Charge fluctuations in cuprate superconductors

Zhongqing Wu[1] and Xuanjia Zhang[2]
[1]*Department of Physics,Tsinghua University, Beijing 100084,China*
[2]*Department of Physics, Zhejiang University, Hangzhou 310027, China*
(Dated: January 26, 2014)

The effect of the lattice periodic potential on superconductivity which was ignored by BCS theory has been investigated. According to the effective mass approximation of band theory, the effect of lattice periodic potential can be embodied in the effective mass m^* of the Ginzburg-Landau (GL) equations. A special property of m^* is that it can be negative. Negative effective mass leads to many unusual phenomena. The superconducting order parameter shows the period distribution. Its modulate wavevector is proportional to the condensed carrier density, which explains the linear relation between the magnetic peaks displacement ϵ and x for $La_{2-x}Sr_xCuO_4$. The superconducting phase is always local and separated originally and evolves into global superconducting phase at the certain pairs concentration, which explains why the cuprate superconductors must be insulator at low doped. The doped concentrations of insulator to superconductor transition for $La_{2-x}Sr_xCuO_4$ is consistent with the experiment results. The relation of the superconducting gap (SG) and the pseudogap (PG) was discussed.
Keywords: Stripes; Ginzburg-Landau theory; Superconductivity; Charge fluctuations.

Since the high temperature superconductor (HTS) was found in 1986, HTS has been one of the most attractive field in condensed matter physics. Almost any physical properties about HTS have been intensely studied and many anomalous properties have been found. which make many people believe that the BCS theory and Fermi liquid theory are no longer fit for HTS. The most striking of all anomalous properties are the stripe phase and pseudogap (PG). Unlike conventional metals in which the charge distribution is homogenous, the charge carriers are segregated into one-dimensional stripe in HTS, which was predicted by t-j model[1] and then supported by many experiment[2,3,4,5,6,7,8]. The relations of many physical properties such as Knight Shifts[9], NMR relaxation rates[10], DC conductivity[11], with the temperature in normal state of HTS do not conform to Fermi liquid theory, which has been valid in the conventional metal. The temperature at which these physical properties begin to depart from Fermi liquid theory are almost the same. Some experiments such as angle-resolved photoemission, tunnelling spectroscopy indicate that the density of states (DOS) in Fermi surface begin to decrease and an PG open at this temperature. The PG is of the same size and k dependence as superconducting gap (SG). The microscope mechanism of PG is still unclear. In superconducting states of HTS, anomalous properties have also been found. For example, the ratio of the energy gap in 0K $\Delta(0)$ with the superconducting phase transition temperature T_c ($2\Delta(0)/k_BT_c \approx 8 \sim 9$) far more than BCS theory' prediction ($2\Delta(0)/k_BT_c = 3.53$)

Some people believe that these anomalous properties result from the correlation effect between electrons, which has been overlook by BCS and Fermi liquid theory. Many model have been proposed for the study of correlation effects. However up to now, there is a lack of the breakthrough in this aspect.

Another important effect that has also been overlook by BCS theory is the lattice periodic potential. The band theory that describes the effect forms the basis of the modern theory of electron in solids. According to the effective mass approximation of band theory, the effect can be included in BCS theory if we substitute the effective mass m^* for mass of bare electron. m^* should be negative for HTS, as will be discussed in the end of our paper. Since Ginzburg-Landau (GL) equations can be derived from the BCS theory, the mass in equation should be also negative for HTS. Negative effective mass will lead to extraordinary spatial distribution of the order parameter, which can well illuminate many anomalous properties.

