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THE HUBBARD MODEL FOR LARGE U

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Abstract: We review the present understanding of the physics of the Hubbard model in the strong coupling limit, with a special emphasis on the two-dimensional square lattice.

I - Introduction

The Hubbard model describes fermions on a lattice, with only one orbital degree of freedom and spin 1/2, subject to an on site-repulsion U. If $c^+_{i\sigma}$ denotes the fermion creation operator on site i with spin $\sigma = \pm 1/2$ and t the nearest neighbour hopping integral, the Hubbard Hamiltonian takes the form

$$H = -t \sum_{<ij>} (c^+_{i\sigma} c_{j\sigma} + h.c.) + U \sum_i n_{i\uparrow} n_{i\downarrow} \qquad (I - 1)$$

This Hamiltonian was introduced in 1963 by Hubbard[1] and others[2,3] as a theoretical way to capture the main effects of correlations in narrow d-bands of transition metals. The first term represents the ordinary band energies of the electrons (for instance $\varepsilon_k = -2t\,(\cos k_x + \cos k_y)$ on the two-dimensional square lattice with lattice spacing a=1). The local interaction term represents the Coulomb repulsion between localized Wannier states on the same site. Thanks to the Pauli principle, it acts only between electrons of different spin. The other matrix elements

of the long range Coulomb interaction are completely neglected in the model. Some justification for the validity of this approximation in real life may be found in Hubbard's first paper. At zero temperature, the model depends only on 2 parameters: t/U the ratio of the kinetic bandwidth over the interaction strength, and $n = \frac{N_\uparrow + N_\downarrow}{L}$ the average site occupancy, to be noted in the following as $1-\delta$.

In spite of its apparent simplicity and an exact solution in 1D[4], properties of the Hubbard model for $d > 1$ are hardly understood. Interest in the 2D-case was naturally boosted up by Anderson's suggestion[5] that it might be relevant to understand the physics of high Tc superconductors. An important issue is therefore to know whether the groundstate of Hamiltonian (I-1) can be superconducting in some region of the parameter space $(t/U,\delta)$. But there are many other interesting problems like the interplay between itinerant ferromagnetism, antiferromagnetism and paramagnetism or the possibility of metal-insulator transition[6] by correlation effects... At the present time, we are certainly still ignorant of the full richness of the Hubbard model and to draw even an approximate phase diagram appears like a very risky task! In these introductory notes, I shall rather try to give a simple acount of the various physical phenomena which happen in the limit of large U and small δ. Some of them are known since a long time, others were discovered recently. For simplicity, we will concentrate our attention to zero temperature properties on the square lattice in 2D, although it is clear that many effects to be discussed in the following find an extension to higher dimensions or other lattices.

II- **Strong coupling expansion**

In the large U limit, difficulties arise when the density n of fermions becomes comparable to 1. Indeed, when $n \ll 1$, the fermions can be seen as a dilute gas with an effective interaction renormalized from U to some two-body scattering metrix of

order t^3: one therefore expects the formation of a featureless paramagnetic liquid at low enough density. On the other hand, while approaching half filling (n=1), correlations between spins $\uparrow$ and $\downarrow$ become very strong and fermions tend to localize. On bipartite lattices, there is an electron-hole symmetry which allows to relate the properties of the system at $1<n<2$ to those at $n<1$. Let us indeed rewrite H as

$$H = -t \sum_{<ij>} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} (n_{i\uparrow}-1/2)(n_{i\downarrow}-1/2) - U \left(\frac{L}{4} - \frac{N}{2}\right) \qquad \text{(II-1)}$$

and make the substitution $c^{+}_{i\sigma} \rightarrow \eta_i c_{i\sigma}$ where $\eta_i=+1$ on sublattice A and -1 on sublattice B. It turns out that the first two terms are invariant in this transformation. This implies in particular for the energy

$$E(n) = \frac{<H>}{L} = E(2-n) + U(n-1) \qquad \text{(II-2)}$$

Therefore, it is enough to study the $n<1$ part of the phase diagram of the Hubbard model (corresponding to the introduction of holes in a half-filled band).

