Incommensurate Charge and Spin Fluctuations in d-wave Superconductors

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We show analytic results for the irreducible charge and spin susceptibilities, \(\chi_0(\omega, \mathbf{Q})\), where \(\mathbf{Q}\) is the momentum transfer between the nodes in d-wave superconductors. Using the BCS theory and a circular Fermi surface, we find that the singular behavior of the irreducible charge susceptibility leads to the dynamic incommensurate charge collective modes. The peaks in the charge structure factor occur at a set of wave vectors which form an ellipse around \(\mathbf{Q}_s = (\pi, \pi)\) and \(\mathbf{Q}_0 = (0, 0)\) in momentum space with momentum dependent spectral weight. It is also found that, due to the non-singular irreducible spin susceptibility, an extremely strong interaction via random phase approximation is required to support the magnetic peaks near \(\mathbf{Q}_s\). Under certain conditions, the peaks in the magnetic structure factor occur near \(\mathbf{Q} = (\pi, (1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi)\).

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The neutron scattering measurements provide the direct information about the wavevector and frequency dependence of the dynamic spin susceptibility. On the other hand the inelastic x-ray or electron scattering can measure the dynamic charge susceptibility. These informations are particularly important in the cuprate superconductors because of the intimate interplay between the spin and charge dynamics which may be related to the mechanism of the high temperature superconductivity.

The neutron scattering experiments on \(La_{2-x}Sr_xCuO_4\) (LSCO) \(^\[1\,2\]\) found the inelastic incommensurate peaks near \(\mathbf{Q}_s = (\pi, \pi)\) in the superconducting state as well as in the normal state \(^\[3\]\). The collective modes occur at \(\mathbf{Q} = (\pi, (1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi)\) for low frequencies. Recently, a lot of effort was put forward to investigate the spin dynamics in \(YBa_2Cu_3O_7-y\) (YBCO) \(^\[3,4\]\). In earlier works, the incommensurate peaks were reported in the scan along the zone diagonal direction \(^\[5\]\). Later it was found that the locations of the higher intensity peaks are the same as those of LSCO; \((\pi, (1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi)\) \(^\[6\]\).

On the theoretical front, there have been two different approaches to explain the incommensurate peaks. The numerical studies of one- and three-band Hubbard models found that the incommensurate peaks occur as the dynamical response of a spatially homogeneous system with a nearly nested Fermi surface. \(^\[5\]\) It was also pointed out that the nesting peaks are at \((\pi(1 \pm \delta), \pi(1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi(1 \mp \delta))\) in YBCO due to the 45 degree rotation of the Fermi surface. \(^\[7\]\) From a different viewpoint, it was proposed that the magnetic incommensurate peaks are induced by the dynamic charge stripes in a spatially inhomogeneous system. \(^\[7\]\) The static charge ordering can occur in the relatively bad metal due to the pinning of the charge stripes. On the other hand, the dynamic fluctuations of the charge stripes result in the phase coherence of the superconducting state.

Recently, Tranquada \(et\ al\) found, in the neutron diffraction measurements, the incommensurate elastic magnetic peaks at \(\mathbf{Q} = (\pi, (1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi)\) in \(La_{1.6-x}Nd_{0.4}Sr_xCuO_4\). \(^\[8\]\) They interpreted these peaks as the evidence for the static stripe order of charge and spins. It was also shown that the superconducting transition temperature increases as the peak splitting parameter, \(\delta\), increases. This may imply that the charge and spin stripes are intimately related to the superconductivity.

These elastic and inelastic neutron scattering experiments motivated us to investigate the incommensurate charge and spin fluctuations in the superconducting state. In particular, since the inelastic experiment on YBCO found the incommensurate peaks at the same positions as those of LSCO, these may not be related to the details of the Fermi surface shape. Thus, as a first step, it is worthwhile to understand the charge and spin dynamics within the BCS theory with a simple Fermi surface. This would provide an important information which should be compared with any new theoretical proposal-either Fermi surface effect or the charge stripes.

