Dynamical t/U Expansion of the Doped Hubbard Model

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We construct a new $U(1)$ slave-spin representation for the single-band Hubbard model in the large-U limit. The mean-field theory in this representation is more amenable to describe both the spin-charge-separation physics of the Mott insulator at half-filling and the strange metal behavior at finite doping. By employing a dynamical Green's function theory for slave spins, we calculate the single-particle spectral function of electrons. The result is comparable to that in dynamical mean field theories. We then formulate a dynamical t/U expansion for the doped Hubbard model that reproduces the mean-field results at the lowest order of expansion. To the next order of expansion, it naturally yields an effective low-energy theory of a t–J model for spinons self-consistently coupled to an XXZ model for the slave spins. We show that the superexchange J is renormalized by doping, in agreement with the Gutzwiller approximation. Surprisingly, we find a new *ferromagnetic* channel of exchange interactions which survives in the infinite U limit, as a manifestation of the Nagaoka ferromagnetism.

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Although parent cuprates are genuine three-band, charge-transfer insulators,[1] it is widely accepted that the high-T_c superconductivity[2] and associated anomalies in the normal state can be adequately described within a doped single-band Hubbard model (HM)[3] with a large onsite repulsion U and its descendent low-energy effective model, the t–J model.[4–6]

The t–J model is usually obtained from the HM by performing a Schrieffer–Wolff-type transformation,[7,8] which can be considered as a type of t/U expansion. However, it is known that certain aspects of the HM are not captured by the t–J model. For example, Nagaoka ferromagnetism[9] and its possible survival at a large-but-finite-U limit is still under debate. Moreover, to be consistent with experimental observations, both the hopping amplitude and superexchange interaction in the t–J model have to be rescaled by the doping level δ empirically, known as the Gutzwiller approximation.[10] However, certain dynamical effects are not captured within the standard Gutzwiller-projected t–J model.[6,11–13]

A more formal approach to construct a low-energy effective theory for the HM would be from either a dynamical t/U perturbative series expansion in terms of Green's functions[14,15] or a cumulant expansion.[16] However, both are generically difficult due to the *noncanonical* nature of the atomic basis when doping is finite. It is possible to describe the dynamics of noncanonical theories via the Schwinger equations-of-motion (SEoM) approach, which is known as the *extremely correlated Fermi liquid* (ECFL) theory,[17] but it is still unclear how the t/U expansion can be performed using the exact SEoM of the HM. A feasible way would be to start with a slave-boson-type representation that can both faithfully reproduce the local single-particle spectrum of the HM and fulfill the spectral sum rule of Green's functions. Then use the path integral method to dynamically integrate out the high-energy degrees of freedom to obtain the corresponding low-energy effective theory. Such a dynamical theory has been obtained at half filling via a slave rotor representation.[16] Unfortunately it cannot be applied to finite doping due to the limited Hilbert space of the rotors. On the other hand, the $U(1)$ slave-spin representation[18] has a larger Hilbert space and would be suitable for the dynamical t/U expansion at finite doping. However, a major obstacle lies in the redundant spin $SU(2)$ symmetry in both the slave-spin and fermionic spinon sectors in its conventional construction.

In this work, we introduce a new $U(1)$ slave-spin representation that better describes the spin-charge separation in a Mott insulator. In light of this convenient representation, we construct a dynamical t/U expansion for the doped HM by employing a perturbative SEoM theory for the slave spins. This enables us to calculate electronic spectral functions, which agree with the cellular dynamical mean field theory (CDMFT)[19] results and the ECFL[17] results obtained by SEoM for the t–J model ($U \to \infty$) on the pole structure and spectral weight distribution, despite the mean field nature of our theory. We further compute the spin-spin interaction strength up to the $O(t/U)$ order of the expansion beyond the saddle point. An effective t–J model with rescaling factors that agrees with those in the Gutzwiller approximation naturally emerges in our theory. In addition to the antiferromagnetic superexchange coupling, we find a ferromagnetic exchange coupling surviving up to $U \to \infty$, which connects to the Nagaoka ferromagnetism. We finally discuss the implication of our theory and future prospects of our new approach to the HM.

