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Checkerboard density of states in strong-coupling superconductors

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The Bogoliubov-de Gennes (BdG) equations are solved in the strong-coupling limit, where real-space (preformed) pairs bose-condense with finite center-of-mass momenta. There are two energy scales in this regime, a temperature independent incoherent gap Δ_p and a temperature dependent coherent gap $\Delta_c(T)$, modulated in real space. The single-particle density of states (DOS) reveals checkerboard modulations similar to the tunnelling DOS in cuprates.

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Many independent observations show that the superconducting state of cuprates is as anomalous as the normal state. In particular, there is strong evidence for a *d*-like order parameter, which changes sign when the CuO_2 plane is rotated by $\pi/2$ [1]. A few phase-sensitive experiments [2] provide unambiguous evidence in this direction. A *d*-wave BCS gap could appear in the two-dimensional Hubbard model near half filling, as suggested by Scalapino, Loh, and Hirsch [3] concurrently with the discovery of novel superconductors. On the other hand, *c*-axis Josephson tunnelling [4], high-precision magnetic measurements [5], photo-excited quasi-particle relaxation dynamics [6] and some other experiments [7] support more conventional anisotropic *s*-like gap.

In fact, there are stronger deviations from the conventional Fermi/BCS-liquid behaviour than the gap symmetry. There is now convincing evidence for pairing of carriers well above T$_c$ as predicted by the bipolaron theory [8], the clearest one is provided by the uniform magnetic susceptibility [9, 10], tunnelling, and photoemission. The tunnelling and photoemission gap is almost temperature independent below T$_c$ [11, 12] and exists above T$_c$ [11, 13, 14] with its maximum several times larger than expected in the weak and intermediate-coupling [15] BCS theory. Kinetic [16] and thermodynamic [17] data suggest that the gap opens both in charge and spin channels at any relevant temperature in a wide range of doping. A plausible explanation is that the normal state (pseudo)gap, Δ_p, is half of the bipolaron binding energy [18], although alternative models have been proposed [19].

Further studies of the gap function revealed even more complicated physics. Reflection experiments, in which an incoming electron from the normal side of a normal/superconducting contact is reflected as a hole along the same trajectory [20], showed a much smaller gap edge than the bias at the tunnelling conductance maxima [21]. Two distinctly different gaps with different magnetic field and temperature dependence were observed in the c-axis I(V) characteristics [22]. They were also observed with the femtosecond time-resolved optical spectroscopy [23]. More recent STM experiments revealed checkerboard spatial modulations of the tunnelling DOS, with [24] and without [25, 26] applied magnetic fields.

We have proposed a simple model [27] explaining two different gaps in cuprates. The main assumption, supported by a parameter-free estimate of the Fermi energy [28], is that the attractive potential is large compared with the renormalised Fermi energy, so that the ground state is the Bose-Einstein condensate of tightly bound real-space pairs. In this letter I calculate the single particle DOS of strong-coupling (bosonic) superconductors by solving the inhomogeneous BdG equations. When pairs are Bose-condensed with finite center-of-mass momenta, I obtain a checkerboard DOS reminiscent of the tunnelling DOS in cuprates.

The anomalous Bogoliubov-Gor'kov average

$$F_{ss'}(\mathbf{r}_1,\mathbf{r}_2)=\left\langle \hat{\Psi}_s(\mathbf{r}_1)\hat{\Psi}_{s'}(\mathbf{r}_2)\right\rangle,$$

is the superconducting order parameter both in the weak and strong-coupling regimes. It depends on the relative coordinate $\rho=\mathbf{r}_1-\mathbf{r}_2$ of two electrons (holes), described by field operators $\hat{\Psi}_s(\mathbf{r})$, and on the center-of-mass coordinate $\mathbf{R}=(\mathbf{r}_1+\mathbf{r}_2)/2$. Its Fourier transform, $f(\mathbf{k},\mathbf{K})$, depends on the relative momentum $\mathbf{k}$ and on the center-of-mass momentum $\mathbf{K}$. In the BCS theory $\mathbf{K}=0$, and the Fourier transform of the order parameter is proportional to the gap in the quasi-particle excitation spectrum, $f(\mathbf{k},\mathbf{K})\propto\Delta_{\mathbf{k}}$. Hence the symmetry of the order parameter and the symmetry of the gap are the same in the weak-coupling regime. Under the rotation of the coordinate system, $\Delta_{\mathbf{k}}$ changes its sign, if the Cooper pairing appears in the d-channel. The Cooper pairing might also take place with finite center-of-mass momentum, if electrons are spin polarized [29].

