bulk of experimental tunneling data supports a picture in which there is a single excitation gap feature $\Delta$ although there are some reports of multiple gap structures in c-axis intrinsic tunneling spectroscopy. At $T = T_c$, the extrinsic superconducting gap closes and the densities of states for the two schools become quite similar, save for the pinning of the gap minimum to the Fermi surface in the intrinsic case.

We turn now to impurity effects which, just as in the BCS case, are not expected to change the formal structure of our mean field theory. The greatest complication is associated with the impurity-renormalized $\Delta_{pg}$, calculated from all possible diagrammatic insertions of the impurity vertex into the particle-hole and particle-particle susceptibilities [see Eqs. (5) and (6)]. A detailed study of these effects in the intrinsic case appears in Ref. [15], although here we will proceed more phenomenologically within both schools. We base the present treatment on analogs of the clean limit mean field gap equations Eqs. (11) and (12) with substitutions $\Delta_{sc} \rightarrow \Delta_{pg}$, $\Delta_{pg} \rightarrow \Delta_{pg}$, $\omega_n \rightarrow \omega_n$, and $\mu \rightarrow \mu$. At the phenomenological level the $T$-dependence of the intrinsic pseudogap is given by

$$\tilde{\Delta}_{pg}(T) = \tilde{\Delta}(T_c) \left( \frac{T}{T_c} \right)^{3/2}, \quad T \leq T_c,$$

and for the extrinsic case,

$$\tilde{\Delta}_{pg}(T) = \tilde{\Delta}(T_c), \quad T \leq T_c,$$

where, in both schools, the excitation gap $\tilde{\Delta}(T_c)$, is presumed to be determined from experiment.

To compute the renormalized frequency $i\tilde{\omega}(i\omega_n)$ and chemical potential $\tilde{\mu}(i\omega_n)$, we follow the usual impurity $T$-matrix approach. We assume an s-wave short-range impurity potential $V(r) = u\delta(r - r_0)$. The impurity scattering matrix $\hat{T}(\omega_n)$ in Nambu space satisfies the Lippman-Schwinger equation: $\hat{T}(\omega_n) = u\delta(\omega - \omega_n)$, where $\hat{g}$ is the impurity-dressed Green’s function.

$$\hat{g}(k, i\omega_n) = \frac{i\tilde{\omega}_n \sigma_0 + \tilde{\Delta}(k) \sigma_1 + (\epsilon_k - \tilde{\mu}) \sigma_3}{(i\tilde{\omega}_n)^2 - E_k^2},$$

Here $\tilde{\Delta}$ is either the full gap or superconducting order parameter in the intrinsic and extrinsic cases, respectively, and $\sigma_i$ are Pauli matrices. Here we suppress the band index in the extrinsic case. Labeling components as $\hat{g} = \sum_i g_i \sigma_i$, the regular and anomalous Green’s functions are $\tilde{G} = g_0 + g_3$, $\tilde{F} = -g_1$. The frequency and chemical potential are renormalized through impurity self-energy $\tilde{\Sigma} = n_i \tilde{g}$, and $i\tilde{\omega}_n = i\omega_n - \Sigma_0$, $\tilde{\mu} = \mu - \Sigma_3$, where $n_i$ is the number of impurities per unit cell. We note that the $T$-matrix for the extrinsic school depends only on the band structure and is independent of the specific type of extrinsic order.

The components of the self-energy are given by

$$\Sigma_0 = \frac{n_i g_0}{(1/u - g_3)^2 - g_0}, \quad \Sigma_3 = \frac{n_i (1/u - g_3)}{(1/u - g_3)^2 - g_0},$$

and

$$g_0 = \sum_i \frac{i\tilde{\omega}_n}{(i\tilde{\omega}_n)^2 - E_k^2}, \quad g_3 = \sum_i \frac{\epsilon_k - \tilde{\mu}}{(i\tilde{\omega}_n)^2 - E_k^2}.$$

There is no frequency-dependent self-energy associated with gap renormalization due to d-wave symmetry. Finally, the magnitudes of $\tilde{\Delta}$, $\Delta_{sc}$, and $\Delta_{pg}$ can be obtained.
using Eqs. (1),(2) and (6), presuming that the excitation gap \( \xi \) is taken from experiment. Here we take the bare lattice dispersion \( \epsilon_0 = -2t_\parallel (\cos k_x + \cos k_y) - 2t_\perp \cos k_z \) so that the dimensionless coupling constant is given by \( g/4t_\parallel \).

The DOS is centered around the Fermi energy.

![FIG. 3: Intrinsic DOS for the clean and dirty cases at \( T = 0 \). The DOS is centered around the Fermi energy.](image1)

![FIG. 4: Extrinsic DOS for the clean and dirty cases at \( T = 0 \). The DOS is centered around \(-\mu\).](image2)

In the remainder of this paper we focus on the behavior of \( T_c \) (and \( T^* \)) and the appropriate generalization of AG theory in the presence of a pseudogap. For definiteness, we consider Zn doping experiments where we exploit the experimental observation that the excitation gap \( \Delta \) at \( T_c \) is relatively unaffected by Zn impurities. We focus here on the unitary limit \((1/u = 0)\), which is regarded as relevant to Zn doping in the cuprates.

