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Extended Hubbard model in two dimensions

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Abstract. The extended Hubbard model with nearest neighbour inter-site correlations has been studied by mapping it onto a spin-Hamiltonian. In the case of a half-filled band the problem is equivalent to that of an anisotropic Heisenberg model in the absence of a field. The phases in the U–Q plane obtained here are in good agreement with those obtained by Monte Carlo simulation. The antiferromagnetic XY-ordered phase of the model is shown to be very similar to an RVB phase. Extending the analogy away from half-filling, a possible dependence of the critical temperature T_c with the doping concentration δ in a high-T_c system is suggested.

1. Introduction

The Hubbard model [1] defined on a two-dimensional lattice has attracted a lot of attention as a possible model for high-T_c superconductors [2]. In the last two decades this model has been extensively studied for itinerant antiferromagnetism as well as for a description of the metal–insulator transition.

Experimentally, it is known that the precursor Cu–O-based insulators show magnetic long-range order in two dimensions [3], while the RVB phase of Anderson does not. Pure La_2CuO_4 has been shown to exhibit meta-magnetism. Further, studies in the Er–Ba–Cu–O system indicate that with an increase in the concentration of dopants, the behaviour of the system shows a cross-over from an Ising-like insulating phase to an XY-like metallic (superconducting) phase. This suggests that the model Hamiltonian used to describe such systems should take account of the anisotropic spin–spin interaction. The half-filled Hubbard model can be mapped on to an isotropic Heisenberg model for $U \gg t$. Using a transformation due to Shiba [4] and Robaszkiewicz *et al* [5] it is possible to transform the extended Hubbard model into an interacting spin system with anisotropic spin–spin interaction. Varma [6] has recently used such a model to obtain insulating behaviour near half-filling and superconductivity away from it, in agreement with the experimental properties of systems such as $BaPb_xBi_{1-x}$. Another point in favour of the extended Hubbard model is that the superconducting transitions in the systems mentioned above, as well as that in systems like Y–Ba–Cu–O, occur near the metal–insulator transition. The Hubbard model with intra-site Coulomb repulsion leads only to a continuous transition [7]. It has been suggested [8] that in the limit $U \gg t$, the inter-site term Q_{ij} may lead to a discontinuous transition.

It may be appropriate here to comment on the relative strengths of the parameters U and Q. Recent estimates suggest that the inter-site interaction strength may even be as much as fifty percent of the intra-site strength causing serious errors in calculations

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where such terms are omitted. Additionally, the in-plane coherence length in these materials is of the order of a few lattice spacings [9].

Recently, Callaway and Zhang [10] have studied the extended Hubbard model using a Monte Carlo technique. For the half-filled case, they obtain a phase diagram in the Q–U plane showing antiferromagnetic (AFM), charge density wave (CDW) and singlet-pairing states.

In the following, we consider the extended Hubbard model and using a canonical transformation map it onto a spin-$\frac{1}{2}$ anisotropic Heisenberg model. It may be remarked that any transformation of this type breaks the spherical symmetry of the original model. Thus while mapping back the conclusions from the anisotropic Heisenberg model to the original model it must be noted that magnetization could point in any direction restoring the spherical symmetry. Within the resulting theory, we obtain a phase diagram which is in agreement with the Monte Carlo results of Zhang and Callaway. Away from half-filling, the problem is equivalent to that of an antiferromagnet in an external field. The Kosterlitz–Thouless phase of the anisotropic model is identified with an X–Y-ordered RVB-like phase. As the occupancy parameter δ is varied, there is an insulator–metal transition. The relevance of these to T versus δ phase diagrams of the high-T_c oxides away from half-filling is also indicated. For certain values of U and Q, there is an indication of ferromagnetic phase, which is of interest [11].

