Phonons, charge and spin in correlated systems
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Chapter 1

Introduction

1.1 Strongly Correlated Systems

The first striking success of the quantum theory of solids was the classification of crystals into metals and insulators as a function of the occupation of the electronic bands. According to band theory a crystal is a metal if the last band is partially occupied and an insulator otherwise. The band theory assumes that every electron is moving in a periodic potential created by the positive ions and by the other electrons. In this one electron picture, every electron is sensitive only to the average properties of the surrounding environment, any correlation being neglected. The eigenstates of this one-particle problem, with the corresponding energies taking continuous values on some distinct intervals, constitute the bands.

Even though band theory has been successful in many respects, shortly after its appearance, de Boer and Verwey [1] reported that many properties of transition-metal oxides are in total disagreement with the band structure calculations. As a result of partially occupied $d$ type band, a metallic behavior was expected. In fact, these materials are insulators with a conductivity gap an order of magnitude larger then the maximum gap derived even with the most sophisticated band structure calculation techniques. Mott and Peierls [2] were the first to suggest that the reason for the band theory failure might be the neglect of the repulsive Coulomb interaction between electrons on the $d$ orbitals. Later on, Mott [3–5] and Hubbard [6, 7] showed that if the repulsion is larger than the bare electron bandwidth the Fermi level will be located inside a gap and the system will be indeed an insulator.

In the last decades an impressive number of novel materials, poorly described by conventional techniques and displaying a rich variety of properties, were discovered. Among them, in order of both practical and theoretical importance, the transitional-metal oxides and especially the cuprate superconductors occupy a leading position. A common characteristic of transitional-metal compounds is the essential contribution of the $3d$ orbitals to the electronic properties. The $3d$ orbitals are special in the sense that they have a small spatial extent (much smaller than the extent of the ligand $p$ orbitals) and therefore retain much of the initial atomic properties as the strong Coulomb repulsion between two electrons on the same ion. This unscreened short-ranged repulsion makes the correlations
play a predominant role in the underlying physics *, resulting in a large number of physical properties, which are unfortunately not well understood from the theoretical point of view.

The conventional treatment of systems with interacting electrons, valid in many cases, was developed by Landau. The main assumption of his Fermi-liquid theory is a one to one correspondence between the interacting and the noninteracting ground state and low-energy excitations. The interacting ground state is still assumed to have a sharp Fermi surface, which results in well defined quasiparticles close to the Fermi level. This is due to Pauli principle which blocks the scattering inside the Fermi sea (the only allowed scattering mechanism is by creating electron-hole pairs), resulting in a quasiparticle lifetime which is much longer than the inverse of the excitation energy. The quasiparticles behave like electrons in a noninteracting system, and as a consequence, the Fermi-liquid properties are described by the same expressions as the corresponding Fermi-gas ones. Thus it is possible to account for the effect of interaction only by renormalizing a few parameters, such as the effective mass.

The experimental study of the correlated materials show that they exhibit “strange” behavior, which cannot be understood in the framework of Fermi-liquid theory. At present, good theories which treat properly the correlations effects are missing. No one knows a reliable way to deal with the problems where both the kinetic part and the interaction part of the Hamiltonian are of the same order of importance. Besides the strong electronic interaction, another common characteristic of many strongly correlated materials is the low dimensionality (quasi-two or quasi-one dimensional). This implies strong quantum fluctuations, making the theoretical treatment even more difficult.

In the last years, a large number of analytical approaches, which use more or less uncontrollable approximations, were applied to strongly correlated systems, giving sometimes contradictory results. Besides those, numerical algorithms, as unbiased methods to solve the model Hamiltonians, acknowledged a huge development. However these numerical techniques have several shortcomings too. They are not able to deal with large systems, making the extrapolation of the results to the thermodynamic limit unreliable. Nevertheless, we believe that the new cluster mean-field methods, which treat numerically exact the short-range correlations inside a cluster and at the mean field level the physics on longer length scales, should give good results provided only the short-range correlations are important.

