Phase diagram of the Hubbard model on a square lattice: 
A cluster slave-spin Study

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The cluster slave-spin method is employed to investigate systematically the ground state properties of the Hubbard model on a square lattice with doping $\delta$ and coupling strength $U$ being its parameters. At half-filling, a relation between the staggered magnetization $M$ and the antiferromagnetic (AFM) gap $\Delta_{AFM}$ is established in the small $U$ limit to compare with that from the Hartree-Fock theory, and a first-order metal-insulator Mott transition in the paramagnetic state is substantiated, which is characterized by discontinuities and hystereses at $U_{Mott} = 10t$. The interaction $U_c$ for the crossover in the AFM state, separating the weak- and strong-coupling regimes, is found to remain almost unchanged with large dopings, and smaller than $U_{Mott}$ at half-filling because of long range AFM correlations. Finally, an overall phase diagram in the $U$-$\delta$ plane is presented, which is composed of four regimes: the AFM metal at half-filling, the AFM metal with the compressibility $\kappa > 0$ or $\kappa < 0$, and the paramagnetic metal, as well as three phase transitions: (i) From the AFM metal to the paramagnetic metal, (ii) between the AFM metal phases with positive and negative $\kappa$, and (iii) separating the AFM insulating phase at $\delta = 0$ from the AFM metal phase for $\delta > 0$.

I. INTRODUCTION

Because of its intimate relation to the high-$T_c$ unconventional superconductivity based on cuprate oxides, the one-band Hubbard model on a square lattice has been extensively studied through many theoretical approaches — Green’s function methods, variational methods, renormalization-group methods, and numerical methods such as the Quantum Monte Carlo (QMC) simulations, cluster dynamical mean-field theory (CDMFT), density matrix embedding theory (DMET), etc. Up till now, some consensuses about this model have been reached, e.g., the first-order metal-insulator Mott transition in the half-filled paramagnetic (PM) state, and an infinitesimal critical coupling strength for the antiferromagnetic (AFM) phase at half-filling because of the nested Fermi surface in the square lattice. Even if the Mott transition in the half-filled PM system transforms into a crossover in the AFM state, the relationship between them has not yet been understood thoroughly. There are two types of phase separation: the one with hole-rich and hole-poor regions and that with incommensurate AFM at small and intermediate $U$. While the earlier works present the phase separation as a mixture of AFM and FM states in the large $U$ limit, we find that the phase separation happens easier when doping the AFM Slatter insulator. It is worthy of noticing that the theoretical and numerical results can not be compared with experiments on the cuprate oxides directly because some crucial simplifications have been made in the Hubbard model by neglecting the long-range Coulomb interaction, the hopping matrix elements further than the nearest neighbors, and the inter-layer correlations, which have made the phase diagram of the two-dimensional (2D) Hubbard model qualitatively different from that of high-$T_c$ cuprate superconductors. However, recent experimental improvement on the ultracold atoms to lower the local temperature of the optical lattice beyond the exchange energy $J$ make it possible to observe the spatial charge and spin correlations even beyond the nearest neighbors. Thus, the optical lattice platform could not only help us unveil the phase diagram in the intriguing regime where the kinetic energy and interaction potential become comparable, but also examine the validity of various theoretical methods based on different approximations. Meanwhile, more reliable results of the model ought to be needed to provide guidelines for experimental researches.

Although the QMC method have succeeded in coping with the half-filled bipartite lattice, the sign problem for the doped fermion systems and the finite size effect make its predictions for non-half-filled systems at least questionable. In these cases, some nonperturbative semi-analytic methods based on slave-variable representations have been introduced to throw some light on the regime with modest coupling strengths, where the conventional perturbative techniques fail to give rise to correct solutions. Among all the slave-particle approaches, slave-boson method has been applied to the single band and multiorbital systems successfully. Earlier, Kotliar and Rukenstein have proven that the saddle point approximation within the slave-boson approach could reproduce the Gutzwiller approximation’s results of the half-filled PM state, and high-energy excitations can be taken into account by the fluctuations around the saddle point. Nevertheless, as the dimension of degrees of freedom increases, the exponentially growing number of bosonic slave variables makes the slave boson approach particularly inapplicable to multiorbital systems and cluster mean-field theories. For the large $U$ Hubbard model, a fermion-spin transformation has been developed to implement the charge-spin separation.

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in its equivalent, $t$-$J$ model, where the charge degree of freedom is represented by a spinless fermion while the spin degree of freedom by a hard-core boson. Within this scheme and its development, both the normal state properties and superconductivity mechanism of doped cuprates has been investigated extensively.

Recently, the slave-spin approach\textsuperscript{54–57} has been devised to study the half-filled multiorbital Hubbard model, where the slave spin is introduced to represent the charge sector of an electron. The difficulty mentioned above has been overcome because only one slave variable is needed for each degree of freedom. After that, the slave-spin method was improved by Hassan and de’ Medici\textsuperscript{7} to deal with the non-half-filled systems, known as the $Z_2$ slave-spin theory. However, it has been proven that the $Z_2$ slave-spin theory fails to reproduce the noninteracting dispersion of the multi-orbital Hamiltonian because of the non-zero orbit-dependent Lagrange multipliers. The $U(1)$ slave-spin theory\textsuperscript{8} can not only produce the same results as the $Z_2$ theory’s when the on-site interaction is on, but also capture the correct dispersion in the noninteracting limit by the extra orbit-dependent effective chemical potential, which is identical to the Lagrange multiplier at $U=0$ [see Appendix. C for details]. A recently generalized cluster slave-spin method\textsuperscript{9} has succeeded in describing the crossover of the AFM gap $\Delta_{AFM}$ and obtaining the correct quasi-particle residue that is consistent with the theory’s when the on-site interaction is off, but also the compressibility, has been observed in the regions with positive and negative compressibility, and the PM metal.

