Superconducting state with a finite-momentum pairing mechanism in zero external magnetic field

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In the BCS theory of superconductivity, one assumes that all Cooper pairs have the same center-of-mass momentum. This is indeed enforced by self-consistency if the pairing interaction is momentum independent. Here, we show that for an attractive nearest-neighbor interaction, this is different. In this case, stable solutions with pairs with momenta \( \mathbf{q} \) and \(-\mathbf{q}\) coexist and, for a sufficiently strong interaction, one of these states becomes the ground state of the superconductor. The possibility for a finite-momentum pairing state emerges only for nodal superconductors and is accompanied by a charge order with wave vector \( 2\mathbf{q} \). For a weak pairing interaction, the ground state is a \( d \)-wave superconductor.

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In the original formulation of the BCS theory of superconductivity,\(^1\) all Cooper pairs are assumed to have the same center-of-mass momentum \( \mathbf{q} \). One possible generalization of this theory is to introduce a pair amplitude for each center-of-mass momentum separately. In the BCS theory for conventional superconductors, only one of these order parameters (OPs) is selected and the stable state is the one where all pairs have the same momentum and form the BCS condensate. For films in an external magnetic field, Fulde and Ferrell\(^2\) and, independently, Larkin and Ovchinnikov\(^3\) introduced a superconducting (SC) state with coexisting pair momenta \( \mathbf{q} \) and \(-\mathbf{q}\), a state that explicitly breaks time inversion symmetry. For unconventional pairing symmetries, the competition between pair momenta is more complex and it has remained unresolved whether a bulk SC ground state with different pair momenta may exist without magnetic field.\(^4\) A SC state with different coexisting pair momenta generally exhibits a spatially inhomogeneous charge density. One example of a superconductor of this type is the recently proposed “pair density-wave” (PDW) state.\(^5–7\) It is characterized in real space by a two-component order parameter

\[
\Delta(r) = \Delta_{\mathbf{q}e^{i\mathbf{q}r}} + \Delta_{-\mathbf{q}e^{-i\mathbf{q}r}}.
\]

This structure bears some resemblance to the Larkin-Ovchinnikov state, but it preserves time inversion symmetry. The PDW is accompanied by a charge-density pattern with wave vector \( 2\mathbf{q} \). For this reason the PDW state has been proposed to describe the SC state of high-\( T_c \) cuprates with coexisting stripe order,\(^8\) especially Nd-doped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) (Ref. 8) and \( \text{La}_{2-x}\text{Ba}_x\text{CuO}_4 \) for \( x=1/8 \).\(^9–12\) In particular, the recent experiments on the 1/8-doped material stimulated further theoretical studies to resolve the nature and the origin of the SC state in the charge ordered phase.\(^13\) The PDW might be a candidate state, but so far a microscopic model that yields the PDW as its ground state is lacking.

In this Rapid Communication, rather than attempting a microscopic theory for striped cuprates, we address the general question of whether finite-momentum pairing in zero magnetic field can exist in the ground state of a microscopic pairing Hamiltonian. We formulate an extended version of the BCS theory using Gor'kov’s equations and explicitly allow for the coexistence of different finite-momentum pairing amplitudes. We identify conditions for a ground-state solution with finite OPs for the pair momenta \( \mathbf{q} \) and \(-\mathbf{q}\). This pairing state is realized beyond a critical interaction strength \( V_c \) for an attractive nearest-neighbor interaction, and it is characterized by a charge stripe order, a gapless density of states (DOS), and a partially reconstructed Fermi surface. On the other hand, for \( V < V_c \), the \( d \)-wave superconductor is the stable ground state.

We start from a tight-binding Hamiltonian on a square lattice with \( N \) sites and periodic boundary conditions,

\[
\mathcal{H} = \sum_{\mathbf{k},s} \varepsilon_{\mathbf{k}} c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s} + \frac{1}{N} \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k'}, s, s'} V(\mathbf{k}, \mathbf{k'}, \mathbf{q}) c_{\mathbf{k}s}^\dagger c_{\mathbf{k}s}^\dagger c_{\mathbf{k}+\mathbf{q}s'} c_{\mathbf{k}+\mathbf{q}s'}.
\]

With nearest- and next-nearest-neighbor hopping amplitudes \( t \) and \( t' \), respectively, the single-electron dispersion has the form

\[
\varepsilon_{\mathbf{k}} = -2t [\cos k_x + \cos k_y] + 4t' \cos k_x \cos k_y - \mu,
\]

where \( \mu \) is the chemical potential.