On the other hand, the symmetry of the order parameter could be different from the 'internal' symmetry of the pair wave-function, and from the symmetry of a single-particle excitation gap in the strong-coupling regime [8]. Real-space pairs might have an unconventional symmetry due to a specific symmetry of the pairing potential as in the case of the Cooper pairs [3]. The d-wave symmetry of the ground state could be also due to a topological degeneracy of inter-site pairs on a square lattice [30], as proposed in Ref. [31]. But in any case the ground state and DOS are homogeneous, if pairs are condensed with $\mathbf{K} = 0$. However, if a pair band dispersion has its minima at finite $\mathbf{K}$ in the center-of-mass Brillouin zone, the Bose condensate is inhomogeneous. In particular, the center-of-mass bipolaron energy bands could have their minima at the Brillouin zone boundaries at $\mathbf{K} = (\pi, 0)$ and three other equivalent momenta [32] (here and further I take the lattice constant $a = 1$, and $\hbar = 1$). These four states are degenerate, so that the condensate wave function $\psi(\mathbf{m})$ in the real (Wannier) space, $\mathbf{m} = (m_x, m_y)$, is their superposition,

$$\psi(\mathbf{m}) = \sum_{\mathbf{K}=(\pm\pi,0),(0,\pm\pi)} b_{\mathbf{K}} e^{-i\mathbf{K}\cdot\mathbf{m}}, \quad (1)$$

where $b_{\mathbf{K}} = \pm\sqrt{n_c}/2$ are c-numbers, and $n_c(T)$ is the atomic density of the Bose-condensate. The superposition, Eq.(1), respects the time-reversal and parity symmetries, if

$$\psi(\mathbf{m}) = \sqrt{n_c}\left[\cos(\pi m_x) \pm \cos(\pi m_y)\right]. \quad (2)$$

Two order parameters, Eq.(2), are physically identical because they are related by the translation transformation. They have d-wave symmetry changing sign in the real space, when the lattice is rotated by $\pi/2$. This symmetry is entirely due to the pair-band energy dispersion with four minima at $\mathbf{K} \neq 0$, rather than due a specific pairing potential. It reveals itself as a *checkerboard* modulation of the hole density with two-dimensional patterns, oriented along the diagonals. From this insight one can expect a fundamental connection between stripes detected by different techniques [33, 34] and the symmetry of the order parameter in cuprates [32].

Now let us take into account that in the superconducting state ($T < T_c$) single-particle excitations interact with the pair condensate via the same short-range attractive potential, which forms the pairs [27]. The Hamiltonian describing the interaction of excitations with the pair Bose-condensate in the Wannier representation is

$$\begin{aligned} H &= -\sum_{s,\mathbf{m},\mathbf{n}} [t(\mathbf{m}-\mathbf{n}) + \mu\delta_{\mathbf{m},\mathbf{n}}] c^{\dagger}_{s\mathbf{m}} c_{s\mathbf{n}} \\ &+ \sum_{\mathbf{m}} [\Delta(\mathbf{m}) c^{\dagger}_{\uparrow\mathbf{m}} c^{}_{\downarrow\mathbf{m}} + H.c.], \end{aligned} \quad (3)$$

where $s =\uparrow,\downarrow$ is the spin, $t(\mathbf{m})$ and μ are hopping integrals and the chemical potential, respectively, $c^{\dagger}_{s\mathbf{m}}$ and $c_{s\mathbf{m}}$ create (annihilate) an electron or hole at site $\mathbf{m}$, and $\Delta(\mathbf{m}) \propto \psi(\mathbf{m})$. Applying equations of motion for the Heisenberg operators $\tilde{c}^{\dagger}_{s\mathbf{m}}(t)$ and $\tilde{c}_{s\mathbf{m}}(t)$, and the Bogoliubov transformation [35]

$$\tilde{c}_{\uparrow\mathbf{m}}(t) = \sum_{\nu}[u_\nu(\mathbf{m})\alpha_\nu e^{-i\epsilon_\nu t} + v^*_\nu(\mathbf{m})\beta^{\dagger}_\nu e^{i\epsilon_\nu t}], \quad (4)$$

$$\tilde{c}_{\downarrow\mathbf{m}}(t) = \sum_{\nu}[u_\nu(\mathbf{m})\beta_\nu e^{-i\epsilon_\nu t} - v^*_\nu(\mathbf{m})\alpha^{\dagger}_\nu e^{i\epsilon_\nu t}], \quad (5)$$

one obtains BdG equations describing the single-particle excitation spectrum,

$$\epsilon u(\mathbf{m}) = -\sum_{\mathbf{n}}[t(\mathbf{m}-\mathbf{n}) + \mu\delta_{\mathbf{m},\mathbf{n}}]u(\mathbf{n}) + \Delta(\mathbf{m})v(\mathbf{m}), \quad (6)$$