In the slave-spin method, the electron operator $c_{\alpha}$ is decomposed into the product of a fermionic spinon and a slave spin with $S=\frac{1}{2}$ which represents the physical spin and charge degrees of freedom, respectively,

$$c_{\alpha}^\dagger = S_{\alpha}^f f_{\alpha}^\dagger .$$

With the constraint $a_{\alpha}^\dagger b_{\alpha} + b_{\alpha}^\dagger a_{\alpha} = 1$, the slave-spin operator is rewritten in the Schewinger boson representation

$$S_{\alpha}^f = a_{\alpha}^\dagger b_{\alpha} , \quad S_{\alpha}^- = \frac{1}{2} (a_{\alpha}^\dagger a_{\alpha} - b_{\alpha}^\dagger b_{\alpha}) ,$$

which has been utilized to describe the metal-insulator Mott transition in the multiorbital Hubbard model\textsuperscript{8}. In the slave-spin formalism, the original Hillbert space of a single degree of freedom with the basis $\{|n_{\alpha}\} = \{|0\}, |1\rangle$ is enlarged to $\{|n_{\alpha}^f, S_{\alpha}^f\} = \{|0,\frac{1}{2}\}, |\frac{1}{2}, -\frac{1}{2}\rangle, |\frac{1}{2}, \frac{1}{2}\rangle, |1, -\frac{1}{2}\rangle, |1, \frac{1}{2}\rangle\}$. Thus, the following constraint is enforced to project out the unphysical states $\{|0,\frac{1}{2}\}, |\frac{1}{2}, -\frac{1}{2}\rangle$:

$$S_{\alpha}^f = f_{\alpha}^\dagger f_{\alpha} - \frac{1}{2} .$$

However, according to Kotliar and Ruckenstein\textsuperscript{5}, the slave-spin operators defined in Eq. (3) need to be dressed to ensure the correct behavior in the noninteracting limit

$$\tilde{S}_{\alpha}^f = P_{\alpha} P_{\alpha}^\dagger a_{\alpha}^\dagger b_{\alpha} , \quad P_{\alpha} = \frac{1}{\sqrt{1+2 S_{\alpha}^-}}$$

Then, in the slave-spin method, the Hamiltonian (1) can be rewritten as

$$H = -t \sum_{\langle i,j\rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.C.}) + U \sum_{\sigma} n_{\sigma}^\dagger n_{\sigma} - \mu \sum_{\sigma} n_{\sigma} + U \Delta_{AFM}$$

$$- \sum_{\sigma} \Delta_{\alpha\sigma} (f_{i\sigma}^\dagger f_{\sigma} - S_{i\sigma}^- - \frac{1}{2})$$

$$+ \frac{U}{2} \sum_{\sigma} (S_{i\sigma}^f + \frac{1}{2})(S_{i\sigma}^- + \frac{1}{2}) ,$$

II. FORMALISM

We start from the standard single-band fermionic Hubbard model\textsuperscript{1} defined by

$$H = -t \sum_{\langle i,j\rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.C.}) + U \sum_{\sigma} n_{\sigma}^\dagger n_{\sigma} - \mu \sum_{\sigma} n_{\sigma} + U \Delta_{AFM}$$

where $t$, $U$, $\mu$ are the nearest hopping constant, the on-site Coulomb repulsion energy and the chemical potential, respectively. $\langle i,j \rangle$ represents that the sum is over the nearest neighbors, and $c_{i\sigma}(c_{i\sigma}^\dagger)$ annihilates (creates) an electron at site $i$ with spin $\sigma = \uparrow, \downarrow$, and the number operator $n_{\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$.

In Sec. III C, $M$, $\Delta_{AFM}$, and the compressibility $\kappa$ as functions of $U$ and $\delta$ are studied thoroughly, and an overall phase diagram in the $U$-$\delta$ plane is presented.
where the constraint (4) is taken care of by introducing a Lagrange multiplier $\lambda_{i\sigma}$. Under the two-site cluster approximation sketched in Fig. 1(a), Eq. (6) can be decomposed into a fermionic spinon Hamiltonian and a composite boson fields $\tilde{\lambda}_{i\sigma}$ the quasi-particle residue $Z$ as $tZ$. Second, the Hamiltonian (8) in the slave-spin sector is a repulsively interacting Bose-Hubbard model for bosons $a_{i\sigma}$ and $b_{i\sigma}$ in the staggered external field $\lambda_{A\sigma}$ and $\lambda_{B\sigma}$. When the composite boson fields $\tilde{z}_{i\sigma}$ condensate, i.e., $\langle \tilde{z}_{i\sigma} \rangle \neq 0$ below the critical coupling strength $U_{\text{Mott}}$ for the metal-insulator transition in the PM state, the system changes from the insulating phase to a metallic one. Moreover, when $U$ is strong enough to make $\lambda_{A\sigma} \neq \lambda_{B\sigma}$, i.e., $\lambda_{\sigma} \neq 0$, the system will transit into the AFM state from the PM state. Thus, the Hamiltonian (7) and (8) can describe both the Mott transition at $U = U_{\text{Mott}}$ in the PM phase and the PM-to-AFM transition at $U_M$.

It has been proven that the four-site cluster approximation makes a great improvement compared to the two-site one by including more inter-site fluctuations. Thus, except Figs. 2 and 9, all our results are obtained in the four-site cluster approximation as illustrated in Fig. 1(b), whose mean-field fermionic spinon Hamiltonian remains the same as Eq. (7), and the cluster slave-spin Hamiltonian reads:

$$H_{4\text{-site}}^{S} = H_{\chi}^{S} + H_{U}^{S} + H_{K}^{S},$$

where

$$H_{\chi}^{S} = \sum_{\lambda_{1\sigma}} \lambda_{1\sigma} S_{\lambda_{1\sigma}}^{\uparrow},$$

$$H_{U}^{S} = \sum_{l} U(S_{\lambda_{l\sigma}}^{\uparrow} + \frac{1}{2})(S_{\lambda_{l\sigma}}^{\uparrow} + \frac{1}{2}),$$

$$H_{K}^{S} = \sum_{\sigma} \left\{ \epsilon_{\sigma}^{x} (z_{1\sigma}^{\dagger} z_{2\sigma}^{\dagger} z_{3\sigma} + z_{2\sigma}^{\dagger} z_{4\sigma} + z_{3\sigma}^{\dagger} z_{4\sigma}) + \epsilon_{\sigma}^{y} (z_{1\sigma}^{\dagger} z_{2\sigma}^{\dagger} z_{3\sigma} + z_{2\sigma}^{\dagger} z_{4\sigma} + z_{3\sigma}^{\dagger} z_{4\sigma}) + \epsilon_{\sigma}^{z} (z_{1\sigma}^{\dagger} z_{2\sigma}^{\dagger} z_{3\sigma} + z_{2\sigma}^{\dagger} z_{4\sigma} + z_{3\sigma}^{\dagger} z_{4\sigma}) \right\}.$$ (15)

