

Universality class of quantum criticality in the two-dimensional Hubbard model at intermediate temperatures ($t^2/U \ll T \ll t$)

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By using numerically exact determinantal Monte Carlo we show that the dilute Fermi gas quantum critical theory quantitatively describes the behavior of the density and compressibility along the Mott/metal crossover in the two-dimensional Hubbard model for temperatures somewhat less than (roughly half) the tunneling but greater than (roughly twice) the superexchange energy. In contrast, we find that other observables such as the kinetic energy, doubly occupied sites, and magnetization in a finite Zeeman field are poorly described by the same dilute Fermi gas universality class. In addition to these findings' fundamental interest, they are relevant to cold atom systems, where the intermediate temperature regime is currently in experimental reach.

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I. INTRODUCTION

The crossover between a Mott insulator (MI) and a metal in strongly correlated materials is an incredibly rich problem.¹ At least two key factors play a role: The emergence of a charge gap and the onset of magnetic order due to superexchange. The role of each was debated originally by Slater and Mott in the 1940s and 1950s. Reference 2 gives some history and a modern perspective. These intertwined effects—the former of which is in general indescribable by a local order parameter—give small energy scales at the transition and excitations proliferate, impeding a full theoretical treatment. A quantum critical perspective frequently has been applied to the two-dimensional Hubbard model, the simplest canonical model that includes MI and metallic states. At temperatures low compared to the superexchange temperature there are numerous proposed scenarios, some (suggested) to explain the strange metal or pseudogap behavior, but few definitive conclusions, and, more basically, even the *phases* at zero temperature are unknown. Moreover, open questions remain for even the simplest quantum critical scenarios (e.g., Refs. 3 and 4).

We address the related question at temperatures *above* the superexchange scale, showing that for appropriate parameters and observables the “dilute Fermi gas” (DFG) universality class *quantitatively* describes the low energy behavior. This is part of a broad set of questions regarding manifestations of “criticality” even when a low temperature transition is avoided (e.g., Ref. 5) or has different character at low and intermediate temperatures,⁶ and of an even broader set of questions connecting quantum critical behavior to microscopic models, from high-temperature superconductors³ and heavy fermion materials⁷ to string theory,⁸ non-Abelian gauge theories in high energy physics,⁹ and even black hole structure¹⁰ and cosmic inflation in astrophysics.¹¹ Although the physics at temperatures above the superexchange energy is simpler than at low temperatures, it has remained uncertain whether and in what regime universal physics manifests, and even less clear which universality class describes the behavior.^{1,12–14} Our results are also directly related to present day and near-term future experiments with ultracold fermions in optical lattices.¹⁵ Although a common scenario of the doping-driven MI/metal crossover at these temperatures involves the DFG

theory where the effective number of carriers vanishes at the (avoided or fictional) zero-temperature transition, such behavior has *not* been verified with exact calculations.¹ Other possibilities exist, for example a diverging effective mass at the transition. Another possibility comes from zero-temperature determinantal quantum Monte Carlo, which finds a dynamic critical exponent $z = 4$, in contrast to $z = 2$ expected for the DFG and other theories.^{1,16} However, the intermediate temperature universal behavior has remained neglected, although the $z = 4$ scaling has been conjectured to persist up to temperatures above the superexchange scale.¹ We show through analysis of numerically exact determinantal quantum Monte Carlo calculations that the $z = 2$ DFG quantitatively describes the density equation of state in an appropriate intermediate temperature regime, complementing the zero temperature findings.^{1,16}

We consider the two-dimensional square lattice Hubbard model defined by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle, \sigma} f_{i\sigma}^\dagger f_{j\sigma} + \sum_i \left[\frac{U}{2} n_i(n_i - 1) - \mu n_i + h s_{iz} \right], \quad (1)$$

with $f_{i\sigma}$ and $f_{i\sigma}^\dagger$ fermionic annihilation and creation operators for states at site i and spin state $\sigma \in \{\uparrow, \downarrow\}$, $n_{i\sigma} \equiv f_{i\sigma}^\dagger f_{i\sigma}$, $n_i \equiv n_{i\uparrow} + n_{i\downarrow}$, $s_{iz} \equiv n_{i\uparrow} - n_{i\downarrow}$, and the sum $\sum_{\langle i,j \rangle}$ is over nearest neighbor sites i and j . The energy scales are tunneling t , interaction U , chemical potential μ , and Zeeman field h . We defined the chemical potential such that the center of the half-filling ($n = 1$) MI occurs at $\mu = 0$.

