Quantum Lifshitz Point in the Infinite-Dimensional Hubbard Model

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We show that the Gutzwiller variational wave function is very accurate for the computation of magnetic phase boundaries in the infinite-dimensional Hubbard model. This allows us to substantially extend known phase diagrams. For both the half-hypercubic and the hypercubic lattice, a large part of the phase diagram is occupied by an incommensurate phase, intermediate between the ferromagnetic and the paramagnetic phase. In case of the hypercubic lattice, the three phases join at a new quantum Lifshitz point at which the order parameter is critical and the stiffness vanishes.

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The Hubbard model was originally introduced to study ferromagnetism in strongly correlated metals [1–3]. This phenomenon as prototypically realized in Fe, Co, and Ni is one of the oldest phenomena investigated in solid state theory. A related problem is incommensurate spin-density-wave order as manifested in Cr and its alloys [4]. Also various transition metal oxides show incommensurate magnetic phases (often accompanied by charge order), like cuprates [5], nickelates [6], and manganites [7].

Despite decades of investigation, not much is known about the magnetic phase diagram of the Hubbard model. The simplest treatments [8,9] partition the zero temperature phase diagram in three regions: antiferromagnetic (AFM) close to $n = 1$ particles per atom, ferromagnetic (FM) at large interaction and far from $n = 1$, and paramagnetic (PM) at small interaction and/or close to $n = 0$, 2. More sophisticated treatments include in addition incommensurate (IC) phases [10,11].

Infinite-dimensional lattices offer a unique opportunity to study the competition between PM and FM keeping the problem tractable and, at the same time, retaining much of the physics expected in three-dimensional lattices [12]. Here we investigate the Hubbard model in the limit of infinite dimension $\mathcal{D}$ using the Gutzwiller variational wave function (GWF) [13]. Instabilities of the FM and PM ground state are systematically studied as a function of momentum, doping, and interaction strength using a random-phase-approximation (RPA) like expansion [14,15]. In principle, the model can be solved exactly in this limit by using dynamical mean-field theory (DMFT) which maps the problem to an impurity problem amenable of numerical solution [12]. Limitations on the numerical algorithm, however, have prevented for an extensive zero temperature investigation of the phase diagram. A study by Uhrig on the stability of the FM phase in an infinite-dimensional generalization of the fcc lattice, the so-called half-hypercubic (hhc) lattice, is one of the few cases where the $T = 0$ self-consistent DMFT problem has been solved exactly [16].

Here we show, comparing with exact results when available, that the GWF is surprisingly accurate for the determination of magnetic phase boundaries in infinite-dimensional lattices. In addition, we significantly extend the computation of the $T = 0$ magnetic phase diagram to regions in parameter space yet poorly explored by DMFT. More specifically, for the hhc, we show that the GWF FM instability line agrees with the exact computation by Uhrig [16]. In addition, we present the first systematic investigation of the stability of the PM state in this lattice and find that the PM and FM never meet but are separated by an IC phase (Fig. 2). A similar systematic study of the hypercubic lattice (hc) shows also a large region of, yet poorly studied, IC order (Fig. 3). In contrast to the hhc case, PM and FM phases have a common phase boundary. The IC phase, the FM phase, and the PM phase join in a quantum version of the multicritical Lifshitz point (LP). Classical LP are interesting because they are associated with unusual critical exponents [17]. We anticipate unusual critical behavior for a quantum LP (QLP) shall it occur at physical dimensions.