We begin with the intrinsic school, where the sensitivity of \( T_c \) and \( T^* \) to the impurity concentration \( n_i \) can be studied as a function of a single coupling constant \( g = g_{sc} \), which we presume to be unaffected by the addition of impurities. Figure 3 shows the behavior of the excitation gap \( \Delta(T) \) vs temperature normalized to its clean limit value, obtained using the impurity-generalized form of Eqs. (1a) and (1b). The figure should be viewed as extending above \( T_c \) only in the sense that it provides a reasonable extrapolation to both the impurity concentration and gaps are normalized to the zero-temperature values in the clean limit \( \Delta_0 \).

![FIG. 5: Temperature dependencies of the full excitation gaps for the intrinsic case at strong \((g/4t_\parallel = -1.2)\) and weak coupling \((g/4t_\parallel = -0.15, \text{inset})\), in the unitary limit at different impurity densities. Temperatures are normalized to the clean limit \( T_0 \) and gaps are normalized to the zero-temperature values in the clean limit \( \Delta_0 \).](image3)

![FIG. 5: Temperature dependencies of the full excitation gaps for the intrinsic case at strong \((g/4t_\parallel = -1.2)\) and weak coupling \((g/4t_\parallel = -0.15, \text{inset})\), in the unitary limit at different impurity densities. Temperatures are normalized to the clean limit \( T_0 \) and gaps are normalized to the zero-temperature values in the clean limit \( \Delta_0 \).](image4)

physically affected by pair-breaking, while the pseudogap peaks remain relatively robust. It can be inferred from these figures that with increasing disorder the differences in the two schools diminish, from the perspective of the density of states, except that the position of the minimum in the extrinsic case is not tied to the Fermi energy. Physical differences, however, remain profound, particu-
at the appropriate $T_c$ is relatively independent of impurity concentration. It can be seen that the suppression rate increases as the coupling becomes stronger, or effectively as $\Delta(T_c)$ increases. Similar results for the extrinsic case were obtained in Ref. 4. This faster $T_c$ suppression in the strong coupling regime can be understood through a simple physical picture. Impurity scattering will produce states which fill in the gap and eventually destroy superconducting coherence. In the strong coupling (pseudogap) regime, where the normal state already has a gap, fewer impurities are required to restore the system to the “normal” state.

We turn now to calculations which can be directly compared with experiment and plot the normalized slopes of $T^*$ and $T_c$, with respect to increasing Zn concentration, for varying hole concentration $x$, first for the intrinsic case. To convert from the coupling constant parameter $g$ to $x$ we take as input the experimentally measured values of $p_g(x,0)$ and the measured excitation gap at $T_c$. Here it is adequate to choose these values corresponding to the pristine case, and presume that Zn doping does not affect the excitation gap at $T_c$. Figure 6 indicates the initial slope ($1/T_0 dT/dn_i$, where $T_0$ is the appropriate clean limit temperature) for $T^*$ (dashed line) or $T_c$ (solid line). In the overdoped limit, the theory is asymptotically equivalent to standard AG theory, in which also $T^* = T_c$. For smaller values of $x$ the slope decreases so that $T^*$ is only weakly dependent on impurity concentration. By contrast, the initial $T_c$ slope (solid line) shows a very different hole concentration dependence. As the hole concentration decreases, the slope decreases. However, in the very underdoped regime, where the pseudogap is well established, the curve turns around and rapidly increases. The inset presents a comparison of theory and experiment of $\eta = (dT_c/dn_i)/(dT_c/dn_i, x = 0.20)$ vs $z = \Delta_{pg}(T_c)/(\Delta_{pg}(T_c), x = 0.05)$, where the agreement appears to be reasonable. There are fewer systematic studies of impurity-induced changes in $T^*$; however, the small effect found here at low $x$ appears to be compatible with the data.

Finally in Fig. 8 we present the counterpart plots of the initial slopes for $T_c$ and $T^*$ in the extrinsic case. $T_c$ is computed as in the intrinsic case by assuming $\Delta_{pg}(T_c)$ is relatively insensitive to impurities. Impurity renormalizations are determined through Eqs. (11) and (12) while the suppression of $T^*$ is calculated via Eqs. (1b) and (16), extended to include appropriate impurity renormalizations. The inset shows the clean phase diagram which forms the basis for these calculations. Our fit to the published form $\Delta/T_0$ of this phase diagram provided values for the coupling constants $g\Delta_{pg}/4t = -0.4$ and $g\Delta_{pg}/4t = -0.375$. To make contact with experiment we chose a parameter set in which $T_c/T^*$ and $n_x/\Delta(0)$ were reasonably well fit to experiment in the underdoped regime. As is similar to the intrinsic case, there is a dramatic increase in the slope of $T_c$ as the insulator is
approached. This increase is associated with the onset of the pseudogap which occurs for $x \lesssim 0.15$. Above this critical concentration $T^*$ is zero, and the system becomes a conventional dirty BCS superconductor. In this way, the intrinsic and extrinsic schools differ, since for the former at large $x$, $T^* \rightarrow T_c$.

