Quantum Lifshitz point in the infinite dimensional Hubbard model

F. Günther,1 G. Seibold,1 and J. Lorenzana2

1Institut für Physik BTU Cottbus, P.O. Box 101344, 03013 Cottbus
2SMC-INFM, ISC-CNR, Dipartimento di Fisica,
Università di Roma La Sapienza, P. Aldo Moro 2, 00185 Roma, Italy
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We show that the Gutzwiller variational wave function is surprisingly 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 metals1 2 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 alloys4. Also various transition metal oxides show incommensurate magnetic phases which are often accompanied by charge order, like cuprates5, nickelates6 and manganites7.

Despite decades of investigation not much is known about the magnetic phase diagram of the Hubbard model. The simplest treatments8 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) phases10 11.

Infinite dimensional lattices offer an 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 lattices12. Here we investigate the Hubbard model in the limit of infinite dimension \( D \) using the Gutzwiller variational wave function (GWF)12. 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 expansion13 14 15. In principle the model can be solved exactly14. Here we show, comparing with exact results when available, that the celebrated 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 methods. More specifically, for the hhc, we show that the GWF FM instability line agrees with the exact computation by Uhrig14. 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 exponents16. We anticipate unusual critical behavior for a quantum LP (QLP) shall it occur at physical dimensions.

We start from the Hubbard Hamiltonian1 2 3

\[
H = \sum_{i,j,\sigma} t_{ij} \hat{c}_{i\sigma}^\dagger \hat{c}_{j\sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},
\]

where \( \hat{c}_{i\sigma}^\dagger (\hat{c}_{i\sigma}) \) destroys (creates) an electron with spin \( \sigma \) at site \( i \). \( U \) is the on-site Hubbard interaction and \( t_{ij} \) denotes the hopping parameter between sites \( i \) and \( j \).

The energy of the model is evaluated within the GWF for polarized and unpolarized phases. In the limit \( D \to \infty \) the Gutzwiller approximation (GA) to the variational problem becomes exact20 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 \cite{21} 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 \cite{22}. Basically we compute the dynamic spin susceptibility $\chi_{ij}(\omega) = -\frac{1}{N} \int e^{i\omega t} \langle T S^+_i(t) S^-_j(0) \rangle$ 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. \cite{17}. For simplicity we neglect macroscopic phase separation \cite{9,11} which, in any case, would be frustrated if the long-range Coulomb interaction were taken into account \cite{10}.

We consider the hypercubic lattice and the half-hypercubic lattice. The latter can be obtained from the hypercubic lattice by removing all the even sites. For the hhc case we consider hopping restricted to $t_{ij} = t/D$ for nearest neighbor sites and $t_{ij} = t/(2D)$ for next-nearest neighbor sites \cite{14}. For the hypercubic lattice we keep only nearest-neighbor hopping $t_{ij} = t/\sqrt{2D}$. In the latter case it has been shown \cite{23} that all the momentum dependence of correlation functions is contained in the factor

$$\eta_q = \frac{1}{D} \sum_{i=1}^{D} \cos(q_i),$$

which can be parametrized by a value between 1 and –1 corresponding to a scan along the zone diagonal from $q = (0, \ldots, 0)$ to $q = (\pi, \ldots, \pi)$, 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 $\eta_q^2$ which varies from 1 to 0 corresponding to a scan from $q = (0, \ldots, 0)$ to $q = (\pi/2, \ldots, \pi/2)$, respectively \cite{23}.

The hhc lattice is non-bipartite, 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 $\delta$. 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 $U_{BR} \equiv -8\tau$ with $\tau$ the noninteracting kinetic energy at half-filling \cite{22}.

Fig. 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 $1 - \eta_q(q)$ for small $q$ and shows a Goldstone mode at $q = 0$. As $U$ is decreased the excitation energy becomes negative first at $q = 0$ 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.

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 $\delta$ \cite{14} 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 $q$. In the figure we indicate by arrows the value of $\eta_q$ for the unstable modes. The instability occurs at $\eta_q \rightarrow 0$ for small $\delta$, consistent with the wave vector $q = (\pi/2, \ldots, \pi/2)$ and gradually shifts to $\eta_q = 1$ for $\delta = 1$ as expected for the instability toward the FM phase ($q = 0$).

Both instability lines indicate that there is an IC phase

![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 $U > 0.98U_{BR}$.](image1)

![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. [14]. In the inset a scaled representation of the FM stability limit is shown with $U_{red} = U/(U + U_{BR})$ and $U_{BR} = 6.86$. Dashed line: limit of stability of the PM phase. The arrows indicate the value of $\eta_q$ parameterizing the momentum of the unstable mode.](image2)
The present FM boundary practically coincides with the T = 0 extrapolated results of Ref. [24] while a substantial portion of the PM range of Ref. [24] 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 of the FM phase obtained in Ref. [25] within an approximate solution of the DMFT equations. Dotted lines are levels of constant magnetization. Energies are in units of $U_{BR} = 6.38 t$.

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 $\eta$ for the unstable mode of the PM phase. The stars correspond to the limit of stability of the FM phase obtained in Ref. [22] within an approximate solution of the DMFT equations.
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 $D$ 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 $D = 4$. Cuprates may be not so far from this phenomenology since at low temperatures and as a function of $\delta$ they show a transition from an AFM state to a paramagnet/superconductor which in addition often shows IC behavior. 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 that the system is also close to a FM instability which suggests the proximity to a IC-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. In all these cases, however, disorder effects appear to be quite relevant. Another system where one may hope to find a QLP are 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.

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 $D \rightarrow \infty$ magnetic phase diagram of the Hubbard model. We find that quite generically incommensurate phases appear as intermediate phases between strongly polarized FM phases 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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