We use determinantal quantum Monte Carlo (DQMC)¹⁷ to compute spin densities $n_\sigma = \langle n_{\sigma,i} \rangle$, compressibility $\kappa = \partial n / \partial \mu$, kinetic energy (divided by t) $K = -(1/2) \sum_{\langle j \rangle, \sigma} [(f_{i\sigma}^\dagger f_{j\sigma}) + \text{H.c.}]$ (sum is over neighbors j of arbitrary site i), doubly occupied site fraction $D = \langle n_{i\uparrow} n_{i\downarrow} \rangle$, and the nearest-neighbor spin correlator $X = \langle s_{iz} s_{jz} \rangle$ with i and j nearest neighbors. We will show that for $h = 0$, small enough t/U , and T in the window $t^2/U \lesssim T \lesssim t$ (we set $k_B = 1$), the DFG universality class quantitatively describes the μ dependence of the density near the MI/metal crossover for several U/t and T/t . We also show that other observables

and the Zeeman field dependence of all observables is not well described by the DFG or any $z = 2$ universality class, and perhaps is described by another universal theory.

Many of these observables can be measured in cold fermionic atoms trapped in optical lattices,¹⁵ which are already in the $T \sim t$ regime. One can apply a similar analysis to that carried out here to the experimental data. In the present region one can use the comparison to validate the faithful emulation of the Hubbard Hamiltonian. As these experiments achieve somewhat colder temperatures, they will be able to explore more exotic quantum criticality inaccessible to DQMC,¹⁸ including the low-temperature $z = 4$ criticality observed in Ref. 16.

II. SCALING

For conventional quantum phase transitions described by symmetry breaking of a bosonic order parameter, observables \mathcal{O} take the form¹⁹ $\mathcal{O}(g, T, \dots) = \mathcal{O}_r(g, T, \dots) + T^{1+d/z-1/(zv_\mathcal{O})} \Psi_\mathcal{O}[(g - g_c)/T^{1/(zv_g)}]$, where g is a relevant coupling, the “...” of the argument indicate irrelevant couplings, $v_\mathcal{O}$ and v_g are, possibly nontrivial, scaling dimensions, d is the spatial dimension, and z is the dynamic critical exponent. The function \mathcal{O}_r is analytic and $\Psi_\mathcal{O}$ is a singular, universal contribution. The definition of “universality” is that the only dependence of $\Psi_\mathcal{O}$ on the irrelevant variables is to change the dimensional constant in $\Psi_\mathcal{O}$ that converts $\frac{g-g_c}{T^{1/(zv_g)}}$ into a dimensionless constant. These constants for $z = 1$ and $z = 2$ theories have the interpretation of an effective sound speed and excitation mass, respectively. We have assumed g is the only relevant coupling. Generally there can be more than one relevant variable, but frequently there are only one or two.

For conserved observables \mathcal{O} such as density and magnetization’s dependence on variables coupling to these quantities, the scaling structure simplifies to²⁰

$$\mathcal{O}(\mu, h, T, \dots) = \mathcal{O}_r(\mu, h, T, \dots) + T^x \Psi_\mathcal{O}\left(\frac{\mu - \mu_c}{T}, \frac{h - h_c}{T}\right), \quad (2)$$

where $x = d/z$ for $\mathcal{O} = n_\sigma$ and $x = d/z - 1$ for $\mathcal{O} = \kappa$. Here we include two relevant couplings, h and μ , the only two relevant couplings for the DFG universality class discussed below. Close to critical point one can Taylor expand the regular piece $n_{\sigma,r}$ and keep only the constant term, which we denote $n_\sigma^{(0)}$. For the MI/metal crossover we will find $n^{(0)} = 1$, as intuitively expected.

This scaling structure also applies to some more general transitions than symmetry breaking bosonic ones, including the DFG transition of interest here.¹⁹ This universality class is defined by the Hamiltonian

$$H_{\text{DFG}} = \sum_{\mathbf{k}, \sigma} \left(\frac{\hbar^2 k^2}{2m^*} - \mu^* \right) \rho_{\mathbf{k}\sigma} + \sum_{\mathbf{k}} h^* (\rho_{\mathbf{k}\uparrow} - \rho_{\mathbf{k}\downarrow}) + \frac{g}{2} \sum_{\mathbf{p}, \mathbf{k}, \mathbf{q}} c_{\mathbf{k}, \uparrow}^\dagger c_{\mathbf{p}, \downarrow}^\dagger c_{\mathbf{p}-\mathbf{q}, \downarrow} c_{\mathbf{k}+\mathbf{q}, \uparrow}, \quad (3)$$