1.2 High $T_c$ Superconductors

In 1986 Bednorz and Müller [9] discovered a new type superconductor, based on Cu and O, with a surprisingly then high critical temperature ($\approx 30$ K). Their discovery has been one of the most important discovery in condensed matter physics of the second half of the last century. Soon after their discovery, a large number of similar materials (called generic cuprates) were synthesized, having the critical temperature above the

*By definition everything beyond the Hartree-Fock approximation (i.e. beyond the one-particle picture) is a correlation effect.
boiling point of liquid nitrogen (77 K) * and therefore opening enormous opportunities for technological applications. The common belief is that the understanding of these materials could provide the knowledge for growing room temperature superconductors. Thus, since their discovery, the cuprates have been under an extraordinary intensive, both experimental and theoretical, investigation.

However, the results so far are modest comparative to the invested effort. After more than fifteen years of intensive research, the cuprates are far from being understood. As veritable strongly correlated systems, they exhibit many “anomalous” properties, imposing severe constrains on any reasonable theory.

Despite of their different chemical composition, the cuprates superconductors have many common characteristics, and it is natural to assume that these characteristics determine the basics physics. The high $T_c$ superconductors are layered materials, containing quasi-two-dimensional $CuO_2$ planes sandwiched between block layers. The generic structure is illustrated in Fig. 1.1, but it also should be said that some materials have more 

*Nowadays the highest $T_c$ under normal pressure conditions is around 130 K and, under high pressure, around 160 K.
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Figure 1.2: Generic phase diagram of cuprates superconductors [8].

The electronic states close to the Fermi level are contained in the $CuO_2$ planes. The block layers play the role of charge reservoirs, controlling the number of charge carries in the conduction planes upon chemical doping. Consequently, theoretical models designed to describe the physics of a single $CuO_2$ plane for different electronic concentrations were proposed for the cuprates. However, there is no general agreement on what should be the minimal model which captures the basic physics of a $CuO_2$ plane. The photoemission experiments show that the first electron removal states have O $p$ origin, unlike the first electron addition states which have Cu $d$ character, placing the cuprates in the charge-transfer regime of Zaanen-Sawatzky-Allen scheme [10]. It is believed that the only Cu orbital which participates to low-energy physics is the $d_{x^2-y^2}$ one. It couples to the in-plane oxygen $p$ orbitals, and therefore the first models contained all these degrees of freedom ($d$ and $p$). However, based on the strong Cu-O hybridization, many physicists believe that one step further can be taken and a reduction to a one-band Hamiltonian which contains only the $d_{x^2-y^2}$ orbitals can be done. But there is no general agreement on that, and
1.2. High $T_c$ Superconductors

some authors consider the oxygen orbitals as essential for explaining the properties of the phase diagram, such as the pseudogap for example [11, 12].

The common physical properties of cuprates can be summarized in the generic phase diagram presented in Fig. 1.2 [8]. The undoped materials are antiferromagnetic insulators. Upon doping the antiferromagnetism is quickly destroyed. For the doping range approximatively in between 5% and 30%, the cuprates become superconductors at low temperature. The doping value where the $T_c$ is maximum (around 15%) is called optimal doping. The lower and higher doping regime are called underdoped and respectively overdoped regimes. Unlike in the conventional superconductors, the superconducting gap in the cuprates has $d$-wave symmetry, with nodes along the diagonal directions and changing the sign upon a $\pi/2$ rotation [13–16]. In the overdoped region, above $T_c$ the system is a Fermi-liquid metal. But the most intriguing physics occurs in the underdoped region, in the proximity to the antiferromagnetic phase. The majority of physicists believe that the understanding of the underdoped normal state would provide the key for elucidating the superconductivity mechanism.

Almost all the quantities measured on underdoped samples exhibit “anomalous” behavior. The most remarkable anomaly is the pseudogap, and many other “strange” properties are believed to be related to it. The pseudogap is a depletion in the density of states close to the chemical potential, noticed below a characteristic temperature, $T^*$. The earliest indications of the pseudogap were found in NMR experiments [17–19] where the spin susceptibility measured by the Knight-shift was seen to decrease strongly below $T^*$. Many other measurements like heat capacity [20], resistivity [21, 22], infrared absorption [23–25], neutron scattering [26], and tunneling [27, 28] show also evidences of pseudogap. However, the most direct and unambiguous evidence comes from the angle-resolved photoemission spectroscopy (ARPES) [29, 30]. At least for the hole doped systems, the ARPES spectra show that the pseudogap is well developed at the zone boundary and vanishes along the diagonal directions, suggesting the same symmetry as the superconducting gap. Therefore, in many scenarios suggested by the theorists the pseudogap is considered as the precursor of the superconducting gap.

