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Antiferromagnetism and superconductivity in a quasi two-dimensional electron gas.
Scaling theory of a generic Hubbard model

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Résumé.- Nous étudions un modèle de Hubbard bi-dimensionnel, dans une limite de coupage faible. Le modèle générique a des intégrales de recouvrement entre premiers voisins, mais aussi entre seconds voisins. Le modèle peut être pertinent pour les oxydes supraconducteurs à haute $T_c$. Nous développons pour le cas générique une théorie d'échelle mise au point pour le cas d'une surface de Fermi carrée à demi remplissage. Nous traitons de manière cohérente les singularités en $\ln^2(T)$ et en $\ln(T)$ qui proviennent des fonctions de corrélations d'onde de densité ou de paires de Cooper. Lorsque l'emboîtement de la surface de Fermi est suffisamment mauvais, la supraconductivité singlet de symétrie orbitale d, renforcée par les fluctuations de spin antiferromagnétiques, gagne la compétition avec ces dernières même lorsque le niveau de Fermi est à la singularité de Van Hove. Nous trouvons que la température de supraconductivité $T_{SC}$ est de l'ordre de la température de Néel du modèle à emboîtement parfait dans une part significative du diagramme de phase. La diffusion des électrons sur des impuretés normales peut être efficace pour supprimer la supraconductivité. La température de Néel peut être maximum ailleurs qu'au demi remplissage, et l'antiferromagnétisme est facilement supprimé par de faibles variations du nombre de porteurs. Nous discutons de la pertinence de nos résultats pour les oxydes supraconducteurs.

Abstract.- We study the two dimensional Hubbard model in the weak coupling limit, in the vicinity of half band filling, for a generic model which has nearest neighbour as well as next nearest neighbour overlap integrals. The model is hoped to be relevant to the new high $T_c$ superconducting oxides. A scaling theory, previously studied for the case of perfectly nested square Fermi surface at half band filling, is developed for the generic case, and allows a consistent treatment of the coupled $\ln^2(T)$ and $\ln(T)$ singularities arising from density wave and Cooper pair fluctuations. When violation of perfect nesting is sufficient, d type singlet superconductivity, induced by antiferromagnetic spin fluctuations, overwhelms the latter even when the Fermi level is at the Van Hove singularity. We find that the superconducting temperature $T_{SC}$ is of the order of the Néel temperature of the perfectly nested model in a sizeable part of the phase diagram. We also find that normal impurity scattering, when sufficiently strong, may be efficient in suppressing superconductivity. The maximum Néel temperature, in the antiferromagnetic part of the phase diagram may occur away from half band filling, and antiferromagnetism is easily suppressed by small changes in carrier concentration. The relevance of our results to actual high $T_c$ superconducting oxides is discussed.

The existence of antiferromagnetism in La$_2$CuO$_{4-\delta}$ compounds is a strong indication that the mechanism of superconductivity in the new high $T_c$ oxides has to do with electron electron interactions in a non conventional way [1 to 4].

One crucial point is the nature of antiferromagnetic order, which seems to be experimentally con-
nected to an insulating phase of the above mentioned compounds. The debate between strongly correlated models starting from a Mott Hubbard insulator or weakly correlated models which stress the importance of two dimensional nesting of the Fermi surface in a half filled Cu d-band has been reviewed recently [5].

Our motivation here is a recent result : the Néel temperature $T_N$ is found to increase by almost an order of magnitude as $\delta$ increases from zero to about $3 \times 10^{-2}$. The spin density per site increases by about 100% in the same concentration range, from $\sim 0.2 \mu_B$ to $\sim 0.4 \mu_B$. The smooth variation of $T_N$ with oxygen vacancy concentration seems to show that magnetism is a fairly homogeneous property of the material under the annealing conditions described in references [2 - 4].

Within a strongly correlated model, $T_N$ is maximum at $\delta = 0$ and one expects at low oxygen vacancy concentration a variation $\delta T_N / T_N \sim \delta$ for $\delta << t/U$ where $t$ is the nearest neighbour overlap integral and $U$ the intra atomic Coulomb integral. Antiferromagnetism vanishes when $\delta/4 \sim t/U$. This criterion is obtained as follows : the maximum kinetic energy gain for a carrier when the spin configuration in a square lattice changes from antiferromagnetic to ferromagnetic [6] is $zt \left[ 1 - (2/z) \left( \frac{z-1}{2} \right)^{1/2} \right]$, to be balanced against the exchange term $zt^2/U$, with $z = 4$. If $t = 0.5$ eV, experiment requires $U = 66$ eV, about one order of magnitude larger than reasonable estimates. On the other hand a weakly correlated model, based on the simplest tight binding picture, which has perfect nesting for a half filled band easily accounts for the observed order of magnitude of $T_N$ variation with $\delta$ [7].