where m^* is the effective mass, g is the effective interaction, μ^* is the effective chemical potential, h^* is the effective magnetic field, $c_{\mathbf{k}\sigma}$ ($c_{\mathbf{k}\sigma}^\dagger$) are fermionic annihilation (creation) operators

for momentum \mathbf{k} and spin σ , and $\rho_{\mathbf{k}\sigma} \equiv c_{\mathbf{k}\sigma}^\dagger c_{\mathbf{k}\sigma}$. For the present case it can be shown that $\mu^* = \mu - \mu_c$ and $h^* = h - h_c$. The interaction term is the only relevant coupling in $d < 2$ and is marginal in $d = 2$. We stress that this is a (candidate) effective model only near the quantum critical crossover, and there is no simple relationship between the renormalized parameters g and m^* and the microscopic parameters U , μ , h , and t .

Despite the simple nature of the Hamiltonian in Eq. (3), it displays a quantum phase transition with much of the phenomenology of general quantum critical behavior. The $T = 0$ phase transition is tuned by μ and occurs at $\mu_c = 0$. For $\mu^* < 0$ the zero temperature system is a vacuum of no particles, and at temperatures $T \ll |\mu^*|$ is a dilute classical gas. For $\mu^* > 0$ the zero-temperature system is a Fermi liquid, and low finite temperatures $T \ll |\mu^*|$ add dilute quasiparticle excitations. At finite temperatures satisfying $T \gtrsim |\mu^*|$, an intervening “quantum critical” region occurs, and the spatial separation between excitations is comparable to their thermal de Broglie wavelength.

If we ignore the marginal interaction term, the DFG observables are simply those of a noninteracting gas:

$$\rho_\sigma(\mu, h, T) = \frac{m^* T}{2\pi\hbar^2} \log(1 + e^{\beta(\mu + \sigma h)}), \quad (4)$$

with $\beta = 1/T$, and σ in the exponential takes values $\{+1, -1\}$ for $\sigma = \{\uparrow, \downarrow\}$. We expect the interactions to give logarithmic corrections in $d = 2$, but we find that these are negligible in the regime considered herein.

III. RESULTS

We compute several observables, enumerated below, with DQMC for each value of μ and h (see Appendices A and E for numerical details). To determine μ_c and $n_\sigma^{(0)}$, and $\kappa^{(0)}$, we have plotted, for example, κ versus μ (for the $h = 0$ calculations), as illustrated in Fig. 1 (bottom inset). Equations (2) imply that for observables in the scaling region, the resulting curves should cross at $\mu = \mu_c$ with the crossing value giving $\mathcal{O}^{(0)}$. From this we find that $n^{(0)} = 1$, $\kappa^{(0)} = 0$, and $\mu_c/t = \{0, -0.83, -1.2, -3\}$ for $U/t = \{4, 6, 8, 12\}$. Note that the $U/t = 4$ value of μ_c is likely nonzero, but is zero within our error bars. The μ_c/t used in Fig. 1 are slightly different, namely $\mu_c/t = \{-0.3, -0.8, -1.3, -3.2\}$, found by adjusting to get best agreement with DFG theory. These roughly agree with the crossing points, but shifted by $\delta(\mu_c/t) \lesssim 0.3$. The difference between the two methods is likely due to the fact the crossing is influenced by data from nonuniversal temperatures. We emphasize that these μ_c are that of a *fictional* $T = 0$ Mott/metal transition, which may actually be shifted from any true $T = 0$ transition. It is nevertheless worth comparing these values of μ_c/t to naive expectations for the $T = 0$ transition in the small- and large- t/U limits. Note the trend of decreasing μ_c for increasing t : As expected, the MI regime shrinks as t increases. For small t/U , a simple model of Hubbard bands with width $8t$ gives that $\mu_c/t = -U/(2t) + 4$, so $\mu_c/t = -2$ for our smallest $t/U = 1/12$, in rough agreement with our observations. At $t/U = 1/4$, the RPA result (accurate for large t/U) $\mu_c \approx -t e^{-2\pi\sqrt{t/U}} \approx -0.04$ compares favorably with our results, although $t/U = 1/4$ is far from the $U \rightarrow 0$ limit. We emphasize that the comparison with the RPA is

