Insulating spin liquid in the lightly doped two-dimensional Hubbard model

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We calculate the charge compressibility and uniform spin susceptibility for the two-dimensional (2D) Hubbard model slightly away from half-filling within a two-loop renormalization group scheme. We find numerically that both those quantities flow to zero as we increase the initial interaction strength from weak to intermediate couplings. This result implies gap openings in both charge and spin excitation spectra for the latter interaction regime. When this occurs, the ground state of the lightly doped 2D Hubbard model may be interpreted as an insulating spin liquid as opposed to a Mott insulating state.

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After two decades of intensive research on the high-Tc superconductors, physicists are still puzzled by some of their very unusual electronic properties. The prominent example is given by the cuprates. At zero doping, despite the fact that their highest occupied band is half-filled, they are charge insulators, and display antiferromagnetic long-range order. For this reason, they are said to be Mott insulators. As soon as one starts doping those compounds with holes, the long-range magnetic order becomes rapidly suppressed, and there are experimental evidences of an emergence of a spin gap in their corresponding excitation spectra. A charge gap is also observed by ARPES experiments in such lightly-doped systems. Moreover, at finite temperatures, they turn themselves into poor conductors with electronic properties differing considerably from the predictions of Landau’s Fermi liquid theory. This scenario configures the so-called pseudogap regime. Although this phase continues to be not well understood, it is widely acknowledged to play a fundamental role in the underlying microscopic mechanism of such high-Tc superconductors. Indeed, upon some further doping, those poor metals become superconducting with d-wave symmetry up to relatively high temperatures around the optimal doping level.

From the theoretical viewpoint, it is widely accepted that the appropriate model for describing such systems is the two-dimensional (2D) Hubbard model (HM), since it is known to have a Mott insulating phase at half-filling, and is expected to become a d-wave superconductor at larger doping. However, its intermediate doping regime, which could provide some insight to understand the physical nature of the pseudogap state, still remains elusive to this date. In this Letter we intend to address this question using renormalization group (RG) techniques in order to infer about the ground state of such model for electron densities slightly away from the half-filling limit.

Our considerations here will be based on a complete two-loop RG calculation of the uniform charge (CS) and spin (SS) susceptibilities of the 2D HM, taking into account simultaneously both the renormalization of the couplings, and the self-energy effects. (The CS is also called the charge compressibility of the system.) To best of our knowledge, it is the first time that such a full two-loop RG calculation is performed for the 2D lightly-doped RG model, since previous estimates of the uniform susceptibilities followed random phase approximation (RPA) schemes.

In momentum space, the 2D Hubbard Hamiltonian on a square lattice is given by

\[ H = \sum_{\mathbf{k},\sigma} \xi_{\mathbf{k}} \psi_{\mathbf{k}\sigma}^\dagger \psi_{\mathbf{k}\sigma} + \frac{U}{N_{\text{sites}}} \sum_{\mathbf{p},\mathbf{q}} \psi_{\mathbf{p}\uparrow}^\dagger \psi_{\mathbf{p}\downarrow}^\dagger \psi_{\mathbf{q}\downarrow} \psi_{\mathbf{q}\uparrow}, \]

where the energy dispersion is simply \( \xi_{\mathbf{k}} = -2t [\cos(k_x a) + \cos(k_y a)] - \mu \), and \( \psi_{\mathbf{k}\sigma}^\dagger \) and \( \psi_{\mathbf{k}\sigma} \) are the usual creation and annihilation operators of electrons with momentum \( \mathbf{k} \) and spin projection \( \sigma = \uparrow, \downarrow \). Besides, \( \mu \) stands for the chemical potential, whereas \( a \) is the square lattice spacing. Another important parameter here is the width of the noninteracting band, which is given by \( W = 8t \). This model describes a system with many electrons interacting mutually via a local repulsive interaction \( U \), and with a total number \( N_{\text{sites}} \) of lattice sites. The electron band filling of the system is controlled by the ratio \( \mu/t \). When \( \mu/t = 0 \) the system is exactly at half-filling. As we start doping it with holes, \( \mu/t \) takes slightly negative values.

![FIG. 1: (Color online) (a) The half-filled Fermi surface (FS) of the 2D Hubbard model (dashed line), the lightly hole-doped FS (blue solid line), and (b) the latter FS after a rotation of the axes by 45° degrees.](image-url)
Our starting point is a 2D nearly flat Fermi surface (FS) with no van Hove singularities (see Fig. 1). It correctly describes the 2D HM slightly away from the half-filling case. A similar FS has already been used by other groups to investigate the leading instabilities within either a parquet or, equivalently, a one-loop RG approach. All those investigations find diverging susceptibilities at finite energies (or finite temperatures) with the dominant instability being always the spin density wave (SDW). Their interpretation is that this implies a spontaneous symmetry breaking in the system, and the onset of a long-range ordered antiferromagnetic state.