The spinon part is readily Fourier transformed into $k$-space:

$$H_{MF}^{f} = \sum_{k,\sigma} (\xi_{k\sigma} f_{k\sigma}^\dagger f_{k\sigma} + \Delta_{\sigma} f_{k\sigma}^\dagger f_{k+Q\sigma}),$$

where

$$\xi_{k\sigma} = -4tZ\gamma_k - \mu_{\sigma}^{\text{eff}}, \quad \gamma_k = \frac{1}{2}(\cos k_x + \cos k_y),$$

$$\mu_{\sigma}^{\text{eff}} = \mu - \frac{1}{2}(\mu_{A\sigma} - \lambda_{A\sigma} + \mu_{B\sigma} - \lambda_{B\sigma}) ,$$

$$\Delta_{\sigma} = \frac{1}{2}(\mu_{A\sigma} - \lambda_{A\sigma} - \mu_{B\sigma} + \lambda_{B\sigma}).$$

Noticing that $\Delta_{\sigma} = -\Delta_{-\sigma}$ in the AFM state, the PM state can be reached by simply forcing the AFM gap $\Delta_{\text{AFM}} = |\Delta_{\sigma}| = 0$.

Still, there are two key points needed to be cleared. First, the fermionic spinon Hamiltonian (7) is very similar to that in the Hartree-Fock (HF) approximation except the hopping constant $t$ is renormalized by the quasi-particle residue $Z$ as $tZ$. Second, the Hamiltonian (8) in the slave-spin sector is a repulsively interacting Bose-Hubbard model for bosons $a_{i\sigma}$ and $b_{i\sigma}$ in the staggered external field $\lambda_{A\sigma}$ and $\lambda_{B\sigma}$. When the composite boson fields $\tilde{z}_{i\sigma}$ condensate, i.e., $\langle \tilde{z}_{i\sigma} \rangle \neq 0$ below the critical coupling strength $U_{\text{Mott}}$ for the metal-insulator transition in the PM state, the system changes from the insulating phase to a metallic one. Moreover, when $U$ is strong enough to make $\lambda_{A\sigma} \neq \lambda_{B\sigma}$, i.e., $\lambda_{\sigma} \neq 0$, the system will transit into the AFM state from the PM state. Thus, the Hamiltonian (7) and (8) can describe both the Mott transition at $U = U_{\text{Mott}}$ in the PM phase and the PM-to-AFM transition at $U_M$.

It has been proven that the four-site cluster approximation makes a great improvement compared to the two-site one by including more inter-site fluctuations. Thus, except Figs. 2 and 9, all our results are obtained in the four-site cluster approximation as illustrated in Fig. 1(b), whose mean-field fermionic spinon Hamiltonian remains the same as Eq. (7), and the cluster slave-spin Hamiltonian reads:

$$H_{4\text{-site}}^{S} = H_{\chi}^{S} + H_{U}^{S} + H_{K}^{S},$$

where

$$H_{\chi}^{S} = \sum_{l=1\sigma}^{4} \lambda_{l\sigma} S_{l\sigma}^{\uparrow},$$

$$H_{U}^{S} = \sum_{l} U(S_{l\sigma}^{\uparrow} + \frac{1}{2})(S_{l\sigma}^{\uparrow} + \frac{1}{2}),$$

$$H_{K}^{S} = \sum_{\sigma} \left\{ \epsilon_{\sigma}^{x} (z_{1\sigma}^{\dagger} z_{2\sigma}^{\dagger} z_{3\sigma} + z_{2\sigma}^{\dagger} z_{4\sigma} + z_{3\sigma}^{\dagger} z_{4\sigma}) + \epsilon_{\sigma}^{y} (z_{1\sigma}^{\dagger} z_{2\sigma}^{\dagger} z_{3\sigma} + z_{2\sigma}^{\dagger} z_{4\sigma} + z_{3\sigma}^{\dagger} z_{4\sigma}) + \epsilon_{\sigma}^{z} (z_{1\sigma}^{\dagger} z_{2\sigma}^{\dagger} z_{3\sigma} + z_{2\sigma}^{\dagger} z_{4\sigma} + z_{3\sigma}^{\dagger} z_{4\sigma}) \right\}.$$ (15)

In this work, we only investigate the ground state properties of the system and will adopt the following density of states in all computations to avoid the finite size effect,

$$D(\gamma) = \frac{1}{N} \sum_{k} \delta(\gamma - \gamma_k) = \frac{2}{\pi} K(\sqrt{1-\gamma^2}),$$

where $K(x)$ is the complete elliptical function of the first kind.

### III. RESULTS AND DISCUSSIONS

#### A. SYSTEMS WITH FINITE DOPING

We analyze the quasi-particle residue $Z$, the generalized Gutzwiller factor $g_t$, the AFM gap $\Delta_{\text{AFM}}$, the staggered magnetization $M$, the holodouble correlators between the nearest neighbors $C_{12}$.
The results are as follows: (i) In Fig. 2(a), we find that $Z$’s behave similarly with $g_{\uparrow \downarrow}$ in both the two- and four-site cluster approximations, and it is suppressed drastically when extra inter-site fluctuations are taken into account as the cluster size is enlarged from two to four. (ii) In Fig. 2(b), the crossover $U_c$ separating the weak- and strong-coupling regime in the AFM state is defined by the peak position of $\Delta_{\text{AFM}}$, which decreases from 12.9$t$ (2-site) to 8.9$t$ (4-site). Both $\Delta_{\text{AFM}}$ and $M$ [Fig. 2(c)] are restrained appreciably by the inter-site fluctuations. One observes that $M$ from the cluster slave-spin approximation and the HF theory are consistent when $U$ is small. (iii) In Fig. 2(d), a maximum of $C_{14}$ around $U \sim 20t$ can be identified as one of the features of the strong correlation, the reason for which has been analyzed in Appendix A. (iv) In Fig. 2(e), $\langle H_{\text{S-site}} \rangle/n/2$ in the AFM states declines suddenly at $U \sim U_M \approx t$, which is caused by the decrease of the interaction potential compared to the PM state in this region [cf. Fig. 3 (f)], and behaves as $-1/U$ at large $U$, which is similar to $\Delta_{\text{AFM}}/t$. (v) In Fig. 2(f), as $U$ goes up, the double occupancy decreases monotonically, which probably tends to zero as $U$ goes to infinity. Finally, we find that the difference between the results from two approximations is much smaller in the small and large $U$ limit than those at intermediate $U$’s, which necessitates enlarging the cluster size to study the properties of Hubbard model with moderate coupling strengths.