Within a weakly correlated model, it is in fact almost unavoidable that, as a function of doping, $T_N$ is maximum away from half band filling. In the simplest tight binding picture the Fermi surface shown in figure 1 has the perfect nesting property at half band filling ($\mu = 0$) for $Q_0 = \left( \pm \pi, \pm \frac{\pi}{2} \right)$, as well as the well known saddle points at $k = \left( \pm \frac{\pi}{2}, 0 \right)$ and $k = \left( 0, \pm \frac{\pi}{2} \right)$. This leads to the $\ln^2 T$ divergences in Spin Density Wave (SDW) and Cooper pair response functions [8] ... However any correcting term to the simplest tight binding model (such as second nearest neighbour overlap terms) leads to qualitative differences with the zero order model. Consider for example the electronic dispersion law :

$$\epsilon(k) = -2t \left( \cos k_x a + \cos k_y a \right) + 4t_2 \cos k_x a \cos k_y a - \mu. \quad (1)$$

With a finite next nearest neighbour $t_2 \neq 0$, nesting is imperfect and the Fermi surface does not go through the saddle points if $\mu = 0$.

Various authors have stressed that the strong antiferromagnetic fluctuations which arise when $\mu = t_2 = 0$ may give rise to an attractive coupling between electrons provided that the orbital symmetry of the singlet pair is of d type, so as to minimize the repulsive interaction at the origin [9 - 18] . When $t_2 = 0$, Schulz [19] has remarked that the RPA approximation to derive the phase diagram of (2) may be in error because the electron-hole and Cooper pair channels are coupled together ; he has set up a simple scaling theory which allows to treat those on the same footing. The phase diagram he derives has a maximum of $T_N(\mu)$ at $\mu = 0$ and an anisotropic singlet d superconducting phase which overwhelms the antiferromagnetic order when $\mu > T_N(\mu = 0)$.

On the other hand, Lin and Hirsch [20] have stressed that the model (Eq. (2)) which they studied for its magnetic properties is pathological at $t_2 = 0$ and that the generic model has $t_2 \neq 0$. Indeed band calculations [21] yield $t_2 \sim 0.03 t$.

Lin and Hirsch [20] show that within Hartree-
Fock approximation, one finds a SDW instability with a maximum of $T_N$ away from $\mu = 0$. This is straightforward with equation (1) since at $\mu = -4t_2$ the Fermi level sits at the Van Hove singularity and, as shown by Rice and Scott [22], this leads to a divergent spin susceptibility for the wavevector which connects the saddle points while the same response is bounded at $\mu = 0$. However this Hartree-Fock result is not confirmed by a Monte Carlo computation, which always yield a maximum of $T_N$ at $\mu = 0$ [20].

We have thus decided to visit again the generic model, i.e. that with $t_2 \neq 0$, and $t_2/t < 1$; we have extended the scaling approach [19] to that situation: at first, the chemical potential is adjusted so that the Fermi surface sits at the Van Hove singularity, i.e. $\mu_o = -4t_2$. In that case the normalized SDW susceptibility is

$$\chi(Q_0, T) = \begin{cases} \frac{1}{2\pi} \left( \frac{\ln^2 \pi^2 t}{2T} - \frac{\ln^2 \pi^2 t}{\varepsilon_c} \right) ; & \varepsilon_c > 4t_2 \\ \frac{1}{2\pi} \frac{\ln^2 \pi^2 t}{4t_2} \left( \frac{\ln^2 \pi^2 t}{2T} - \frac{\ln^2 \pi^2 t}{\varepsilon_c} \right) ; & \varepsilon_c < 4t_2 \end{cases}$$

(3)

where $\varepsilon_c$ is an ultraviolet cutoff. In the second line the logarithmically divergent terms (with $T$ or $\varepsilon_c$) come from the Van Hove singularity while the coefficient in front reflects the violation of perfect nesting.