At present, with respect to the cuprates physics in general and pseudogap in particular, there is a great disagreement between theorists, and perhaps there are as many theories as there are the groups investigating the problem. However, in the following we introduce briefly some of the most important ideas and scenarios which have appeared since the high $T_c$ discovery.

Based on the vicinity of the underdoped region to the antiferromagnetic phase, some scenarios assume that the pseudogap appears as a result of coupling of quasiparticles to sharp antiferromagnetic spin fluctuations peaked at $(\pi, \pi)$ [31]. With reducing the doping, the pseudogap will evolve into the full spin-density-wave gap characteristic to undoped antiferromagnets with nested Fermi surface.

There are another scenarios which assume that in the pseudogap region the pairs are already formed. The formation of pairs starts at the pseudogap temperature, $T^*$, and $T_c$ is the temperature where the phase coherence occurs [32]. The bipolaron superconductivity theory, which we discuss in the next section (Section 1.3), should also be included in this category.

Theories based on resonating valence bond (RVB) and spin-charge separation are also
popular in the field [33, 34]. Here the spins pair into short-ranged singlets when $T < T^*$, resulting in a gap in the spin excitation spectrum which is assimilated to the pseudogap. The elementary excitations are not quasiparticles but *spinons* which are charge neutral fermions with spin $1/2$ and *holons* which are charged bosons with spin $0$. At $T_c$ the holons condensate and recombine with the spinons giving rise to superconductivity.

Other authors relate the pseudogap to the existence of a quantum critical point close to the optimal doping and identify the pseudogap as a region characterized by circulating currents and time-reversal broken symmetry [11].

Because the physics of the normal and of the superconducting state is so unconventional, it is rather widely believed that phonons do not play an essential role in the superconductivity mechanism. Nevertheless, there is strong experimental evidence showing
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that the electron-lattice coupling is strong [35–38], beyond the applicability of the conventional theories which describe the electron-phonon interacting systems. Consequently, other authors [35, 39] claim that the superconductivity is driven by the phonons as in the conventional superconductors, the difference being only the strength of the coupling between charge carriers and phonons.

Before ending this section, we would like to stress another important characteristic of cuprates, namely the asymmetric behavior of the electron and hole doped samples. The asymmetry can be seen from the experimentally determined phase diagram presented in Fig. 1.3. In the electron doped materials the antiferromagnetism survives up to a larger critical doping while the opposite thing can be said about the superconductivity. However, the recent angle-resolved photoemission data on electron-doped materials [40], which exhibit a pseudogap around $(\pi/2, \pi/2)$ and well defined quasiparticles at the zone boundary show that this asymmetry is more profound. In the case that the superconducting gap in the electronic doped systems has still $x^2 - y^2$ symmetry (as our calculations suggest), these results would question the assumption that the pseudogap is a precursor of the superconducting gap. Nevertheless, there is no agreement so far about the symmetry of the superconducting gap in electron doped materials, some experiments indicating a $s$-wave symmetry and others a $d$-wave symmetry. Nevertheless, the electron doped materials are much less studied than the hole doped ones, due to the difficulty encountered in the preparation of good samples.

### 1.3 Electron-Phonon Interaction and Superconductivity

The interaction between electrons and lattice degrees of freedom plays a crucial role in understanding the properties of many materials and results in a multitude of physical phenomena. Structural transitions like Jahn-Teller distortion in perovskite or Peierls dimerization in one-dimensional systems, the pairing and the condensation of the charge carriers resulting in superconductivity are some of the most spectacular effects which originate from electron-lattice interaction. Even in situations where no real phase transitions take place the transport properties in crystals are largely influenced by the interaction of the charge carriers with the lattice. Not only does the inelastic scattering of the electrons with the impurities or with the thermally activated phonons determine the carriers mobility but also the formation of low-energy coherent states which result in a fundamental change of the charge carriers properties. These states are called polarons, a concept introduced long time ago by Landau (1933) [41] which describes a charge carrier which carries with it a lattice deformation. Besides dressing the charge carriers, the phonons also induce an effective attraction between them. As Bardeen, Cooper and Schrieffer (BCS) showed [42], even a weak attraction is enough to make a Fermi liquid state instable towards electron pairing. The electrons form pairs in momentum space close to the Fermi level (Cooper pairs). The condensation of the Cooper pairs leads the system to the superconducting phase. However if the electron-phonon attraction is too strong the result may be different, now two electrons forming a strong bound pair of small size in real space. Such an entity is called a small bipolaron and can be identified with a hard
core charged boson. If the density of charge carries is small the physics can be considered as being well described by a liquid of bipolarons which suffers Bose-Einstein condensation resulting also in superconductivity.