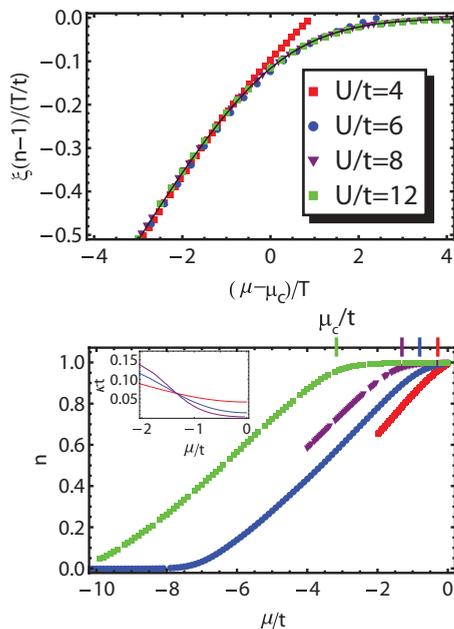


FIG. 1. (Color online) Top: Universal μ dependence of the density for several tunneling rates and interaction strengths (t/U). Data are for $T = t/3$, except for $U/t = 12$ for which $T = t/2.5$. We observe excellent universal collapse for all data at $U/t = 6, 8, 12$ and also for all but very low hole densities at $U/t = 4$. Details: $(n-1)\xi/T$ vs $(\mu - \mu_c)/T$ for $h = 0$, where $\xi \propto m^*a^2/(2\pi\hbar^2)$ is a nonuniversal factor related to the effective m^* . We fit the nonuniversal scaling factor ξ to obtain collapse with the dilute Fermi gas critical theory prediction, Eq. (4) (thin black line). Agreement is so good that the line is mostly obscured by the data. Because we are doping the Mott insulator with holes rather than particles, the chemical potential μ and effective mass m^* have their sign flipped relative to Eq. (4). Bottom: Same data (legend same as top panel) showing filling n vs μ/t without any scaling. Vertical ticks on upper axis show μ_c/t for each U/t . Inset shows an example of how we determine μ_c by the crossing of κ as a function of μ ($T/t = 0.33, 0.5, 1$, steeper to flatter curves, at $U/t = 8$).

provided only to illustrate consistency between our results with zero temperature theory. For example, the RPA μ_c is always so small that in the temperature range we consider, it would give results nearly identical to a $\mu_c = 0$ transition.²¹

This is why spin correlations being negligible in our temperature regime is consistent with them being responsible for making μ_c nonzero in the RPA.

Figure 1 shows that the density is a universal function of μ for temperatures around $T = t/3$. More precisely, this means that the rescaled density $(n-1)/T$ is a universal function of $(\mu - \mu_c)/T$, up to a vertical rescaling.²² It shows appropriately rescaled observables for $t/U = 1/4, 1/6, 1/8$, and $1/12$. The collapse indicates $z = 2$ scaling behavior for several t/U at $t/T = 1/3$. Furthermore, Fig. 1 shows quite remarkably that the noninteracting DFG [Eq. (4)] quantitatively describes the density scaling function of the Hubbard model. The DFG (thin black line) quantitatively describes the data, despite the underlying state of a strongly correlated Mott insulator and associated short range particle-hole and spin correlations. Although in $d = 2$ we expect logarithmic corrections to the noninteracting scaling functions, these are unobservably small.

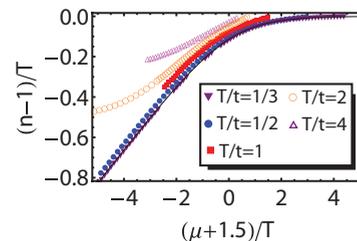


FIG. 2. (Color online) Universal μ dependence of the densities for $U/t = 8$. Universality breaks down outside of $t^2/U \lesssim T \lesssim t$ window, but is excellent in this regime. Additionally, the universal scaling function obtained is in quantitative agreement with the dilute Fermi gas critical theory prediction, Eq. (4) (thin black line) in the intermediate temperature regime. (We set $t = 1$ in figure labels.)

We note that the DFG universality class is analogous to the dilute Bose gas universality class governing the filling controlled Bose-Hubbard model's MI/superfluid transition, and the analysis techniques used to diagnose it here are similar to Ref. 18.