For large U, real doubly occupied sites are energetically very unfavourable. One natural way of describing the low energy physics of the Hubbard model consists in writing an effective Hamiltonian within the subspace of no doubly occupied sites[7-10]. Admixture of virtual doubly occupied sites will result in successive corrections to the Hamiltonian in powers of t/U. To see how this really works, let us separate in the hopping processes of (II-1) the ones which do not change the number of doubly occupied sites

$$H^{o}_{t} = -t \sum_{\substack{<ij> \\ \sigma}} \left\{ (1-n_{i-\sigma})\, c^{+}_{i\sigma} c_{j\sigma}\, (1-n_{j-\sigma}) + n_{i-\sigma}\, c^{+}_{i\sigma}\, c_{j\sigma}\, n_{j-\sigma} + \text{h.c.} \right\} \qquad \text{(II-3)}$$

from those which destroy or create a doubly occupied site (to be called hereafter mixing terms)

$$H_t^+ + H_t^- = -t \sum_{<ij>} \left\{ n_{i-\sigma} c_{i\sigma}^+ c_{j\sigma} (1-n_{j-\sigma}) + (1-n_{i-\sigma}) c_{i\sigma}^+ c_{j\sigma} n_{j-\sigma} + h.c. \right\} \qquad (II-4)$$

One then performs a unitary transformation which to lowest order in t/U eliminates the troublesome part of the Hamiltonian $H_t^+ + H_t^-$

$$H_{eff} = e^{iS} H e^{-iS} = H + i[S,H] + i^2/2\,[S,[S,H]] + \ldots \qquad (II-5)$$

The condition that $H_t^+ + H_t^- = -i\,[S,H_0]$ yields at once $S = -i/U\,(H_t^+ - H_t^-)$, up to corrections of order $(t/U)^2$ and leads to

$$H_{eff} = H_t^o - 1/U\,[H_t^-, H_t^+] \qquad (II-6)$$

New mixing terms have appeared in H_{eff} beside the result (II-6) but they are of order t/U compared to the initial ones. Clearly the procedure can go on recursively by expanding S in powers of t/U. Although there is no proof of the convergence of this infinite perturbation series, it is generally believed that H_{eff} in (II-6) is a good approximation to the Hubbard Hamiltonian , provided that $U > zt$ (where z is the coordination number of the lattice).

Let us now make more explicit the expression of H_{eff} acting on the subspace of no doubly occupied sites. One gets

$$H_{eff} = -t \sum_{\substack{<i,j> \\ \sigma}} (\tilde{c}_{j\sigma}^+ \tilde{c}_{i\sigma} + h.c.) + 4t^2/U \sum_{<ij>} (\vec{S}_i \cdot \vec{S}_j - \frac{n_i n_j}{4})$$

$$-t^2/U \sum_{\substack{<i,j,k> \\ \sigma}} (\tilde{c}_{k\sigma}^+ n_{j-\sigma} \tilde{c}_{i\sigma} - \tilde{c}_{k\sigma}^+ c_{j-\sigma}^+ c_{j\sigma} \tilde{c}_{k-\sigma} + h.c.) \qquad (II-3)$$

where the operators $\tilde{c}_{i\sigma}=c_{i\sigma}(1-n_{i-\sigma})$ are fermion annihilation operators projected on the subspace of no doubly occupied sites and $\vec{S}_i$ is the spin operator $1/2[c^{+}_{i\sigma}\vec{\tau}_{\sigma\sigma'}c_{i\sigma'}]$.

The first term describes direct hopping between nearest neighbours. The third one corresponds to an indirect hopping process between next nearest neighbours. It involves the virtual creation at the intermediate site j, of a $\uparrow\downarrow$ pair, which then releases one of the spins $\uparrow$ or $\downarrow$ to site i. These hopping terms become meaningful only at nonzero δ, since at half-filling electrons cannot move without violating the constraint. The third term is usually not retained in the so-called t-J model, because it is t/U smaller than the leading hopping term.

In the half filled case, H_{eff} reduces to the antiferromagnetic Heisenberg Hamiltonian with nearest neighbours coupling constant $J=4t^2/U$. This exchange interaction first obtained by Anderson[11] has the same physical origin as the last part of H_{eff}. Neighbouring antiparalell spins can lower their energy by virtually sharing the same site. This favours the formation of local singlet pairs (with energy -3/4 J). The nature of the groundstate of a quantum antiferromagnet is not as simple as for a quantum ferromagnet, because the classical Néel state with staggered spin order is not an eigenstate of the Hamiltonian. Whether or not the ground state for spin 1/2 possesses long range spin order in 2D has been a highly debated matter these recent years, following the suggestion by Anderson[5] that strong quantum fluctuations could rather favour the formation of a spin liquid state, in contrast to the "crystalline" Néel state. We shall come back to this question in the next section. It is worth noting that the tendency towards antiferromagnetism is also observed in the weak coupling limit (U/t «1) and that it occurs at infinitesimal values of U on bipartite lattices due to the perfect nesting properties of the Fermi surface[12,13].