In the last years there is growing experimental evidence that in the fashionable strongly correlated materials like manganese and copper oxides, aside from the unscreened Coulomb repulsion, the electron-lattice interaction is also extremely important [43–50]. The electron-phonon coupling strength is usually of intermediate strength so that neither the weak-coupling nor the strong-coupling theories work. Therefore numerical solutions for models which address the electron-phonon interaction in this difficult region of parameter space are highly desirable. Aside from a realistic (and difficult) multi-electron problem solution, for a basic understanding of the underlying physics special interest should be paid to simpler problems which address the effect of a polarizable medium (lattice) on a single charge carrier (polaron problem) and the phonon induced pairing mechanism of two electrons (or holes) in a lattice (bipolaron formation problem).

**Electron-phonon interaction** In general, the lattice is considered as a set of linear oscillators, being modeled by

$$H_{ph} = \sum_{q,\nu} \omega_{\nu}(q) b_{q,\nu}^\dagger b_{q,\nu}$$  \hspace{1cm} (1.1)

where $b_{q,\nu}^\dagger$ ($b_{q,\nu}$) is the creation (annihilation) operator of a phonon with momentum $q$ and $\nu$ is the vibration branch index. The electrons interacting with the lattice potential are described by

$$H_1 = H_{el} + H_{el-ph} = \sum_{i=1}^{N_e} \frac{p_i^2}{2m_e} + V(r_i)$$  \hspace{1cm} (1.2)

where $N_e$ is the total number of electrons and

$$V(r_i) = \sum_{l} v(r_i - R_i)$$  \hspace{1cm} (1.3)

is the crystal field potential. $R_i$ is the position of the $i$-th ion, and in general its deviation, $x_l$, from the equilibrium position, $R_{0l}$, is small, so we can write

$$v(r_i - R_i) \approx v(r_i - R_{0l}) + \frac{\partial v}{\partial R}(r_i - R_{0l}) x_l$$  \hspace{1cm} (1.4)

The contribution of the first term of Eq. 1.4 in Eq. 1.2 results in a Hamiltonian which describes the interaction of electrons with a periodic potential, thus producing noninteracting Bloch states. In the second quantization formalism it can be written as

$$H_{el} = \sum_{k\sigma} \varepsilon(k) c_{k\sigma}^\dagger c_{k\sigma}$$  \hspace{1cm} (1.5)

where $c_{k\sigma}^\dagger$ ($c_{k\sigma}$) is the creation (annihilation) operator of a electron state with momentum $k$ and spin $\sigma$. Taking into account that the Fourier transform of the displacement $x_l$ is

$$x_q \propto \sum_{\nu} \sqrt{\frac{1}{\omega_{\nu}(q)}} (b_{q,\nu}^\dagger + b_{q,\nu})$$  \hspace{1cm} (1.6)
frequency \(|\varepsilon - \mu| \approx \omega\). The quasiparticle close to the Fermi level is an electron carrying a phononic cloud (which results in an increase of its effective mass, \(m^*\)) being similar to a polaron and the high energy quasiparticle is a free electron like \([35, 52]\). The effective mass ratio

\[
\frac{m^*}{m} = 1 + \lambda
\]

which can be determined by measuring the quasiparticles dispersion provides a means of calculating the electron-phonon coupling strength, \(\lambda\), in materials. Here \(\lambda\) is the BCS like defined electron-phonon coupling, i.e. \(\lambda = V N(0) \approx 2 g^2 \omega N(0)\) where \(N(0)\) is the density of states at the Fermi level and \(V\) the effective electron-electron attraction induced by the phonons.

The poles of the phonon propagator \(\mathcal{D}\) give for small momentum phonon the renormalized dispersion \([35, 53]\)

\[
\tilde{\omega}(q) = \omega(q)\sqrt{1 - 2\lambda}
\]

which shows that Migdal’s theorem fails when the electron-phonon coupling \(\lambda > 1/2\). A strong electron-phonon interaction changes the ions equilibrium position (as the strong coupling perturbation theory shows) driving a phonon vacuum instability resulting in the breakdown of the Migdal approximation.