For the superconducting state with singlet pairing, we use the BCS-type mean-field decoupling scheme and approximate

\[
\langle c_{\mathbf{k}s}^\dagger c_{\mathbf{k'-q}s'}^\dagger c_{\mathbf{k'+q}s'} c_{\mathbf{k}s} \rangle \approx \langle c_{\mathbf{k}s}^\dagger c_{\mathbf{k'-q}s'}^\dagger c_{\mathbf{k}+\mathbf{q}s'} c_{\mathbf{k}s} \rangle.
\]

The system is then represented by the spin-independent imaginary time Green’s function \( \tilde{\mathcal{G}}(\mathbf{k}, \mathbf{k'}, \tau) = -\langle T_\tau \mathcal{F}(\mathbf{k}+\tau) (\mathbf{k}+\tau) \mathcal{F}(\mathbf{k}, \mathbf{k'}, 0) \rangle \) and the anomalous propagators

\[
\tilde{\mathcal{F}}(\mathbf{k}, \mathbf{k'}, \tau) = \langle T_\tau \mathcal{F}(\mathbf{k}+\tau) (\mathbf{k}+\tau) \mathcal{F}(\mathbf{k}, \mathbf{k'}, 0) \rangle \quad \text{and} \quad \tilde{\mathcal{F}}^*(\mathbf{k}, \mathbf{k'}, \tau) = \langle T_\tau \mathcal{F}^*(\mathbf{k}+\tau) (\mathbf{k}+\tau) \mathcal{F}(\mathbf{k}, \mathbf{k'}, 0) \rangle \quad \text{for} \quad s \neq s'.
\]

The Heisenberg equations of motion for the normal and anomalous Green’s functions lead to the following Gor’kov equations:\(^14\)

\[
\tilde{\mathcal{G}}(\mathbf{k}, \mathbf{k'}, \omega_n) = \tilde{\mathcal{G}}_0(\mathbf{k}, \omega_n) \times \left[ \delta_{\mathbf{k}, \mathbf{k'}} - \sum_\mathbf{q} \Delta(\mathbf{k}, \mathbf{q}) \tilde{\mathcal{F}}^*(\mathbf{k} - \mathbf{q}, \mathbf{k'}, \omega_n) \right]^{-1},
\]
\begin{equation}
\mathcal{F}(\mathbf{k}, \mathbf{k}', \omega_n) = G_0(\mathbf{k}, \omega_n) \sum_q \Delta(\mathbf{k}, \mathbf{q}) G(-\mathbf{k}', -\mathbf{k} + \mathbf{q}, -\omega_n),
\end{equation}

where \( G_0(\mathbf{k}, \omega_n) = [i\omega_n - \varepsilon_k]^{-1} \) is the Green’s function in the normal state and \( \omega_n = (2n+1)\pi T \) is the fermion Matsubara frequency for temperature \( T \). The order parameter \( \Delta(\mathbf{k}, \mathbf{q}) \) is determined by the self-consistency condition

\begin{equation}
\Delta(\mathbf{k}, \mathbf{q}) = -\frac{T}{N} \sum_n \sum_{\mathbf{k}'} V(\mathbf{k}, \mathbf{k}', \mathbf{q}) \mathcal{F}(\mathbf{k}', \mathbf{k}' - \mathbf{q}, \omega_n). 
\end{equation}

For the interaction, we choose a simple ansatz that allows for unconventional pairing; we assume an attractive interaction between electrons on neighboring sites. The Fourier transform of this attractive interaction can be decomposed into \( s, p, \) and \( d \) pairing channels. With the restriction to singlet pairing only the \( s \) and \( d \) channels remain, which is equivalent to the interaction \( V(\mathbf{k}, \mathbf{k}', \mathbf{q}) = V_s(\mathbf{k}, \mathbf{k}', \mathbf{q}) + V_d(\mathbf{k}, \mathbf{k}', \mathbf{q}) \) in momentum space, with factorizable extended \( s \)- and \( d \)-wave components \( V_s(\mathbf{k}, \mathbf{k}', \mathbf{q}) \) and \( V_d(\mathbf{k}, \mathbf{k}', \mathbf{q}) \), where

\begin{equation}
V_{s,d}(\mathbf{k}, \mathbf{k}', \mathbf{q}) = V_{s,d}(\mathbf{k} - \mathbf{q}/2) g_{s,d}(\mathbf{k}' - \mathbf{q}/2). 
\end{equation}

