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Enhancement of superconductivity by local inhomogeneities

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We study the effect of inhomogeneity of the pairing interaction or the background potential on the superconducting transition temperature, T_c. In the weak coupling BCS regime, we find that inhomogeneity, which is incommensurate with the Fermi surface nesting vectors, *enhances* T_c relative to its value for the uniform system. For a fixed modulation strength we find that the highest T_c is reached when the characteristic modulation length scale is of the order of the superconducting coherence length.

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Many strongly correlated superconductors, and in particular high-temperature superconducting (HTSC) cuprates, exhibit inhomogeneous electronic and/or structural phases at the nanoscale.[1–3] The coexistence of HTSC and inhomogeneity suggests that the underlying inhomogeneities could be at least partially responsible for the high value of the superconducting transition temperature. Emery and Kivelson proposed that HTSC is related to frustrated electronic phase separation, commonly expected in strongly correlated systems.[4] These ideas for inhomogeneous superconductivity have been further developed in the context of stripes.[5,6] It is important to distinguish these and related scenarios for superconductivity creation or enhancement by inhomogeneity from the conventional weak-coupling coexistence of superconductivity and various density waves.[7–10] In the latter case, the density-wave order inevitably suppresses superconductivity due to the competition for the Fermi surface electrons.

It is therefore important to understand the nature of the interplay between superconductivity and inhomogeneities. A complete description of the interplay is clearly impossible. However, in the case in which the characteristic energy scale responsible for the formation of the inhomogeneity is much larger than the superconducting energy scale (the gap Δ), and where the residual interactions are weak, a description based on the BCS theory should be reliable. The purpose of this paper is to study the effect of such imposed inhomogeneity on superconductivity within the BCS framework. The origin of the inhomogeneity could be either electronic, as in the frustrated phase separation scenario, or structural, that is, caused by local lattice distortions or nonuniform carrier concentration due to doping irregularities. We will assume that these structures do not cause Fermi surface nesting either due to the lack of periodicity (e.g., random doping profile) or due to the periodicity being incommensurate with the nested momentum transfers (e.g., frustrated phase separation, or stripes). Under these conditions we generically find that inhomogeneity *enhances* the global superconducting transition temperature, T_c. At the mean-field level, the maximum T_c is achieved when the characteristic length scale of the inhomogeneities, L, is large, in which case the transition temperature is that of the regions with the highest local T_c. Upon including the effects of phase fluctuations, we find that T_c is maximized when L is comparable to the superconducting coherence length $\xi \sim v_F/T_c$. The increase of the transition temperature occurs at the expense of the superfluid density, which is reduced in inhomogeneous superconductors relative to their homogeneous counterparts.

Inhomogeneous pairing: mean-field treatment. As a first example we consider a Hubbard model with an inhomogeneous attractive potential $U(\mathbf{r})>0$,

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_U\\ \mathcal{H}_0 &= \sum_{\mathbf{k}\sigma} \xi_{\mathbf{k}} c^{\dagger}{}_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma}\\ \mathcal{H}_U &= -\sum_{\mathbf{r}} U(\mathbf{r}) n_{\uparrow}(\mathbf{r}) n_{\downarrow}(\mathbf{r}),\end{aligned} \tag{1}$$

where $\xi_{\mathbf{k}}=\epsilon_{\mathbf{k}}-\mu$ and $n_\sigma(\mathbf{r})=c^{\dagger}{}_{\sigma}(\mathbf{r})c_\sigma(\mathbf{r})$ is the occupation number of electrons of spin σ at position $\mathbf{r}$. Within this model, our goal is to understand whether for a *fixed average* pairing strength $\overline{U(\mathbf{r})}$, a uniform or nonuniform $U(\mathbf{r})$ yields a higher transition temperature, T_c. In the weak-coupling limit, we can derive the BCS condition for the onset of superconductivity from the Hamiltonian (1),