In this Letter we argue that is not necessarily true since this result may also be an indicative of the limitations of the one-loop RG scheme. In low-dimensional systems, large quantum fluctuations are expected to suppress long-range order. The more those effects are taken into account, the more likely those long-range ordered states are transformed into short-range magnetically ordered phases. This also becomes clear as a result of our work. Taking into account quantum fluctuation effects up to two-loop order in our RG scheme, we are able to show that, for moderate coupling regimes, both charge compressibility and uniform spin susceptibility are strongly suppressed and flow unequivocally to zero. This behavior implies that there are gaps for both charge and spin excitations, and no trace of long-range symmetry breaking order in those cases. Such a state with a fully gapped charge and spin spectra is usually denominated the insulating spin liquid (ISL). The ISL is an example of a short-range resonant valence bond state, which was first proposed for a $S=1/2$ Heisenberg model of a short-range resonant valence bond state, which was an insulating spin liquid (ISL). The ISL is an example of a short-range resonant valence bond state, which was first proposed for a $S=1/2$ Heisenberg model, and clearly revealed in even-leg Hubbard ladders by both RG and bosonization approaches.

In order to implement a full RG calculation of the uniform susceptibilities, it is essential to consider at least two-loop order contributions. This is due to the fact that, at one-loop level, there is not a single infrared (IR) divergent diagram in the calculation of the so-called uniform response functions. In contrast, there are several of those diagrams in two loops (the nonparquet diagrams), and, as a result, one can reliably begin to derive appropriate RG flow equations for those quantities at that order of perturbation theory.

To keep a closer contact with well-known works in one-dimensional systems, we divide the FS into four different regions (two sets of solid and dashed line patches). Here we restrict the momenta at the FS to the flat parts only. The interaction processes connecting parallel patches of the FS are always logarithmically IR divergent due to quantum fluctuations. In contrast, those connecting perpendicular patches always remain finite, and do not contribute to the RG flow equations in our approach. For convenience, we restrict ourselves to one-electron states labeled by the momenta $p_\parallel = k_x$ and $p_\perp = k_y$ associated with one of the two sets of perpendicular patches. The momenta parallel to the FS are restricted to the interval $-\Delta \leq p_\parallel \leq \Delta$, with $2\Delta$ being essentially the size of the flat patches. The energy dispersion of the single-particle states is given by $\varepsilon_a(p) = v_F (|p_\perp| - k_F)$, and depends only on the momenta perpendicular to the FS. The label $a = \pm$ refers to the flat sectors at $p_\perp = \pm k_F$, respectively. In addition, we take $k_F - \lambda \leq |p_\perp| \leq k_F + \lambda$, where $\lambda$ is a fixed ultraviolet (UV) microscopic momentum cut-off.

We now write down the Lagrangian of the 2D HM as

$$L = \sum_{\mathbf{p}, \sigma, a=\pm} \psi_{(a)\sigma}^\dagger (\mathbf{p}) [i\partial_t - v_F (|p_\perp| - k_F)] \psi_{(a)\sigma} (\mathbf{p}) - \frac{1}{V} \sum_{\mathbf{p}, \mathbf{q}, \mathbf{k}, \alpha, \beta, \gamma} \sum_{\sigma, \delta, \epsilon} [g_2 \delta_{\alpha \delta} \delta_{\beta \gamma} - g_1 \delta_{\alpha \gamma} \delta_{\beta \delta}] \times \psi_{(+\delta)}^\dagger (\mathbf{p} + \mathbf{q} - \mathbf{k}) \psi_{(-\gamma)} (\mathbf{k}) \psi_{(-\beta)} (\mathbf{q}) \psi_{(+\alpha)} (\mathbf{p}),$$