2. Equivalent Hamiltonian

The extended Hubbard model in two dimensions is defined by the Hamiltonian

$$H = -t \sum_{\substack{\langle ij \rangle \\ \sigma}} C^{\dagger}_{i\sigma} C_{j\sigma} + U \sum_{i\sigma} n_{i\sigma} n_{i\bar{\sigma}} + Q \sum_{\substack{\langle ij \rangle \\ \sigma\sigma'}} n_{i\sigma} n_{j\sigma'} \tag{1}$$

where $\langle ij \rangle$ denotes sum over nearest neighbour sites i and j on a two-dimensional square lattice, and σ is the spin index. Adler [12] included the effect of the inter-site term by decoupling the last term within the mean field approximation. This has the effect of converting this term to a purely single-site term which leaves out the crucial many-body effect contained therein. Eapen *et al* [13] have solved this model in the Hubbard III approximation, which includes finite lifetime effects [7]. They obtain three bands centred at t, $t + Un_\sigma + QnZ$ and $t + U + QnZ$. For $Q = 0$, however, there are only two bands as the strength associated with the third band vanishes. As Q and U are varied, three bands coalesce into two bands for values of $QZ/U > 0.5$. This situation prevails in the two-dimensional high-T_c oxides, as well as in the three-dimensional $BaBiO_3$-based materials.

Hence, it is appropriate to work in the two-band regime. Further, we restrict ourselves to the singly-occupied states as t/U is assumed small. This is done by using a projection technique due to Chao *et al* [14] to define two operators P_1 and P_2 which respectively project out the singly-occupied and the doubly-occupied states. The effect of the former type of operators is to replace the operators $C_{i\sigma}$ by $C_{i\sigma}(1 - n_{i\bar{\sigma}})$ while that of the latter is to replace $C_{i\sigma}$ by $C_{i\sigma} n_{i\bar{\sigma}}$. To the lowest order in t/U, the transformed Hamiltonian is given by

$$\tilde{H} = P_1 H P_1 + P_2 H P_2 - \frac{(P_1 H P_2 H P_1 - P_2 H P_1 H P_2)}{U_{\text{eff}}} \tag{2}$$

where $U_{\text{eff}} = U + QnZ$ is the effective separation between the sub-bands. For the Hamiltonian (1), one obtains the following relations:

$$\begin{aligned}
P_1HP_1 &= -t\sum_{\substack{\langle ij\rangle\\ \sigma}}(1-n_{i\bar\sigma})C^\dagger_{i\sigma}C_{j\sigma}(1-n_{j\bar\sigma}) + Q\sum_{\substack{\langle ij\rangle\\ \sigma\sigma'}}(1-n_{i\bar\sigma})n_{i\sigma}n_{j\sigma'}(1-n_{j\bar\sigma'})\\
P_1HP_2 &= -t\sum_{\substack{\langle ij\rangle\\ \sigma}}(1-n_{i\bar\sigma})C^\dagger_{i\sigma}C_{j\sigma}n_{j\bar\sigma} + Q\sum_{\substack{\langle ij\rangle\\ \sigma\sigma'}}(1-n_{i\bar\sigma})n_{i\sigma}n_{j\sigma'}n_{j\bar\sigma'}\\
P_2HP_1 &= -t\sum_{\substack{\langle ij\rangle\\ \sigma}}n_{i\bar\sigma}C^\dagger_{i\sigma}C_{j\sigma}(1-n_{j\bar\sigma}) + Q\sum_{\substack{\langle ij\rangle\\ \sigma\sigma'}}n_{i\bar\sigma}n_{i\sigma}n_{j\sigma'}(1-n_{j\bar\sigma'})\\
P_2HP_2 &= -t\sum_{\substack{\langle ij\rangle\\ \sigma}}n_{i\bar\sigma}C^\dagger_{i\sigma}C_{j\sigma}n_{j\bar\sigma} + U\sum_{i\sigma}n_{i\bar\sigma}n_{i\sigma} + Q\sum_{\substack{\langle ij\rangle\\ \sigma\sigma'}}n_{i\bar\sigma}n_{i\sigma}n_{j\sigma'}n_{j\bar\sigma'}).
\end{aligned} \tag{3}$$

We define spin operators in the standard fermion representation

$$\begin{aligned}
S_i^+ &= C^\dagger_{i\uparrow}C_{i\downarrow}\\
S_i^- &= C^\dagger_{i\downarrow}C_{i\uparrow}\\
S_i^z &= (n_{i\uparrow}-n_{i\downarrow})/2.
\end{aligned} \tag{4}$$