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$U(1)$ Slave-Spin Representation of the Hubbard Model. We rewrite the physical electron operators $d_{i\sigma}$ and $d^\dagger_{i\sigma}$ as

$$d^\dagger_{i\sigma} = (S^+_{ia} + S^+_{ib}) f^\dagger_{i\sigma}/\sqrt{2},$$
$$d_{i\sigma} = (S^-_{ia} + S^-_{ib}) f_{i\sigma}/\sqrt{2}, \tag{1}$$

where $S^\pm_{ia}$ represents ladder operators of $S = 1/2$ slave spins, and $f_{i\sigma}$ is a fermionic spinon operator. In contrast to previous slave-spin constructions,[18,20] in this representation, the slave-spin indices a and b are no longer associated with the physical spin index σ, so that the slave spins and spinons respectively carry the charge and spin degrees of freedom, indicating a full charge-spin separation. The constraint becomes $\sum_{l=a,\,b} S^z_{is} = \sum_{\sigma=\uparrow,\downarrow}(f^\dagger_{i\sigma} f_{i\sigma} - \frac{1}{2})$, in contrast to previous constructions in which the constraint is for each spin flavor. The Hamiltonian of the single-band HM in this slave-spin representation is written as

$$H = H_{S,0} + H_{f,0} + H_t, \tag{2}$$

with $H_{S,\,0} = \frac{U}{2}\sum_i(\sum_s S^z_{is})^2 + h\sum_{is} S^z_{is}$, $H_t = -\sum_{ij\sigma}\frac{t_{ij}}{2}(S^+_{ia} + S^+_{ib})(S^-_{ja} + S^-_{jb}) f^\dagger_{i\sigma} f_{j\sigma}$, $H_{f,\,0} = (-h - \mu)\sum_{i\sigma} n^f_{i\sigma}$. Here, μ is the chemical potential and h is a Lagrangian multiplier to implement the constraint. Within this work, we consider the model on the square lattice with only nearest neighbor (nn) hopping.

As we shall demonstrate later, this representation reproduces Green's function of a Mott insulator in a slave rotor representation,[21,22] which has been shown to have captured the impurity physics of a Mott insulator.[23] This representation hence provides a better description of the Mott insulating phase at half filling. Meanwhile, at the mean-field level it retains the capability of describing the phases at finite doping just as in previous works.[18] In this work, we focus on the dynamical properties and the low-energy effective theory obtained beyond the mean-field level at finite doping where dynamical fluctuations are taken into account.

The Atomic Limit. To study the dynamical properties of slave spins, we use the SEoM method, which converts the Heisenberg equations of motion of the operators into exact equations of motion of Green's functions or propagators of these operators. This is formally carried out via a perturbation theory on an effective XXZ spin model under transverse and longitudinal fields, which is similar to those developed for Heisenberg models.[24–29] The details on the perturbation approach will be presented elsewhere.[30] For simplicity, we only show main results here.

Slave-spin Green's function is defined as

$$G^{\alpha\bar{\alpha}'}_{\eta,B,S,ss'}[i,\,f] = \langle \mathcal{T}[S^\alpha_{is}(t_i), S^{\bar{\alpha}'}_{fs'}(t_f)]_\eta\rangle - c_\eta\langle S^\alpha_{is}\rangle\langle S^{\bar{\alpha}'}_{fs'}\rangle, \tag{3}$$

with $\alpha = +$ or $-$, $s = a$ or b, $\eta = B$ or F representing the sign of the time-ordering and $c_B = 1$ and $c_F = 0$. Throughout this work, we use the labels $[i,\,f]$ to denote the space-time coordinates of the initial and final states $[x_i,\,t_i; x_f,\,t_f]$. To simplify the notation, from now on we drop the slave-spin index s so that $G^{\alpha\bar{\alpha}'}_{\eta,\,S}$ indicates a form of 2×2 matrix in spin space. One may freely choose to use either bosonic (B) or fermionic (F) Green's functions in the calculation because each will give a complete set of equations. Here we only show results for $G^{\alpha\bar{\alpha}'}_{B,\,B,\,S,\,ss'}$ and present the form of $G^{\alpha\bar{\alpha}'}_{F,\,Sss'}$ in the Supplementary Material (SM) as needed.