where $\psi_{(\pm)}^\dagger$ and $\psi_{(\pm)}$ are now fermionic fields associated to electrons located at the $\pm$ patches. The summation over momenta must be appropriately understood as $\sum_{\mathbf{p}} = V/(2\pi)^2 \int d^2p$ in the thermodynamic limit. We linearized the energy dispersion about the lightly-doped FS, and the interaction term was parametrized in a manifestly SU(2) invariant form. Here we follow the well-known g-ology notation, with $g_1$ and $g_2$ standing for backscattering and forward scattering couplings, respectively. Since this should represent the 2D HM, these couplings must be initially defined as $g_1 = g_2 = (V/4N_{\text{sites}})U$. In addition, we do not include Umklapp
processes since we are not at half-filling, and our FS does not intersect the so-called Umklapp surface at any point (see Fig. 1(a)). Consequently, our result is different from another evidence of ISL behavior reported in the literature in the context of the $t - t'$ 2D HM. In their case, the FS intersects the Umklapp surface even away from half-filling, and, for this reason, Umklapp processes become an essential ingredient for the correct description of the system at the lightly-doped regime. Moreover, their estimates of the uniform susceptibilities follow the already mentioned RPA-like scheme.

Since the HM is a microscopic model, all terms in the Lagrangian are defined at a scale of a few lattice spacings in real space (i.e at the UV cutoff scale in momentum space). These parameters are often inaccessible to every day experiments, since the latter probe only the low-energy and the long-wavelength dynamics of a given system. In RG theory, these unobserved quantities are known as the bare parameters. In fact, if one attempts to construct naive perturbative calculations with such parameters, one will obtain IR divergent Feynman diagrams in the computation of several quantities such as, e.g., the backscattering and the forward scattering four-point vertices, and the single-particle Green’s function. These divergences mean that the perturbation theory setup is not appropriately formulated. To solve this problem, one can redefine the perturbation scheme in a such a way as to circumvent these infinite results in the calculation of observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities. This is the strategy of the so-called renormalized perturbation theory. Thus, one rewrites all observable quantities.

As we explained in our previous paper, when one deals with this FS problem, the counterterms needed to renormalize the theory turn out to be continuous functions of the three momenta parallel to the FS, rather than being simply infinite constants. In addition, we computed the RG flow equations for the coupling functions and the quasiparticle weight up to two-loop order, and showed that they were in fact coupled integro-differential equations. We solved those equations self-consistently and, as a result, we found out for an intermediate coupling regime a possibly new physical regime, which was characterized by a strongly suppressed quasiparticle weight. Here we continue to explore this intermediate coupling regime, and our present calculation shows that the resulting quantum state may in fact be interpreted as an ISL.

To obtain the uniform susceptibilities of this system, we must first calculate the linear response due to an infinitesimal external field perturbation that couples to both charge and spin number operators. We do this by adding to the Lagrangian the new term

$$-h_{\text{external}} \sum_{\mathbf{p}, \alpha} T_B^{\alpha \alpha}(\mathbf{p}) \psi_{(\alpha)\alpha}^{R \dagger}(\mathbf{p}) \psi_{(\alpha)\alpha}^{R}(\mathbf{p}),$$

where $B$ stands for the bare quantities. This will generate an additional vertex (the one-particle irreducible function $\Gamma^{(2,1)}(\mathbf{p}, \mathbf{q} \approx 0)$), which will in turn be afflicted by new IR divergences (see the nonparquet diagrams in Fig. 2). As a result, we must rewrite the bare quantity $T_B^{\alpha \alpha}$ in terms of its renormalized counterpart (henceforth called $\bar{T}_R^{\alpha \alpha}$), and an appropriate counterterm $\Delta \bar{T}_R^{\alpha \alpha}$, i.e.

$$\bar{T}_B^{\alpha \alpha}(p_{\parallel}) = Z^{-1}(p_{\parallel}) \left[ T_R^{\alpha \alpha}(p_{\parallel}) + \Delta \bar{T}_R^{\alpha \alpha}(p_{\parallel}) \right].$$

The quasiparticle weight $Z$ factor comes from the renormalization of the fermionic fields, which must be also taken into account in order to include the feedback of the self-energy effects into the RG flow equations. The $Z$ function is calculated explicitly in Ref. As was mentioned before, $\Delta \bar{T}_R^{\alpha \alpha}$ must cancel exactly the divergences generated by the nonparquet diagrams. However, there are still several ways of choosing that counterterm. To solve this ambiguity, we must make a prescription establishing precisely that the $\bar{T}_R^{\alpha \alpha}$ is the experimentally observable response, i.e., $\Gamma^{(2,1)}(p_{\parallel}, p_0 = \omega, p_{\perp} = k_F; q \approx 0) = -i \bar{T}_R^{\alpha \alpha}(p_{\parallel}, \omega)$, where $\omega$ is the RG energy scale parameter that denotes the proximity of the renormalized theory to the FS. In this way, to flow towards the FS we let $\omega \to 0$.