Here, \( V > 0 \) is the attractive pairing interaction strength and \( g_s(\mathbf{k}) = \cos k_x + \cos k_y \) and \( g_d(\mathbf{k}) = \cos k_x - \cos k_y \). Thus,

\begin{equation}
\Delta(\mathbf{k}, \mathbf{q}) = \Delta_s(\mathbf{q}) g_s(\mathbf{k} - \mathbf{q}/2) + \Delta_d(\mathbf{q}) g_d(\mathbf{k} - \mathbf{q}/2).
\end{equation}

The vector \( \mathbf{q} \) labels mean-field solutions that correspond to order parameters in real space with phase winding numbers \( q_j \) and \( q_x \) in \( x \) and \( y \) directions, respectively.

If \( \Delta(\mathbf{k}, \mathbf{q}) \neq 0 \) for a single momentum \( \mathbf{q} \neq 0 \), then \( \mathcal{F}(\mathbf{k}, \mathbf{k}', \omega_n) \) and \( \mathcal{F}(\mathbf{k}, \mathbf{k}', \omega_n) \) have off-diagonal terms in momentum space, but \( G(\mathbf{k}, \mathbf{k}', \omega_n) \) is still diagonal. If \( \Delta(\mathbf{k}, \mathbf{q}) \neq 0 \) for at least two different momenta \( \mathbf{q} \), then also \( G(\mathbf{k}, \mathbf{k}', \omega_n) \) has off-diagonal terms and the discrete translational invariance is broken. The charge density is obtained from \( \rho(r) = \frac{1}{N} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{r}} n(\mathbf{k}, \mathbf{k}') \), where \( n(\mathbf{k}, \mathbf{k}') = 2T \sum_{\omega_n} G(\mathbf{k}, \mathbf{k}', \omega_n) \). Thus, there are charge modulations whenever \( G(\mathbf{k}, \mathbf{k}', \omega_n) \) has off-diagonal terms.

Inserting Eq. (4) into Eq. (3) leads to a system of coupled equations for the Green’s function \( G(\mathbf{k}, \mathbf{k}', \omega_n) \). Assuming that \( n(\mathbf{k}, \mathbf{k}') \neq n(\mathbf{k}) \) for \( \mathbf{k} \neq \mathbf{k}' \), \( \mathcal{F}(\mathbf{k}, \mathbf{k} + \mathbf{q}, \omega_n) \) and \( \mathcal{F}(\mathbf{k} + \mathbf{q}, \mathbf{k}, \omega_n) \) are approximately kept only the term proportional to \( G(\mathbf{k}, \mathbf{k} + \mathbf{q}, \mathbf{k}, \omega_n) \) in the sum in Eq. (4). This approximation in Eqs. (3) and (4) leads to an analytical solution of the Gor’kov equations to leading order in \( n(\mathbf{k}, \mathbf{k}') \) for \( \mathbf{k} \neq \mathbf{k}' \). The quantitative validity of this approximation will be verified \textit{a posteriori}.

In an ansatz for a self-consistent solution of the Gor’kov equations (3) and (4), we choose \( Q \) trial vectors \( \mathbf{q}_1, \ldots, \mathbf{q}_Q \) and set \( \Delta(\mathbf{k}, \mathbf{q}) = 0 \) for all other values of \( \mathbf{q} \neq \mathbf{q}_j \). Thereby we test selected combinations of \( \mathbf{q} \) vectors for self-consistent solutions. With this ansatz, the energy spectrum of the system consists of \( Q + 1 \) bands \( E_\alpha(\mathbf{k}) \), where \( \alpha = 0, \ldots, Q \). The conventional BCS solution is realized for \( Q = 1 \) with just two quasiparticle bands and \( \mathbf{q} = 0 \). Generally, one obtains a set of \( 2Q \) coupled self-consistency equations for \( \Delta_s(\mathbf{q}_j) \) and \( \Delta_d(\mathbf{q}_j) \).
the ground state. The optimal pair and, consequently, the finite-momentum pairing state is
modulations in the above approximation for a posteriori which three lattice constants. The charge modulation in the SC state
as in Fig. 1. The coherence peaks of the $q=0$ state are split due to the Van Hove singularity of the two-dimensional tight-binding dispersion.