Using these, the transformed Hamiltonian becomes, after considerable algebra,

$$\begin{aligned}
\tilde H = {} & -t\sum_{\langle ij\rangle}(1-n_{i\bar\sigma})C^\dagger_{i\sigma}C_{j\sigma}(1-n_{j\bar\sigma}) + \frac{4t^2}{U_{\text{eff}}}\sum_{\langle ij\rangle}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{n_in_j}{4}\right)\\
& + Q\sum_{\substack{\langle ij\rangle\\ \sigma\sigma'}}(1-n_{i\bar\sigma})n_{i\sigma}n_{j\sigma'}(1-n_{j\bar\sigma'}) + Q\sum_{\substack{\langle ij\rangle\\ \sigma\sigma'}}n_{i\bar\sigma}n_{i\sigma}n_{j\sigma'}n_{j\bar\sigma'}\\
& - \frac{2Q^2}{U+QnZ}\sum_{\substack{\langle ij\rangle\\ \sigma}}(n_{i\bar\sigma}n_{i\sigma}n_{j\sigma}n_{j\bar\sigma} - C^\dagger_{i\bar\sigma}C_{j\bar\sigma}n_{i\sigma}n_{j\sigma}).
\end{aligned} \tag{5}$$

Except for the hopping described by the first term of (5), one can get an effective spin Hamiltonian by using (4) in (5) through relations of following type:

$$\begin{aligned}
\sum_{\substack{\langle ij\rangle\\ \sigma}}n_{i\sigma}n_{j\sigma} &= 2\sum_{\langle ij\rangle}S_i^zS_j^z + \frac{1}{2}\sum_{\langle ij\rangle}n_in_j\\
\sum_{i\sigma}n_{i\bar\sigma}n_{i\sigma} &= -\frac{4}{3}\sum_i(\boldsymbol{S}_i)^2 + \sum_{i\sigma}n_{i\sigma}.
\end{aligned} \tag{6}$$

Further, we replace $\sum_{\substack{\langle ij\rangle\\ \sigma}} C^\dagger_{i\bar\sigma}C_{j\bar\sigma}n_{i\sigma}n_{j\sigma}$ by $2p\sum_{\langle ij\rangle}[\boldsymbol{S}_i\cdot\boldsymbol{S}_j - S_i^zS_j^z]$, its approximate value. Here $p = \langle C^\dagger_{i\sigma}C_{j\sigma}\rangle$ is assumed independent of σ. The value of p depends

only on the distance $|i-j|$. Following Adler [15], we have performed a preliminary calculation which indicates that p oscillates with distance and changes sign at around the nearest neighbour separation. It may be noted that the first of the equations (6) is responsible for breaking the spin-rotational symmetry of the original model. Similar transformations have been used by Robaszkiewicz *et al* [5] and Varma [6]. However, these authors obtain, in addition, an external field term because they use a Jordan–Wigner type of transformation to spin variables.

In addition, for $S=\frac{1}{2}$, one can replace [16]

$$-J\sum_{(ij)}[\boldsymbol{S}_i\cdot\boldsymbol{S}_j+\alpha(\boldsymbol{S}_i\cdot\boldsymbol{S}_j)^2]$$

by

$$-J\sum_{(ij)}\left(1-\frac{\alpha}{2}\right)\boldsymbol{S}_i\cdot\boldsymbol{S}_j\,.$$

The final transformed Hamiltonian is

$$\begin{aligned}\tilde{H}=&-t\sum_{(ij)_\sigma}(1-n_{i\sigma})C^\dagger i\sigma C_{j\sigma}(1-n_{j\bar{\sigma}})+J_z\sum_{(ij)}S_i^zS_j^z\\&+J_{xy}\sum_{(ij)}(S_i^+S_j^-+S_i^-S_j^+)+J_2\sum_i(\boldsymbol{S}_i)^2+J_3\sum_{(ij)}n_in_j\end{aligned}\tag{7}$$

where

$$\begin{aligned}J_z&=\frac{4t^2}{U+QnZ}-\frac{8Q}{9}+\frac{16Q^2}{U+QnZ}\\J_{xy}&=\frac{1}{2}\left[J_z+\frac{4Q^2p}{U+QnZ}\right]\\J_2&=-\frac{4}{3}QnZ\\J_3&=\left[Q-\frac{t^2}{U+Qn\bar{z}}\right].\end{aligned}\tag{8}$$