In the atomic limit (corresponding to Ising slave spins), we can obtain exact dynamical Green's function (also see the SM).[30] An arbitrary state (not necessarily an eigenstate) of $H_{S,\,0}$ can be fully characterized by the set of parameters $(M,\ m,\ \Delta m^2)$, where $M = \langle S^z_a + S^z_b\rangle$, $m = \langle S^z_a - S^z_b\rangle$, $\Delta m^2 = \langle (S^z_a - S^z_b)^2\rangle$. Solving $H_{S,\,0}$ at half filling (see the SM and Ref. [30]) we find $h = 0$, $M = 0$, $m^2 + \Delta m^2 = 1$. Here the uncertainty of m and Δm^2 reflects the spin degeneracy at the atomic limit. Choosing $m = 1$, we get (also see the SM)[30]

$$G^{\alpha\bar{\alpha}'}_{B,S} = \frac{\alpha\delta_{\alpha\alpha'}\sigma_z}{\omega - \alpha\sigma_z U/2}. \tag{4}$$

Switching to imaginary frequency $\omega \to i\nu$, we can recover slave-rotor Green's function $G_X[\nu]$ at half-filling $(G^{+-}_{B,\,S,\,aa} + G^{+-}_{B,\,S,\,bb})/2 \to G_X[\nu] = (\nu^2/U + U/4)^{-1}$, consistent with previous works.[16,21,22]

Effective Theory at Saddle-Point Level. Following the construction of Ref. [16], when the hopping is turned on, at the saddle-point level the theory is decoupled into an effective slave-spin theory

$$H_{S,\text{eff}} = H_{S,0} + H_{S,t}, \tag{5}$$

with $H_{S,\,t} = -\sum_{ij,\,ss'}(Q_{f,\,ij} S^+_{is} S^-_{js'} + \text{h.c.})$, and an effective f-spinon theory

$$H_{f,\text{eff}} = H_{f,0} + H_{f,t} \tag{6}$$

with $H_{f,\,t} = -\sum_{ij\sigma}(Q_{S,\,ij} f^\dagger_{i\sigma} f_{j\sigma} + \text{h.c.})$. The parameters $Q_{f,\,ij} = \sum_\sigma t_{ij}\langle f^\dagger_{i\sigma} f_{j\sigma}\rangle$, $Q_{S,\,ij} = \sum_{ss'} t_{ij}\langle S^+_{is} S^-_{js'}\rangle$ are self-consistently determined. In this theory the quasiparticle spectral weight is defined as $Z = \langle S_x\rangle^2$. The Mott insulator at half filling is described by a paramagnetic state of the slave spins with $\langle S_x\rangle = 0$. Doping the Mott insulator drives the system to a metallic state, in which the slave spins form long-range order $\langle S_x\rangle \neq 0$. When only the nn hopping is taken into account, $Q_{f,\,ij}$ is determined by the spinon density (that equals the electron density) and is independent of $Q_{S,\,ij}$. With this, the self-consistency at the saddle point is trivially achieved at finite doping δ. For simplicity, in the rest of this work, we restrict to the cases $\delta \sim 0$ where a perturbation theory is presumably valid.

At the saddle-point level, the slave-spin Hamiltonian can be solved by implementing a Weiss mean-field approximation to $H_{S,\,t}$, which has been widely adopted in previous works for single- and multi-orbital systems.[18,20,31–34] In this approximation,

$$H_{S,t} \approx H_{S,tMF} = -\sum_{is}\Big[\Big(\sum_{\langle ij\rangle s'} Q_{f,\,ij}\langle S^-_{js'}\rangle\Big) S^+_{is} + \text{h.c.}\Big]. \tag{7}$$

The $U(1)$ symmetry of the slave spins is broken and we choose $\langle S^+_{is}\rangle = \langle S^-_{is}\rangle = \langle S^x_{is}\rangle = M_x$. On a 2D square lattice with only nn hopping, $Q_{f,\,ij} = Q_f$ so that the mean-field Hamiltonian $H_{S,\,MF} = H_{S,\,0} + H_{S,\,tMF}$ becomes a local Hamiltonian. It can be solved by exact diagonalization and one finds $Z \propto \delta \simeq Q_{S,\,ij}$. The same result can

be alternatively arrived from lowest-order Green's function $G^{\alpha\alpha'}_{B,0}[\omega]$ in our dynamical perturbation theory in the limit of small doping δ (see the SM).