To understand how the quantities discussed in Fig. 2 evolve with the increase of $U$ at different doping levels, their dependence on $U$ at a set of dopings $\delta^P = 0.02$, $\delta^A = 0.02$, 0.05, 0.1, 0.2 are plotted in Fig. 3, where $A$ and $P$ denote the AFM or PM state, respectively. First, in Fig. 3(a), we find that $Z$ in the PM state is larger than its counterpart in the AFM state when $U < 6t$, or otherwise when $U > 6t$, and the quasi-particle weight in the PM state decreases more dramatically than that in the AFM state around $U \sim U_{\text{Mott}} = 10t$ at $\delta = 0.02$. Moreover, the increase of $Z$ with doping in the AFM state is observed at all $U$’s, signifying the system’s tendency towards a correlated metal. Second, the $\Delta_{\text{AFM}}$ at all dopings present a crossover behavior at $U_c$, and then reaches a finite value except for $\delta = 0.2$ whose $\Delta_{\text{AFM}}$ vanishes at $U = 26t$ in Fig. 3(b). The reason for this unusual behavior may be that at $\delta = 0.2$, the system is an AFM metal, whereas the increased $U$ makes the system more localized which is unfavorable to the itinerant AFM. It is worth mentioning that $\Delta_{\text{AFM}}$ shows a nonmonotonic behavior with the increase of doping when $U > U_{\text{Mott}}$. Third, as shown in Fig. 3(c), $M$ decreases monotonically with doping and like $\Delta_{\text{AFM}}$ at $\delta = 0.2$, the staggered magnetization also vanishes after reaching its maximum at $U_c$. The same picture has been observed in the recent DMET calculation\textsuperscript{32} and some earlier work by Kotliar and Ruckenstein$^5$. The holon-doublon correlator $C_{12}$ and double occupancy $\langle D \rangle$ as functions of $U$ are depicted in Fig. 3(d) and (e), respectively, both of which decrease monotonically with $\delta$. $C_{14}$ in the PM state is smaller than that in the AFM state when $U < U_c$ (8.9$t$ for $\delta = 0.02$), or otherwise in the case of $U > U_c$, while the opposite is true for $\langle D \rangle$. Furthermore, the ground state energy of the cluster slave-spin Hamiltonian (12) $\langle H_{\text{S-site}} \rangle/2$ is plotted in Fig. 3(f). There are three key points needed to be addressed: (i) According to Fig. 3(e), compared to the PM state, it is the decrease of the interaction potential that makes $\langle H_{\text{S-site}} \rangle/2$ decline rapidly upon entering the AFM state. (ii) For $U \lesssim U_{\text{Mott}} = 10t$, $\langle H_{\text{4-site}} \rangle/2$ increases monotonically with doping, while it presents a nonmonotonic behavior when $U \gtrsim U_{\text{Mott}}$. (iii) In contrast to the PM state, $\langle D \rangle$ and $\langle H_{\text{S-site}} \rangle/2$ diminish drastically as the AFM emerges, which can be understood through $\langle D \rangle = (1 - \delta)/2 - 2\langle M_f \rangle^2$ with $M_f = \langle n_{\uparrow \uparrow} - n_{\downarrow \downarrow} \rangle/2$. We now discuss the difference of the energetics of the slave-spin Hamiltonian (12) between the AFM and PM
FIG. 3. (a) The quasiparticle weight $Z$, (b) the AFM energy gap $\Delta_{AFM}/t$, (c) the staggered magnetization $M$, (d) the holondouble correlator between the nearest neighbors $C_{12}$, (e) the double occupancy per site, and (f) the expectation value of the cluster slave-spin Hamiltonian as functions of $U$ at a set of doping concentrations $\delta = 0.02$ (red), 0.05 (green), 0.1 (blue), 0.2 (violet) in the AFM state and $\delta = 0.02$ (black) in the PM state obtained by the four-site cluster.

states, as well as the electron momentum distribution and the hopping probability between the nearest and next nearest neighbors.

The differences of the kinetic energy $E_K$, interaction potential $E_U$ and their summation $E_{Total}$ of the approximate Hamiltonian (12) between the AFM and PM states ($\Delta E = E^{(A)} - E^{(P)}$) as functions of $U$ are plotted in Fig. 4. We observe a region around $6.5t < U < 8.94t$ separating the weak- and strong-coupling regimes in the AFM state$^{21,22,26,29,59}$. When $U < 6.5t$ or $U > 8.94t$, the AFM state in the system is governed by the interaction potential gain supporting the Slater mechanism or the kinetic energy gain that favors the super-exchange mechanism, respectively$^{21,30,59}$. However, a sharp crossover is observed at $U_{Mott}$ in the recent CDMFT calculation of the half-filled Hubbard model$^{30}$.