The Cooper pair bubble, on the other hand, is:

$$\Pi(0, T) = \frac{1}{2\pi} \left( \frac{\ln^2 \pi^2 t}{2t} - \frac{\ln^2 \pi^2 t}{\varepsilon_c} \right)$$

(4)

We neglect here other contributions such as for example $\chi(Q = 0, T)$ or $\Pi(Q, T)$ because, although they are logarithmically divergent, they have a small prefactor compared to $\ln \pi^2 t/4t_2$ (See Appendix A).

Finally, when $|\mu - \mu_o|$ is larger than $|4t_2|$, we have:

$$\chi(Q_0, T) \simeq \frac{1}{2\pi} \frac{\ln^2 \pi^2 t}{[\mu - \mu_o]} ; \varepsilon_c > 4t_2$$

$$\Pi(0, T) \simeq \frac{1}{2\pi} \frac{\ln^2 \pi^2 t}{[\mu - \mu_o]} \ln \frac{\pi^2 t}{4t_2}$$

(5)

As in reference [19] we consider only interactions between states near the corners of the Fermi surface, which are labelled by 1, 2. The following interactions are considered:

$$G_1 : (1, 2) \rightarrow (2, 1) ; \quad G_2 : (1, 1) \rightarrow (1, 1)$$

$$G_3 : (1, 1) \rightarrow (2, 2) ; \quad G_4 : (1, 2) \rightarrow (1, 2)$$

In the Hubbard model $G_i = U/4\pi t$.

At high cutoff energy $\varepsilon_c$, there are $\ln^2$ corrections from e-e and from e-h diagrams in the perturbation expansion of the electron-electron vertices $\Gamma_i$ [19]. We rewrite them here, specifying the contributions from e-e ($\Pi$) or e-h ($\chi$) diagrams. We have:

$$\begin{align*}
\Gamma_1 &= G_1 - 2 \left( G_1^2 - G_1G_4 \right) \\
\Gamma_2 &= G_2 - \left( G_2^2 + G_2G_1 \right) \\
\Gamma_3 &= G_3 - 2G_2G_3+G_2 + 2 \left( 2G_3G_4 - G_4G_1 \right) \\
\Gamma_4 &= G_4 + \left( G_4^2 + G_4G_1 \right)
\end{align*}$$

(6)

In the Appendix A, we derive more complete equations which take into account the other logarithmic fluctuations. At low cutoff energy, equation (6) still holds, but with the low energy expression of $\chi$ replacing its high energy form. Likewise when $|\mu - \mu_o| > 4t_2$ and $\varepsilon_c < 4t_2$, equation (5) prevails in (6).

Following references [19, 23], we write the Lie equation for the renormalized couplings, setting $l = \ln \left( \pi^2 t/\varepsilon_c \right) / (2\pi)^{1/2}$ and $l_0 = \ln \left( \pi^2 t/4t_2 \right) / (2\pi)^{1/2}$

$$\begin{align*}
G_1' &= 2G_1 (G_4 - G_1) l_o \\
G_2' &= -2 \left( G_2^2 + G_2G_1 \right) l \\
G_3' &= -4G_2G_3 + 2G_3 \left( 2G_4 - G_1 \right) l_0 \\
G_4' &= \left( G_4^2 + G_4G_1 \right) l_0
\end{align*}$$

(7)

(The validity of the approach is doubtful beyond 2nd order in $G_i$s)

The RPA couplings are [19]:

* $-2 (G_2 + G_3)$ for singlet s-type superconductivity.
* $-2 (G_2 - G_3)$ for singlet d-type superconductivity.
* $2 (G_3 + G_4)$ for Spin Density Wave (SDW) antiferromagnetism.
* $-2 (2G_1 + G_3 - G_4)$ for Charge Density Wave (CD W) instability.

At high energy ($\varepsilon_c > 4t_2$), $l_0$ has to be replaced by $2l$ in (7), thereby retrieving the original equations in reference (19) for $t_2 = 0$.

We have solved numerically equation (7) by starting the renormalization procedures at $l = 0$ until $l = l_0$, and then going over to equation (7) using the renormalised values $G_i (l_0)$ as bare couplings for the new problem.