In the presence of perturbations, the lowest-order effect is that the ground state $|\psi(M,\ m,\ \Delta m)\rangle$ is renormalized. Hence, $G^{\alpha\alpha'}_{B,0}[\omega]$ for arbitrary states under the evolution of $H_{S,0}$ takes the following form:

$$G^{\alpha\bar{\alpha}}_{B,S,0}[\omega] = \sigma_0 \frac{X(\omega+\alpha h)+[M+\alpha(1-X)]U/2}{(\omega+\alpha h)^2-U^2/4}, \quad (8)$$

where $X = 1-\Delta m^2$. In the above expression, we already made use of the following properties: (i) $m = 0$ in the onset of transverse field; (ii) $\Delta m^2 \simeq 1$ near the doping-driven-Mott-insulator-to-metal transition, so that X is also a small parameter. Numerical calculations find $X = c_0\delta$ in this mean-field approximation where c_0 runs from about 1.3 near U_c to 1 for $U\to\infty$.

Perturbative Correction to Slave-Spin Green's Functions. Consider the perturbation to slave spin Green's functions of $H_{S,MF}$ as follows:

$$G^{\alpha\bar{\alpha}'}_{B,S}[\omega] \simeq G^{\alpha\bar{\alpha}'}_{B,S,0}[\omega] + G^{\alpha\bar{\alpha}'}_{B,S,1}[\omega], \quad (9)$$

where $G^{\alpha\bar{\alpha}'}_{B,1}[\omega]$ is the lowest-order correction of $G^{\alpha\bar{\alpha}'}_{B}[\omega]$ (other than the change in wavefunction under the evolution of H_0). The SEoM theory gives

$$\begin{aligned} G^{\alpha\bar{\alpha}'}_{B,S,1,ss'}[\omega] = \frac{\alpha}{\omega+\alpha h}\Big[&\frac{\alpha'(U\langle S^x_s\rangle + h_x)I_x}{2} \\ &+ \sum_{\alpha''}\frac{\alpha'' h_x}{2\omega}\big(U\langle S^x_\sigma\rangle G^{\alpha''\bar{\alpha}'}_{B,S,0,\bar{s}s'}[\omega] \\ &+ h_x G^{\alpha''\bar{\alpha}'}_{B,S,0,ss'}[\omega]\big)\Big], \end{aligned} \quad (10)$$

where $I_x = \sigma_0\langle M_x\rangle$. Although the bare first-order perturbation to $G^{\alpha\bar{\alpha}'}_{B,S}$ yields correct results for observables, such as second-order correction to $\langle S_z\rangle$, it violates the spectral weight sum rule significantly, especially when U is large. In principle, this can be fixed by going to higher-order perturbations. Here we adopt a simple random-phase approximation (RPA) to the diagonal (in both the slave spin flavor index and the α superscript index for which $+-$ or $-+$ is considered diagonal) components of $G^{\alpha\bar{\alpha}'}_{B,S}$:

$$G^{+-(-+)}_{B,S,ss}[\omega] \simeq \Big(G^{+-(-+)}_{B,S,0,ss}[\omega]^{-1} - G^{+-(-+)}_{B,S,1,ss}[\omega]\Big)^{-1}, \quad (11)$$

whereas the off-diagonal components are left the same. As we will show below, the spectral sum rule approximately holds by taking this RPA form of Green's functions at small dopings.