**Migdal-Eliashberg’s approach to superconductivity** The Eliashberg’s theory of superconductivity \([54, 55]\) is an extension of Migdal’s treatment for the normal state of electron-phonon coupled systems to the superconductivity phase. It uses the same approximation which neglects the electron-phonon vertex corrections and therefore it is expected to work only at small and intermediate coupling values. From another perspective it is a generalization of the BCS theory which allows a proper treatment of the retardation effects and to include realistic phonon dispersion and electron-phonon interaction matrix.

The difference from the normal state treatment is that now (as in the BCS approach) the anomalous averages \(\langle c^\dagger c^\dagger \rangle\) are allowed to take a nonzero value. In order to do that the electron Green’s function is defined as a \(2 \times 2\) matrix

\[
G(k, \tau) = \begin{pmatrix}
T^r(c^\dagger_k(\tau)c^\dagger_k(\tau)) & T^r(c^\dagger_k(\tau)c^\dagger_{-k}) \\
T^r(c^\dagger_{-k}(\tau)c^\dagger_k) & T^r(c^\dagger_{-k}(\tau)c^\dagger_{-k})
\end{pmatrix}
\]

In zero order the off-diagonal elements (the anomalous averages) are zero. The Green’s function is calculated by summing the same set of diagrams as in the Migdal’s normal state approach (Eq. 1.10) but now a \(2 \times 2\) matrix corresponds to every propagator and also to the electron-phonon vertex \([56, 57]\). The phonon propagator

\[
\mathcal{D}(k, \omega) = \mathcal{D}(k, \omega) \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\]

and the electron-phonon vertex

\[
g(q) = g(q) \begin{pmatrix}
1 & 0 \\
0 & -1
\end{pmatrix}
\]
are diagonal matrices. The Green’s function propagator is the Fourier transform of Eq. 1.16. The self-consistent solution of (Eq. 1.10) shows that at low temperature the off-diagonal elements of the Green’s function are nonzero. An important result is that this happens only when all the noncrossing diagrams are summed up. In any finite order of the perturbation theory the Green’s function is a diagonal matrix, thus the superconductivity is a nonperturbative effect. The Eliashberg’s approach reproduces the BCS results if the same approximation is made for the phonon propagator (i.e. $D(q, \omega) = -1$ for $\omega < \omega_D$ and zero otherwise). The critical superconductivity temperature is defined as the temperature where the anomalous averages vanish. The BCS value is

$$T_c = 1.13 \omega_D e^{-\frac{1}{\lambda}}$$

(1.19)

One of the great advantages of Eliashberg’s formulation is the possibility to include the Coulomb repulsion in the same framework. Even though there is no adiabatic parameter for the Coulomb interaction, the neglect of vertex corrections corresponds to Random Phase Approximation (RPA) and provides good results for a qualitative analysis. A remarkable result is obtained. At the Fermi surface the relevant parameter introduced by the screened Coulomb repulsion, $V(q)$, will be $\mu_c$ defined as

$$\mu_c = V(q_F) N(0)$$

(1.20)

The electron-electron repulsion competes with the phonon induced attraction, but the critical temperature will be

$$T_c = \frac{2\omega_D}{\pi} e^{-\frac{1}{\lambda - \mu_c^*}}$$

(1.21)

where $\mu_c^*$ is the Coulomb pseudopotential, defined as

$$\mu_c^* = \frac{\mu_c}{1 + \mu_c \ln(\epsilon_F/\omega_D)}$$

(1.22)

The remarkable thing is that the Coulomb repulsion effect enters only through the strongly suppressed pseudopotential $\mu_c^*$. It means that even a strong repulsion does not destroy the superconductivity or implicitly the pairing. This happens due to the fact that aside from the sign the two competing interactions are fundamentally different. The attractive interaction is retarded, being defined in a small frequency window of the order $\omega_D$, which means that it still acts for a period of time after two electrons meet another. On the other hand the Coulomb repulsion acts on a much larger frequency window, of the order of $\epsilon_F$, being more or less instantaneous. When two electrons meet they separate quickly at a distance where the repulsion becomes small but the retarded attraction delayed in time will be still effective there, making the pairing possible.