When $Q=0$, $J_z=2J_{xy}=-4J_3=4t^2/U$, so that equation (7) leads to Anderson's result away from half-filling [2]

$$\tilde{H}=-t\sum_{(ij)_\sigma}(1-n_{i\bar{\sigma}})C_{i\sigma}^\dagger C_{j\sigma}(1-n_{j\bar{\sigma}})+J\sum_{(ij)}\left(\boldsymbol{S}_i\cdot\boldsymbol{S}_j-\tfrac{1}{4}n_in_j\right).\tag{9}$$

In the exactly half-filled case, $n_i=n_j=1$, $\sum(\boldsymbol{S}_i)^2$ is a c number and $n_{i\sigma}=1-n_{i\bar{\sigma}}$. From equation (7) one then has,

$$\tilde{H}=J_z\sum_{(ij)}S_i^zS_i^z+J_{xy}\sum_{(ij)}(S_i^+S_j^-+S_i^-S_j^+)\tag{10a}$$

which can be rewritten as

$$\tilde{H} = \alpha J_z \sum_{\langle ij \rangle} (\boldsymbol{S}_i \cdot \boldsymbol{S}_j) + J_z(1-\alpha) \sum_{\langle ij \rangle} S_i^z S_j^z \tag{10b}$$

where

$$\alpha = 1 + \frac{36Q^2 p}{36t^2 - 8QU - 16Q^2}. \tag{10c}$$

The canonical transformation is thus seen to produce two effects. In addition to renormalizing Anderson's exchange constant J to αJ_z, it also breaks the spin-rotational symmetry of the original model Hamiltonian given in equation (1) except in the special case of $n = 1$ and $Q = 0$. As we have remarked earlier, this is not that serious since the rotational symmetry could be obtained back when one performs the inverse transformation [6] and quantities like magnetization could point in any direction. The same deficiency, incidentally, is inherent in most treatments of the Hubbard model using a functional integral approach where the Hamiltonian is usually expressed in terms of $(S_z)^2$. The system with Hamiltonian given by equation (10) is known to exhibit magnetic long-range order in two dimensions [17]. The undoped insulator is thus characterized by the two-dimensional LRO in accordance with the experimental observation.

3. Discussions and results

For the Hamiltonian described by equation (10), it can be seen that there exists a gap between $S^z = 0$ and $S^z = \pm 1$ excitation spectrum given by

$$\begin{aligned} \Delta &= E(S^z = \pm 1) - E(S^z = 0) \\ &= J_z(1-\alpha)/2 \\ &= -\frac{2Q^2 p}{U + 4Q}. \end{aligned} \tag{11}$$

As p is negative, the state with $S^z = 0$ lies lower in energy. For $Q = 0$, equation (11) gives $\Delta = 0$, showing that the triplets are degenerate, as is expected for the isotropic Heisenberg model.

From equation (11), it is seen that as Q tends to zero, the gap Δ closes in a continuous fashion, indicating that the ordering transition at $\alpha = 1$ is continuous, in agreement with the indications available from the numerical results of Barnes *et al* [18].

Let us consider some special cases.

(i) $U > 0$, $Q > 0$: for both U and Q positive and large compared to t, and $U \gg Q$, we have

$$J_z = \frac{36t^2 - 8QU - 16Q^2}{9(U + 4Q)} \approx \frac{-8Q(U + 2Q)}{9(U + 4Q)}$$

$$\alpha = 1 + \frac{36Q^2 p}{36t^2 - 8QU - 16Q^2} \approx 1 - \frac{9Qp}{2(U + 2Q)}.$$

We find that J_z is negative while α is positive and greater than 1. Notice that the above result assumes $Q \gg t$ and hence the conclusions are not valid in the limit of Q going to zero. In this case we have a ferromagnetic Heisenberg model with exchange constant αJ_z in the presence of an additional antiferromagnetic Ising interaction of strength $J_z(1-\alpha) > 0$. The spin spectrum has a gap with the triplets being separated from the singlet by $J_z(1+\alpha)/2$.