In this paper, we compute analytically the irreducible charge and spin susceptibilities in the BCS d-wave superconducting state with a circular Fermi surface. We found that the incommensurate charge collective modes occur at a set of wave vectors. The wave vectors form an ellipse around \(\mathbf{Q}_s = (\pi, \pi)\) in momentum space. The spectral weight also depends on the wave vectors. It is found that the incommensurate spin collective mode can occur near \(\mathbf{Q} = (\pi, (1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi)\) only when an extremely strong interaction is assumed via the random phase approximation. Using the analytic form of the irreducible spin susceptibility, we also examine the NMR relaxation rate \(1/T_1\) for low temperatures and found that \((T_1 T)^{-1} \sim T^2/(\Delta E_F)^2\). We also analyze the quasiparticle lifetime for small frequencies at the nodes; \(1/\tau \sim V^2 \omega^3/(\Delta E_F)^2\), where \(V\) is the interaction.
Let us consider the simplest model for the electronic energy with a circular Fermi-surface of radius $k_F$.

$$\xi_k = \epsilon_k - \mu = \frac{k^2}{2m} + \frac{k_y^2}{2m} - \frac{k_z^2}{2m},$$

(1)

The lowest order charge, $\chi_0^c$, and spin susceptibilities, $\chi_0^s$, for momentum $Q$ and energy $\omega$ at $T = 0$ are given by

$$\chi_0^c(\omega, Q) = -\frac{1}{2} \sum_k \left(1 - \frac{\xi_k + q \xi_k + \Delta_k + q \Delta_k}{E_{k+Q} E_k}\right) \left(\frac{1}{\omega + E_{k+Q} + E_k + i\eta} - \frac{1}{\omega - E_{k+Q} - E_k + i\eta}\right),$$

(2)

$$\chi_0^s(\omega, Q) = -\frac{1}{2} \sum_k \left(1 - \frac{\xi_k + q \xi_k + \Delta_k + q \Delta_k}{E_{k+Q} E_k}\right) \left(\frac{1}{\omega + E_{k+Q} + E_k + i\eta} - \frac{1}{\omega - E_{k+Q} - E_k + i\eta}\right),$$

(3)

where $E_k = \sqrt{\xi_k^2 + \Delta_k^2}$ with $\Delta_k = \Delta \cos 2\phi$. The different coherence factors in the charge and spin susceptibilities in Eq. (3) come from the fact that the magnetic scattering is odd with respect to the time reversal symmetry while the charge scattering is even.

Let us examine the momentum transfer near $Q_x = (\sqrt{2}k_F, \sqrt{2}k_F)$ or $(\pi, \pi)$ shown in Fig. 1. Near the nodes, we expand the electronic dispersion relation and the amplitude of the gap. We find the following for $|p| + |q| < k_F/\sqrt{2}$.

$$\xi_k \simeq -\sqrt{2}v_F(p_x + p_y), \quad \Delta_k \simeq -\sqrt{2}\Delta(p_x - p_y)/k_F,$$

$$\xi_{k+Q} \simeq \sqrt{2}v_F(p_x + q_x + p_y + q_y), \quad \Delta_{k+Q} \simeq \sqrt{2}\Delta(p_x + q_x - p_y - q_y)/k_F.$$  

(4)

Here $p = k - k_0$ and $q = Q - Q_x$, where $k_0$ denotes the node of d-wave superconductors. Note also that one obtains the same dispersion relations near $(\pi, \pi)$ in the tight binding model with $1/m = ta^2$ and $\sqrt{2}k_F = \pi/2a$ [11], where $t$ is the hopping amplitude and $a$ is the lattice spacing. Then, the Dirac dispersion for the quasiparticle is found near the nodes:

$$E_k = \sqrt{2E_F^2 p_+^2 + 2\Delta^2 p_-^2},$$

$$E_{k+Q} = \sqrt{2E_F^2 (p_x + q_x)^2 + 2\Delta (p_- + q_-)^2},$$

(5)

where

$$p_\pm = (p_x \pm p_y)/k_F, \quad q_\pm = (q_x \pm q_y)/k_F.$$  

(6)

Evaluating Eq. (2) with Eq. (3), the imaginary part of the charge susceptibilities is found for $\omega_\eta \leq \omega < \Delta$,

$$\text{Im} \chi_0^c(\omega, Q) = \frac{1}{32\Delta E_F} \frac{\omega^2 - (\sqrt{2}E_F q_\eta)^2}{\sqrt{\omega^2 - \omega_\eta^2}},$$

(7)

where

$$\omega_\eta^2 = 2E^2 q_\eta^2 + 2\Delta^2 q_-^2.$$  

(8)

It can be seen in Eq. (3) that the charge susceptibility diverges as $\omega$ approaches $\omega_\eta$ and has the following scaling form:

$$\text{Im} \chi_0^c(\omega, Q) = \frac{\omega}{32\Delta E_F} f\left(\frac{\sqrt{2}E_F q_+}{\omega}, \frac{\sqrt{2}\Delta q_-}{\omega}\right),$$