The theoretical machinery that we have set up has strong similarities to an approach taken by Loram and collaborators, extended further to the disordered case. It should be stressed, though, that their approach is a hybrid of extrinsic and intrinsic pseudogap theories, where the temperature dependence of the various gap parameters corresponds to the extrinsic case (shown in Fig. 1b), whereas the dispersion and superfluid density corresponds to an intrinsic pseudogap. As shown in this paper, pair-breaking effects on $T_c$ can be successfully addressed at a semi-quantitative level both in intrinsic and extrinsic models. It should be noted that the rather strikingly different sensitivities of $T^*$ and $T_c$ to impurity concentration which are found experimentally, are often taken as an indication that the cuprate pseudogap cannot be intrinsic, i.e., related to the superconductivity, itself. Indeed similar results are found in the presence of magnetic field pair-breaking and it should be viewed as one of the fundamental results of this paper that this inference is incorrect. The differences lie in the fact that an excitation gap is present when $T_c$ is established, but not at $T^*$, and it is this gap in the density of states that contributes to the stronger pair-breaking effects on $T_c$. Indeed, it is precisely this excitation gap which invalidates the results of conventional AG theory. It may be necessary eventually to incorporate an even more local treatment of pair-breaking than that discussed here, but such a Bogoliubov-de Gennes generalization must include pseudogap effects. Indeed, the very basis for a more local treatment of impurities is the observed small coherence lengths, which are the heart of the present “intrinsic” pseudogap theory.

In summary, in this paper we find within two diametrically opposed pseudogap schools, that pseudogap effects at and below $T_c$ must play an essential role in pair-breaking. While there is no definitive experiment to distinguish between these two schools, we have argued elsewhere that the intrinsic dispersion leads to smaller and more benign modifications of BCS theory. In both theoretical approaches, the rather robust behavior for $T^*$ and the associated excitation gap in the underdoped regime, found in the presence of impurities may be associated with the widely observed superconductor-insulator transition. Superconducting coherence is more readily destroyed than is the excitation gap (and $T^*$), thereby leading to an insulating state when $T_c$ is suppressed to zero, in much the same way as in the presence of applied magnetic field. While there are clear differences, seen particularly in electrodynamical calculations (as well as density of states effects) between the intrinsic and extrinsic pseudogap schools, the impurity sensitivities of $T_c$ within these two different approaches are quite similar, and reasonably consistent with experiment. This similarity derives from the fact that both mean field theoretic calculations of $T_c$ have a general BCS-like character, except for the presence of a (pseudo) gap at the onset of superconductivity. For $T^*$ the differences are more apparent in the overdoped regime and this, in turn, reflects the fact that $T^* \rightarrow 0$ in one case (extrinsic), whereas $T^* \rightarrow T_c$ in another (intrinsc). In this paper we have set the stage for a computation of transport properties which require as an essential input, an understanding of impurity effects. The generalization of AG theory presented here should help to clarify the important role played by pseudogap effects, at $T_c$ and their relation to impurity-induced pair-breaking.

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In the intrinsic model, the distinction between the superconducting order parameter and the pseudogap below $T_c$ can only be observed through the different lifetime of the condensate and the finite-momentum excitations. See Ref. 27.

31. W. Kim, J.-X. Zhu, J. P. Carbotte, and C. S. Ting, Phys. Rev. B 65, 064502 (2002).
32. C. Renner, B. Revaz, K. Kadowaki, I. Maggio-Aprile, and O. Fischer, Phys. Rev. Lett. 80, 3606 (1998).
33. N. Miyakawa, J. Zasadzinski, L. Ozyuzer, P. Guptasarma, D. G. Hinks, C. Kendziora, and K. E. Gray, Phys. Rev. Lett. 83, 1018 (1999).
34. V. M. Krasnov et al., Phys. Rev. Lett. 84, 5860 (2000).
35. J. Stajic, A. Iyengar, K. Levin, B. R. Boyce, and T. Lemberger, cond-mat/0205497.
36. A. P. Iyengar, J. Stajic, Y.-J. Kao, and K. Levin, cond-mat/0208203.
37. J. Maly, B. Janko, and K. Levin, Phys. Rev. B 59, 1354 (1999).
38. Y.-J. Kao, A. P. Iyengar, Q. J. Chen, and K. Levin, Phys. Rev. B 64, 140505 (2001).