We start from the Hubbard Hamiltonian [1–3] with onsite interaction U and hopping matrix element t_{ij} between sites i and j. The energy of the model is evaluated within the GWF for polarized and unpolarized phases. In the limit $\mathcal{D} \to \infty$ the Gutzwiller approximation (GA) to the variational problem becomes exact [18] which greatly simplifies the computations. The stability of these solutions is studied by an RPA analysis at different momenta. By construction, the limits of stability thus obtained correspond to the point where a more stable variational solution would be found in a fully unrestricted computation of the GWF energy. This requires a rotationally invariant formulation of the GA energy functional [19] and to take into account the change in the double occupancy for small quasistatic changes of the charge and spin distribution as in Vollhardt's GA-based Fermi liquid computation [20]. Basically we compute the dynamic spin susceptibility $\chi_q(\omega) = -\frac{1}{N}\int e^{i\omega t}\langle \mathcal{T} S^+_q(t) S^-_{-q}(0)\rangle$ in both para- and

FM states which can be obtained from a density expansion of the Gutzwiller energy functional. Details of the formalism are given in Ref. [15]. For simplicity, we neglect macroscopic phase separation [9,11] which, in any case, would be frustrated if the long-range Coulomb interaction were taken into account [21].

We consider the hypercubic lattice and the half-hypercubic lattice. The latter can be obtained from the hc lattice by removing all the even sites. For the hhc case we consider hopping restricted to $t_{ij} = t/\mathcal{D}$ for nearest-neighbor sites and $t_{ij} = t/(2\mathcal{D})$ for next-nearest-neighbor sites [16]. For the hypercubic lattice we keep only nearest-neighbor hopping $t_{ij} = t/\sqrt{2\mathcal{D}}$. In the latter case it has been shown [22] that all the momentum dependence of correlation functions is contained in the factor $\eta_{\mathbf{q}} = \frac{1}{\mathcal{D}} \times \sum_{i=1}^{\mathcal{D}} \cos(q_i)$, which can be parametrized by a value between 1 and -1 corresponding to a scan along the zone diagonal from $\mathbf{q} = (0, \ldots, 0)$ to $\mathbf{q} = (\pi, \ldots, \pi)$, respectively. On the other hand, for the half-hypercubic lattice the Brillouin zone is cut in half and the momentum dependence is contained in the factor $\eta_{\mathbf{q}}^2$ which varies from 1 to 0 corresponding to a scan from $\mathbf{q} = (0, \ldots, 0)$ to $\mathbf{q} = (\pi/2, \ldots, \pi/2)$, respectively [22].

The hhc lattice is nonbipartite; therefore, antiferromagnetism is frustrated. In addition, it has a density of states with a square root divergence at a lower band edge that makes ferromagnetism stable for large U and large δ. Here $\delta \equiv 1 - n$ is the density deviation from half filling and n is the density. For convenience we define the Brinkmann-Rice critical U value $U_{\mathrm{BR}} \equiv -8\bar{\epsilon}$ with $\bar{\epsilon}$ the noninteracting kinetic energy at half filling [20].

Figure 1 shows the transverse magnon dispersion computed on top of a saturated FM solution at $\delta = 0.3$ in the hhc for different values of U which as expected is linear (quadratic) in $1 - \eta_{\mathbf{q}}$ ($\mathbf{q}$) for small $\mathbf{q}$ and shows a Goldstone mode at $\mathbf{q} = \mathbf{0}$. As U is decreased, the excitation energy becomes negative first at $\mathbf{q} = 0$ and then also at finite momentum, signaling an instability due to a change of sign in the stiffness of the magnetization. Since this is a transverse excitation, the ferromagnet tends to become a spiral.

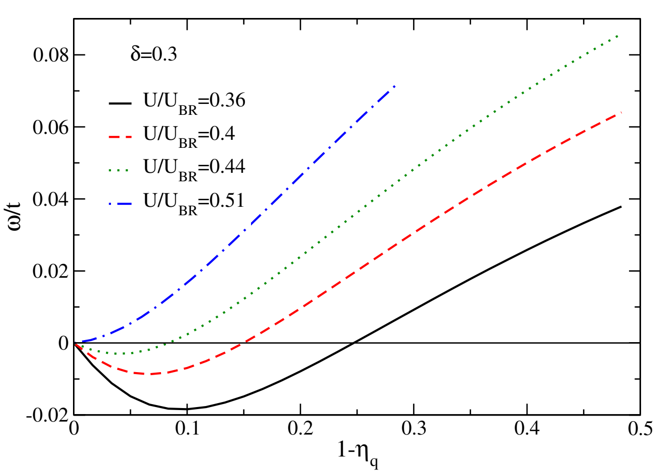

FIG. 1 (color online). Magnon dispersions for the (fully polarized) ferromagnet in the half-hypercubic lattice for $\delta = 0.3$. At this doping the FM solution is stable for $U > 0.49U_{\mathrm{BR}}$.