In eq.(II-7), the projected operators $\tilde{c}^{+}_{i\sigma}$ and $\tilde{c}_{i\sigma}$ are rather awkward operators which do not have good commutation rules on the same site. This makes diagrammatic expansions in terms of these operators very complicated. An elegant way to bypass this problem consists in the introduction of auxiliary fields which keep track of the empty sites, in the same spirit as the slave boson approach[14] in the mixed valence problem. In the present case, two ways are opened: either occupied sites are described by fermions $c^{+}_{i\sigma}$ and empty sites by a boson b^{+}_{i}, with the constraint that at each site the number of bosons and fermions be equal to 1. The physical electron (as involved in hopping events) is then represented by the composite operator $c^{+}_{i\sigma}b_i$. Alternatively, one can describe spins by Schwinger bosons operators[15] $\vec{S}_i=1/2(b^{+}_{i\sigma}\vec{\tau}_{\sigma\sigma'}b_{i\sigma'})$ and holes by a spinless fermion operator ψ^{+}_{i} with the same constraint as before. In the first formulation , the t-J hamiltonian reads

$$-t\sum_{\substack{ij\\\sigma}} b_j\, c^{+}_{j\sigma}\, c_{i\sigma}\, b^{+}_{i} - J/2 \sum_{<ij>} \left\{(c^{+}_{i\sigma}c_{j\sigma})(c^{+}_{j\sigma'}c_{i\sigma'})+b^{+}_{i}b_i b^{+}_{j}b_j\right\}+\sum_i \lambda_i\Big(\sum_\sigma c^{+}_{i\sigma}c_{i\sigma}+b^{+}_{i}b_i-1\Big) \quad \text{(II-8)}$$

The Lagrange multiplier λ_i enforces the constraint at each site, while the remaining part of the Hamiltonian evolves obviously inside the restricted subspace. A similar expression is obtained in the second formulation with appropriate changes of operators. Note that now charge and spin degrees of freedom are clearly disentangled, but strongly coupled by the hopping term.

Although both formulations are exact, they lead to very different physics, once approximate treatments are introduced. The Schwinger bosons approach gives certainly a more physical way to deal with spin variables (which applies to arbitrary values of the spin) . The fermionic approach, on the other hand, may become more useful at relatively high hole concentration, where it allows to recover quite naturally a Fermi liquid picture.

III- **Half-filled band**

The only physical processes left in this limit are spin exchanges. It is now widely accepted that the ground state of a S=1/2 quantum antiferromagnet possesses long range order on the square lattice. Moreover, usual bosonic spin waves are thought to give a good description of the elementary excitations.

Evidence for long range order comes from exact diagonalization on finite clusters[16-18], Monte Carlo calculations[19], Monte Carlo variational methods[18,20,21] or renormalization group analysis[22]. To get some feeling of the problem, it is instructive to look briefly at the different wave functions that have been considered in the third class of approach. On a bipartite lattice, according to a theorem by Lieb, Schultz and Mattis[23], the ground state wave function ψ_0 is a spin singlet. The central question is to know whether the spin-spin correlation function $|\langle \vec{S}_0 . \vec{S}_R \rangle|$ vanishes or tends to a finite value at large distances. Marshall[24] has proven that ψ_0 may be chosen to be real in the basis of the eigenstates of the individual S_i^z. In addition, ψ_0 changes sign upon exchange of any nearest neighbour pair of antiparalell spins. The Marshall sign rule can be enforced by seeking ψ_0 in the form

$$|\psi_0\rangle = \sum_{\{\sigma\}} c\{\sigma\}\, e^{\,i\pi \sum_{i\in B}(1/2-S_i^z)}\, |\sigma_1 \ldots \sigma_N\rangle \quad \text{with} \quad c\{\sigma\}>0 \qquad \text{(III-1)}$$

where the lattice has been divided into two sublattices A and B and $\{\sigma\}$ represents the 2^N possible spin configurations. The classical Néel state $\langle S_i^x \rangle = \pm 1/2$ is obtained for constant weights $c\{\sigma\}$. Quantum corrections to the classical wave function may be introduced by taking $c\{\sigma\} \sim \exp - [\sum_{i,j} K(r_{ij})\, S_i^z S_j^z]$ [25,18,20]. Usually, the wave functions obtained in this way are not singlet states. They rather describe broken symmetry states, with a finite staggered

magnetization along the x direction. Very good values of the energy were obtained in ref.20, by allowing long range distribution of the two-spin interactions $K(r_{ij})$ ($E \approx -0.3319J$ per bond, to be compared to series estimates $-0.334J$ [26]).