The electron momentum distribution $n_d(k)$ calculated in Appendix B are plotted in Fig. 5(a) and (b). The overall feature is that the on-site interaction transfers
The hopping probability between the nearest neighbor $|\langle c_{i\sigma}^\dagger c_{i+\delta}\rangle|^2 \approx Z^2 |\langle f_{i\sigma} f_{i+\delta}\rangle|^2$ and its derivative are plotted in Fig. 6(a) and (b). $|\langle c_{i\sigma}^\dagger c_{i+\delta}\rangle|^2$ is smaller in the AFM state than in the PM state when $U_M < U < U_c$, because the AFM state is driven by the interaction potential gain at small $U$ [see Fig. 4] that suppresses the double occupancy, leading to the same effect on $|\langle c_{i\sigma}^\dagger c_{i+\delta}\rangle|^2$ [compare Fig. 3(e) and Fig. 6(a)]. However, the opposite is true when $U > U_c$ because the AFM state is stabilized by the super-exchange mechanism at large $U$. Accordingly, the gradient of $|\langle c_{i\sigma}^\dagger c_{i+\delta}\rangle|^2$ with respect to $U$ has a minimum at $U = 3.0t$, $7.4t$ in the AFM and PM states, respectively, signifying that the long range AFM order suppresses the hopping probability between the nearest neighbors noticeably for small $U$.

The hopping probability between the next nearest neighbors $|\langle c_{i\sigma}^\dagger c_{i+\delta}\rangle|^2$ ($i \in A$) $\approx |\langle \tilde{z}_{A}\rangle|^4 |\langle f_{i\sigma} f_{i+\delta}\rangle|^2$ and its derivative are shown in Fig. 7(a) and (b). In the AFM state, $|\langle c_{i\sigma}^\dagger c_{i+\delta}\rangle|^2$ depends either on site $i$ or on spin $\sigma$, and varies nonmonotonically — remaining small when $U < U_M$, then zooming up at $U = U_M$, and vanishing when $U > U_{Mott}$ after reaching its maximum at $U \sim 3t$. However, in the PM state, it decreases to zero monotonically as $U$ increases.

### B. HALF-FILLED SYSTEM

By diagonalizing the spinon Hamiltonian (10), the self-consistent parameters $n_{A/B\sigma}^i = \langle f_{A/B\sigma}^i f_{A/B\sigma}^\dagger \rangle$ and $\epsilon_{\sigma}^0$ can...
To establish the relation between $M$ and $\Delta_{AFM}$ in the small $U$ limit, we expand asymptotically the integrals $I_c(\lambda)$ and $I_f(\lambda)$ as $\lambda \to \infty$:

$$
\epsilon \sim -t \left[ \frac{2}{\pi^2} \Delta^2 \ln \Delta - \left( \frac{1}{2\pi^2} - \frac{3\ln 2}{\pi^2} \right) \Delta^2 \ln \Delta + \left( \frac{1}{4\pi^2} + \frac{3\ln 2}{2\pi^2} - \frac{9(\ln 2)^2}{2\pi^2} \right) \Delta^2 \right],
$$

(22)

$$
\langle S^z_{A/B\sigma} \rangle \sim (-/+) \operatorname{sgn}(\Delta_{\sigma}) \left[ \frac{1}{\pi^2} \Delta^2 \ln \Delta - \frac{6\ln 2}{\pi^2} \Delta \ln \Delta + \frac{9(\ln 2)^2}{\pi^2} \Delta \right],
$$

(23)

with $\Delta = \lambda^{-1} = \Delta_{AFM}/(4tZ)$, resulting in

$$
M = \frac{1}{2} \left| \langle S^z_{A\sigma} \rangle - \langle S^z_{B\sigma} \rangle \right|
$$

$$
\sim \frac{1}{\pi^2} \Delta^2 \ln \Delta - \frac{6\ln 2}{\pi^2} \Delta \ln \Delta + \frac{9(\ln 2)^2}{\pi^2} \Delta.
$$

(24)

Therefore, the simple HF relation of $\Delta_{AFM} = UM$ (Ref. 20) needs to be corrected. By adopting the $U$ dependent form of the AFM gap

$$
\Delta_{AFM} = A\sqrt{U} e^{-B\sqrt{\frac{\pi}{2}}},
$$

(25)

which has been verified by the QMC method, we fit our self-consistent data to obtain

$$
\left\{ \begin{array}{l}
A = 0.02086 \pm 0.00418, \\
B = 1.90604 \pm 0.06189,
\end{array} \right.
$$

(26)

as shown in Fig. 8 (a). Then, the result is substituted into Eq. (24) to recover perfectly the data of $M$ shown Fig. 8 (b).

Moreover, the AFM gap $\Delta_{AFM}$, starting from an infinitesimal $U$, should also present in the spectrum function of the electron. In the slave-spin method, the spectrum function of the electron Green’s function can be expressed as

$$
A(q, \omega) = \int_0^\omega d\Omega A_{e\text{-spin}}(q-k, \omega - \Omega) A_{\text{fermion}}(k, \Omega).
$$

(27)

Assuming a gap $\Delta_{AFM}$ in the fermionic spinon sector of Hamiltonian (1), $A_{\text{fermion}}(k, \Omega < \Delta_{AFM}) = 0$, it is easy to understand that the electron spectrum function $A(q, \omega)$ will vanish when $\omega$ is smaller than $\Delta_{AFM}$.

Additionally, $Z$, $C_{12/14}$, $(H^2_{4\text{-site}})/2$, and $(D)$ as functions of $U$ are plotted in Fig. 9. The overall features are similar to those with $\delta = 0.02$ [cf. Fig. 2] for comparison except two critical distinctions. First, in the PM state, the first-order Mott transition occurs at $U_{\text{Mott}} = 10t$, characterized by the discontinuity and hysteresis behavior of these quantities. Compared to the AFM’s $U_c=8.2t$ shown in Fig. 8(a), we find that the AFM correlations significantly reduce the coupling strength which separates the weak- and strong-coupling regimes. This is consistent with the CDMFT...
In the following, we combine the results of the staggered magnetization $M$ (Fig. 11), the AFM gap $\Delta_{AFM}$ (Fig. 12), and the compressibility $\kappa$ (Fig. 13) to present an overall phase diagram for the Hubbard model (Fig. 15).

The staggered magnetization $M$ with $\delta$ and $U$ being its parameters is plotted in Fig. 11, where the phase boundary between the AFM and PM states is denoted by $\delta_M(U)$. First, the staggered magnetization always saturates at a certain value when $U > U_{Mott}$, while decreases monotonically with $\delta$. Second, marked by the dense contours around $\delta_M(U)$, the staggered magnetization decreases continuously to zero as $\delta$ approaches $\delta_M(U)$, signifying the second-order transition between the AFM and the PM phases. Third, $\delta_M(U)$ shows a nonmonotonic behavior with $U$ (Ref. 31), which is consistent with the re-entrance of $M$ with $U$ at $\delta = 0.2$, as shown in Fig. 3(c).