$$\Delta_{\mathbf{q}} = \int \frac{d^d p}{(2\pi)^d} U(\mathbf{q}-\mathbf{p}) K(\mathbf{p}) \Delta_{\mathbf{p}}, \tag{2}$$

where $\Delta_{\mathbf{q}}=\Sigma_{\mathbf{k}\ \mathbf{p}} U(\mathbf{k})\langle c_{\mathbf{q}/2-\mathbf{k}/2+\mathbf{p}\uparrow} c_{\mathbf{q}/2-\mathbf{k}/2-\mathbf{p}\downarrow}\rangle$, $U(\mathbf{k})$ is the Fourier transform of the pairing interaction, and $K(\mathbf{p})$ is the pairing kernel. The pairing kernel depends on temperature T and the mean-field (MF) superconducting transition is defined by the temperature at which the integral equation has a nontrivial solution. The kernel can be calculated from the normal state electron Green functions[11]

$$K(\mathbf{p}) \approx N_f \ln\left[\frac{2\gamma\omega_D}{\pi\sqrt{T^2+(v_f p)^2}}\right]\Theta(\omega_D - |v_f p|), \tag{3}$$

where N_f is the density of states at the Fermi surface, v_f is the Fermi velocity, T is temperature, and $\ln \gamma \approx 0.577$ is Euler's constant. Here we also introduced an explicit high-energy cutoff for the attraction, ω_D. For $T \gg v_f p$ this expression reduces to the well-known homogeneous result, $K \sim N_f \ln[2\gamma\omega_D/(\pi T)]$.

The modulation of the pairing interaction leads to the mixing between Cooper pairs with different center-of-mass momenta. For simplicity we first assume a harmonic modulation ($Q \equiv 2\pi/L$) of the pairing, $U(\mathbf{r}) = \bar{U} + U_Q \cos(\mathbf{Q}\cdot\mathbf{r})$. In this case the integral equation (2) reduces to a system of linear equations $\Delta_n = \bar{U}K_n\Delta_n + (U_Q/2)[K_{n-1}\Delta_{n-1} + K_{n+1}\Delta_{n+1}] \equiv \mathcal{M}_{nm}\Delta_m$, where $\Delta_n \equiv \Delta(n\mathbf{Q}+q_0)$ and $K_n \equiv K(n\mathbf{Q}+q_0)$. The "parent" momentum q_0 defines the minimal momentum of a Cooper pair in the connected family $\Delta(n\mathbf{Q}+q_0)$.

The paring instability occurs at the temperature T_c, such that the largest eigenvalue of matrix $\mathcal{M}$ is equal to 1. In the uniform case, $U_Q=0$, this condition is $\bar{U}K(0)=1$. We will now prove that the mean-field transition temperature is greater than in the uniform case, $U_Q=0$. Consider the $q_0=0$ family and without loss of generality, take $U_Q>0$. Since all of the matrix elements of $\mathcal{M}$ are non-negative, by Perron's theorem,[12] the maximal eigenvalue is a positive number that is larger than any diagonal matrix element, including $\bar{U}K(0)$. Thus, generically, the superconducting onset temperature T_c is increased whenever $U_Q \neq 0$.

This result can be understood from an analogy with a quantum mechanical particle in a tight-binding chain. Defining a variable $\Lambda_n = \bar{U}K_n\Delta_n$, the BCS condition takes a simple symmetric form, $\Lambda_n = (1/\bar{U}K_n)\Lambda_n - (U_Q/2\bar{U})(\Lambda_{n+1} + \Lambda_{n-1})$. The "hopping" term delocalizes the particle and thus reduces the "energy" below its minimal on-site value $(1/\bar{U}K_0)$. Clearly, this leads to a relative increase of T_c, even in the case of multi-Q modulation.