(9)

where

$$f(a, b) = \frac{1 - a^2}{\sqrt{1 - a^2 - b^2}}.$$  

(10)

Note that the incommensurate collective modes occur with a set of wave vectors. The wave vectors form an ellipse around $Q_x = (\pi, \pi)$ in momentum space for the energy $\omega_\eta$. The eccentricity of the ellipse is determined by the
ratio of $\Delta$ and $E_F$. Since $E_F$ is typically larger than $\Delta$ ($E_F/\Delta = 5 \sim 10$), the ellipse is elongated along the direction perpendicular to the zone diagonal. This result is a consequence of the anisotropic Dirac dispersion relation of the quasiparticles near the node. The Eq. (10) implies that the spectral weight of the incommensurate collective mode depends on the wave vectors. In particular, the spectral weight of the collective mode vanishes at two points in the zone diagonal direction. It is found that the charge susceptibility in the random phase approximation, $\chi^c(\omega, q) = \chi^c_0(\omega) \frac{1}{\pi} \left( 1 + \frac{1}{q^a q^b} \right)$, is almost the same as the irreducible susceptibility, $\chi^c_0(\omega)$, for quite large range of the interaction strength if one assumes $V(\omega, q) = V$. If $E_F \sim 10\Delta$, $V \sim E_F$, and $\Delta \sim 30meV$, the correction to the position of the singularity, $\omega_q \sim 20meV$, is of order of $10^{-2}meV$. Thus $\chi^c_0$ is enough to describe the charge susceptibility as far as the most singular part is concerned.

In the lattice, the Umklapp scattering is present and it leads to an additional contribution to the susceptibility. This contribution provides another collective modes with the energy, $\omega_q = 2E_F q^2 + 2\Delta q^2$. As a result, the imaginary part of the susceptibility becomes

$$\text{Im}\chi^c_0(\omega, q) = \frac{1}{32\Delta E_F} \left[ \frac{\omega^2 - (\sqrt{2}E_Fq_+)^2}{\omega^2 - \omega_q^2} + \frac{\omega^2 - (\sqrt{2}E_Fq_-)^2}{\omega^2 - \omega_q^2} \right].$$

(11)

One can see that the shape of the structure factor depends on the ratio of the Fermi energy, $E_F$, and the maximum amplitude of the gap, $\Delta$. In Fig. 2, we show the imaginary part of the charge susceptibility for $E_F/\Delta = 7$ and 2. It is usually assumed that the ratio of the Fermi energy and the gap is order of 5 $\sim 10$ because of the short coherence length though it has not been confirmed. In a recent tunneling experiment, it was claimed that the ratio might be order of one in the case of Bi2Sr2CaCu2O8+q (BiSCCO). As $E_F/\Delta$ gets bigger, the anisotropy of the structure factor becomes stronger as shown in Fig. 2. If one could detect the charge collective modes by inelastic x-ray or electron scattering, it would provide the ratio of the Fermi energy and the gap of the cuprates.

The charge susceptibility in the real space is found from the Fourier transform of Eq. (7) as

$$\text{Im}\chi^c_0(\omega, x, y) = \frac{1}{64\sqrt{2}\pi E_F} \frac{(\omega r)^{3/2}}{r^3} J_{1/2}(\omega r) + \left( \frac{1}{2} - r_+^2 J_{1/2}(\omega r) + \frac{1}{2} - r_-^2 J_{1/2}(\omega r) \right).$$

(12)

where $J_r(x)$ is the Bessel function and $r^2 = r_+^2 + r_-^2$. Here $r_+ = (x + y)/(2\sqrt{2}E_F)$ and $r_- = (x - y)/(2\sqrt{2}\Delta)$. Since the periodicity of the oscillation depends on the ratio $E_F/\Delta$, the shape of the structure factor in the real space is elongated along the $r_-$ direction for $E_F > \Delta$ shown in Fig. 3.

Let us now study the spin susceptibility for the momentum transfer near $Q_\pi = (\pi, \pi)$. We found

$$\text{Im}\chi^s_0(\omega, Q) = \frac{1}{16\Delta E_F} \sqrt{\omega^2 - \omega_q^2},$$

(13)

It can be clearly seen in Eqs. (7) and (13) that the spin susceptibility is smooth while the charge susceptibility diverges as mentioned above. The difference between the charge and spin susceptibilities comes from the coherence factors. The spin susceptibility has the maximum at $Q_\pi$ ($\omega_q = 0$) for a given frequency $\omega$ and decreases as $\omega_q$ approaches $\omega$. One can show that when $\omega_q$ becomes larger than $\omega$ the imaginary part of the irreducible spin susceptibility is negligible. On the other hand, the real part of the irreducible spin susceptibility is $(16\Delta E_F)^{-1}\sqrt{\omega^2 - \omega_q^2}$ for $\omega_q > \omega$.