In Fig. 2 we show the limit of stability of the saturated FM phase thus obtained (full line) and the exact computation by Uhrig (asterisks). Only in the region where bound states appear for small δ [16] significant deviations appear as shown in the inset which indicates that the GWF energy is quite accurate. We also show in Fig. 2 the stability limit of the PM phase (dashed line). The first excited state of the paramagnet is a triplet with z component of the spin $m = -1, 0, 1$. Spin rotational invariance requires that the longitudinal ($m = 0$) and transverse ($m = -1, 1$) excitations are degenerate and indeed all three become soft at the boundary at some finite $\mathbf{q}$. In the figure, we indicate by arrows the value of $\eta_{\mathbf{q}}$ for the unstable modes. The instability occurs at $\eta_{\mathbf{q}} \to 0$ for small δ [wave vector $\mathbf{q} = (\pi/2, \ldots, \pi/2)$] and gradually shifts to $\eta_{\mathbf{q}} = 1$ for $\delta = 1$ as expected for the instability toward the FM phase ($\mathbf{q} = 0$).

Both instability lines indicate that there is an IC phase intermediate between the FM phase and the PM phase. This does not show up in the DMFT numerical study of Ref. [23] because it is restricted to $\mathbf{q} = 0$ instabilities. The present FM boundary practically coincides with the $T = 0$ extrapolated results of Ref. [23] while a substantial portion of the PM range of Ref. [23] is instead occupied by IC phases in the present computation.

Encouraged by these results which show the accuracy of the Gutzwiller variational energy to determine the phase boundaries, we consider the hc lattice. The limit of stability

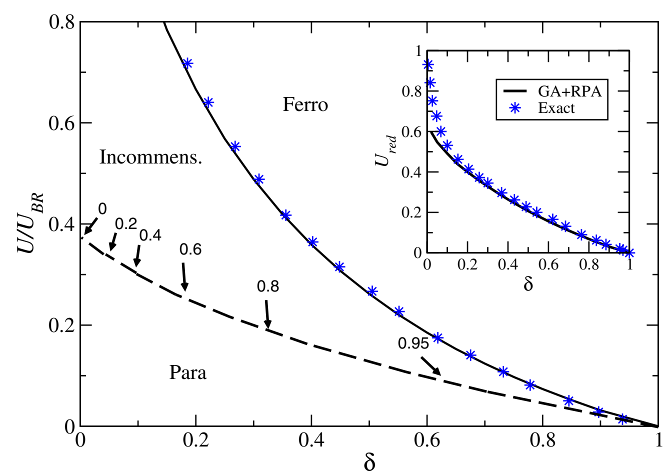

FIG. 2 (color online). Full line: limit of stability of the FM phase within the Gutzwiller wave function for the hhc lattice. The asterisks are the exact result from Ref. [16]. In the inset, a scaled representation of the FM stability limit is shown with $U_{\mathrm{red}} = U/(U + U_{\mathrm{BR}})$ and $U_{\mathrm{BR}} = 6.86t$. Dashed line: limit of stability of the PM phase. The arrows indicate the value of $\eta_{\mathbf{q}}$ parametrizing the momentum of the unstable mode.