The divergence of coupling constants at $l^*$ is interpreted [19] as a phase transition at a temperature $T_c = \pi^2 t/4 \exp -\sqrt{2\pi} l^*$. Within the simple treatment we describe here, it is clear that as long as $4t_2 < T_{SDW}^0$ (where $T_{SDW}^0$ is the SDW transition temperature for $t_2 = 0$), the second regime does not come into play, i.e. the instability is a SDW one [19], with dominant SDW fluctuations in the metallic phase. When $4t_2 > T_{SDW}^0$, the winning instability is the anisotropic singlet d-type superconductivity, with a much slower decrease of $T_{SC}$ as a function of $\mu$ along the line $\mu = -4t_2$ than along the line $t_2 = 0$. The trajectories for the renormalized couplings cross at a finite value $l_*$, which defines a cross over temperature in the metallic phase between
a regime dominated by SDW fluctuations and one dominated by SCd fluctuations near the SC transition temperature.

One feature of our results is that, at fixed $t_2$, the superconducting transition $T_{SC}(t_2, \mu)$ does not vary much with $|\mu - \mu_0| < T_{SDW}(t_2, \mu_0)$. In particular, when $4t_2 \sim T_{SDW}$, there is a whole range of chemical potential variation such that $T_{SC}(t_2, \mu) \sim T_{SDW}$. The order of magnitude of the variation of carrier concentration $x$ over which $T_{SDW}$ does not vary much (for $4t_2 < T_{SDW}$) is

$$x = \int_{\mu_0}^{\mu_0 + T_{SDW}} n(E) dE = \frac{T_{SDW}}{2\pi^2 t} \left( 1 + \ln \frac{\pi^2 t}{T_{SDW}} \right)$$

with $t = 0.5$ eV one finds $x \sim 7 \times 10^{-3}$ for $T_{SDW} \equiv 100$ K i.e. $T_{SDW}$ vanishes for $x \sim 10^{-2}$. Introducing $m^*/m \approx 5$ as in reference [17] yields $\delta \approx 2.5 \times 10^{-2}$.

Remark: An interesting feature of the model is that normal impurities act as efficient pair breaking mechanism for singlet d type superconductivity when $1/\tau > T_{SC}$, because the SDW fluctuations saturate when this happens $(\tau$ is the electronic relaxation time due to normal impurity scattering). Indeed, when $\epsilon_c < \min(1/\tau, 4t_2)$ then $x(Q, T) = \frac{1}{2\pi} \ln \frac{\pi^2 t}{4t_2} \ln \frac{x^2 t}{\epsilon_c}$ and $\Pi(0, T) = \frac{1}{2\pi} \ln x^2 t \ln \frac{\epsilon_c}{\pi^2 t}$, so that one recovers the regime studied in reference [19] for $\mu > T_{SDW}$, with exponentially smaller $T_{SC}$ at large enough $x^{-1}$. This confirms a remark in reference [17].

Conclusion.

We have discussed a scaling theory for a generic model of a two dimensional tight binding electron gas in a square lattice, including next nearest neighbour overlap integrals. Our main results are: the maximum of $T_{SDW}$ as a function of doping may occur away from half band filling in the weak coupling limit, in agreement with the RPA result and in apparent contradiction with strong coupling theories; the range of stability of antiferromagnetism with doping is comparable to that found within RPA and agrees with experiment; when $4t_2$ exceeds $T_{SDW}$, d type singlet superconductivity, induced by antiferromagnetic fluctuations, overwhelms the latter even when the Fermi level is at the Van Hove singularity; we find that the superconducting temperature $T_{SC}$ is of the order of the Néel temperature of the perfectly nested model in a sizeable part of the phase diagram; normal impurity scattering, when sufficiently strong, may be efficient in suppressing superconductivity. There may exist other explanations for the apparent maximum of $T_N$ away from stoichiometry: for example a partial overlap of La d-bands with Cu-O p-d bands or defects in stoichiometry. This would leave as a difficulty for strong coupling theories the rapid variation of $T_N$ with oxygen vacancy concentration.