We emphasize that, although the universal scaling curves are well-described by the noninteracting DFG theory, the system is in fact strongly correlated in several strong senses. The DFG describes emergent fermionic excitations, not the underlying fermions in the Hamiltonian, and we will soon argue these emergent excitations are *not* even adiabatically connected to the bare fermions. One obvious manifestation of correlations is that we find (not shown) a large suppression of double occupancies, as well as some small spin-spin correlations (Fig. 3). A more dramatic sign of strong correlations is that the DFG Fermi surface violates Luttinger's theorem.²³ Luttinger's theorem, valid for any state adiabatically connected to the $U = 0$ Fermi liquid, says that the volume of the Fermi surface is given by the particle density. The particle density n_{DFG} in the DFG is the number of holes or particles “on top of” the Mott insulator. For example, for doping the Mott insulator with particles, $n_{\text{DFG}} = n - 1$ (in lattice units), so that Luttinger's theorem is enormously violated, with a defect of one particle per site. This shows that the emergent DFG fermions are *not* adiabatically connected to a $U = 0$ Fermi gas.

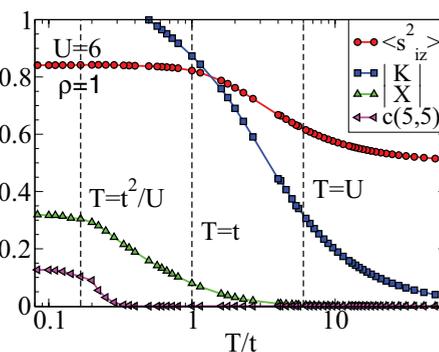


FIG. 3. (Color online) Observables illustrating various temperature regimes: Squared moment ($\langle s_{iz}^2 \rangle$), kinetic energy (in tunneling units) K , nearest neighbor spin-spin correlation magnitude $|X|$, and spin-spin correlation separated by the vector (5,5), in lattice units (maximum separation for a 10×10 lattice with periodic boundary conditions). (We set $t = 1$ in figure labels.)

While Fig. 1 shows the universal collapse fixing T and varying U/t , Fig. 2 shows collapse of data fixing U/t and varying T . We find that the DFG (thin black line) *quantitatively* describes the μ dependence for temperatures satisfying $t^2/U \lesssim T \lesssim t$. As shown in Fig. 3, in this regime the spin moment has fully developed but long range spin correlations are playing a secondary role. The $T = t/3$ results in Fig. 1 are also in this temperature window. We also have checked that, in contrast to the plots of rescaled variables [e.g., $(n - 1)/T$ vs $(\mu - \mu_c)/T$], plotting variables without rescaling or rescaling according to other z (e.g. $z = 1$ or $z = 4$) fails to give good collapse [see Fig. 1 (bottom) and Appendices].

The data collapse observed for $t^2/U \lesssim T \lesssim t$ breaks down for both lower and higher temperatures. At higher temperatures this is natural because the excitations begin to probe energy scales beyond the bottom of the excitation band, where the dispersion is well described by $\epsilon_k = \hbar^2 k^2 / (2m^*)$, and begin to see the microscopic band structure. At lower temperatures $T \lesssim t^2/U$ the spin correlations modify the behavior, in contrast to higher T where they give only small, nonuniversal contributions that are irrelevant to the universal physics. These correlations at high temperatures depend on microscopic details governing superexchange physics. Only at much lower temperatures ($T \ll t^2/U$) will universal behavior recover, and it likely will be more exotic, for example one of the scenarios referenced in the Introduction.

We emphasize that the observed collapse is compelling evidence for some underlying universality and not a result of gratuitous fitting. First, we note that *two* different temperatures ($T = t/2$ and $T = t/3$) at $U = 8t$ collapse quantitatively onto the dilute Fermi gas prediction, with a third temperature ($T = t$) collapsing quite accurately as well. All of these curves collapse with two total parameters $n_c = 1$ and $\mu_c = -1.5$ trivially shifting the horizontal and vertical position, with a third m^* controlling the linear asymptote for negative μ . However, none of these parameters tune the width of the crossover between the asymptotes. In light of this, the collapse of multiple temperatures is even more remarkable. That each U also collapses onto the same shape after fitting m^* and μ_c is equally remarkable.