Localized holes organize into one-dimensional structures, which has been observed in HTS in many experiments[3,7,8,12,13]. The spin modulation also shows one-dimensional properties. Neutron scattering studies reveal that there are two types of twin domains and spin modulation is one dimensional in each domain for $La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_6.6$[4,14]. We think that these one-dimensional properities result from the one-directional modulation of order parameter. Then with no magnetic field considered, the first equation of GL can be written as

$$\alpha\psi + \beta|\psi|^2\psi - \frac{\hbar^2}{2m_l^*}\frac{\partial^2\psi}{\partial l^2} = 0, \tag{1}$$

where m_l^* is the component of the effective mass in l direction, $\psi = \sqrt{n_s(r)}e^{i\phi(r)}$ is the order parameter, which only vary along l and is equal in direction perpendicular to l, where $n_s(r)$ is the local condensed carrier density and ϕ is the phase of the effective wave function.

Taking $f = \frac{\psi}{\psi_0}$ as the dimensionless effective wave function where $|\psi_0|^2 = -\frac{\alpha}{\beta}$, under the condition $m_l^* < 0$, the equation (1) reduces to

$$\xi^2\frac{\partial^2 f}{\partial l^2} = f(1-f^2), \tag{2}$$

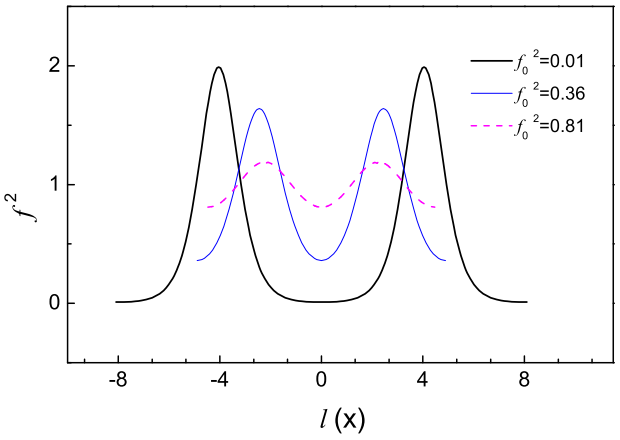

FIG. 1: $f^2 = \frac{|\psi|^2}{|\psi_0|^2}$ as a function of space coordinate l (in units of ξ) for $f_0^2 = 0.01, 0.36, 0.81$

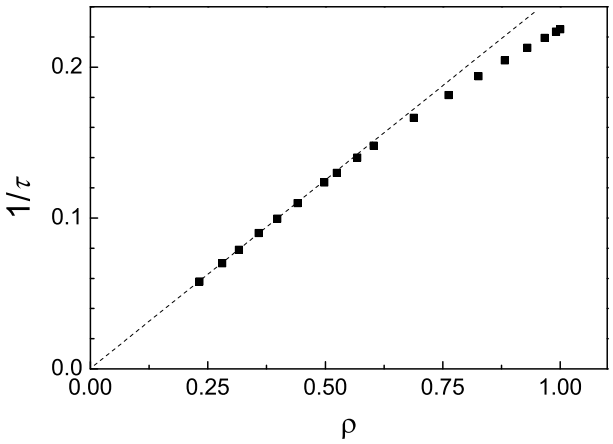

FIG. 2: The dependence of inverse of charge modulation period $\frac{1}{\tau}$(in units of $\frac{1}{\xi}$) on the condensed carrier density ρ (in units of $|\psi_0|^2$).

where $\xi^2 = \frac{\hbar^2}{|2m_l^*\alpha|}$. The corresponding equation for $m_l^* > 0$ can be obtain as long as the left side of equation (2) multiply by -1. As will be shown later, just above difference between equation for $m_l^* > 0$ and $m_l^* < 0$ leads to that they have very different spatial distribution of the order parameter. Since the coefficient of each term in equation (2) does not include the variable l, the origin can be arbitrary for the infinity system. Therefore we choose the origin where f has the minimum. Then the boundary condition is