In a RVB-type approach, Liang et al.[21] studied singlet wave functions of a Jastrow-type

$$|\psi_1> = \sum_{\substack{i\alpha\in A \\ j\beta\in B}} h(i_1-j_1) \ldots h(i_n-j_n)(i_1,j_1) \ldots (i_n,j_n) \qquad \text{(III-2)}$$

where $(i,j) = |i\uparrow j\downarrow> - |i\downarrow j\uparrow>$ is a singlet bond between a A-site and a B-site and the summation is over all possible coverings of the lattice by such bonds. The Marshall sign rule is obeyed if $h(i-j)>0$ at all distances. If $h(i-j)\neq 0$ only for nearest neighbours, one recovers the dimer wave function introduced by Sutherland[27], which is known to have very short range AF order[28]. If on the contrary $h(l)$ does not depend at all on the bond length , it can be shown that ψ_1 describes a classic Néel state averaged on all spin directions. In ref.21, the best variational states ($E \approx -0.3344J$ per bond) were obtained when including long bonds with a power law decrease of $h(l)$ and these states displayed long range order. However, disordered states with only short bonds were found to lie very close in energy ($E \approx -0.3338J$).

Beside variational approaches, renormalization group study of the long wave length action of Heisenberg antiferromagnet[22] strongly suggests that $S=1/2$ is above the critical value S_c where spins disorder because of zero point quantum fluctuations. The same conclusion was reached by a mean field theory[15], based on the Schwinger bosons representation, which decouples the spin interaction in a BCS-like approximation by introducing the order parameter $D_{\hat{\eta}} = <b^A_{i\uparrow} b^B_{i+\hat{\eta}\downarrow} - b^A_{i\downarrow} b^B_{i+\hat{\eta}\uparrow}>$ on each bond. In this approach, S_c was found to be of order 0.19. For $S<S_c$, there is a gap in the mean field

boson (triplet) excitation spectrum and the spin-spin correlation length is finite. For $S>S_c$, the gap closes, which means long range antiferromagnetic order. In this regime, the low energy excitations are well described by usual spin wave theory around a broken symmetry Néel state.

In contrast to the bosonic theories, approaches based on fermions unavoidably lead to disordered spin liquids. The Princeton group[29] introduced as a candidate for the description of a quantum spin liquid the Gutzwiller wave function[30]

$$|\psi> = P_G \prod_{\varepsilon_k \leq \varepsilon_f} c^+_{k\uparrow} c^+_{k\downarrow} |0> \qquad \text{(III-3)}$$

where P_G is the so-called Gutzwiller projector on the space of no doubly occupied sites. Here, P_G is applied to the Fermi sea of tight binding electrons at half filling (described by the energy dispersion $\varepsilon_k \approx -2t(\cos k_x + \cos k_y)$). This wave function is known to give good results in 1D for the energy and the spin-spin correlations[31]. ψ in (III-3) is obviously a singlet wave function (the property is true for the independent electrons wave function and is preserved in the Gutzwiller projection).In 2D, ψ turns out to be not so satisfactory[33]. Within this family of RVB-wave functions, better results are obtained when one forms Slater determinants with eigenstates of tight-binding electrons moving in a magnetic field of flux π per plaquette, which creates two subbands of energy $\varepsilon_k = \pm 2t\sqrt{\cos^2 k_x + \cos^2 k_y}$. This is the flux phase, first discovered by Affleck, Marston[34] and Kotliar[35]. It is worth mentioning at this point, that there is a close paralell between these variational wave functions and Hartree-like factorizations of the Heisenberg Hamiltonian in fermionic variables[29,34,35]

$$H = \sum_{<ij>} \left[\Delta_{ij}(c^{+}_{j\uparrow}c_{i\uparrow}+c^{+}_{j\downarrow}c_{i\downarrow}) + h.c. - \frac{|\Delta ij|^2}{J} \right] \qquad \text{(III-4)}$$

where the order parameter $\Delta ij=<c^{+}_{j\uparrow}c_{i\uparrow}+c^{+}_{j\downarrow}c_{i\downarrow}>$ is a complex number measuring the formation of singlet bonds between neighbouring sites.