Large **Q** *limit.* In this limit, the quickly oscillating coupling is ineffective at mixing different modes, so that the off-diagonal terms in $\mathcal{M}$ are rapidly decaying with n. We are then justified in keeping only a small portion of the matrix surrounding the $n=0$ term. The lowest order correction to the homogeneous result is obtained by considering couplings between Δ_0 and $\Delta_{\pm 1}$. The largest eigenvalue in this case is

$$\lambda_{\max} = \frac{\bar{U}}{2}\left[K_0 + K_1 + \sqrt{(K_0 - K_1)^2 + \frac{2K_0K_1{U_Q}^2}{\bar{U}^2}}\right].$$

Given the separation of energy scales, $T_c \ll v_f Q \ll \omega_D$, we obtain T_c by solving $\lambda_{\max}=1$,

$$T_c = \frac{2\gamma}{\pi}\omega_D \exp[-1/N_f(\bar{U} + \eta)], \tag{4}$$

where $\eta = {U_Q}^2 K_1/[2(1-\bar{U}K_1)]$. While η is positive, and since $K_1 \sim \ln[\omega_D/v_f Q]$ decreases with increasing Q, so does η. For $v_F Q > \omega_D$, Cooper pairs can no longer scatter off the quickly oscillating coupling landscape, and we recover the critical temperature for the homogeneous case.

Small **Q** *limit.* In the limit $Q\xi \ll 1$, the global MF transition temperature is determined by the regions with the strongest pairing interaction, $T_c \approx (2\gamma/\pi)\omega_D \exp[-1/N_f(\bar{U} + |U_Q|)]$. The deviations from this result due to finite Q and the effects of the phase fluctuations are discussed below.

Electron density modulation. Before going further, let us in parallel consider the case of homogeneous coupling $U(\mathbf{r}) = \bar{U}$, with inhomogeneity caused by a background potential variation. In the simplest case of the harmonic modulation, the additional contribution to the Hamiltonian (1) is

$$\mathcal{H}_\rho = \rho \sum_{i\sigma} c^{\dagger}{}_{i\sigma} c_{i\sigma} \cos \mathbf{Q}\cdot\mathbf{r}_i. \tag{5}$$

It is easy to see that for particle-hole symmetric density of states (DOS), the linear in ρ contributions to the BCS instability condition equations vanish identically. For small values of **Q**, the modulation acts as a slowly varying shift in the local chemical potential with the amplitude proportional to $|\rho|$. Thus, we only get a linear in ρ contribution for *asymmetric* DOS, $N(\epsilon) = N_f + N'(\epsilon - \epsilon_F)$. We then find that the BCS equations are identical to the case of inhomogeneous pairing interaction with the modulation strength

$${U_Q}^{\text{eff}} = -\bar{U}\frac{N'\rho}{N_f}. \tag{6}$$

Ginzburg-Landau analysis ($Q\xi \ll 1$). We now consider the general case of slow variation of the pairing strength and/or background potential. The Ginzburg-Landau free energy functional in the presence of inhomogeneity is

$$F = -\int d\mathbf{r}\, d\mathbf{r}' K(\mathbf{r}-\mathbf{r}')\Delta(\mathbf{r})\Delta(\mathbf{r}') + \int d\mathbf{r}\frac{\Delta(\mathbf{r})^2}{U(\mathbf{r})} + \alpha\int d\mathbf{r}\rho(\mathbf{r})\Delta(\mathbf{r})^2 + \frac{\beta}{2}\int d\mathbf{r}\Delta(\mathbf{r})^4. \tag{7}$$

Here we assumed that the order parameter remains real even in the presence of inhomogeneity. We include both the coupling of the superconducting order parameter to a density wave, as well as the inhomogeneity of the pairing interaction. For small amplitude modulation of the pairing interaction, $U(\mathbf{r}) = \bar{U} + \delta U(\mathbf{r})$ with $|\delta U(\mathbf{r})| < \bar{U}$, the two mechanisms are formally equivalent. For particle-hole asymmetric DOS, from the above considerations, $\alpha = -\bar{U}N'/N_f$. For simplicity, we only consider the inhomogeneous $U(\mathbf{r})$ case here. The pair susceptibility kernel is given by Eq. (3). In the long wave length limit,