The Electronic Spectral Functions. Knowing Green's function of slave spins, the single-electron spectral function at finite doping is readily calculated. Here we discuss the local spectral function of electrons within the above mean-field approach. From Eq. (1), electronic Green's function $iG_d[i,\ f] \simeq (\sum_{ss'} iG^{-+}_{B,B,S,S,ss'}[i,\ f])(iG_f[i,\ f])$, which leads to the electronic spectral function

$$\rho_d[\omega,\ x] = \int d\omega'\Big(\sum_{ss'}\rho^{-+}_{B,B,S,S,ss'}[\omega+\omega',\ x]\Big)\rho_f[\omega'], \quad (12)$$

where the slave-spin spectral function $\rho^{-+}_{B,B,S,S,ss'}[\omega,\ x] = -\pi^{-1}\Im m[G^{-+}_{B,B,S,S,ss'}[\omega - i\eta^+\mathrm{sgn}[\omega]]]$. At the mean-field level, we take $\rho_f[\omega'] \simeq (\pi)^{-1}\delta(\omega')$, and Eq. (12) becomes

$$\rho^{MF}_d[\omega,\ x] \simeq \sum_{ss'}\rho^{-+}_{B,B,S,ss'}[\omega,\ x]. \quad (13)$$

Note that slave-spin Green's function in Eq. (9) is also local, so that $\rho^{MF}_d[\omega,\ x] = \rho^{MF}_d[\omega]$. Although the rigorous $\rho_f[\omega']$ does have k-dependence, the local nature of the slave-spin part ensures that such k-dependence has no interesting structure other than the free electron dispersion within the regime of this work. See the SM for a detailed discussion.

We show the evolution of the local electron spectral function with doping level δ in Fig. 1(a), from which we can identify four distinct poles, labeled as W_i, $(i = 1,\ldots,4)$, respectively. The doping dependence of the calculated spectral weight at each pole W_i is shown in Fig. 1(b). We also plot together the quarter of total spectral weight $W_{\rm total}/4 = \sum_i W_i/4$, which indicates that the spectral weight sum rule is conserved up to an error of the perturbation theory $\mathcal{O}(h_x)$, much smaller than the doping level δ.

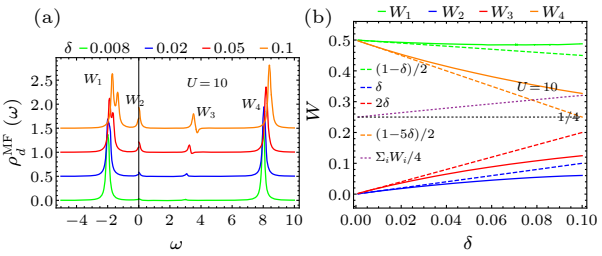

Fig. 1. (a) local electronic spectral functions for $\delta = 0.008,\ 0.02,\ 0.05,\ 0.1$ with a 0.5 shifting for each curve; (b) the spectral weights for each pole as a function of δ and compared with the corresponding asymptotic behaviors. The average spectral weight $\sum_i W_i/4$ of the poles is shown, which indicates approximate conservation of the total spectral weight (see text). A Lorentzian broadening factor $\eta^+ = 0.1$ is used in each curve in (a), and $\eta^+ = 0.01$ is used in (b).

By using the bare first-order perturbation results, we identify that the poles of $\rho^{MF}_d[\omega]$ are approximately located at $\omega_i \in \{h-U/2,\ 0,\ h,\ U/2+h\}$. The corresponding linear fittings for the spectral weight at these poles (dashed lines) are $\{(1-\delta)/2,\ \delta,\ 2\delta,\ (1-5\delta)/2\}$. These results clearly show that the poles respectively correspond to the lower Hubbard band (LHB), Fermi energy, mid-gap states, upper Hubbard band (UHB), and the spectral weight redistribution among them with doping.

For $U\to\infty$, it has been understood that the spectral weights of the four poles should be $\{W_1 = (1-\delta)/2,\ W_2 + W_3 = \delta,\ W_4 = (1-\delta)/2\}$. At finite U, it has be found that there is a correction due to a finite probability of double occupancy. For example, the CDMFT results in Ref. [19] identified that $\{W_1 = (1-\delta)/2,\ W_2 = \delta,\ W_3 = n_{\rm doublon},\ W_4 = (1-\delta-2\ n_{\rm doublon})/2\}$. Accordingly, our results give a doublon density $n_{\rm doublon} = 2\delta$ at $U = 10t$.