Both Monte-Carlo calculations[36] and mean field theories favour the flux phase , whose energy however remains rather far from the estimates for the true ground state. In the mean field approach (which becomes exact in the formal limit of a large number of fermion colours), the best choice for the Δ_{ij} happens to be a dimer phase (where each site is linked to only one of its neighbours so that there is no bond overlap). The flux phase was even shown to be unstable against dimerization[37].This trend could signify the inadequacy of fermionic variables for representing spins at dimensions greater than 1. It has been argued in ref.38 that the fermionic theories (with their prediction of dimer phases) may give a good description of strongly disordered spin liquids.

IV- **The infinite U limit**

In this limit, Heff reduces to the nearest neighbour hopping term. Spins have no dynamics by their own, they move only through collisions with holes. At half filling, the ground state has a 2^N degeneracy corresponding to the two possible spin orientations per site.

IV-a) One hole problem

There is a theorem by Nagaoka[39], which states that the ground state is ferromagnetic on bipartite lattices, i.e. it has the maximum total spin $S=\frac{L-1}{2}$. This result can be understood as follows: the vacancy, by hopping from site to site, scrambles the spins behind it and usually leaves after running along a closed loop a final configuration of spins orthogonal to the initial one. So a

disordered spin configuration destroys the coherence of Bloch states and reduces the effective bandwidth of the vacancy. It is only in a perfect ferromagnetic environment that a vacancy can take its minimal kinetic energy -zt.

This band narrowing was studied by Brinkman and Rice[40] in various spin configurations. In the case of Néel order, they used a retraceable path approximation, which turned out to be very accurate and found an incoherent band of width $24R(z-1)\,t < 2zt$, except in 1D where $z=2$ (the absence of band-narrowing in this last case is an exact result: at infinite U, fermions cannot cross and are therefore insensitive to their spin degrees of freedom in 1D). As discussed in ref.41, the Brinkman Rice approximation amounts to neglect any overlap between the various strings of overturned spins that the hole leaves behind its path. It was noticed in ref.42, that this assumption fails as soon as the hole goes around a loop one and a half times but these paths become significant at relatively high energy compared to the bottom of the band.

Nagaoka's theorem raises the important question of the domain of stability of the ferromagnetic phase in function of the concentration of holes. At high density of holes ($n \ll 1$), it is clear that a paramagnetic phase will appear since it costs a lot of kinetic energy to align all the spins. Estimations for the instability threshold from the paramagnetic side are difficult and not very reliable because of the strong correlations . From the ferromagnetic side, one may look at the local stability with respect to the reversal of one spin (creation of a magnon): even if the problem looks simpler, it is yet unsolved. The reversed spin acts as a scatterer for the holes, which keeps a memory of the collisions through its position. Recently Shastry et al.[43] approached the problem by using a variational wave function which overturns an up spin electron at the Fermi surface and places it at the bottom of a down spin band narrowed by correlation effects. More precisely, they considered the trial wave function

$$|\chi v\rangle = (L)^{-1/2} \sum_m e^{i\vec{q}\cdot\vec{r}_m} c^+_{m\downarrow} (1-n_{m\uparrow}) c_{kF\uparrow} |F\rangle \qquad \text{(IV-1)}$$

where $|F\rangle$ is the ferromagnetic Nagaoka state $\prod_{\varepsilon_k \leq \varepsilon_f} c^+_{k\uparrow}|0\rangle$. They proved the instability for $\delta > 0.49$ on the square lattice,which is of the order of mean-field estimates[3,44]. However, there is some suspicion at the present time that more exotic physics may happen well before reaching these high densities.