$$-\epsilon v(\mathbf{m}) = -\sum_{\mathbf{n}}[t(\mathbf{m}-\mathbf{n}) + \mu\delta_{\mathbf{m},\mathbf{n}}]v(\mathbf{n}) + \Delta(\mathbf{m})u(\mathbf{m}), \quad (7)$$

where excitation quantum numbers ν are omitted for transparency. These equations are supplemented by the sum rule $\sum_\nu[u_\nu(\mathbf{m})u^*_\nu(\mathbf{n}) + v_\nu(\mathbf{m})v^*_\nu(\mathbf{n})] = \delta_{\mathbf{m},\mathbf{n}}$, which provides the Fermi statistics of single particle excitations α and β. Different from the conventional BdG equations in the weak-coupling limit, there is virtually no feedback of single particle excitations on the off-diagonal potential, $\Delta(\mathbf{m})$, in the strong-coupling regime. The number of these excitations is low at temperatures below Δ_p/k_B, so that the coherent potential $\Delta(\mathbf{m})$ is an external (rather than a self-consistent) field, solely determined by the pair Bose condensate [27].

While the analytical solution is not possible for any arbitrary off-diagonal interaction $\Delta(\mathbf{m})$, one can readily solve the infinite system of discrete equations (6,7) for a periodic $\Delta(\mathbf{m})$ with a period commensurate with the lattice constant, for example

$$\Delta(\mathbf{m}) = \Delta_c[e^{i\pi m_x} - e^{i\pi m_y}], \quad (8)$$

which corresponds to the pair condensate at $\mathbf{K} = (\pm\pi, 0)$ and $(0, \pm\pi)$, Eq.(2), with a temperature dependent (coherent) $\Delta_c \propto \sqrt{n_c(T)}$. In this case the quasi-momentum $\mathbf{k}$ is the proper quantum number, $\nu = \mathbf{k}$, and the excitation wave-function is a superposition of plane waves,

$$\begin{aligned} u_\nu(\mathbf{m}) &= u_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{m}} + \tilde{u}_{\mathbf{k}} e^{i(\mathbf{k}-\mathbf{g})\cdot\mathbf{m}}, && (9) \\ v_\nu(\mathbf{m}) &= v_{\mathbf{k}} e^{i(\mathbf{k}-\mathbf{g}_x)\cdot\mathbf{m}} + \tilde{v}_{\mathbf{k}} e^{i(\mathbf{k}-\mathbf{g}_y)\cdot\mathbf{m}}. && (10) \end{aligned}$$

Here $\mathbf{g}_x = (\pi, 0)$, $\mathbf{g}_y = (0, \pi)$, and $\mathbf{g} = (\pi, \pi)$ are reciprocal doubled lattice vectors. Substituting Eqs.(9) and (10) into Eqs.(6,7) one obtains four coupled algebraic equations,

$$\begin{aligned} \epsilon_{\mathbf{k}} u_{\mathbf{k}} &= \xi_{\mathbf{k}} u_{\mathbf{k}} - \Delta_c(v_{\mathbf{k}} - \tilde{v}_{\mathbf{k}}), && (11) \\ \epsilon_{\mathbf{k}} \tilde{u}_{\mathbf{k}} &= \xi_{\mathbf{k}-\mathbf{g}} \tilde{u}_{\mathbf{k}} + \Delta_c(v_{\mathbf{k}} - \tilde{v}_{\mathbf{k}}), && (12) \\ -\epsilon_{\mathbf{k}} v_{\mathbf{k}} &= \xi_{\mathbf{k}-\mathbf{g}_x} v_{\mathbf{k}} + \Delta_c(u_{\mathbf{k}} - \tilde{u}_{\mathbf{k}}), && (13) \\ -\epsilon_{\mathbf{k}} \tilde{v}_{\mathbf{k}} &= \xi_{\mathbf{k}-\mathbf{g}_y} \tilde{v}_{\mathbf{k}} - \Delta_c(u_{\mathbf{k}} - \tilde{u}_{\mathbf{k}}), && (14) \end{aligned}$$

where $\xi_{\mathbf{k}} = -\sum_{\mathbf{n}} t(\mathbf{n}) e^{i\mathbf{k}\cdot\mathbf{n}} - \mu$. The determinant of the system (11-14) yields the following equation for the energy spectrum ϵ:

$$\begin{aligned} &(\epsilon - \xi_{\mathbf{k}})(\epsilon - \xi_{\mathbf{k}-\mathbf{g}})(\epsilon + \xi_{\mathbf{k}-\mathbf{g}_x})(\epsilon + \xi_{\mathbf{k}-\mathbf{g}_y}) \\ &= \Delta_c^2(2\epsilon + \xi_{\mathbf{k}-\mathbf{g}_x} + \xi_{\mathbf{k}-\mathbf{g}_y})(2\epsilon - \xi_{\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{g}}). \end{aligned} \quad (15)$$