For all analyzed parameter sets, which led to stable ground-state solutions with finite-momentum pairing, the relative
competition and their coexistence demands that those regions in momentum space with maximum pairing amplitude of either
of the two are optimally separated. We emphasize that this mechanism for the stabilization of the finite-momentum pairing state is not possible for isotropic superconductors.

For the finite-$q$ ground-state solutions the charge density $\rho(r)$ has an oscillatory part arising from the off-diagonal
terms of the Green’s function. For the $q=(\pm q,0)$ state the charge density forms a sinusoidal stripe pattern with wave
number $2q$. Correspondingly, the charge density varies as

$$\rho(r) = \rho + \rho_1 \cos(2q x).$$

For all analyzed parameter sets, which led to stable ground-state solutions with finite-momentum pairing, the relative
charge modulation with an amplitude $\rho_1/\rho$ was near 2%, which a posteriori justifies the assumption of small charge
modulations in the above approximation for $\mathcal{F}(k,k',\omega_n)$. For $q=\pi/3$, the wavelength of the stripe pattern is therefore
three lattice constants. The charge modulation in the SC state suggests us to include a self-consistent charge-density-wave
(CDW) OP in the mean-field decoupling scheme of the Hamiltonian (1). We have analyzed this extension with coexisting OPs for SC and CDW orders for selected cases. The CDW OP tends to stabilize the state with finite-momentum pairing but it remains small and does not change the solutions qualitatively. Also arbitrary orientations of the Cooper pair’s center-of-mass momenta were considered, but in all cases the lowest-energy solutions were obtained for momenta in (10) and (01) directions.

The finite-momentum pairing state has further characteristic properties that are at variance with a BCS-like
$d$-wave superconductor (with $q=0$). The DOS $D(E)$

$$= 1/N \sum_q n(k)$$

Above $V_c$, the potential-energy gain from pairing overcomes the concomitant increase in the kinetic energy due to the finite center-of-mass momentum of each pair and, consequently, the finite-momentum pairing state is the ground state. The optimal $q=q_{\text{min}}(1,0)$ or $q=q_{\text{min}}(0,1)$ sensitively depends on $V$, $t'$, and $\rho$, but it is typically found in between $q_1 \approx \pi/8$ and $q_2 \approx \pi/2$ for a wide parameter range. $q_{\text{min}}$ is near the maximum distance between the nodes on the Fermi surface of the two order parameters $\Delta(k,q)$ and $\Delta(k,-q)$. This suggests that the two order parameters are in competition and their coexistence demands that those regions in momentum space with maximum pairing amplitude of either of the two are optimally separated. We emphasize that this mechanism for the stabilization of the finite-momentum pairing state is not possible for isotropic superconductors.

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sensitively on the band filling.

Fermi-surface reconstruction. The zero-energy states
neous formation of electron pairs with center-of-mass mo-
tion provides self-consistent solutions with the simulta-
extended BCS theory with attractive nearest-neighbor inter-
paired electrons.

gendered by the striped superconductor La$_{15}$
charge-density modulation with wave vector 2
for nodal superconductors. Due to the concomitant striped
finite-momentum pairing amplitudes for center-of-mass mo-
ments $q=\pm q$; these solutions are absent for an
attractive contact interaction and their possibility arises only
for nodal superconductors. Due to the concomitant striped
charge-density modulation with wave vector $2q$, a connec-
tion to the striped superconductor La$_{15/8}$Ba$_{1/8}$CuO$_4$ appears
tempting. However, without the inclusion of additional cor-
relation effects as the source for a possible spin order pattern,
we consider it premature to draw conclusions about the fa-
vorable wavelength of the stripes.

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