To compare scaling functions obtained with DQMC to the DFG theory, one requires a single nonuniversal scaling factor, the DFG effective mass in Eq. (4). From this we find the ratios of m^* for $t/U = 1/4, 1/6, 1/8, 1/12$ are $1 : 1.7 : 2.4 : 4.1$, increasing as t/U decreases. The ratios assuming $m^* \propto 1/t$ would be $1 : 1.5 : 2 : 3$, so we see that roughly $m^* \propto 1/t$ for small t . This is what is expected from a simple picture of “upper and lower Hubbard bands” governing weakly interacting “doublons” (doubly occupied sites) and “holons” (vacancies in the Mott insulator), where the phase transition is driven by varying the chemical potential through the edge of one of the bands. We note that even in the strong coupling limit $U/t \rightarrow \infty$ in this Hubbard band picture the effective mass is simply given by the tunneling t . Our rough agreement with this prediction further supports the Hubbard band picture as a starting point for considering the problem.

Figures 1 and 2 illustrate that universal scaling is best for small values of t/U , becoming quantitative over the full visible range for $t/U \lesssim 1/8$. This is natural since only for

small t/U is there a large separation between the t^2/U and t temperature scales that must hold in order for the temperature to satisfy $t^2/U \ll T \ll t$. In contrast, we have seen that other observables do not appear universal, checking the nearest neighbor spin correlations, doubly occupied sites, and kinetic energy (see Appendix C).

We also find that the DFG fails to capture the h dependence of the spin densities. The reason is that in addition to the itinerant charge carriers governed by the DFG, there is a Mott background with spin degrees of freedom. For $t/U \ll 1$ this background is described by a high temperature $T \gg t^2/U$ Heisenberg model, which reduces to a single site problem. The spin densities from this background are $n_\uparrow = 1/(1 + e^{2\beta h})$ and $n_\downarrow = 1/(1 + e^{-2\beta h})$. At $T = 0$ these are singular (step functions) at $h = 0$, indicating a nonanalytic contribution to the spin densities that is not captured by the dilute Fermi gas theory. Thus at $\mu = \mu_c$ for $h = 0$ there are coinciding singularities from this “background” and DFG contributions. (More details are in Appendix D.)

IV. SUMMARY AND DISCUSSION

We have computed the density, compressibility, fraction of doubly occupied sites, kinetic energy, and nearest neighbor spin correlations of the two-dimensional square lattice Hubbard model with determinantal quantum Monte Carlo near the Mott/metal crossover. In the language introduced in Ref. 24, we find that although prior work shows the $T = 0$ quantum critical point obeys universal $z = 4$ “marginal quantum critical” scaling, this crosses over to universal $z = 2$ (nonmarginal) dilute Fermi gas quantum critical scaling at intermediate temperatures. Specifically, we find the dilute Fermi gas theory *quantitatively* gives the scaling functions for the density at $h = 0$ for a range of $t/U \lesssim 1/6$ and temperatures $t^2/U \lesssim T \lesssim t$. In contrast, we find that there is no apparent universality for other observables, and also that for $h \neq 0$, the singular contribution from the nonitinerant spin degrees of freedom invalidates the dilute Fermi gas theory.

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APPENDIX A: NUMERICAL DETAILS

We calculate observables with determinantal quantum Monte Carlo for a $L \times L$ lattice with $L = 10$, discretizing imaginary time evolution into Trotter steps of size $\delta\tau = 1/(12t)$, running 1000 Monte Carlo equilibration steps, followed by 100 000 steps for statistical sampling. The one exception is the $t/U = 1/12$, $T/t = 1/3$ calculation, for which 500 000 statistical sampling steps were necessary to get sufficiently accurate results. Typical statistical error bars for the density, not shown, are less than a tenth of a percent, smaller than the point size. We have checked convergence in each of

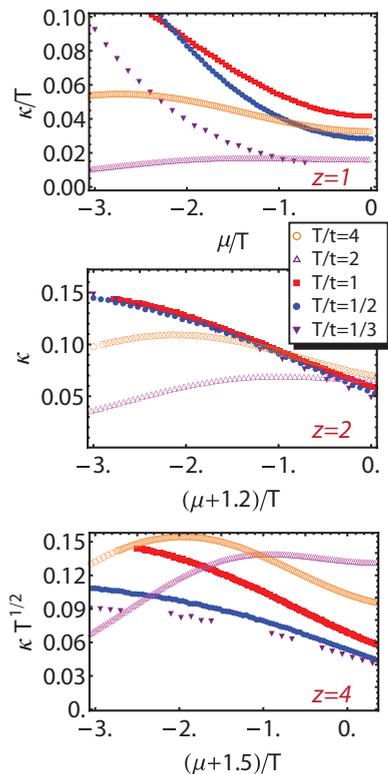


FIG. 4. (Color online) Rescaled compressibility (κ/T^{x-1} with $x = d/z$) vs rescaled chemical potential $(\mu - \mu_c)/T$ for $U/t = 8$ and dynamic exponent $z = 1, 2, 4$, top to bottom. The $z = 2$ rescaling obtains good collapse while the $z = 1$ and $z = 4$ both fail to give any significant collapse. The other values of U/t we considered show similar results. (We set $t = 1$ in figure labels.)