$$f(0) = f_0,$$

$$\left.\frac{\partial f}{\partial l}\right|_{l=0} = 0. \tag{3}$$

The dependence of f^2 on the space coordinate l is shown in Fig. 1. The spatial distribution of the order parameter is sensitive to f_0^2. When f_0^2 is close to 1, the condensed carrier density fluctuation is similar to the charge density wave. When f_0^2 is close to 0, the phase separation is obvious. The condensed carriers get together and form periodically charged stripes. Between the charged stripes are regions where few condensed carrier can be found and the microscope composition is similar with the parent compounds of HTS. We call these regions antiferromagnetic (AF) stripes. It is shown that AF stripes are wider than charge stripes when $f_0^2 = 0.01$ in Fig. 1, which is more distinct when further decreasing f_0^2. The stripes have been observed by many experiments in HTS and their structure change with the doped concentration. The low-energy neutron-scattering studies performed on $La_{2-x-y}Nd_ySr_xCuO_4$ by Yamada *et al*[5] have demonstrated that the charge modulation wavevector ϵ initially increases linearly with x before saturating for $x > 1/8$.

In order to compare with the results of the low-energy neutron-scattering studies, we investigated the relation of the average condensed carrier density with the order parameter modulation wavevector. The average condensed carrier density is defined as

$$\rho = \frac{1}{\tau}\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} |\psi|^2 dl = \frac{1}{\tau}|\psi_0|^2 \int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} |f|^2 dl, \tag{4}$$

where τ is the order parameter modulation period. The dependence of ρ on $\frac{1}{\tau}$ is shown in Fig. 2. ρ varies linearly with $\frac{1}{\tau}$ as

$$\rho = \frac{\xi|\psi_0|^2}{k}\frac{1}{\tau} \tag{5}$$

for $\rho < 0.6|\psi_0|^2$, where $k = \frac{4}{15}$ is the slope of the broken line. Because that the modulation wavevector ϵ is proportional to the inverse of the charge modulation period and the average condensed carrier density ρ is proportional to Sr concentration x for $La_{2-x}Sr_xCuO_4$ if all of carrier condensed, the equation (5) denotes

$$\epsilon \propto x \tag{6}$$

when $\rho < 0.6|\psi_0|^2$. Furthermore, the modulation wavevector ϵ reaches the maximum when the order parameter is homogenous distribution. These results accord well with the neutron scattering measurements on $La_{2-x-y}Nd_ySr_xCuO_4$[5,6].

Fig. 1 indicates that there are two kinds of the spatial distribution of the condensed carriers density: One is the global distribution, the other shows that the condensed carriers is local and separate each other. The kind of the distribution can be determined by whether f_0^2 is close to 0 and should be close correlative with the average condensed carrier density ρ. The relation of f_0^2 with ρ is shown in Fig. 3. When ρ is smaller than $\rho_c = 0.35|\psi_0|^2$, f_0^2 is almost 0 and the superconducting phase is local

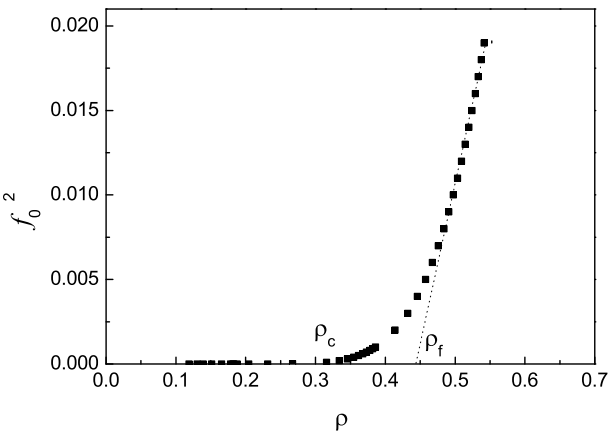

FIG. 3: f_0^2 as a function of the condensed carrier density ρ (in units of $|\psi_0|^2$)