It is well known that the Ising limit of the model, in which only an FM interaction is taken into account, corresponds to the classical lattice-gas model with attractive interaction between nearest neighbour atoms. The XY part of the Hamiltonian takes into account quantum hopping between nearest neighbours. The parameter p, which depends on the distance $|i-j|$, can be varied by external factors like application of pressure or change in dopant concentration. For positive p, the ground state belongs to $S=1, S^z=1$, i.e. it is a triplet. As p is varied by changing the external parameters, the spin gap reduces and for some critical value of the parameter, the ground state shows a cross-over to the $S=1$, $S^z=0$ state corresponding to an unsaturated ferromagnet. In this region, the dominant term in the Hamiltonian becomes XY-like.

However, for sufficiently small Q, the original expressions for J_z and α need to be used, which implies $J_z > 0$ for U and $Q > 0$. For $p > 0$, i.e. for $\alpha > 1$, the ground state has AFM X–Y ordering of the spins. This phase is very similar to the RVB phase of Baskaran *et al* [2] in that it has a gapless spin excitation spectrum [18] and it does not have antiferromagnetic long-range order (except possibly topological long-range order of the Kosterlitz–Thouless type). With a small amount of doping, we would then have appreciable singlet-pairing correlations, in agreement with the Monte Carlo simulation results of Callaway *et al* [10].

However, in the region of p where $\overline{p_c} = [(4/9)+(2U/9Q)-(t/Q)^2] < p < 0$ we have $0 < \alpha < 1$, so one has an AFM Z-ordered ground state. Varying p by changing the external parameters, we have $\alpha < 0$ when $p < \overline{p_c}$, and this case describes the situation in which one has co-existent sublattice AFM LRO of the Z-component (corresponding to CDW) and FM order of the XY-components, in qualitative agreement with MC simulation.

(ii) $U > 0$, $Q < 0$: for $(U+4Q)$ positive, one has $J_z > 0$ and in the region of p where $p_c = [-2(U+2Q)/9Q] < p < 0$ one has AFM LRO of the Z-components. In classical models, the system shows LRO, but for spin $S = \frac{1}{2}$ models, quantum fluctuations destroy this order [19]. If one now moves away from the half-filled case by doping, the system will behave like an AFM in a field, and in the region of doping concentration (field values) where quantum fluctuations are suppressed, the system shows sublattice LRO. The X–Y phase can be stabilized by varying the parameter p and this phase corresponds to the Kosterlitz–Thouless phase of the anisotropic AFM.

However, for $-U/2 < Q < -U/4$, $J_z < 0$ and for $p_c < p < 0$ we have $0 < \alpha < 1$ so that the ground state is a triplet and belongs to $S=1, S^z=1$.

If p is now decreased, α switches sign when $p < p_c$, and so one has a XX–Z model. For bipartite lattices and in the absence of transverse fields, the Hamiltonian is invariant under the change $J_z \rightarrow -J_z$, and one has an AFM model. In this case, all that was remarked for the case $(U+4Q) > 0$, $0 < \alpha < 1$ remains valid. For non-bipartite lattices, however, one interesting realization is that the system with $J_z < 0$ and $J_z\alpha/2 > 0$ can be interpreted as a quantum lattice-gas with repulsive quantum exchange and an attractive interaction between neighbouring atoms. In this situation, one has a phase where co-existence of the FM order of the Z-component and the AFM order of the XY-components is found; this may be a model of co-existence of diagonal

and off-diagonal LRO in quantum spin systems.