these parameters. In particular, for finite size effects, we found that the results were unchanged roughly within statistical error bars going from $L = 8$ to $L = 16$ for the $t/U = 1/4$ case where we expect the finite-size effects to be most important. We similarly found for the Trotter step $\delta\tau$ no change within statistical error bars from decreasing it to $\delta\tau = 1/(16t)$.

APPENDIX B: COMPARISON OF RESCALING FOR $z = 1, z = 2$, AND $z = 4$

Figure 4 illustrates that the $z = 2$ rescalings offer a good universal collapse of the data, while other candidate z fails. We show $z = 1$ and $z = 4$ but have examined others. We determined μ_c from the best crossing point of $n/T^{d/z}$, but for $z = 1$ and $z = 4$ there were no good crossings ($\mu_c = 0$ and $\mu_c = -1.5$, respectively, were the best or at least as good as any others, but still failed to show crossings). Note that in the main text, the presented data used μ_c determined to give good collapse of the low-temperature data to the dilute Fermi gas theory, and the resulting value of μ_c was slightly different than with the crossing method (e.g., $\mu_c = -1.5$ instead of $\mu_c = -1.2$ for the $z = 2$ rescaling of the $U/t = 8$ data). Since we have no natural theory to use for comparison in the $z = 1$ and $z = 4$ cases, determining μ_c by the crossing points was more fair for the comparison of Fig. 4.

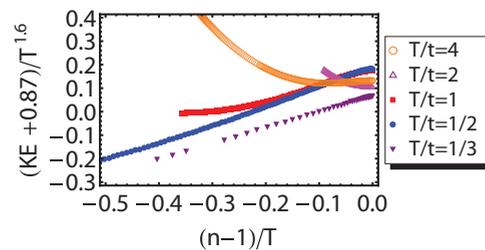


FIG. 5. (Color online) Rescaled kinetic energy $(K + 0.87)/(T/t)^{1.6}$ vs rescaled density $(n - 1)/T$, for $t/U = 1/8$. We have adjusted the offset (0.87) and the exponent (1.6) to find the best collapse for the two lowest temperature curves, but collapse is still poor. (We set $t = 1$ in figure labels.)

APPENDIX C: FAILURE OF NONUNIVERSAL OBSERVABLES TO RESCALE

As discussed in the main text, besides the μ derivatives of the free energy, densities, and compressibilities, we find no other static universal observables. We calculated the kinetic energy K , nearest neighbor spin correlator X , and double occupation probability D . This remains the case, even if we allow the nonuniversal constant $D(T = 0, \mu = \mu_c)$ and the scaling exponent to take arbitrary values. Figure 5 illustrates the best collapse we could obtain for the kinetic energy at $t/U = 1/8$, found by matching the small hole density behavior of the two lowest temperature curves. We find poor collapse. These results are typical.

APPENDIX D: h DEPENDENCE OF OBSERVABLES DISAGREES WITH DFG THEORY

We have noted that μ and h are (the only) relevant tuning parameters within the dilute Fermi gas (DFG) theory. Thus we might expect the DFG to govern the universal h dependence of observables. However, we have computed the spin-up and spin-down densities of the Hubbard model as a function of h for $\mu = \mu_c$ and $t/U = 1/8$ and find that the DFG theory does not adequately describe these observables. More strongly, no scaling collapse is obtained for $z = 2$, ruling out not only the DFG universality class, but any $z = 2$ theory. Figure 6 (top panel) demonstrates the lack of $z = 2$ scaling, and the middle panel shows the DFG theory curves for comparison.

To understand this lack of collapse, we reconsider the physical picture leading to the application of the dilute Fermi gas theory. We also note that no formal justification has to this point been available, so that we must rely on our physical intuition. The basic picture was of itinerant dopants governed by the DFG theory coupled to an essentially inert Mott background. The Mott background's only effect was to renormalize the DFG parameters and provide a nonuniversal, nonsingular contribution to the observables, which was irrelevant near the quantum critical point.