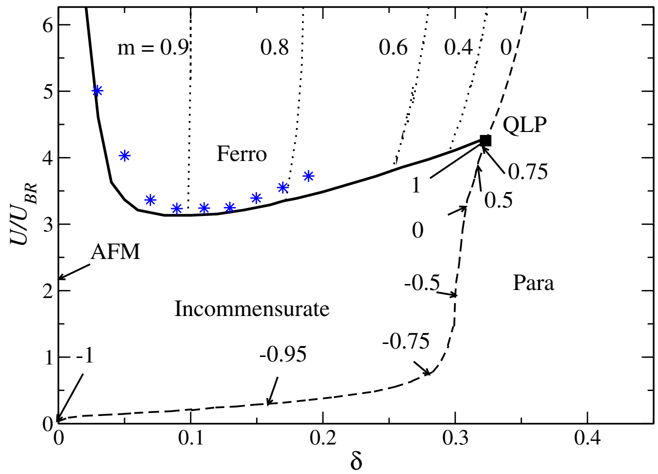

FIG. 3 (color online). Limit of stability of the FM (full line) and PM (dashed line) phases for the hc lattice. Arrows indicate the value of $\eta_{\mathbf{q}}$ for the unstable mode of the PM phase. The stars correspond to the limit of stability of the FM phase obtained in Ref. [24] within an approximate solution of the DMFT equations. Dotted lines are levels of constant magnetization. Energies are in units of $U_{\mathrm{BR}} = 6.38t$.

of the FM phase and of the PM phase are shown in Fig. 3. Since the hc lattice has perfect nesting the instability towards antiferromagnetism ($\eta_{\mathbf{q}} = -1$) sets in at $U/t = 0$ for $\delta = 0$ [9,11]. For $\delta > 0$ an IC phase emerges with $\eta_{\mathbf{q}}$ gradually increasing. Decreasing U at finite δ the FM phase becomes unstable at the full line due to a change of sign in the stiffness of the magnetization as for the hhc lattice. Finally at the QLP the PM instability mode becomes uniform ($\eta_{\mathbf{q}} = 1$) and one has a transition to a weak (partially polarized) FM phase.

The dotted lines in Fig. 3 are level curves of constant magnetization m. The density of states of the $\mathcal{D} = \infty$ hypercubic lattice is a Gaussian. Because of the Gaussian tails an infinite splitting of the minority and majority bands, i.e., $U \to \infty$, is required to produce a fully polarized state. For finite U one has a magnetization of the FM state that increases from zero as δ decreases from the PM boundary (dashed line) and becomes logarithmically saturated for small δ.

The limit of stability of the FM phase in Fig. 3 is in good agreement with the FM phase boundary for the hypercubic lattice obtained in a DMFT study based on a large U expansion and the no crossing approximation as impurity solver (asterisks) [24]. This again points to a good accuracy of the GWF.

The magnetic phase diagram of the $\mathcal{D} = \infty$ hc lattice has been studied at finite temperature by Freericks and Jarrell using DMFT [25]. The finite temperature instabilities are towards a commensurate AFM and become IC only at the lowest temperature which does not allow for a reliable $T = 0$ extrapolation of the PM-IC phase boundary. If we restrict to the AFM instability of the GWF we find an instability line in the U-δ plane (not shown) which is in good agreement with the $T = 0$ extrapolated phase diagram of Ref. [25]. This is probably due to the fact that the extrapolation is dominated by the high temperature commensurate data. In the present phase diagram, the IC phase occupies a larger region.

At the QLP the IC, PM, and FM phases meet. This behavior is the quantum analogue of the classical LP observed in MnP where the same phases meet but at finite temperature and in the presence of an external field [26].

On general grounds regarding the proximity of $\mathcal{D} = 3$ systems to infinite-dimensional systems [12], we expect the phase diagram of Fig. 3 to resemble that of the cubic lattice. It is then worth speculating on the behavior of a QLP shall it occur at finite $\mathcal{D}$. In analogy with a classical LP, also for a QLP we expect anomalous critical behavior.

The $T = 0$ PM-FM transition and PM-IC transition are the first studied examples of quantum critical behavior [27–32]. The transition is characterized by a dynamical exponent $z = 3$ ($z = 2$) for the PM-FM (PM-IC) and the upper critical spatial dimension is $4 - z$. Therefore, in many cases of interest the theory is Gaussian. It was pointed out that in the case of FM transitions, because the magnetization is a conserved quantity, long-range interactions appear and the critical exponents change [30].