Two positive roots for ϵ describe the single-particle excitation spectrum. Their calculation is rather cumbersome,

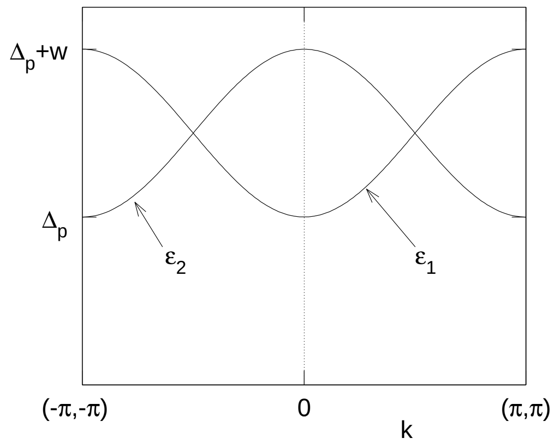

FIG. 1: Single-particle excitation energy spectrum (arb. units) along the diagonal direction of the two-dimensional Brillouin zone

but not in the extreme strong-coupling limit, where the pair binding energy $2\Delta_p$ is large compared with Δ_c and with the single-particle bandwidth w. The chemical potential in this limit is pinned below a single-particle band edge, so that $\mu = -(\Delta_p + w/2)$ is negative, and its magnitude is large compared with Δ_c. Then the right hand side in Eq.(15) is a perturbation, and the spectrum is

$$\epsilon_{1\mathbf{k}} \approx \xi_{\mathbf{k}} - \frac{\Delta_c^2}{\mu}, \tag{16}$$

$$\epsilon_{2\mathbf{k}} \approx \xi_{\mathbf{k}-\mathbf{g}} - \frac{\Delta_c^2}{\mu}, \tag{17}$$

Its dispersion along the diagonal direction is shown in Fig.1 in the nearest neighbor approximation for the hopping integrals on a square lattice.

If a metallic tip is placed at the point $\mathbf{m}$ above the surface of a sample, the STM current $I(V, \mathbf{m})$ creates an electron (or hole) at this point. Applying the Fermi-Dirac golden rule and the Bogoliubov transformation, Eq.(4,5), and assuming that the temperature is much lower than Δ_p/k_B one readily obtains the tunnelling conductance

$$\sigma(V, \mathbf{m}) \equiv \frac{dI(V, \mathbf{m})}{dV} \propto \sum_{\nu} |u_\nu(\mathbf{m})|^2 \delta(eV - \epsilon_\nu), \tag{18}$$

which is a local excitation DOS. The solution Eq.(9) leads to a spatially modulated conductance,

$$\sigma(V, \mathbf{m}) = \sigma_{reg}(V) + \sigma_{mod}(V)\cos(\pi m_x + \pi m_y). \tag{19}$$

The smooth (regular) contribution is

$$\sigma_{reg}(V) = \sigma_0 \sum_{\mathbf{k}, r=1,2} (u_{r\mathbf{k}}^2 + \tilde{u}_{r\mathbf{k}}^2)\delta(eV - \epsilon_{r\mathbf{k}}), \tag{20}$$

and the amplitude of the modulated contribution is

$$\sigma_{mod}(V) = 2\sigma_0 \sum_{\mathbf{k}, r=1,2} u_{r\mathbf{k}} \tilde{u}_{r\mathbf{k}} \delta(eV - \epsilon_{r\mathbf{k}}), \tag{21}$$

where σ_0 is a constant. Conductance modulations reveal a checkerboard pattern, as the Bose condensate itself, Eq.(2),

$$\frac{\sigma - \sigma_{reg}}{\sigma_{reg}} = A\cos(\pi m_x + \pi m_y), \tag{22}$$

where

$$A = 2\sum_{\mathbf{k}} \left[u_{1\mathbf{k}}\tilde{u}_{1\mathbf{k}}\delta(eV - \epsilon_{1\mathbf{k}}) + u_{2\mathbf{k}}\tilde{u}_{2\mathbf{k}}\delta(eV - \epsilon_{2\mathbf{k}})\right] / \sum_{\mathbf{k}} \left[(u_{1\mathbf{k}}^2 + \tilde{u}_{1\mathbf{k}}^2)\delta(eV - \epsilon_{1\mathbf{k}}) + (\tilde{u}_{2\mathbf{k}}^2 + u_{2\mathbf{k}}^2)\delta(eV - \epsilon_{2\mathbf{k}})\right]$$