However, when a magnetic field is applied, treating the Mott background as inert is dangerous. To see this, consider the case where there are *no* itinerant charge carriers and thus the DFG plays no role. The Mott background may be described by a Heisenberg model, and since we are in the high temperature limit $T \gg t^2/U$, this reduces to a single site problem. In this

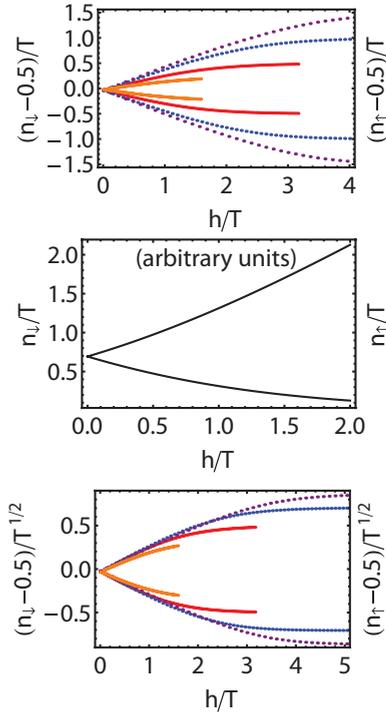


FIG. 6. (Color online) Top: Determinantal quantum Monte Carlo data for spin-down density (top curves) and spin-up density (bottom curves) rescaled at $U/t = 8$, assuming a dynamical critical exponent $z = 2$. Going from “inner curves” to “outer curves,” the temperatures are $T/t = 2, 1, 1/2, 1/3$. No scaling collapse is observed. Middle: Dilute Fermi gas theory predictions for comparison. Bottom: Same as top, but results rescaled according to $z = 4$. (We set $t = 1$ in figure labels.)

case, the spin densities are $n_{\uparrow} = e^{-\beta h} / (e^{-\beta h} + e^{\beta h})$ and $n_{\downarrow} = e^{\beta h} / (e^{-\beta h} + e^{\beta h})$. We see these are singular (step functions) at $h = 0$ and $T = 0$, so that the “Mott background” gives a singular contribution here, rather than a regular contribution as in the $h = 0$ case, tuning μ . This indicates that the singular contribution will include both a universal contribution from the DFG theory and from the “background.” The extent to and way in which these two pieces of physics couple at $h \neq 0$ is a complicated issue that we leave to future work.

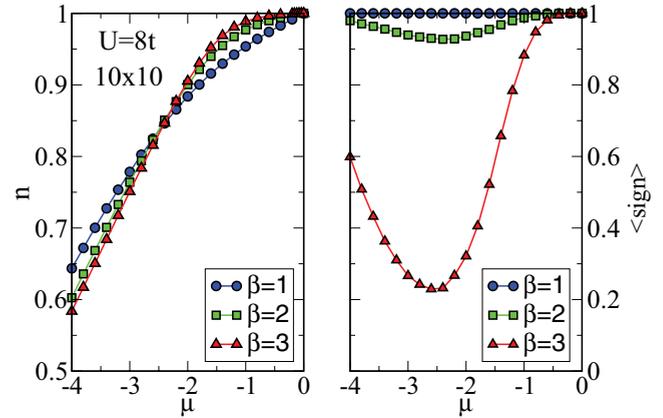


FIG. 7. (Color online) Filling (left) and average determinantal sign (right) as a function of μ for several inverse temperatures β . Chemical potential and temperature are in units of the tunneling t .

Interestingly, we do observe rather good collapse for $z = 4$, reminiscent of the $z = 4$ exponent found at $T = 0$ where magnetic physics, including superexchange, is certainly relevant.¹ However, we emphasize we are well above the superexchange temperature. It would be intriguing to understand this result better, and in particular if it is accidental or if it indicates a new universality class governing the $t^2/U \ll T \ll t$ Hubbard model. Presumably such a universality class would consist of free spins coupled to a DFG in some way, although to be consistent with our results in the main text it must reduce to the DFG universality class when $h = 0$.

APPENDIX E: AVERAGE DETERMINANTAL SIGN AND COMPUTATIONAL EFFICIENCY

Figure 7 shows the average sign of the determinants sampled by the determinantal quantum Monte Carlo, as well as the density, as a function of μ for several inverse temperatures β . The “sign problem” manifests as the average sign goes to zero and there is much cancellation in the sampled terms. We see the sign problem becomes worse for lower temperature and intermediate fillings, $n \sim 0.8$.

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