IV-b) Two holes problem

Indeed Nagaoka's theorem fails already for two holes on a finite lattice. This was first observed in exact diagonalization studies on small clusters[45], which showed that the ground state in this case is a spin singlet. The underlying physics has been convincingly explained in ref.46: two holes can overcome the cost in kinetic energy due to the Pauli principle, by taking advantage of the spin texture around them, which helps them to mimic hard core bosons. To understand qualitatively how this can be achieved, let us come back to the t-J Hamiltonian in the Schwinger bosons formulation at J=0. The spins are treated at a mean-field level and we consider a static spin configuration described by a slowly varying unit vector $\hat{\Omega}(\vec{r})$. If θ and φ are the Euler angles of $\hat{\Omega}$, then the spinor $b = (b\uparrow, b\downarrow)$ may be parametrized as $(\cos\theta/2, \sin\theta/2 e^{-i\varphi})$ and for two neighbouring sites, the spin-spin overlap intervening in the hopping term takes the form

$$b^+_j b_i = \sqrt{\frac{1+\hat{\Omega}_i\cdot\hat{\Omega}_j}{2}}\, e^{i\varphi_i}, \qquad \varphi_{ij} \approx \sin^2\theta/2\, \vec{r}_{ij}\cdot\vec{\nabla}\varphi \qquad \text{(IV-2)}$$

We see that the spin distortion reduces the effective hopping metrix but also gives a phase to it, similarly to the Aharonov-Bohm effect in a magnetic field.

For topologically non trivial spin configurations like the skyrmion[47], which wraps the order parameter sphere once, a net flux of 2π is produced, which affects the hole spectrum. A detailed calculation[46] shows that one can build variational wave functions along these lines, which have a lower energy than the Nagaoka state with two holes.

To which extent this argument can be extended to finite hole density and favour "flux phases" over the ferromagnetic state, is not yet entirely clear. The only firm result concerns tight binding electrons in an external uniform magnetic field. It has been shown numerically[48] and more recently analytically[49] that on a lattice the total electron energy reaches an absolute minimum, when the flux per plaquette is 2π times the density, as had been conjectured by Anderson and Wiegman[50]. This gain in energy should be compared to the kinetic bandwidth reduction resulting from eq. (IV-2). It may also be necessary in the present problem to go beyond mean-field level and to take into account spin-backflow effects[49].

V- **One hole at finite U**

This is a highly non trivial problem, because the hole moves rapidly and is strongly coupled to the spin waves. Considerable physical insight has been gained by first treating the Ising limit ($J_\perp = 0$), where the quantum spin fluctuations are frozen[41,51], or the slow hole limit ($t<J$)[52]. For the real problem of the Heisenberg interaction with $t \gg J$, the general conclusion is that a quasiparticle band should form at dimensions ≥ 2 [42,52-54] of width scaling like J rather than t. The energy minima are found in numerical work[42,56-58] to lie at the AF zone face center $\vec{k}=(\pm\pi/2,\pm\pi/2)$ (with a possible shift to $(0,\pi)$ above $t/J \sim 4$).

V-a) Ising limit

In the very large U limit, Nagaoka's theorem tells us that the hole prefers to live in a ferromagnetic environment. However, at finite J, one single hole can order the spins only in a finite area to avoid a too large cost in magnetic energy . The size of the ferromagnetic region is such as to balance the localization energy $\sim t/R^2$ against the exchange energy $\sim JR^2$. A precise calculation (assuming sharp polaron walls) gives in 2D the energy

$$E_0 = -4t + 8.5(Jt)^{1/2} + 0(J) \qquad (V\text{-}1)$$

Note that the inclusion of $J_\perp$would modify the numerical coefficient of the second term but not the basic physics. This magnetic polaron is a very heavy object which can move only through the diffusion of magnetization across its area. In the domain of very low values of J/t where this object may appear (see below), it is energetically advantageous for many holes to share the same polaron, so that there is a phase separation between an antiferromagnetic phase without holes and a ferromagnetic one rich in holes[60].

At lower values of t/J, a string-like picture seems more appropriate. In the space of random walks of the Brinkman Rice approximation, the Ising part of the exchange hamiltonian provides a confining potential roughly scaling like Jl, where l is the number of steps (or of overturned spins). As a consequence, the eigenstates become discrete with an energy spacing $t(J/t)^{2/3}$. In ref.41, the hole energy was predicted to be

$$E_1 = -2\sqrt{3}\,t + 2.74t(J/t)^{2/3} \qquad (V\text{-}2)$$

in rather good agreement with recent exact diagonalization results[61]. As argued in ref.41, $E_1 < E_0$ provided $J/t < .005$, so that the string polaron replaces very rapidly the Nagaoka's one. These states are tied to an origin and do not

form delocalized Bloch states. No binding between two such objects was found at energy scales $t(J/t)^{2/3}$, as an effect of Pauli statistics.