The AFM gap $\Delta_{AFM}$ in the same parameter space is plotted in Fig. 12, where the previous boundary $\delta_M(U)$ still holds for $\Delta_{AFM}$. When $U > U_{Mott}$, the maximum of $\Delta_{AFM}$ occurs at $\delta \approx 0.05$, leading to the interesting vertical re-entrance behavior as $\delta$ increases, which reflects that the AFM gap at half-filling vanishes in the large $U$ limit.

Figure 13 shows the results for the compressibility $\kappa = n^{-2}\partial n/\partial \mu$. The staircase in this figure obviously is an artifact because of discrete $U$’s adopted to calculate $\kappa$, i.e., $\Delta U = t$ when $U \leq 12t$ and $\Delta U = 2t$ when $12t < U \leq 20t$, which can only be eliminated in the $\Delta U \to 0$ limit. As shown in Fig. 13, there exist two phase boundaries delineated by the midpoints of these steps: (i) $\delta^1_\kappa(U)$, between the regions with positive (red) and negative (blue) compressibility. (ii) $\delta^2_\kappa(U)$, from the region with $\kappa < -0.5$ (blue) to $0.2 < \kappa < 0.5$ (yellow). As shown in Fig. 14, $\kappa = 0$ at half-filling is disconnected from that at an infinitesimal doping $31$, signifying that the half-filled system in the AFM state is an insulator while the doped one a metal. By Fig. 11 and Fig. 13, the systems with $\delta^1_\kappa(U) < \delta < \delta^2_\kappa(U)$ are AFM metals with negative compressibility, meaning the uniform AFM configuration is not the actual ground state, whereas an inhomogeneous phase with $M \neq 0$ could be the alternative. In addition, the space between $\delta^1_\kappa(U)$ and $\delta^2_\kappa(U)$ shows a broadening-narrowing feature as $U$ increases, and they may merge into one as $U \gg 20t$, implying that this kind of phase separation can not be observed in the large $U$ limit. $21,27,28$. Moreover, $\delta^2_\kappa(U)$ is identical to $\delta_M(U)$, thus, $\delta_M(U)$ is the boundary separating the AFM metal phase with $\kappa < 0$ and the PM metal phase.

By aggregating Figs. 11, 12 and 13, we acquire an overall phase diagram, Fig. 15, of the Hubbard model in the $U$-$\delta$ plane. The boundary $\delta_{HF}(U)$ between the AFM and PM phases within the HF theory is plotted as the dashed line. As expected, the consistency between $\delta_{HF}(U)$ and $\delta_M(U)$ only lies in the small $U$ region.

C. PHASE DIAGRAM

![Graph](image)

**FIG. 8.** (a) the AFM energy gap $\Delta_{AFM}/t$ where the inset shows the same data at small $U$ together with the fitting data (black line) and (b) the staggered magnetization $M$ where the inset shows the same data at small $U$ together with that calculated by Eq. (24) (black line).
which is also the case of $M$ in Fig. 2(c). There exists one crossover $U_c$, separating the weak- and strong-coupling regions, and three transitions in the $U$-$\delta$ plane: (i) between the AFM insulator at $\delta = 0$, marked by the heavy blue line, and the AFM metal for $\delta > 0$; (ii) $\delta_1^A(U)$, separating the AFM phases with the positive and negative compressibility, which may not exist after considering the inhomogeneous phases; (iii) $\delta_2^A(U)$, from the AFM metal with negative compressibility to the PM metal. Thus, we find phase
FIG. 12. The AFM gap $\Delta_{\text{AFM}}$ as functions of $U$ and $\delta$ in the AFM states obtained by the four-site cluster.

FIG. 13. The compressibility $\kappa$ as functions of $U$ and $\delta$ in the AFM states obtained by the four-site cluster. $\kappa$ in the red and blue region are greater than 0.5 and less than -0.5, respectively.

separation at small and intermediate coupling strengths, which is in agreement with the auxiliary-field QMC\textsuperscript{27,28} and variational\textsuperscript{21} studies. However, the phase separation occurs at intermediate doping levels in our work but at small dopings in these QMC studies. This discrepancy most likely results from the fact that the cluster slave-spin mean-field theory exaggerates the system’s tendency towards a uniform AFM state, which may be remedied by enlarging the cluster size and strictly dealing with the constraint $S_\alpha^z = f_\alpha^† f_\alpha - \frac{1}{2}$ locally within the cluster. It should be mentioned that $U_c$’s at all dopings are close to the $U_{\text{Mott}}$ of $\delta = 0$, manifesting that the physics in the AFM state are governed by the underlying Mott transition in the half-filled PM state\textsuperscript{21,30,31}. The reason for the close relationship between the crossover mentioned above and the Mott transition in the PM state is that both phenomena are driven by the competition between the kinetic energy and interaction potential of the Hubbard model.

FIG. 14. The compressibility $\kappa$ as functions of $\delta$ in the AFM state at $U = 5t$, $10t$, and $18t$ obtained by four-site cluster. Red lines are the extrapolated curves from the corresponding self-consistent data using $\kappa_0 + \alpha \delta^2 + \beta \delta^4$. The red circles at $\delta = 0$ denotes the discontinuity of $\kappa = 0$ at $\delta = 0$.