**Nonadiabatic superconductivity** When applied to high $T_c$ materials, there are in principle two reasons for Migdal-Eliashberg’s theory to fail. One is the large value of the electron-phonon coupling which leads to phonon instability (see Eq. 1.15), and we are going to discuss about it in the next paragraph. The other reason is the small Fermi energy ($0.1 - 0.3$ eV) [58, 59] which does not allow the Migdal’s “adiabatic” parameter
$\varepsilon_F/\omega$ to be small. L. Pietroniero et al. [60, 61] pointed out that even for a small electron-phonon coupling the vertex corrections are important, and in some cases can lead to a strong enhancement of $T_c$. In their work they generalized the Eliashberg’s theory to include the first order vertex corrections.

**Alexandrov’s bipolaronic theory of superconductivity** The experimental data [35–38] show that the electron-lattice interaction in high $T_c$ materials is large, being above the applicability range of Migdal’s approximation. Therefore Alexandrov and co-workers [35, 39] proposed a theory based on the strong electron-phonon coupling expansion for explaining the physics of high $T_c$ superconductors.

It is known that when the electron-phonon coupling is large the phonon mediated attraction between electrons leads to the formation of strong bound pairs localized in the real space (bipolarons). Alexandrov argues that the low-energy physics is described by a liquid of bipolarons. At low density, where the overlap of the bipolaron wave functions has a negligible effect, the bipolarons can be treated as charged $2e^-$ bosons which Bose-Einstein condensate and suffer a transition to a superfluid state at the critical temperature $T_c$. The superfluid state of a charged Bose-gas is equivalent to the superconductivity phase.

However some authors raised objections against the bipolaron theory. Chakraverty et al. [62] argued that the bipolarons are much too heavy states to account for the high value of $T_c$ found experimentally in the cuprate materials. From our calculations (see Chapter 4) we also found an exponentially large bipolaron mass for the on-site bipolaron (i.e. a bound state with the electrons residing on the same site) even in the intermediate electron-phonon coupling region. Nevertheless as the strong coupling theory and numerical calculations show [63], the inter-site bipolarons (i.e. bound states with the electrons on neighboring sites) are much lighter states. These are states resulting from a non-localized electron-phonon interaction (unlike the on-site interaction considered in our model). In fact Alexandrov’s proposed bipolaron is an inter-site state with one hole in a $CuO_2$ plane on a oxygen plaquette (formed by the four O atoms around a Cu ion) and with the other hole on the apex O situated above the plaquette. Aside from being a light particle and therefore able to provide a high $T_c$, Alexandrov argues that this particular bipolaron state can also explain another important characteristic of the cuprates superconductors, the $d$-wave symmetry of the order parameter [13–16]. The apex oxygen participates to the bipolaron formation with two orbitals, $p_x$ and $p_y$, resulting in two degenerate bipolaron bands.

$$E_x(k) = -t \cos(k_x) + t' \cos(k_y)$$  \hspace{1cm} (1.23)
$$E_y(k) = t' \cos(k_x) - t \cos(k_y)$$  \hspace{1cm} (1.24)

with $t, t' > 0$ and $t \gg t'$. The bipolaron containing the apical $p_x$ hole has a large dispersion along the $X$ direction because it involves the inter apical oxygens $pp\sigma$ hopping integral and a small dispersion along the $Y$ direction where the $pp\pi$ hopping integral is involved. It is orthogonal to the bipolaron formed with the $p_y$ apical oxygen orbital. The relevant thing is that the energy bands minima are not at $(0,0)$ but at the Brillouin zone boundary points, $(0, \pm \pi)$ for the “along $x$” band and respectively at $(\pm \pi, 0)$ for the “along $y$” band.
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When the bipolaron liquid Bose-Einstein condenses the states situated at these points in the Brillouin Zone will be macroscopically occupied. Alexandrov has proposed the following real-space order parameter function for \( d \)-wave cuprates superconductors [64],

\[
\Psi(r_x, r_y) = \left(\frac{x}{2}\right)^{1/2}(\cos(r_x\pi) - \cos(r_y\pi))
\] (1.25)

constructed by taking a linear combination of the zone boundary condensate states. The symmetry of the order parameter is a result of the bipolaron energy dispersion with the minima at the zone boundary and has nothing to do with the symmetry of the internal wave function of a single bipolaron∗.