As a result, the spin susceptibility in the random phase approximation, $\chi^s(\omega, Q) = \chi^s_0(\omega, Q) / [1 + J(\omega, Q)\chi^s_0(\omega, Q)]$, can support the collective modes if the interaction $J(\omega, Q)J > 16E_F$. The shape of the spin structure factor depends on the ratio $E_F/\Delta$. As mentioned above, the Umklapp scattering provides the additional contribution to the spin susceptibility. After including the Umklapp scattering, we find the following results. The positions of the magnetic peaks are near $(\pi, \pi(1 \pm \delta))$ and $(\pi(1 \pm \delta), \pi)$, where $\delta$ (in units of $2\pi/a$) is given by

$$\delta = \frac{1}{2} \sqrt{\omega^2 - (16\Delta E_F/J)^2} / \sqrt{E_F^2 + \Delta^2}.$$  

(14)

If $\omega < (16\Delta E_F/J)$ and $E_F/\Delta \sim 5 - 10$, the peak splitting parameter, $\delta$, is order of 0.1 and almost independent of the frequency. In the experiments, $\delta$ seems to be frequency independent [12]. Our results imply that the interaction strength, $J$, and the ratio of the Fermi energy and the amplitude of the gap determine the positions of the peaks for low frequencies. The weights of the magnetic peaks are also determined by the interaction strength. For $E_F/\Delta \sim 1$, the magnetic peaks form a circle with the radius $\delta$ given by Eq. (14) which may happen in BiSCCO. However, it is known that the interaction is typically smaller than the Fermi energy in the superconducting state, so that the condition
We can also compute the quasiparticle scattering rate due to the charge fluctuations. We consider only the charge fluctuations because these are more stronger than those of the spin. The lowest order self-energy can be obtained from

\[ \Sigma = iV^2 \int \frac{d^2Q}{(2\pi)^2} \int \frac{d\nu}{2\pi} \frac{\omega + \nu}{(\omega + \nu)^2 - E_{k+Q}^2 + i\eta} \int \frac{dx}{\pi} \frac{\Im \chi_0^{c}(x,Q)}{\omega - x + i\eta}, \]  

(17)

The imaginary part of the self energy in the \( I \) space is found at the node, \( \mathbf{k}_0 \), as

\[ \Im \Sigma(t,\mathbf{k}_0) = V^2 \int_0^{\infty} \frac{dx}{2} \int \frac{d^2Q}{(2\pi)^2} \Im \chi_0^{c}(x,Q) [\delta(\omega + x + E_{k_0+Q}) + \delta(\omega - x - E_{k_0+Q})] \]

\[ \simeq V^2 \frac{\omega^3}{(E_F \Delta)^2}. \]  

(18)

It can be shown that the self energies in the \( \tau_1 \) and \( \tau_3 \) spaces have larger power in \( \omega, \mathcal{O}(\omega^3) \), compared to \( \omega^3 \). Thus, the leading contribution to the quasiparticle scattering rate, \( 1/\tau(\omega) \), is given by

\[ 1/\tau(\omega) \simeq V^2 \frac{\omega^3}{(E_F \Delta)^2}. \]  

(19)

In summary, we presented the analytic results for the dynamic charge and spin susceptibilities near \( \mathbf{Q}_x = (\pi, \pi) \) and \( \mathbf{Q}_0 = (0, 0) \) in the BCS d-wave superconducting state. We found that the presence of the d-wave node leads to the incommensurate charge peaks for a set of wavevectors forming an ellipse near \( \mathbf{Q}_x \) and \( \mathbf{Q}_0 \). We also showed that incommensurate magnetic peaks near \( \mathbf{Q}_x \) can be obtained through the random phase approximation if the extremely strong interaction is assumed. When the Umklapp process is included, higher intensity of the magnetic structure factor would appear at \((\pi, \pi(1 \pm \delta))\) and \((\pi(1 \pm \delta), \pi)\) where the incommensurate magnetic peaks were found in the experiments on \( \text{LSCO} \) and \( \text{YBCO} \). We also compute the NMR relaxation rate going as \( T^3 \) and the quasiparticle scattering rate as \( \omega^3 \) in the superconducting state.