With $Q < -U/4$, $J_z < 0$, and for $p > p_c > 0$, we have $0 < \alpha < 1$, so that we have Ising-like AFM Z-order. If p is now decreased by varying external parameters, α changes sign when p is decreased below p_c. For non-bipartite lattices, it has been shown that even for infinitesimally small $-J_z\alpha/2$, the behaviour of the system resembles that of an XY ferromagnet [20]. Interestingly, this model with $J_z > 0$ and $J_z\alpha/2 < 0$ can be interpreted as a quantum lattice-gas model with attractive quantum exchange $J_z\alpha/2$ and a repulsive interaction J_z; it may be a possible candidate for the co-existence of diagonal and off-diagonal LRO in quantum spin systems. It is likely that the Z-ordered phase will become unstable for some critical value of $J_z\alpha/2 = (J_z\alpha/2)_c$. This will most likely indicate the stability of a superfluid phase for values of $J_z\alpha/2 > (J_z\alpha/2)_c$. We have not succeeded in calculating $(J_z\alpha/2)_c$.

(iii) $U < 0$, $Q > 0$: with U and Q such that $-U/2 > Q$, $-U/4$, $J_z > 0$. For $p > 0$, α becomes greater than 1, so that the ground state is the XY-ordered AFM state. As remarked earlier, this XY phase of the anisotropic AFM is similar to an RVB phase. This would signal the onset of superconductivity caused by Bose–Einstein condensation of pre-existing singlets.

On the other hand, with $Q > -U/2$, one has $J_z < 0$. With $p > p'c = 2(U + 2Q)/9Q$, one has co-existent FM ordering of the Z-component and AFM ordering of the XY-components. This is the so called XX-Z model, and for bipartite lattices, one has an AFM ground state. With decrease in p, α switches sign as p is varied through p'_c . For $0 < p < p_c$, one has an FM Z-ordered phase. For small anisotropy, i.e. for $(1 - \alpha)$ small, we have [21]

$$T_c = \frac{\pi J_z(0)}{2k_B} \frac{1}{\ln\left(\frac{1}{1-\alpha}\right)}. \tag{12}$$

Above T_c, there is an Onsager-like transition in 2D to a phase with paramagnetic ground state. As p is decreased further, α becomes greater than 1, so that the FM XY-ordered state is now the ground state of the system. Here, we have a sort of unsaturated ferromagnetism. For $Q < -U/2$, we have $J_z < 0$. Starting with $p > 0$, we find that with $\alpha > 1$, the FM XY-ordered state is the ground state of the system. Here we again have an unsaturated FM. As p is varied through zero, α becomes less than 1, and in the region of p values satisfying $p_c = -[2(U + 2Q)/9Q] < p < 0$ the ground state belongs to $S = 1$, $S_z = 1$, and one has an FM Z-ordered phase. As p is further decreased, at p''_c, α switches sign, and for values of p less than this critical value, one has the so-called XX-Z model. For bipartite lattices and in the absence of transverse fields, we have an AFM ground state, but for general cases, we have co-existent FM order of the Z-component and AFM order of the XY-components.

(iv) $U < 0$, $Q < 0$: with U and Q negative, J_z is positive. Starting from $p > p_c = (2|U + 2Q|/9|Q|)$, we have $\alpha < 0$. For general non-bipartite lattices, we have co-existence of AFM Z-order (CDW) and FM XY-order (unsaturated FM).

If p is now decreased, but $0 < p < p_c$, we have $0 < \alpha < 1$, and so one has Ising-like sublattice AFM order. Further decrease in p stabilizes the AFM XY-ordered state, and therefore we have a RVB-like ground state. Doping the insulator in this region would result in Bose condensation of the pre-existing singlets, leading to superconductivity. This is in qualitative agreement with Callaway's Monte Carlo simulation, where appreciable singlet correlations are observed in the region of $U < 0$, $Q < 0$ at exactly half-filling.

The non-half-filled case: departure from half-filling is achieved by doping the system with holes. In the corresponding magnetic problem, it corresponds to adding a magnetic field term to the spin Hamiltonian. For values of this field from zero to a critical value given by $H_c = J_z(1-\alpha^2)^{1/2}$, the ground state remains an AFM Z-ordered state when a first-order transition occurs to a state with AFM XY-order [21]. The corresponding hole density is given by