$$K(\mathbf{r}-\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}')N_f\left[\ln\frac{2\gamma\omega_D}{\pi T} + \xi^2\nabla^2\right], \tag{8}$$

where $\xi = v_F/T$. Computing the variation of Eq. (7) with respect to the order parameter, we find the equation for a stationary solution $\Delta(\mathbf{r})$,

$$-\xi^2\nabla^2\Delta(\mathbf{r}) + g(\mathbf{r})\Delta(\mathbf{r}) + \frac{\beta}{N_f}\Delta(\mathbf{r})^3 = 0,$$

$$g(\mathbf{r}) = \frac{1}{N_f U(\mathbf{r})} - \ln\frac{2\gamma\omega_D}{\pi T}. \tag{9}$$

As a first step, we determine the inhomogeneous mean-field (MF) transition temperature for the pairing interaction $U(\mathbf{r}) = \bar{U} + U_Q\cos(\mathbf{Q}\cdot\mathbf{r})$, with $Q\xi \ll 1$. Close to the MF transition, the cubic terms in Eq. (9) can be neglected. Expanding in $U_Q/\bar{U}$, and transforming Eq. (9) to Fourier space, we obtain a system of equations connecting $\Delta(\mathbf{k})$ and $\Delta(\mathbf{k}\pm\mathbf{Q})$. For small Q, $\Delta(\mathbf{k}\pm\mathbf{Q})\approx\Delta(\mathbf{k})$, and after expanding up to the second order in Q, we obtain

$$-g_{\max}\Delta(\mathbf{k}) = (\xi\mathbf{k})^2\Delta(\mathbf{k}) - \frac{1}{2}A^2Q^2\partial_k^2\Delta(\mathbf{k}). \qquad (10)$$

Here $g_{\max}$ denotes $g(\mathbf{r})$ evaluated at $U(\mathbf{r})=\bar{U}+|U_Q|$ and $A=\sqrt{U_Q/(N_f\bar{U}^2)}$ (note that there is no explicit constraint on the value of parameter A since it is a ratio of two small numbers). The MF transition temperature is determined by the smallest eigenvalue of the differential operator on the right-hand side. This eigenvalue corresponds to the "ground-state energy" of a harmonic oscillator, $\xi QA/\sqrt{2}$. The corresponding transition temperature $T_c^{\mathrm{MF}}=T_{\max}^{\mathrm{MF}}\exp(-\xi QA/\sqrt{2})$, is only slightly less than the transition temperature, $T_{\max}^{\mathrm{MF}}$ for a system with a homogeneous pairing interaction $U_{\max}=\bar{U}+|U_Q|$. More importantly, it is easy to see that in the limit of small $Q\xi$, the order parameter is exponentially suppressed in the region of smaller pairing interaction relative to its value at the peak,

$$\Delta_{\min} \sim \Delta_{\max}\exp\{-A(\xi Q)^{-1}\}, \qquad (11)$$

This, in turn, implies that phase fluctuations, which we discuss below, can reduce the global phase coherence temperature significantly below T_c^{MF}.

The expression of Eq. (11) is only valid at the MF transition temperature, where Δ is infinitesimal. To determine Δ below T_c^{MF} we need to solve the nonlinear Eq. (9). In a d-dimensional superconductor, with an arbitrary smooth variation of $U(\mathbf{r})$, the boundary of the "classically forbidden" region, $g(\mathbf{r})>0$, is a $(d-1)$-dimensional surface. Hence, near the boundary the problem is essentially one-dimensional, and in the $g(\mathbf{r})>0$ region we can apply the standard WKB approximation to solve the linearized Eq. (9). The prefactor is fixed by matching the WKB solution to the intermediate asymptotic at the boundary x_0, which can be obtained by solving the full Eq. (9) in a linear potential $g(x)=g'(x_0)(x-x_0)$. We then find that in the particular case of harmonic modulation discussed above, the order parameter distance d away from the boundary is approximately