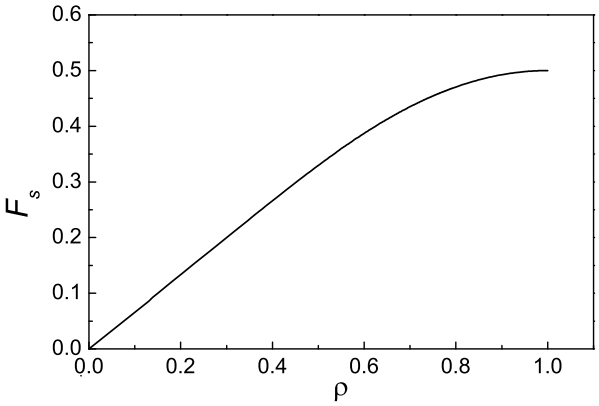

FIG. 4: The dependence of the free energy density F_s (in units of $\alpha|\psi_0|^2$) on the condensed carrier density ρ (in units of $|\psi_0|^2$).

and separated each other, which leads to that the system does not show global superconductivity. It is obvious the temperature of the global superconductivity T_c is determined by the value of f_0^2 at ground state. Expanding T_c with the value of f_0^2 at ground state by Thaler Formula, we have that T_c is proportional to f_0^2 when $f_0^2 << 1$. Because all of carrier condensed at ground state, so $\rho \propto x$. Therefore, in fact, Fig. 3 reveals the dependence of T_c on Sr concentration x. ρ_c just corresponds to the Sr concentration x_c of non-superconductor to superconductor transition. According to the fact that modulated wave vector ϵ has maximum at $\rho = |\psi_0|^2$ in our result and is saturating at $x = 1/8$ by the experiment[5], we evaluated x_c to be about 0.044 for $La_{2-x}Sr_xCuO_4$.

It is well known that the free energy of system must decrease with increasing the condensed carrier density. Obviously, we should make sure whether our free energy meets the above demand. The free energy density of the system

$$F_s = \frac{1}{\tau}\int_{-\frac{\tau}{2}}^{\frac{\tau}{2}} [\alpha|\psi|^2 + \frac{\beta}{2}|\psi|^4 + \frac{1}{2m_l^*}|(-i\hbar\nabla)\psi|^2]dl, \quad (7)$$

where the free energy density in the normal state is taken as zero. The relation of F_s (in units of $\alpha|\psi_0|^2$) and ρ is shown in Fig. 4. F_s decrease monotonously with increasing the condensed carrier density ρ(note: α is negative). It implies that more and more carriers condensed with decreasing the temperature. An intriguing phenomenon is that F_s is weak-dependence on ρ when $\rho \approx 1$, which means that the electron pairs can be excited without energy. Namely, the energy gap has node. At the conventional superconductor, the energy gap is non-zero and manifests itself in exponentially activated temperature dependence of a wide variety of dynamic and thermodynamic properties at low temperature. At HTS the exponentially activated temperature dependence is disappear. Cavity perturbation measurements[15] and muon spin rotation study[16] on high quality $YBa_2Cu_3O_7$ crystals have revealed the linear temperature dependence in the penetration depth λ below 30 K. A linear term in the low temperature thermal conductivity has also been found[17]. Above linear temperature dependence of physical properties indicates non-exponentially activated temperature dependence of the DOS of the quasiparticle excitation, which can appear only when there is node in the energy gap. The presence of a zero-bias conductance peak in tunneling spectroscopy also supports that the energy gap has node[18].

The electrons begin to pair below the superconducting phase transition temperature. But the system does not show the zero-resistance properties because the superconducting phase is local at low pairs concentration. The condensation of electrons leads to the decrease of density of states in Fermi surface, which results in the anomalous of normal state transport properties and the open of the pseudogap (PG). The normal state PG turns into the superconducting gap (SG) when the local superconducting phase evolves into the global one. Therefore it is natural that many experiment, such as angle-resolved photoemission, tunnelling spectroscopy, nuclear magnetic resonance and neutron scattering, reveal that SG emerges from the normal state PG and is of the same size and k dependence as PG[19]. Even all of carriers transform into electron pairs, the superconducting phase is still local and separate for $x < x_c$ (= 0.044 for $La_{2-x}Sr_xCuO_4$). The system does not show global superconductivity at any temperature. They become insulators because the local superconducting phase consumes all of carrier at low temperature. For $x > x_c$, the local superconducting phase can always evolve into the global one at certain temperature. Therefore the x_c is the concentration of insulator to superconductor transition. Since the transition concentration is determined by extending the experiment data of $T_c \neq 0K$, it may be arbitrary a value