is the amplitude of modulations depending on the voltage V and temperature. An analytical result is obtained in the strong-coupling limit with the excitation spectrum given by Eqs. (16,17) for the voltage near the threshold, $eV \approx \Delta_p$. In this case only states near bottoms of each excitation band, Fig.1, contribute to the integrals in Eq.(22), so that

$$\tilde{u}_{1\mathbf{k}} = \frac{\xi_{\mathbf{k}} - \epsilon_{1\mathbf{k}}}{\epsilon_{1\mathbf{k}} - \xi_{\mathbf{k}-\mathbf{g}}} u_{1\mathbf{k}} \approx -u_{1\mathbf{k}}\frac{\Delta_c^2}{\mu w} \ll u_{1\mathbf{k}}, \tag{23}$$

and

$$u_{2\mathbf{k}} = \frac{\xi_{\mathbf{k}-\mathbf{g}} - \epsilon_{2\mathbf{k}}}{\epsilon_{2\mathbf{k}} - \xi_{\mathbf{k}}} \tilde{u}_{2\mathbf{k}} \approx -\tilde{u}_{2\mathbf{k}}\frac{\Delta_c^2}{\mu w} \ll \tilde{u}_{2\mathbf{k}}. \tag{24}$$

Substituting these expressions into A, Eq.(22), yields in the lowest order of Δ_c,

$$A \approx -\frac{2\Delta_c^2}{\mu w}. \tag{25}$$

The result, Eq.(22) generally agrees with the STM experiments [24, 25, 26, 36, 37], where the spatial checkerboard modulations of σ were observed in a few cuprates. The period of the modulations was found either commensurate or non-commensurate depending on a sample composition. In our model the period is determined by the center-of mass wave vectors $\mathbf{K}$ of the Bose-condensed preformed pairs. While the general case has to be solved numerically [38], the perturbation result, Eq.(22) is qualitatively applied for any $\mathbf{K}$ at least close to T_c, where the coherent gap is small, if one replaces $\cos(\pi m_x + \pi m_y)$ by $\cos(K_x m_x + K_y m_y)$. The period of DOS modulations does not depend on the voltage in the perturbation regime, as observed [39], but it could be voltage dependent well below T_c, where higher powers of Δ_c are important. Different from any other scenario, proposed so far [40], the hole density, which is about twice of the condensate density at low temperatures, is spatially modulated with the period determined by the inverse wave vectors corresponding to the center-of-mass pair band-minima. This 'kinetic' interpretation of charge modulations in cuprates, originally proposed [32] before STM results became available, is consistent with the inelastic neutron scattering, where incommensurate inelastic peaks were observed *only* in the *superconducting* state [41]. The vanishing at T_c of the incommensurate peaks is inconsistent with any other stripe picture, where a characteristic distance needs to be observed in the normal state as well. In our model the checkerboard charge modulations should disappear above T_c, where the Bose-condensate evaporates and the coherent gap $\Delta_c(T)$ vanishes, so that $A = 0$ in Eq.(22). While some STM studies [39] report incommensurate DOS modulations somewhat above T_c, they might be due to extrinsic inhomogeneities. In particular, preformed pairs in the surface layer could bose-condense at higher temperatures compared with the bulk T_c. Our model is microscopically derived using the strong-coupling (bipolaron) extension of the BCS theory [8]. If the electron-phonon interaction is strong, such that the BCS coupling constant $\lambda > 1$, electrons form bipolarons above T_c, which are Bose condensed below T_c. The polaron bandwidth is exponentially reduced, which explains a low estimate of the Fermi energy using the experimental London penetration depth in cuprates [28]. Evidence for an exceptionally strong electron-phonon interaction in high-temperature superconductors is now overwhelming (see, for example, [42, 43]). Yet, generally, the model describes charge modulations due to the Bose condensation with non-zero center-of-mass momenta of preformed pairs formed by any pairing interaction.

In conclusion, I solved BdG equations with the periodic off-diagonal potential caused by the Bose condensation of preformed pairs with non-zero center-of-mass momenta, and found the checkerboard modulations of the single-particle DOS similar to those observed in cuprates. The main assumption that the ground state of superconducting cuprates is the Bose-Einstein condensate of preformed pairs, is supported by a growing number of other experiments [8]. The model links charge orders, pairing, and pseudo-gaps as manifestations of a strong attractive interaction in narrow bands.

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