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for the interaction strength to support the collective mode is not realistic. Therefore, it suggests that either the charge fluctuations induce the anomalous interaction or another ingredient is needed to explain the incommensurate magnetic peaks found in the experiments.

In the low energy limit, the susceptibilities for the momentum transfer near \( \mathbf{Q}_0 = (0, 0) \) are also interesting. It is found that

\[ \Im \chi_0^{em}(\omega, \mathbf{Q}) = \frac{1}{32\Delta E_F} \frac{\omega^2 - (\sqrt{2}\Delta\eta-\epsilon_0)^2}{\sqrt{\omega^2 - \omega_\eta^2}}, \]

\[ \Im \chi_0^{sm}(\omega, \mathbf{Q}) = \frac{1}{32\Delta E_F} \frac{\omega_\eta^2}{\sqrt{\omega^2 - \omega_\eta^2}}, \]  

(15)

where \( \mathbf{q} = \mathbf{Q} - \mathbf{Q}_0 \). Note that both the irreducible charge and spin susceptibilities are singular as \( \omega \) approaches \( \omega_\eta \). However, these singularities in the long wavelength limit are likely to be weakened by the vertex corrections. At relatively high frequencies \( \sim 2\Delta \) the charge and spin collective modes were previously found near \( \mathbf{Q} = (2k_F, 0) \) and \( (k_F, k_F) \) respectively.

Using the above information, we compute the lowest order contribution to the NMR relaxation rate \( 1/T_1 \) assuming that the scattering near \( \mathbf{Q}_x \) dominates:

\[ \frac{1}{T_1 T} = \lim_{\omega \to 0} \frac{1}{T} \int \frac{d^2Q}{(2\pi)^2} \Im \chi_0^{em}(\omega, \mathbf{Q}) \simeq \frac{T^2}{(\Delta E_F)^2}. \]  

(16)

Thus the relaxation rate \( 1/T_1 \) goes as \( T^3 \) which is consistent with the numerical calculations and an experiment for a range of the temperatures.

We can also compute the quasiparticle scattering rate due to the charge fluctuations. We consider only the change fluctuations because these are more stronger than those of the spin. The lowest order self-energy can be obtained from

\[ \Sigma = iV^2 \int \frac{d^2Q}{(2\pi)^2} \int \frac{d\nu}{2\pi} \frac{\omega + \nu + \Delta_{k+Q} H_{0} + \Delta_{k+Q} H_{1} E_{k+Q}^2 + i\eta}{(\omega + \nu)^2 - E_{k+Q}^2 + i\eta} \int \frac{dx}{\pi} \frac{\Im \chi_0^{c}(x,Q)}{\omega - x + i\eta}, \]  

(17)

The imaginary part of the self energy in the \( I \) space is found at the node, \( \mathbf{k}_0 \), as

\[ \Im \Sigma(t,\mathbf{k}_0) = V^2 \int_0^{\infty} \frac{dx}{2} \int \frac{d^2Q}{(2\pi)^2} \Im \chi_0^{c}(x,Q) [\delta(\omega + x + E_{k_0+Q}) + \delta(\omega - x - E_{k_0+Q})] \]

\[ \simeq V^2 \frac{\omega^3}{(E_F \Delta)^2}. \]  

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It can be shown that the self energies in the \( \tau_1 \) and \( \tau_3 \) spaces have larger power in \( \omega, \mathcal{O}(\omega^3) \), compared to \( \omega^3 \). Thus, the leading contribution to the quasiparticle scattering rate, \( 1/\tau(\omega) \), is given by

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FIG. 1. The circular Fermi surface with a radius \(k_F\) illustrating the wave vector \(Q_x\). The diamond represents the tight binding Fermi surface at the half-filling. The node positions \((\pm k_F/\sqrt{2}, \pm k_F/\sqrt{2})\) in the case of the circular Fermi surface correspond to \(k_0 = (\pm \pi/2, \pm \pi/2)\) in the tight binding model. As a result, the momentum transfer \((\sqrt{2}k_F, \sqrt{2}k_F)\) corresponds to \(Q_x = (\pi, \pi)\).

FIG. 2. The charge susceptibility for (a) \(E_F/\Delta = 7\) and (b) 2 with the frequency \(0.6\Delta\). \(q_+\) and \(q_-\) are in units of \(2\pi/a\).

FIG. 3. The charge susceptibility in the real space for \(E_F/\Delta = 7\) and the frequency \(0.6\Delta\). \(x\) and \(y\) are in units of \(a\).
Fig. 2
Fig. 3