between ρ_c and ρ_f. This gives out a likely explanation why the insulator-superconductor transition concentration reported by different experiment groups is obvious disagreement. $\rho_c = 0.34|\psi_0|^2$ and $\rho_f = 0.45|\psi_0|^2$ respectively correspond to $x = 0.044$ and $x = 0.056$ for $La_{2-x}Sr_xCuO_4$, which is well consistent with the experiment result $x \approx 0.05 \sim 0.06$[20,21].

Contrary with the common sense, the superconducting phase appears also in insulator. Furthermore the modulate wave vector ϵ in insulator and in superconductor has the same dependence on doped concentration, $\epsilon \propto x$, which is verified by neutron scattering experiment on $La_{2-x}Sr_xCuO_4$[6]. The Josephon effect experiment by Decca *et al*[22] indicates the existence of an anomalously large proximity effect in underdoped insulating $YBa_2Cu_3O_{6+x}$. Our results that insulator has local superconducting phase will be helpful to understand above anomalously large proximity effect.

It is generally perceived that the superconducting phase transition temperature is the temperature T_C at which the resistance disappear. However, according to our result, this view only suits the conventional metals. The genuine phase transition temperature for HTS is the PG temperature T_p where the order parameter has appeared. The zero-resistance temperature T_C is just the temperature at which the local superconducting phase is translated into the globe superconducting phase. It is well known that the gap should vanish and the breaking of the symmetry will happen at the phase transition temperature. However, these phenomena do not occur at the zero-resistance temperature T_C. On the contrary, a breaking of time-reversal symmetry at the PG temperature T_p is recently found by angle-resolved photoemission study[24]. Therefore, at the region between T_p and T_C, the system that has been taken for normal state is actually in superconducting state. Then it is natural that many physical properties at this region do not conform to Fermi liquid theory that describes the normal-state metal. Noting that the physical properties above the PG temperature accord well with Fermi liquid theory, We are sure that Fermi liquid theory is still fit for HTS. The opinion that the PG temperature is superconducting phase transition temperature is helpful to clarify the perplexity that predict of BCS is invalid for HTS. With the PG temperature T_p given by the experiments, the value of $2\Delta(0)/k_BT_p$ is close to the predict of BCS theory.

Although the negative effective mass m^* is general concept in Solid State Physics, it is still necessary to discuss whether the effective mass may be negative in GL theory. GL theory is a phenomenological theory. Considering that GL theory can be derived from the microscopic BCS theory and the meaning of electron mass in BCS theory is clearer than that in GL theory, we first study the electron mass of BCS theory. Ashcroft had put forward that in its simplest form the BCS theory makes a gross oversimplification in the basic Hamitanian that describes the conduction electrons[25]. The conduction electrons are treated in the free electron approximation and the effect of lattice periodic potential (band structure effect) is ignored. The oversimplifications may seem surprising because the band theory that describes the effect forms the basis of the modern theory of electrons in solids. Then the questions why BCS theory that ignores the effect can still explain the conventional superconductivity and whether the effect can be neglected in HTS rise.