At the QLP the critical behavior is expected to be different. Neglecting long-range interactions, the effective action close to the QLP can be written in analogy to a classical LP and the FM QCP [28]:

$$S = \frac{1}{2}\int \frac{d^{\mathcal{D}}\mathbf{q}}{(2\pi)^{\mathcal{D}}} \frac{1}{\beta}\sum_n \left(r + cq^2 + Dq^4 + \gamma\frac{|\omega_n|}{q}\right) \times \vec{\phi}(\mathbf{q}, \omega_n)\cdot\vec{\phi}(-\mathbf{q}, -\omega_n) + u\int d^{\mathcal{D}}\mathbf{x}\int_0^\beta d\tau[\vec{\phi}(\mathbf{x}, \tau)\cdot\vec{\phi}(\mathbf{x}, \tau)]^2. \quad (1)$$

Here $\vec{\phi}(\mathbf{x}, \tau)$ is a vector order parameter defined in space and imaginary time, $\vec{\phi}(\mathbf{q}, \omega_n)$ is the Fourier transform, and ω_n is a bosonic Matsubara frequency. D, u, and γ are positive constants. The parameters r and c are linear functions of δ and U close to the quantum critical point. At mean-field level the QLP is defined by $c = 0$, $r = 0$. At the FM-PM boundary $r = 0$ and $c > 0$, whereas at the PM-IC phase boundary $c < 0$ and $r = c^2/(4D)$ and the unstable mode has momentum $q = \sqrt{-c/(2D)}$. The FM-IC boundary is characterized by $c = 0$, $r < 0$ thus c changes sign at the boundary mimicking the change of sign in the stiffness found in RPA.

As mentioned above, far from the QLP the transitions have a dynamical exponent $z = 2$, 3. At the QLP the dynamical exponent changes to $z = 5$ and the upper critical dimension becomes $8 - z = 3$. Therefore, if a QLP exists at low $\mathcal{D}$ the quartic term is not irrelevant and the theory becomes non-Gaussian or Gaussian with logarithmic corrections in marked contrast with Hertz theory. A full analysis must take into account singular contributions to the coefficients and goes beyond our present scope.

One can also envisage an AFM QLP at which AFM, PM, and IC phases meet. In this case the damping term becomes momentum independent implying $z = 4$ with an upper critical dimension $\mathcal{D} = 4$. Cuprates may be not so far from this phenomenology since at low temperatures and as a function of δ they show a transition from an AFM state to a paramagnet or superconductor which in addition often shows IC behavior [5]. Even more relevant for our discussion may be the low temperature behavior of overdoped cuprates where the IC states turns into a paramagnet. It has been argued [33] that the system is also close to a FM instability which suggests the proximity to a IC-PM-FM QLP. Another interesting system is $CeCu_{6-x}Au_x$ for which an AFM QLP where only one direction becomes soft has been proposed [34]. In all these cases, however, disorder effects appear to be quite relevant. Another system where one may hope to find a QLP is ultracold atoms in optical lattices. In this fascinating realization of the Hubbard model one can fine tune the parameters in the Hamiltonian which may allow for a full exploration of the phase diagram [35].

To conclude, our comparison with DMFT studies shows that the GWF, which played and still plays a fundamental role in understanding strong correlation, is a very convenient and accurate tool to study the magnetic phase diagram of the Hubbard model. Preliminary results in finite dimension point in the same direction [36]. We find that quite generically incommensurate phases appear as intermediate phases between FM and PM phases. This is interesting because, as mentioned in the introduction, IC phases are observed in a variety of systems in physical dimensions. For the hc lattice we find that the weakly polarized FM and the PM phase have a common phase boundary and both meet with the IC phase at a new QLP at which the magnetic order parameter is critical and the stiffness simultaneously vanishes. We speculate that an analogous QLP may exist in lower dimensional systems and we anticipate anomalous quantum critical behavior.

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