$$\Delta(d) \sim T\sqrt{AQ\xi}\exp[-A\sqrt{Q\xi}(d/\xi)^{3/2}]. \qquad (12)$$

This expression is obtained assuming $g'(x_0)\approx A^2Q$, and therefore valid only for the temperatures sufficiently below $T_c^{\mathrm{MF}}\sim T_{\max}^{\mathrm{MF}}$. So long as $T\gg T_{\min}^{\mathrm{MF}}$ ($T_{\min}^{\mathrm{MF}}$ is the uniform T_c of a system with pairing strength $\bar{U}-|U_Q|$), the distance from the turning point to the minimum point of Δ is $d\sim L$. Notice that this expression depends on temperature not only explicitly, but also through $\xi=v_f/T$.

Phase fluctuation effects (still with $Q\xi\ll 1$). A consequence of the large spatial variations in the mean-field $\Delta(\mathbf{r})$ is that fluctuation effects are severe where $\Delta(\mathbf{r})$ is small. Of these, the most important are the thermal fluctuations in the phase of the order parameter, *i.e.*, such that

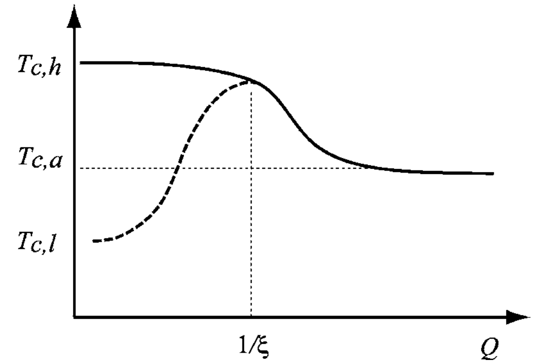

FIG. 1. Critical temperature for the inhomogeneous negative U Hubbard model with coupling $U(x)=\bar{U}+U_Q\cos(Qx)$. The thick line denotes the mean-field result, where $T_{c,a}=(2\gamma/\pi)\omega_D\exp[-1/N_f\bar{U}]$ and $T_{c,h}=(2\gamma/\pi)\omega_D\exp[-1/N_f(\bar{U}+|U_Q|)]$. The dashed line shows the critical temperature once phase fluctuations of the order parameter are included. For $Q\xi\ll 1$, the superconductivity is first established locally in regions where $U(x)$ is large, but macroscopic phase coherence is achieved at a lower temperature, bounded from below by $T_{c,l}=(2\gamma/\pi)\omega_D\exp[-1/N_f(\bar{U}-|U_Q|)]$.

$\Delta(\mathbf{r})=|\Delta_{\mathrm{MF}}(\mathbf{r})|e^{i\theta}$ where $\Delta_{\mathrm{MF}}(\mathbf{r})$ is the solution of Eq. (9), and $\theta(\mathbf{r})$ is a slowly varying function of $\mathbf{r}$. The free energy cost of such phase fluctuations is $F_\theta=\int d\mathbf{r}J(\mathbf{r})(\nabla\theta)^2$, with the local superfluid stiffness $J(\mathbf{r})=N_f\xi^2|\Delta_{\mathrm{MF}}(\mathbf{r})|^2$. In general, the phase-ordering temperature estimated using this as the effective Hamiltonian is reduced from the mean-field transition temperature [i.e., the temperature at which $J(\mathbf{r})$ vanishes], but by an amount that depends on dimensionality, and on the spatial arrangement of the regions of suppressed stiffness.