An interesting and important feature in the spectrum is the asymmetric structure of the pole W_2 about the Fermi

level $\omega = 0$. Though the jump of $\rho_d^{MF}[\omega]$ across $\omega = 0$ is generally an artifact coming from treating the f-spinon density of states as a δ-function, the asymmetry of the spectrum is a physical consequence of the pole of $G^{\alpha\bar{\alpha}'}_{B,S}$. Note that this is a *zero* frequency pole of *time-ordered* Green's function. Thus, it is a dynamical pole whose imaginary part should be interpreted as $\Im m[1/(\omega+i\delta\mathrm{sgn}[\omega])] \propto \partial_\omega\delta(\omega)$. This pole contributes a component $\propto \partial_\omega\rho_f(\omega)$ to $\rho_d(\omega)$ after the convolution. Considering that the f-spinons are treated as canonical fermions whose self-energy is even in ω, a dynamical particle-hole odd component [35] accounting for the asymmetric spectral weight should be incorporated in $\rho_d(\omega)$ through this pole, and this is an important hallmark of strong U correlations in recent microscopic theories including the ECFL theory, [17,35] the hidden Fermi liquid theory, [36,37] as well as dynamical mean field theory results. [38,39]

Spin-Spin Interactions of the Doped Phase. The dynamical expansion allows us to extract the superexchange interactions in terms of the f-spinons:

$$H_J = \frac{J_{ij}}{2} f^\dagger_{i\alpha} f_{i\beta} f^\dagger_{j\beta} f_{j\alpha} \Rightarrow J_{ij}\boldsymbol{S}_i \cdot \boldsymbol{S}_j. \tag{14}$$

Here J_{ij} is obtained by contracting the vertex at one-loop level [16] as

$$J_{ij} = t_{ij}^2 \int \frac{-d\omega}{2\pi} \sum_{ss'll'} G^{+-}_{B,S,ss'}[\omega,\, i,\, i] G^{-+}_{B,S,ll'}[\omega,\, j,\, j]. \tag{15}$$

Plugging in slave-spin Green's function at the atomic limit, we find the superexchange interaction at half filling: $J_0 = 2t_{ij}^2/U$. The missing factor of 2 can be restored when taking into account the fluctuations of the hopping term similarly to Ref. [16].

At finite doping, more channels of spin-spin interactions arise from different dynamical processes. They can be calculated term by term according to Eqs. (15) and (9). Up to the leading orders,

$$J = J^{(0)} + J^{(1)} + \cdots, \tag{16}$$

where $J^{(0)} = -t^2 \int \frac{d\omega}{2\pi} G^{+-}_{B,S,0} G^{-+}_{B,S,0}$ and $J^{(1)} = -t^2 \int \frac{d\omega}{2\pi} (G^{+-}_{B,S,1} G^{-+}_{B,S,0} + G^{+-}_{B,S,0} G^{-+}_{B,S,1})$. $J^{(0)}$ is the superexchange interactions, which is still governed by the virtual transition between the LHB and UHB as $G^{+-(-+)}_{B,S,0}$ only have poles at ω_1 and ω_4. To the lowest order in δ, we have

$$J^{(0)} \simeq J_0^*(1-2\delta), \tag{17}$$

where $a = h/U$ and $J_0^* = J_0(1-4a^2)^{-1}$, which is the bare superexchange interaction strength if only the energy shifting of the LHB and UHB caused by doping is accounted for. $J^{(1)}$ is due to the virtual transitions between LHB and the mid-gap pole W_2. To the lowest order, we have

$$J^{(1)} \simeq -\frac{M_x^2 t^2}{1+4a}, \tag{18}$$

which is ferromagnetic. By extrapolation, we find $M_x^2|_{U\to\infty} \simeq \delta$, which indicates that at finite doping and in the $U \to \infty$ limit only the *ferromagnetic* interaction survives. This links to the Nagaoka ferromagnetism. [9,40] We show the numerical plots of J, $J^{(0)}$, and $-J^{(1)}$ as functions of δ up to $\delta = 0.02$ in Fig. 2.