V-b) Heisenberg limit

The $J_\perp$ part of the Heisenberg interaction is necessary to delocalize these states and give them a dispersion[41,42]. This is easily understood in the small $J_\perp$ limit. The spin flip term is able to repair pairs of overturned spins in the trail of the hole. The action of $J_\perp$ on the first bond of a string attached to some point , makes the new string state look like emanating from one of the eight next nearest neighbours of this point. This simple argument gives

$$E_k \approx J_\perp (\cos kx + \cos ky)^2 \qquad \text{(V-3)}$$

showing that the energy minimum is pushed on the faces of the AF zone. Although this naive result cannot be trusted in the Heisenberg limit, it is suggestive of how a bandwidth of order J may come out, once the energy scale t has been absorbed in the formation of a string-polaron.

In the Heisenberg case, the vacuum is very different from the classical Néel state, because of zero point quantum fluctuations. Furthermore, in contrast to the Ising case, there is no gap in the spin wave excitations. In ref.53, the problem was formulated as an electron-phonon problem and convincing arguments were given for the existence of a quasiparticle pole in the hole Green's function, with a strong renormalization of the mass due to incoherent scattering processes. Nevertheless, the position of the energy minimum in function of t/J,the scaling of the bandwidth with J as well as the relevance of the string picture in the Heisenberg limit are still debated matters[57,58].

V-c) Semiclassical analysis

The far field distortion of the spins around a moving hole can be understood in a transparent way by Shraiman and Siggia's semiclassical analysis[52] of the problem. They consider a small t limit and treat the spins semiclassically. Since Haldane's work on quantum spin chains[62], we know that on a bipartite lattice, the low energy spin fluctuations around the Néel state may be parametrized as

$$\vec{S}^{A(B)}(\vec{r}) = +(-)S\hat{\Omega}_i(\vec{r}) + \vec{M}(\vec{r}) \qquad (V\text{-}4)$$

where $\hat{\Omega}$ is the local staggered order parameter and $\vec{M}$ the local magnetization, which is the conjugate momentum of $\hat{\Omega}$. The exchange energy is given in the long wavelength limit by the non-linear σ Hamiltonian

$$H = 1/2 \int d^2\vec{r} \left[\rho(\vec{\nabla}\hat{\Omega})^2 + \frac{\vec{M}^2}{\chi} \right] \qquad (V\text{-}5)$$

where χ is the susceptibility ~ 1/J and ρ the spin wave stiffness ~JS^2. Keeping only the staggered part of $\vec{S}$ in (V-4) and expanding to lowest order in gradients the hopping term in the t-J Hamiltonian, one gets

$$-t \sum_{i\in A} \left[\sum_{\vec{\delta}=\hat{x},\hat{y}} (\psi^{+}_{i+\vec{\delta}}\psi_i - \psi^{+}_{i-\vec{\delta}}\psi_i)\,\vec{\delta} \right] \cdot S(\vec{\nabla}\theta + i\sin\theta\vec{\nabla}\varphi) + (h.c.) \qquad (V\text{-}6)$$

where θ and φ are the Euler angles of $\hat{\Omega}$. We see that the hole momentum $\vec{p} = (\sin k_x, \sin k_y)$ couples to the background spin current $\hat{\Omega}\wedge\partial_\mu\hat{\Omega}$, like a dipole moment to the electric field in usual electrostatics. It follows that the static spin cloud far from the hole has a dipolar configuration

$$\left[\vec{\Omega}\wedge\partial_\mu\vec{\Omega}\right]_z \approx \frac{(\delta_{\mu\nu} - 2\hat{r}_\mu\hat{r}_\nu)p_\nu(\vec{k})}{r^2} \qquad (V\text{-}7)$$

Beside the coupling to the spin current in (V-6), the hole couples also to the magnetization. This effect, responsible for the formation of the Nagaoka polaron around $\vec{k}=(0,0)$, turns out to be negligible on the AF zone faces. This picture of a long ranged dipolar distortion of the order parameter is expected to hold even in the large t-limit and is confirmed by recent numerical investigations[59]. However, the strength of the effective dipole moment in this limit is not obvious. Note also the importance of the position of the energy minima: at $\vec{k}=(0,\pi)$, $\vec{p}$ vanishes, whereas at $\vec{k}=(\pi/2,\pi/2)$ it points in the (1,1) direction.