$$\delta_0 = (1-\alpha^2)^{1/2}.$$

Physically, for small doping concentration, the holes remain localized and the AFM long-range order (LRO) is maintained. In the usual Hubbard model, in this limit, one would have an RVB phase with only short-range order (SRO). In our model, as the concentration of holes increases, the consequent rise in kinetic energy destroys the LRO, and at $\delta = \delta_0$, the above-mentioned transition takes place. This X–Y ordered phase is the Kosterlitz–Thouless phase of the 2D anisotropic Heisenberg model and has properties similar to the RVB phase. This implies the existence of a superconducting phase near and above a deviation from half-filling δ_0. In this region, T_c is given by Anderson's relation

$$T_c = \frac{2\pi\hbar^2}{m_{\text{eff}}}(\delta - \delta_0).$$

In this region, T_c increases linearly with δ. Experimentally, however, this increase in T_c does not go on indefinitely: it saturates, showing a plateau for some range of δ, finally decreases and goes to zero. This is possibly due to the presence of impurities which provide random fields in the antiferromagnet. In 2D Ising-like systems, such random fields may lead to excessive domain formation which destroys the 2D-LRO. In figure 1 we show the phase diagram on the T–δ plane predicted by our model, depicting the long-range ordered AFM (Ising, I), AFM XY-ordered (singlet superconducting, II) and paramagnetic disordered (metallic, III) phases. It is seen that it reproduces most of the features of the experimental phase diagrams [23]. However, we have not obtained the experimentally observed spin-glass-like phase. Not much is known about this phase, but it is believed to be due to disorder not considered by us. Further, we have not been able to provide even a qualitative explanation for the plateau structure mentioned above.

4. Conclusions

We have considered the effects of including the inter-site correlation terms in the Hubbard model. Our treatment is different from that of Robaszkiewicz *et al* [5] and Varma [6], who have also considered the same model in that these authors map the extended Hubbard model onto an anisotropic Heisenberg model in the presence of an external field while we have mapped it onto a field-free XX–Z model at half-filling. Previous work carried out on this Hamiltonian were either in the mean-field theory or in RPA [5]. The resulting phase diagram shows AFM Z-ordered (charge ordered) region, AFM XY-ordered (singlet superconducting) region and a region of co-existence of these two phases. Varma has recently proposed that this co-existence region can arise as an array of discommensurations in a Z-ordered phase. Disorder can convert

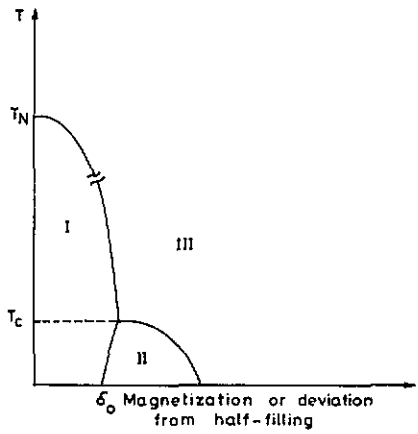

Figure 1. Phase diagram in the δ–T plane. The regions are I: AFM Ising-like, II: AFM XY-ordered, III: disordered paramagnet.

this into a short-ranged CDW. Whether this phase is an artifact of the mean-field-like theories used by these authors needs to be carefully examined. We are led to drastically different results from our strong coupling theory. For the exactly half-filled case, we get an AFM insulator with LRO in agreement with indications obtained from magnetic measurements. Our calculations at and near half-filling are in good qualitative agreement with the Monte Carlo results of Callaway *et al* [10]. For positive U and Q, we find the existence of a ferromagnetic phase. In a small part of the positive U–Q quadrant, we find that the ground state has antiferromagnetic LRO while in the region where the inter-site correlation function p is positive, we get an AFM XY-ordered phase. In this case, doping the insulator will lead to BE condensation of pre-existing singlets.

It may be noticed that in the isotropic model, superconductivity is realized for infinitesimally small doping concentrations since the singlets already exist in the RVB-like phase. Inclusion of inter-site correlations changes this situation drastically in that we get long-range magnetic order for small doping. We believe that quantum fluctuation effects are important in this limit. The increased spectral density of the holes caused by quantum fluctuations is responsible for the destruction of the long-range magnetic order upon doping. Inclusion of weak interplanar coupling can stabilize the phases found above. A qualitative description of the phases as a function of doping has been provided, but a rigorous phase diagram in the U–Q plane has not been attempted.

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