An obvious shortcoming of the present model, as well as that discussed in reference [19] when trying to connect with experiments is that the actual symmetry of La$_2$CuO$_4$ is orthorhombic [24], as well as that of superconducting YBa$_2$Cu$_3$O$_{7-\delta}$ [25]. Then the nearest neighbour overlap integrals $t_x$ and $t_y$ are different. If $|t_x - t_y| > 4t_2$ the situation is somewhat more complicated if $\mu$ is at the Van Hove singularity: singlet d superconducting fluctuations then may be mixed with singlet-s ones, SDW fluctuations are not divergent anymore while ferromagnetic ones are, etc.. This deserves a separate study which is under way and which will be published separately. When $t_2 = \mu = 0$ in the orthorhombic symmetry, the competing fluctuations (e-e and e-h) both diverge as $\ln \pi^2 t/2T$. It is easy to solve the scaling equations in this case: one finds, for obvious reasons (the Fermi surface has perfect nesting) that the SDW instability always dominates; $T_{SDW}$ decreases when $|t_x - t_y| > T_{SDW}$, at a rate intermediate between the two instability lines shown in figure 2. Here again, a non zero $t_2$ ($t_2 > T_{SDW}$) restores the possibility of singlet d superconductivity at $\mu = 0$.

An interesting feature of the model is the existence of a cross over from a strong paraconductive regime to a strong antiferromagnetic spin fluctuation regime in the metallic phase as the temperature increases above $T_{SDW}$; the analysis of magnetoresistance data on YBa$_2$Cu$_3$O$_{7-\delta}$ by Senoussi et al. [26], as well as the remarks by Lee and Read [17] seem to confirm this feature. Anomalies in resistivity which are found around 250 K in LaCuO$_4$ may be a sign of this cross-over line [27].
The coexistence of superconductivity and SDW order is suggested by the simultaneous divergence of both response functions. The electronic states left over in our treatment away from the Fermi surface corners could support the SDW order, as suggested in reference [16].

As already noticed by Hasegawa and Fukuyama [7], the phase diagram of this model always has $T_{SC}$ maximum near the SDW phase. Although at first sight this does not seem to correspond to the experimental phase diagram of $\La_{2-x}\Sr_x\CuO_4$ compounds [28], the observation of superconductivity in $\La_2\CuO_4$[29] might be considered as a support for weak coupling theories even though problems of experimental control of stoechiometry should be clarified.

The relevance of a parameter such as $t_2$ to the physics of $\La_{2-x}\Sr_x\CuO_4$ or $\YBa_2Cu_3O_7$ depends on the comparison with $\hbar/r$. Following reference [17], this sets a lower limit $4t_2 \sim 3T_{SDW}$, i.e. $t_2/t \sim 4 \times 10^{-2}$, of order of the estimate taken from reference [21]. If $t_2$ becomes irrelevant, the weak coupling approach has to argue that actually observed $T_{SC}$ are strongly reduced ones in comparison with ideal ones [17].

We suspect that both strong coupling and weak coupling theories have to face the fact that actual high $T_c$ superconductors are in intermediate situation, as confirmed by the estimate of $U \approx 2.5 \ zt$ in reference [30].

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### Appendix A

In the following, we take into account all divergent logarithmic fluctuations in the scaling equations for the renormalized coupling. Let $\chi(0,T) \equiv F$ and $\Pi (Q_o,T) = S$. Then $F \propto S \propto \ln e_o/2T$ in the first regime, $F \sim S \sim \propto S$ in the second regime.

The generalization of the set of equations (6) is:

$$
\begin{align*}
\Gamma_1 &= G_1 - 2 \left( G_2^2 - G_1G_4 \right) \chi + 2G_1G_2 F - 3G_1G_4 S \\
\Gamma_2 &= G_2 - \left( G_2^2 + G_4^2 \right) \Pi + \\
&\quad + \left( G_1^2 + G_2^2 - 2G_4^2 + 2G_1G_4 \right) F \\
\Gamma_3 &= G_3 - 2G_2G_3 \Pi + 2G_3 \left( 2G_4 - G_1 \right) \chi \\
\Gamma_4 &= G_4 + \left( G_2^2 + G_4^2 \right) \chi - \left( G_1^2 + G_2^2 \right) S + + 2G_2 \left( G_4 - G_1 \right) F
\end{align*}
$$

(A.1)

The numerical results displayed in figure 2 are in fact based on equation (A.1). $T_{SDW}$ is found to be $T_{SDW} = e^{2t_2} \cdot e^{-\left(2\pi/\alpha t_2\right)^{1/2}}$ with $\alpha \approx 4.8$ slightly different from the RPA value 4 or the value found by Schu’s [19].

### References


[27] Tournier, R., private communication.