For concreteness, we consider the case of a two-dimensional (2D) superconductor. At finite temperature, no true long-range order is possible.[13] However, at $T<T_{\mathrm{KT}}$, binding of topological excitations into vortex-antivortex pairs leads to a state with quasi-long-range order, which has a nonzero superfluid stiffness.[14] While for homogeneous BCS superconductors in 2D, the difference between MF and the Kosterlitz-Thouless (KT) transition temperatures is tiny, $(T_c^{\mathrm{MF}}-T_{\mathrm{KT}})/T_c^{\mathrm{MF}}\sim T_c^{\mathrm{MF}}/T_F$ (where T_F is the Fermi temperature), for inhomogeneous superconductors, the suppression of T_{KT}, is generally much larger. For a smooth random distribution of $J(\mathbf{r})$, an estimate of T_{KT} can be made based on the effective superfluid density,

$$T_{\mathrm{KT}} \sim \sqrt{\overline{J(\mathbf{r})}[\overline{1/J(\mathbf{r})}]^{-1}} \approx \sqrt{J_{\min}J_{\max}}. \qquad (13)$$

This expression has a particularly transparent meaning for the unidiretional "stripedlike" variation of $U(\mathbf{r})$ that we treated explicitly when solving the mean-field equations above. There, $J_{\max}$ corresponds to the stiffness along the stripes and $J_{\min}$ perpendicular to the stripes. The corresponding anisotropic XY model directly leads to the result Eq. (13). In this case, we find

$$T_{\mathrm{KT}} \sim \frac{T_f}{T_{\mathrm{KT}}^2} T_c^{\mathrm{MF}} \Delta_{\min}(T_{\mathrm{KT}}).$$

Together with Eq. (12) for $\Delta_{\min}(T_{\mathrm{KT}}) \sim \Delta(L, T_{\mathrm{KT}})$, this equation implicitly defines T_{KT}. With logarithmic accuracy we find that $T_{\mathrm{KT}} \sim \min(T_c^{\mathrm{MF}}, v_f Q/A)$.

In any case, barring certain artificial geometries, it is clear that for a long wave length modulation, $\xi Q \ll 1$, the Kosterlitz-Thouless temperature T_{KT} is exponentially lower than the MF transition temperature; on the other hand, for modulations with $\xi Q \sim 1$, the phase fluctuation region is very narrow and $T_{\mathrm{KT}} \approx T_c^{\mathrm{MF}}$. In this regime, the mean-field superconducting temperature is still exponentially enhanced relative to its value in the uniform state with the same average paring interaction strength, $\bar{U}$. For even faster modulation, $\xi Q \gg 1$, the MF transition temperature drops since the pairings interaction modulation averages out on the length scale of ξ. This trend is presented qualitatively in Fig. 1.

For a "dirty" superconductor with a mean free path shorter than the clean coherence length, $\ell = v_F \tau < \xi$, the effect of phase fluctuations can be estimated in the same way as in the clean limit, with minor changes in prefactors but with the coherence length redefined as $\xi_d = \sqrt{\xi \ell}$.

Summary. We studied the effect of nanoscale inhomogeneity on the superconducting transition temperature, T_c. We considered two possible kinds of inhomogeneity: the modulations of the paring strength and of the background potential. In the weak coupling BCS regime, we find that inhomogeneity, which is incommensurate with the Fermi surface nesting vectors, *enhances* T_c relative to its value for the uniform zero center-of-mass momentum pairing. For a fixed modulation depth we find that the highest T_c is reached when the modulation wavelength is of the order of the superconducting coherence length. For shorter wavelengths, the superconductor cannot take advantage of the locally favorable conditions, while for the longer wavelengths, the global superconductivity is suppressed due to the phase fluctuations on the weak links. Similar results also apply to unconventional superconductors in the presence of smooth (on the $1/k_f$ length scale) inhomogeneities. Clearly oversimplified, the presented picture bears resemblance to the high-temperature superconducting cuprates, where considerable experimental evidence[15] indicates that the maximum T_c occurs at a crossover between a regime where T_c is controlled by the pairing scale and where it is a phase-ordering transition. Evidence for inhomogeneous superconductivity has also been found in several other materials, including $Ba_{1-x}K_xBiO_3$, WO_3, and Pt.[16]

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