We are now ready to define the two different types of uniform response functions, which arise from a symmetrization with respect to the spin projection, namely

$$\bar{T}_{R,CS}(p_{\parallel}, \omega) = \bar{T}_R^{\uparrow \uparrow}(p_{\parallel}, \omega) + \bar{T}_R^{\downarrow \downarrow}(p_{\parallel}, \omega),$$

$$\bar{T}_{R,SS}(p_{\parallel}, \omega) = \bar{T}_R^{\uparrow \downarrow}(p_{\parallel}, \omega) - \bar{T}_R^{\downarrow \uparrow}(p_{\parallel}, \omega),$$

where $\bar{T}_{R,CS}$ and $\bar{T}_{R,SS}$ are the response functions associated with the charge compressibility and spin susceptibility, respectively. In order to compute the RG flow equations for these response functions, one needs to recall that the bare parameters are independent of the renormalization scale $\omega$. Thus, using the RG condition $\omega d \bar{T}_B^{\alpha \alpha} / d\omega = 0$, we obtain

$\text{FIG. 3:}$ Feynman diagram associated with the renormalized charge compressibility and uniform spin susceptibility.
FIG. 4: (Color online) RG flow of both charge compressibility and uniform spin susceptibility as we increase the initial coupling strength given by $U = (g/\pi v_F)\epsilon$.

$$\frac{d}{d\omega} \chi_{R,CS}(p||) = -\frac{1}{\omega} \Delta \chi_{R,CS}(p||) + \gamma(p||) \chi_{R,CS}(p||),$$

$$\frac{d}{d\omega} \chi_{R,SS}(p||) = -\frac{1}{\omega} \Delta \chi_{R,SS}(p||) + \gamma(p||) \chi_{R,SS}(p||),$$

where the anomalous dimension is given by $\gamma(p||) = \omega d \ln Z(p||)/d\omega$. Despite their apparent simplicity, it is impossible to solve these RG equations only by analytical means. To find their solutions, we have again to resort to numerics. Here we use the fourth-order Runge-Kutta numerical method. We discretize the FS continuum replacing the interval $-\Delta \leq p|| \leq \Delta$ by a discrete set of 33 points. We use $\omega = \Omega \exp(-l)$, where $\Omega = 2v_F\lambda$ with $l$ being our RG step. We also choose $\Omega = v_F\Delta < W$. In view of our choice of points for the FS, we are only allowed to go up to $l \approx 2.8$ in the RG flow to avoid the distance to the FS being smaller than the shortest distance between points in our discrete set.

Once the response functions are obtained, we can calculate the flow of the charge compressibility and the uniform spin susceptibility of the system. Using again our diagrammatic convention, it follows from Fig. 3 that they are given by

$$\chi_{CS,SS}(l,\omega) = \frac{1}{4\pi^2 v_F} \int_{-\Delta}^{\Delta} dp|| [\chi_{R,CS}(SS)(p||,\omega)]^2.$$  

To evaluate these quantities we follow the same numerical procedure described above. Our results are displayed in Fig. 4. We note in this plot that both charge and spin susceptibilities flow at the same rate as we approach the FS even though their corresponding response functions have different flow equations. In addition, for initial couplings in which the quasiparticle weight flows to zero, the uniform susceptibilities become strongly suppressed in the low-energy limit. While the former asserts that there are no fermionic quasiparticle excitations present in the system, the latter is related to the complete absence of low-lying bosonic charge and spin collective excitations. Since this resulting state has only gapful excitations, it cannot be related to any broken symmetry state and, as a consequence, should possess only short-range ordering. This quantum state has, therefore, strong similarities with that predicted long ago by Anderson, which is commonly referred to as an ISL. In our present work, it becomes evident that such a state is produced by disordering effects induced by strong quantum fluctuations, and these are approximately taken into account by our two-loop RG scheme. Finally, we call attention to the fact that an insulating behavior in the lightly doped 2D HM was also reported recently in the literature. Our present result is clearly in agreement with their results.

In summary, we examined the flow of both charge compressibility and uniform spin susceptibility in the lightly doped 2D HM as a function of the initial interaction strength within a two-loop RG approach. For moderate interaction regimes, both quantities flow to zero as we approach the initial FS of the system. This is a strong indicative that there are gaps in both charge and spin excitation spectra of the lightly doped 2D HM. Hence the quantum state associated with that regime may be viewed as an ISL as opposed to a Mott insulator. This result may be of relevance for the cuprate high-Tc superconductors in view of the fact that the 2D HM in the intermediate coupling regime is widely believed to be appropriate to describe such compounds in all doping ranges.

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