FIG. 15. The phase diagram of the Hubbard model in the $U$-$\delta$ plane obtained by the four-site cluster, where exist the crossover $U_c$ (red dashed line) dividing the weak- and strong-coupling regimes, at which the $\Delta_{\text{AFM}}$ is maximized, and the AFM for $U < U_c$ and $U > U_c$ is advocated by the interaction potential and kinetic energy gain, respectively. The $U_{\text{Mott}}$ for the Mott transition in the PM state is marked by the red triangle. The half-filling case is highlighted by the heavy blue line, in which the system is an AFM insulator with $\kappa = 0$. Here the black dashed line represents the boundary $\Delta_{\text{MF}}(U)$ between the AFM and PM phases within the HF method.
IV. CONCLUSION

In summary, the cluster slave-spin method has been employed to investigate systematically the ground state properties of the single-band 2D Hubbard model on a square lattice in the parameter space of $U$ and $\delta$. We substantiated that the system presents a broad crossover between the weak- and strong-coupling regimes: (i) The $\Delta_{\text{AFM}}$ increases monotonically with $U$ in the weak-coupling regime, while decreases for large couplings.\(^9\)

(ii) The AFM in the weak-coupling regime is stabilized by the interaction potential gain, while that for large $U$ is supported by the kinetic energy gain.\(^21,30,59\). In Fig. 15, the $U_c$ marked by the red dashed line which is close to $U_{\text{Mott}} = 10t$, signifying that the underlying AFM transition in the half-filled PM state dominates the properties of the AFM states by changing into a crossover\(^21,30,31\) between the weak- and strong-coupling regimes. It is worthy mentioning that $U_c$ at half-filling is smaller than $U_{\text{Mott}}$ because of long range AFM correlations.\(^29\).

For the half-filled system, we analytically calculated in Eq. (24) the relation between $M$ and $\Delta_{\text{AFM}}$ in the small $U$ limit, implying that the one from the HF method needs to be improved to include quantum fluctuations. After fitting the AFM gap of the cluster slave-spin data using the formula from the QMC simulation\(^{20}\), and calculating the dependence of $M$ upon $U$ by Eq. (24), we find the result is in a good agreement with the numerical data as shown in Fig. 8.

The $U$-$\delta$ phase diagram was discussed in Sec. III C, from which we extracted four regimes: AFM insulator at $\delta = 0$, AFM metal with $\kappa > 0$ and $\kappa < 0$, and the PM metal. The second-order transition occurs when the system transits from the AFM metal with $\kappa < 0$ to the PM metal phase, whereas the existence of the transition from the AFM metal phase with $\kappa > 0$ to that with $\kappa < 0$ needs to be proven further by taking the inhomogeneous states into account. Moreover, as shown in Figs. 12 and 15, the crossover, separating the weak- and strong-coupling regimes in the AFM state, always locates around $U_{\text{Mott}}$, and whether this property is specifically associated with the geometry of the square lattice is worthy of subsequent investigations.

According to Figs. 2 and 9, the difference between the two- and four-site cluster results is rather quantitative than qualitative. We believe that the four-site cluster approximation is sufficient to capture the physics because its geometry obeys the same lattice symmetry as the original square lattice, which is very important to extract the reasonable solutions of the system. This conclusion can be reached in our ongoing studies on the honeycomb lattice.

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Appendix A: RELATIONSHIP BETWEEN THE HOLON-DOUBLON CORRELATOR AND THE MOTT TRANSITION

The holon-doublon correlator\(^9\) is defined as

$$C_{ij} = \frac{\langle N_i D_j \rangle - \langle N_i \rangle \langle D_j \rangle}{\langle N_i \rangle \langle D_j \rangle}$$

(A1)

where

$$N_i = (1 - c_{i\sigma}^\dagger c_{i\sigma})(1 - c_{i\sigma}^\dagger c_{i\bar{\sigma}}), \quad D_j = c_{j\sigma}^\dagger c_{j\bar{\sigma}}^\dagger c_{j\sigma} c_{j\bar{\sigma}}$$

(A2)

leading to

$$\langle D_i \rangle \approx \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle = n_{i\uparrow} n_{i\downarrow}$$

(A4)

$$N_i D_j \approx n_{j\sigma} n_{i\bar{\sigma}} (\delta + n_{i\sigma} n_{i\bar{\sigma}}) + \sum_\sigma |\langle c^\dagger_{i\sigma} c_{j\bar{\sigma}} \rangle|^2 \left[ \frac{1}{2} \langle |C^\dagger_{i\sigma} c_j \rangle|^2 + n_{j\bar{\sigma}} (1 - n_{i\sigma}) \right]$$

(A5)

Noticing that there is a simple relation between $\langle N_i \rangle$ and $\langle D_i \rangle$:

$$\langle N_i \rangle = \langle (1 - c_{i\sigma}^\dagger c_{i\sigma})(1 - c_{i\sigma}^\dagger c_{i\bar{\sigma}}) \rangle$$

$$= 1 - \sum_\sigma \langle c_{i\sigma}^\dagger c_{i\sigma} \rangle + \langle c_{i\sigma}^\dagger c_{i\bar{\sigma}}^\dagger c_{i\sigma} c_{i\bar{\sigma}} \rangle$$

$$= \delta + \langle D_i \rangle$$

(A6)

the holon-doublon correlator $C_{ij}$ can thus be rewritten as:

$$C_{ij} \approx \frac{\sum_\sigma |\langle c^\dagger_{i\sigma} c_{j\bar{\sigma}} \rangle|^2 \left[ \frac{1}{2} \langle |C^\dagger_{i\sigma} c_j \rangle|^2 + n_{j\bar{\sigma}} (1 - n_{i\sigma}) \right]}{\langle \delta + \langle D_i \rangle \rangle \langle D_j \rangle}$$

(A7)

We find from Eq. (A7) that when $U \sim U_{\text{Mott}}$, the decrease of the double occupancy will enhance $C_{ij}$ dramatically. In the case of $U \gg U_{\text{Mott}}$, the double occupancy decreases at the same rate as the nearest neighbor hopping probability and more mildly than the next nearest one. Thus, the nearest neighbor holon-doublon correlator will saturate eventually and the next nearest one decrease after reaching its maximum.
Appendix B: ELECTRON-MOMENTUM DISTRIBUTION