Because of the low-dimensionality, the bipolarons localize easily in the presence of random potential wells. Only the non-localized bipolarons participate in the condensate state. The critical temperature \( T_c \) in a quasi-two-dimensional superfluid (but still an anisotropic 3D system) is proportional to the particle density. With increasing the doping the number of localization wells is increasing too and as a result the number of non-localized bipolarons decreases at large doping. The maximum number of non-localized bipolarons (and implicitly the maximum \( T_c \)) will be somewhere around 15% doping [39] in agreement with the experimental phase diagram. Another characteristic feature of cuprates physics, the normal state pseudogap is explained in Alexandrov’s theory as being a result of bipolaron state formation and therefore the pseudogap temperature \( T^* \) should be proportional to the bipolaron binding energy.

The solution to the question whether the high \( T_c \) superconductivity mechanism is a consequence of large electron-phonon interaction or of purely electronic correlation effects is still controversial. More physicists are in favor of the later, believing that the intriguing physics of the cuprates has its origin in the unscreened short range Coulomb repulsion between electrons. However, even if true, there are no priori reasons to neglect the lattice polarization effects and presumably models which include both electron-phonon and electron-electron interaction should be considered. The calculations presented in the last two chapters show that the main characteristics of cuprates superconductors can be obtained neglecting the phonons, but also show that for a better agreement with experiment something else, and we believe that it would be the phonons, should be added to the model.

∗However we believe that strong objections can be raised against Alexandrov’s proposal [65]. First, Eq. 1.25 describes a charge density wave (CDW) of bipolarons, with a \( 2 \times 2 \) supercell, rather than a \( d \)-wave superconductor. The state proposed by Alexandrov is an interesting novel state of matter, but its properties are completely different from superconductors ones. For example we don’t believe that a state described by Eq. 1.25 would exhibit the Andreev reflection phenomenon characteristic to superconductors. Second, we don’t see any reason why the condensation should be in a standing superposition of the condensate states at the zone boundary. A general wave function, with \( N \) bipolarons at \((\pi, 0)\) and \( M \) bipolarons at \((0, \pi)\) should have the form

\[
|\Psi\rangle = (\Psi(\pi, 0) + \Psi(-\pi, 0))^{N}(\Psi(0, \pi) + \Psi(0, -\pi))^{M}|0\rangle
\] (1.26)
1.4 Scope

Since the discovery of high $T_c$ superconductors, the computation tools used for dealing with strongly correlated materials, both analytical and numerical, have developed in an impressive manner. Among them, a new Quantum Monte Carlo method able to calculate exactly the Green's functions, based on the summation of the corresponding Feynman's diagrams, proved to be very powerful for solving polaron like (interaction of a quantum particle with a bosonic environment) and bipolaron like (pairing of two fermions as a result of exchange of bosonic particles) problems. Related to the large electron-lattice coupling encountered in the majority of the correlated materials and especially in high $T_c$ superconductors, the solution to the polaron and bipolaron problems are of a extreme importance in elucidating the properties of quasiparticles and the pairing mechanism, and should be considered as a first step in the understanding of the more complex multi-electron plus phonons problem.

In the last three years, a powerful method for dealing with interacting electrons systems was developed. The technique is called Dynamical Cluster Approximation (DCA) and is an extension of the previous popular Dynamical Mean Field Theory (DMFT). The DMFT maps the lattice problem to an impurity embedded self-consistently in a host and therefore neglects spatial correlations. The DCA maps the lattice to a finite-sized cluster embedded in a host. Non-local correlations up to the cluster size are treated explicitly, while the physics on longer length scales is treated at the mean field level. The rapid development of the computational resources available at the main Supercomputers Centers around the world results in the possibility to increase both the cluster size (i.e. the correlation range) and the number of relevant interactions and degrees of freedoms inside the cluster accordingly, making us to believe that in the very next future many of the intriguing properties of correlated materials will be elucidated through the DCA approach.

Our calculations, which take advantage of the above mentioned techniques, address mainly the physics of high $T_c$ superconductors, even though the polaron and bipolaron concepts have a much larger range of applicability. This thesis can be divided in more or less two independent parts, the first dealing with electron-phonon interaction and the second addressing the Hubbard type Hamiltonians used for modeling the electronic interaction in cuprates superconductors. We consider both parts as absolute necessary steps in solving and understanding of the more realistic problem which consider both electron-lattice and electron-electron interaction at the same time. As we are going to mention at the end of this thesis, this complex problem can be addressed within the DCA framework too, and we plan it as a research project for the next future.