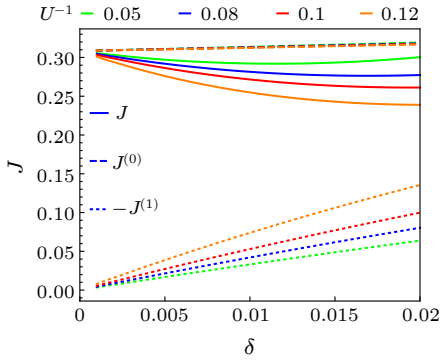

Fig. 2. (i) The total spin-spin interactions strength J (solid lines), (ii) the superexchange interaction strength $J^{(0)}$ (dashed lines), and (iii) the ferromagnetic interaction strength $(-1)\times J^{(1)}$ (dotted lines) plotted as functions of δ.

Effective Theory at First Order in t/U. Based on the above mean-field solution, we can further construct an effective theory for the doped HM in a way similar to Ref. [16]. The resulting theory contains Hamiltonians in both the slave-spin and f-spinon sectors:

$$H_{S,\mathrm{eff}} = H_{S,0} + H_{S,t}, \tag{19}$$

$$H_{f,\mathrm{eff}} = H_{f,t} + H_{f,0} + H_J. \tag{20}$$

$H_{f,\,\mathrm{eff}}$ takes the form of a t–J model and $H_{S,\,\mathrm{eff}}$ takes the form of an XXZ spin model. They are dynamically coupled via self-consistent condition. In our theory the renormalization factors of t and J for the f-spinons, g_t and g_J, are via the slave-spin correlations and no further Gutzwiller projection is necessary. Quantitatively, we find

$$g_t = M_x^2 = 2\delta, \quad g_J = 1-2\delta, \tag{21}$$

which agrees well with those phenomenological values $g_t = 2\delta/(1+\delta)$, $g_J = 1/(1+\delta)^2$ first proposed by Zhang *et al.* [10]

In summary, we propose a slave-spin representation of the HM on a square lattice with nn hoppings and use the SEoM perturbation theory to implement a dynamical t/U expansion in the doped MI. At the saddle-point level, our theory generates nontrivial dynamical properties of single-electron spectrum, including multiple pole structures and spectral weight (re-)distributions with doping, Both features are in excellent agreement with known numerical results despite that our theory is analytic in nature and works directly in the ω–k space. We also derive the exchange interactions among spins. In addition to the usual antiferromagnetic superexchange interactions, we find a new ferromagnetic channel at finite doping and finite U values. This ferromagnetic coupling survives the $U \to \infty$ limit and asymptotically connects to the Nagaoka ferromagnetism. It also provides a viable explanation for recently discovered ferromagnetic order [41] and spin fluctuations [42–44] in cuprates. In general, we find that the low-energy effective theory of the doped MI is a dynamical t–J model with effective renormalization factors in agreement with those proposed phenomenologically based on experimental data and empirical findings. Our

theory thus provides a natural basis and reliable means in understanding the exotic properties of the doped HM.