To answer these questions, we must consider the effect of the lattice periodic potential. The effective mass approximation of band theory shows that the electrons nearby the band gap can be treated as free electrons with the effective mass. The effect of lattice periodic potential is embodied in the effective mass. According to the approximation, if Fermi surface is nearby the band gap, the conduction electrons can be taken as free electron. Then the lattice periodic potential is considered as long as we replace the mass of bare electron with the effective mass m^*. The replacement does not influence the BCS'major equilibrium predictions. It partly explains why BCS theory that ignores the effect of lattice periodic potential can still explain successfully superconductivity. Comparing with bare electron mass, m^* has s special property. It may be negative. For example, the electrons in top of band have the negative m^*, which is a very important conclusion of band theory. GL theory can be derived from the microscopic BCS theory. Therefore its mass may also be negative. The negative m^* only holds true near the top of the band, which means that $|-i\hbar\nabla\psi|^2$ should be limited. We need not be afraid that the minimum of the GL free energy will be unbound from below.

Although the hole description is always introduced when m^* is negative, its application to superconductor is questioned since the hole is the collective behavior of the whole band, whereas electron pairing is only involved in a thin layer of electrons nearby Fermi surface.

Now we can affirm that the lattice periodic potential is very important to HTS. The anomalous properties about HTS are primarily due to this effect. Three striking anomalous properties: the stripe phase, the pseudogap and the energy gap nodes, can been deduce from GL equation if the lattice periodic potential is considered. BCS theory and Fermi liquid theory are still fit for HTS. Some opinions should change. The genuine superconducting phase transition temperature for HTS is the PG temperature T_p where the order parameter has appeared. The zero-resistance temperature T_C is just the temperature at which the local superconducting phase is translated into the globe superconducting phase. The superconducting phase transition happens also in insulator.

[1] J. Zannen, and O. Gunnarsson, Phys. Rev. B **40**, 7391(1989).
[2] P. Dai *et al.*, Science **284**, 265(1999).
[3] T. Noda, H. Eisaki, and S. Uchida, Science **286**, 265(1999).
[4] H. A. Mook, D. Pengcheng, F. Dogan, and R. D. Hunt, Nature **404**, 729(2000).
[5] K. Yamada *et al.*, Physica C. **282 − 287**, 85(1997).
[6] M. Matsuda *et al.*, Phys. Rev. B. **62**, 9148(2000).
[7] J. M. Tranquada *et al.*, Phys. Rev. B. **54**, 7489(1996).
[8] J. M. Tranquada, B. J. Sternlieb, J. D. Axe, Y. Nakamura, and S. Uchida, Nature, **375**, 561(1995).
[9] Walstedt R.E, et. al.,Physical Review B-Condensed Matter,.41,(1990).9574.
[10] K. Ishida, et. al., Phys. Rev. B 58, (1998)R5960
[11] N. Momono, et.al., Physica C 317, (1999)603.
[12] E. Borsa *et al.*, Phys. Rev. B. **52**,7334(1995).
[13] R. P. Sharma *et al.*, Nature, **404**, 736(2000).
[14] J. M. Tranquada, Physica B **241 − 243**, 745(1998).
[15] K. Zhang, D.A. Bonn, et. al., Phys. Rev. Lett 73, 2484(1994).
[16] W. N. Hardy, D.A. Bonn, D. C. Morgan, R. X. Liang and K. Zhang, Phys. Rev. Lett 70, 3999(1993)
[17] K. Krishana, N. P. Ong, et. al., Science 277, 83(1997)
[18] C. R. Hu, Phys. Rev. Lett. 72, 1526(1994).
[19] T. Timusk and B.Statt, Rep. Prog. Phys. **62**, 61(1999).
[20] H.Takagi, T. Ido, S. Ishibashi, M. Uota, and S. Uchida, Phys. Rev. B. **40**, 2254(1989).
[21] B. Ellman *et al.*, Phys. Rev. B. **39**, 9012(1989).
[22] R. S. Decca, H. D. Drew, E. Osquiguil, B. Maiorov, and J. Guimpel, Phys. Rev. Lett. **85**, 3708(2000).
[23] N. Miyakawa *et al.*, Phys.Rev.Lett. **83**, 1018 (1999).
[24] A. Kaminski, et.al., Nature 416, (2002)610.
[25] Neil. W. Ashcroft and N. David Mermin, Solid State Physics (Holt, Rinehart and Winston, New York, 1976).