The manuscript is organized as follows. In Chapter 2 we describe the general principles of the Diagrammatic Quantum Monte Carlo technique used in the next two chapters to solve the polaron and respectively the bipolaron problem. Chapter 3 studies the interaction of a single electron with sharp on-site phonons, addressing both the ground state and the momentum dependent properties of the system. In Chapter 4 the pairing mechanism of two electrons (bipolaron formation) as a function of both electron-lattice coupling and Coulomb repulsion is studied. Chapter 5 gives a short description of the Dynamical Cluster Approximation technique. Using DCA with a $2 \times 2$ cluster, in Chapter 6 we study a five-band Hubbard Hamiltonian, which we consider as a realistic starting point for the
the contribution of the last term of Eq. 1.4 in Eq. 1.2 results in the electron-phonon interaction part of the Hamiltonian

\[
H_{el-ph} = \frac{1}{\sqrt{N}} \sum_{k\sigma,q\nu} g(k, q, \nu) c^\dagger_{k+q\sigma} c_{k\sigma} (b^\dagger_{-q,\nu} + b_{q,\nu})
\]  

(1.7)

The general form of a Hamiltonian which describes both the electrons and the lattice degrees of freedom should be

\[
H = H_{el} + H_{ph} + H_{el-ph} + H_{el-el}
\]  

(1.8)

where \(H_{el-el}\) is a electron-electron interaction term.

The electron-phonon coupling is given by the general matrix \(g(k, q, \nu)\). Several simplified models which consider \(g(k, q, \nu) = g(q)\) like Fröhlich model with \(g(q) \propto \frac{1}{q}\) which is expected for a free or nearly free electron gas and Holstein model with \(g(q) = g = constant\) which is expected if only the on-site energy in a tight binding model is affected, have been under investigation in the course of time.

**Migdal’s approach to normal state** The treatment of systems characterized by a large Fermi surface and a weak to intermediate electron-phonon coupling is greatly simplified following an observation made by Migdal [51] which shows that the renormalization of the electron-phonon interaction is negligible in all orders of perturbation theory. The reason is the Pauli exclusion principle which blocks the scattering inside the Fermi sea, resulting in corrections of the order \(\omega/\varepsilon_F\), where \(\omega\) is the phonon characteristic frequency and \(\varepsilon_F\) is the Fermi energy \(^*\).

Within Migdal’s approximation solving the problem means solving the following system of equations

\[
\Sigma(k, \omega) = \int dq \int d\Omega g(q)^2 D(q, \Omega) G(k - q, \omega - \Omega)
\]  

(1.10)

\[
\Pi(q, \Omega) = \int dk \int d\omega g(q)^2 G(k, \omega) G(k + q, \omega + \Omega)
\]  

(1.11)

where \(G(k, \omega)\) is the electron propagator,

\[
G^{-1}(k, \omega) = G_0^{-1}(k, \omega) - \Sigma(k, \omega)
\]  

(1.12)

and \(D(q, \Omega)\) is the phonon propagator

\[
D^{-1}(q, \Omega) = D_0^{-1}(q, \Omega) - \Pi(q, \Omega)
\]  

(1.13)

The analysis of the real and of the imaginary part of the self-energy shows that well defined quasiparticles exist close to the Fermi surface (when \(|\varepsilon - \mu| < \omega\)) and far from it (when \(|\varepsilon - \mu| >> \omega\)), but not at the excitation energies of the order of the phonon.

\(^*\)This is not true at long wave-length scattering in the systems with optical phonons which are characterized by \(\omega(q = 0) \neq 0\) [52].
description of the cuprates $CuO_2$ plane. The importance of the different oxygen degrees of freedom is studied, as well as the possibility of Hamiltonian reduction from the five-band to a simpler effective one-band model. The electron-hole asymmetry seen in the phase diagram and in the ARPES spectra is discussed too. In Chapter 7 we consider the single-band Hubbard model, both with and without the next-nearest-neighbor hopping integral found previously to be responsible for the electron-hole asymmetry. The calculations are done now on a larger cluster, with 8 sites. The results are compared to the corresponding 4 site cluster ones. We also discuss here the effects introduced by the periodic boundary conditions when are imposed on very small clusters.
References


[65] D. van der Marel, private communications.