V-d) Two holes

The situation is not very clear up to now: exact diagonalization studies[56,57,63] find a spin singlet groundstate with a d_{x2-y2} symmetry and a positive binding energy of order J, for J/t above a critical value of 0.25. This trend is far less conspicuous in the genuine Hubbard model than in the t-J model. The pure long wavelength approach described in the previous paragraph predicts also pairing between holes.

VI- **Finite hole density**

Considering the region in parameter space of small δ and J/t, it is clear that different physics will emerge, depending on the ratio $\frac{t\delta}{J}$. Broadly speaking, if $t\delta \gg J$, the exchange energy can be neglected and one should recover the infinite U physics which was discussed in section IV. For $t\delta \ll J$ on the contrary, the Heisenberg part dominates and antiferromagnetic correlations should persist up to scales at least of the order of the mean hole-hole distance. We do not discuss in this section the very small J/t limit, where a phase separation occurs (defining a first order critical line $\delta_c \sim (J/2\pi t)^{1/2}$). We consider values of

J/t high enough (>0.01) to favour the second type of polaron around each hole. One crude estimate for the boundary between "antiferromagnetic" and "ferromagnetic" behaviours is obtained by comparing the reduction in the hole kinetic energy $(4-2\sqrt{3})t\delta$ to the gain in magnetic energy J. This gives $\delta \sim 2J/t$. It should be noted that this approximate boundary is reached well before the cores around each hole (whose linear extension is of order $(t/J)^{1/6}$ in the Ising limit) percolate. Therefore, if one is interested in understanding the gradual loss of antiferromagnetic correlations upon doping, it seems appropriate to focus on the long wavelength interaction between the heavy quasiparticles which have been found in the 1 hole problem.

The dipolar spin distortions around each hole mediate between them a dipolar interaction of strength ~J, which turns out to have drastic consequences for the spin ordering. It was shown in ref.64 that under certain conditions, a spiral phase may form, in which the order parameter $\hat{\Omega}$ is planar and spirals around a fixed direction, with a pitch scaling like δ. This phase is metallic, with a small hole Fermi surface. In ref.65, a more microscopic mean field theory was elaborated, treating in a better way the quantum spin fluctuations. Beside the single spiral phase, a "double spiral" phase was discovered, in which locally the spins spiral in orthogonal planes in the x and y directions. This phase has a ring of low lying excitations with a radius in $\vec{k}$-space scaling once again like δ and a finite gap at T=0, $\Delta \approx \delta J \exp[-\frac{\delta_c}{\delta}]$, which means that long range order has been lost. Although the double spiral phase has a higher energy than the spiral phase at mean field level, it was argued [65] that fluctuations may help in stabilizing it. Recently, it was shown[66] within Shraiman and Siggia's theory that above a critical strength of the dipolar interaction between holes, the spiral phase is unstable towards the formation of domain walls in the (1,1) or $(1,\overline{1})$ directions on the square lattice. This leads to an insulating modulated spiral phase. Similar predictions for the

appearance of domain walls had been made before within direct Hartree-Fock factorizations of the Hubbard model at strong[67] or weak coupling[68].

We are still lacking a complete understanding of how the introduction of a small density of holes destroys antiferromagnetic correlations. All the propositions dicussed so far, have in common to lead to modulations of the AF order at length scales of order δ^{-1}, much greater than the average distance between holes. The corresponding instabilities arise in 2D at infinitesimal values of the density. It is worth mentioning another work addressing the same problem in a very different spirit: in ref.69, it was argued that holes induce a next nearest neighbour AF spin coupling of order $J\delta$,and the resulting frustrated spin Hamiltonian was shown to have a disordered groundstate above a critical density of holes[70].

If one assumes from the beginning a complete disordering of spins, then the variational Gutzwiller wavefunctions based on the fermionic representation can be thought to give better results in the presence of holes than exactly at half filling. Two possible extensions of the flux phase ($\Phi=\pi$ per plaquette)can be contemplated: either a staggered flux phase which keeps a two-sublattice structure, with an elementary flux smoothly decreasing from π to 0 at a finite value of $\frac{t\delta}{J}$ where one recovers a standard Fermi liquid[33,71]. The other more exotic possibility is a uniform flux phase, with a flux commensurable to the hole density[72,50]. In contrast to the staggered flux phases which have free carriers, the generalized flux phases are insulators, which may be superconducting according to arguments given in ref.72. At the present time, a detailed study of the relative stability in the $(J/t,\delta)$ plane of these various proposals is missing, even at the mean field level.

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