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References

[1] Zaanen J, Sawatzky G A, and Allen J W 1985 *Phys. Rev. Lett.* **55** 418
[2] Bednorz J G and Müller K A 1986 *Z. Phys. B: Condens. Matter* **64** 189
[3] Hubbard J 1963 *Proc. R. Soc. A: Math. Phys. Eng. Sci.* **276** 238
[4] Zhang F C and Rice T M 1988 *Phys. Rev. B* **37** 3759
[5] Dagotto E 1994 *Rev. Mod. Phys.* **66** 763
[6] Lee P A, Nagaosa N, and Wen X G 2006 *Rev. Mod. Phys.* **78** 17
[7] Schrieffer J R and Wolff P A 1966 *Phys. Rev.* **149** 491
[8] MacDonald A H, Girvin S M S, and Yoshioka D 1988 *Phys. Rev. B* **37** 9753
[9] Nagaoka Y 1966 *Phys. Rev.* **147** 392
[10] Zhang F C, Gros C, Rice T M, and Shiba H 1988 *Supercond. Sci. Technol.* **1** 36
[11] Delannoy J Y P, Gingras M J P, Holdsworth P C W, and Tremblay A M S 2005 *Phys. Rev. B* **72** 115114
[12] Anderson P W 2006 *Nat. Phys.* **2** 626
[13] Phillips P 2010 *Rev. Mod. Phys.* **82** 1719
[14] Pairault S, Sénéchal D, and Tremblay A M S 1998 *Phys. Rev. Lett.* **80** 5389
[15] Pairault S, Sénéchal D, and Tremblay A-M S 2000 *Eur. Phys. J. B* **16** 85
[16] Ding W, Yu R, Si Q, and Abrahams E 2019 *Phys. Rev. B* **100** 235113
[17] Shastry B S 2011 *Phys. Rev. Lett.* **107** 056403
[18] Yu R and Si Q 2012 *Phys. Rev. B* **86** 085104
[19] Sakai S, Motome Y, and Imada M 2009 *Phys. Rev. Lett.* **102** 056404
[20] de'Medici L, Georges A, and Biermann S 2005 *Phys. Rev. B* **72** 205124
[21] Florens S and Georges A 2002 *Phys. Rev. B* **66** 165111
[22] Florens S and Georges A 2004 *Phys. Rev. B* **70** 035114
[23] Ding W and Si Q M 2018 arXiv:1810.03309 [cond-mat.str-el]
[24] Kondo J and Yamaji K 1972 *Prog. Theor. Phys.* **47** 807
[25] Shimahara H and Takada S 1991 *J. Phys. Soc. Jpn.* **60** 2394
[26] Gasser W, Heiner E, and Elk K 2001 *Greensche Funktionen in Festkörper-und Vielteilchenphysik* (Weinheim: Wiley-VCH Verlag)
[27] Frobrich P and Kuntz P 2006 *Phys. Rep.* **432** 223
[28] Nolting W and Ramakanth A 2008 *Quantum Theory of Magnetism* (Berlin: Springer)
[29] Majlis N 2007 *The Quantum Theory of Magnetism* (Singerpore: World Scientific) chap 6
[30] Ding W X 2022 arXiv:2202.12082 [quant-ph]
[31] Hassan S R and de'Medici L 2010 *Phys. Rev. B* **81** 035106
[32] Yu R and Si Q M 2011 *Phys. Rev. B* **84** 235115
[33] Lee W C and Lee T K 2017 *Phys. Rev. B* **96** 115114
[34] Lee W C 2016 arXiv:1605.03969 [cond-mat.str-el]
[35] Shastry B S 2012 *Phys. Rev. Lett.* **109** 067004
[36] Anderson P W and Casey P A 2009 *Phys. Rev. B* **80** 094508
[37] Casey P A and Anderson P W 2011 *Phys. Rev. Lett.* **106** 097002
[38] Deng X Y, Mravlje J, Žitko R, Ferrero M, Kotliar G, and Georges A 2013 *Phys. Rev. Lett.* **110** 086401
[39] Xu W H, Haule K, and Kotliar G 2013 *Phys. Rev. Lett.* **111** 036401
[40] Tasaki H 1998 *Prog. Theor. Phys.* **99** 489
[41] Sarkar T, Mandal P R, Poniatowski N R, and Greene R L 2020 arXiv:1902.11235 [cond-mat.supr-con]
[42] Sonier J E, Kaiser C V, Pacradouni V, Sabok-Sayr S A, Cochrane C, MacLaughlin D E, Komiya S, and Hussey N E 2010 *Proc. Natl. Acad. Sci. USA* **107** 17131
[43] Butch N P, Jin K, Kirshenbaum K, Greene R L, and Paglione J 2012 *Proc. Natl. Acad. Sci. USA* **109** 8440
[44] Kurashima K, Adachi T, Suzuki K M, Fukunaga Y, Kawamata T, Noji T, Miyasaka H, Watanabe I, Miyazaki M, Koda A, Kadono R, and Koike Y 2018 *Phys. Rev. Lett.* **121** 057002