Within the cluster slave-spin scheme, the electron momentum distribution \( n_d^{(2)}(k) = \langle d^\dagger_{k\sigma} d_{k\sigma} \rangle \) with respect to 2/4-site cluster approximation are as follows. For the former,

\[
n_d^{(2)}(k) \approx \frac{1}{N} \sum_j \langle f^\dagger_{j\sigma} f_{j\sigma} \rangle 
+ \frac{\langle S^+_{j+\delta\sigma} S^-_{j-\delta\sigma} \rangle}{N} \sum_{j,\delta} e^{i k \cdot \delta} \langle f^\dagger_{j+\delta\sigma} f_{j-\delta\sigma} \rangle 
= 1 - \frac{\delta}{2} - \frac{4Z\epsilon}{t} \gamma_k \, , \tag{B1} \]

and for the latter,

\[
n_d^{(4)}(k) \approx \frac{1}{N} \sum_j \langle f^\dagger_{j\sigma} f_{j\sigma} \rangle 
+ \frac{\langle S^+_{j+\delta\sigma} S^-_{j-\delta\sigma} \rangle}{N} \sum_{j,\delta} e^{i k \cdot \delta} \langle f^\dagger_{j+\delta\sigma} f_{j-\delta\sigma} \rangle 
+ \frac{\langle S^+_{j+\eta\sigma} S^-_{j-\eta\sigma} \rangle}{N} \sum_{j,\eta} e^{i k \cdot \eta} \langle f^\dagger_{j+\eta\sigma} f_{j-\eta\sigma} \rangle 
= 1 - \frac{\delta}{2} - \frac{4Z\epsilon}{t} \gamma_k 
+ \frac{4\gamma_k}{N} \sum_{k' \in RBZ} \gamma_{k'} \left\{ Z_{av} \left[ \theta(-E^+_{k'}) + \theta(-E^-_{k'}) \right] 
+ \frac{Z_\Delta}{\sqrt{(4tZ\gamma_{k'})^2 + \Delta^2}} \left[ \theta(-E^+_{k'}) - \theta(-E^-_{k'}) \right] \right\} \, , \tag{B2} \]

where

\[
\gamma_k = \cos k_x \cos k_y \, , \quad E_{k} = -\mu_{eff} + \sqrt{(4tZ\gamma_k)^2 + \Delta^2} \, , 
Z_{av} = \frac{|\langle \hat{z}_{A}\rangle|^2 + |\langle \hat{z}_{B}\rangle|^2}{2} \, , 
Z_\Delta = \frac{|\langle \hat{z}_{A}\rangle|^2 - |\langle \hat{z}_{B}\rangle|^2}{2} \, .
\]

To understand our present results concerning the negative and beyond unity part of this quantity around \( M \) and \( \Gamma \) point, we refer to the previous work on slave-particle formalism, where a “no-go” theorem has been shown to prevent to obtain a complete correct answer for the electron momentum distribution based merely on a simple decoupling procedure for different degrees of freedom. In the work, the electron momentum distribution is expressed as:

\[
n_c(k, \sigma) = \frac{1 - \delta}{2} + \frac{1}{N} \sum_q n_q a(k + q) n_a(q) \, . \tag{B3} \]

The common feature between Eqs. (B1), (B2), and (B3) is that all of them are corrected from an average occupancy \( n_{\sigma} = \frac{1-\delta}{2} \), and it is easy to check that our results ensure the sum-rule of \( N^{-1} \sum_k n_d(k) = \frac{1-\delta}{2} \).

Appendix C: U(1) SLAVE-SPIN FORMALISM IN THE NONINTERACTING LIMIT

In this Appendix, we prove analytically that in the \( U(1) \) slave-spin theory and within the single-site approximation, the condition \( Z = 1 \) at \( U = 0 \) recovers the correct noninteracting spinon dispersion.

Starting from the approximate Hamiltonian of a multiorbital system in the single-site approximation [Eqs. (15) and (16) in Yu and Si’s work]

\[
H_{S}^{MF} = \sum_{\alpha} \epsilon^\alpha \left( \langle \hat{z}^\dagger_{\alpha} \hat{z}_{\alpha} \rangle + \frac{\Delta}{2} \right) + H_{\text{int}}^S \, , \tag{C2} \]

where

\[
\tilde{z}^\dagger_{\alpha} = \langle P^+_{\alpha} \rangle a^\dagger_{\alpha} b_{\alpha} \langle P^-_{\alpha} \rangle \, , \quad \langle P^+_{\alpha} \rangle = \frac{1}{\sqrt{1/2 + (n^\alpha_{\up} - \frac{1}{2})}} \, , 
\epsilon^\alpha = \sum_{ij} \epsilon_{ij} \langle J_{ij \alpha \sigma} f_{j\sigma} \rangle \, , \quad \epsilon_{ij} = \frac{1}{N} \sum_{ij} \epsilon_{ij} e^{i k \cdot (r_i - r_j)} \, , 
\tilde{\mu}_{\alpha} = 2\tau_{\alpha} \eta_{\alpha} \, , \quad \eta_{\alpha} = \frac{2n^\alpha_{\up} - 1}{4n^\alpha_{\down} (1 - n^\alpha_{\up})} \, , 
\tau_{\alpha} = \sum_{\beta} (\epsilon^\beta \langle \hat{z}^\dagger_{\beta} \rangle \langle \hat{z}_{\beta} \rangle + \text{c.c.}) \, . \tag{C3} \]

Eq. (C2) can be rewritten as

\[
H_{S}^{MF} = \sum_{\alpha} [k_{\alpha} \tilde{z}_{\alpha} + k_{\alpha}^* \tilde{z}^*_{\alpha} + \frac{\lambda}{2} \langle \hat{n}^a_{\alpha} - \hat{n}^b_{\alpha} \rangle] 
+ H_{\text{int}}^S \, , \tag{C4} \]

where \( k_{\alpha} = \sum_{\beta} e^{i \beta_{\alpha} \langle \hat{z}^\dagger_{\beta} \rangle} \). In the noninteracting limit, because of the decoupling of the orbits, we can keep only one degree of freedom in Eq. (C4). After dropping the crystal-field splitting \( \Delta \), and the interaction term, the above Hamiltonians become

\[
H_{S}^{MF} = \sum_{k} \langle \epsilon_k \langle \hat{z}^\dagger \rangle \langle \hat{z} \rangle \rangle + \langle \hat{z}^\dagger \hat{z} \rangle + \frac{\lambda}{2} \langle \hat{n}^a - \hat{n}^b \rangle \, , \tag{C5} \]

where \( \tau = 2\epsilon \langle \hat{z}^\dagger \rangle \langle \hat{z} \rangle \) and \( \tilde{\mu} = 4\epsilon \langle \hat{z}^\dagger \rangle \langle \hat{z} \rangle \).

Under the hard-core boson constraint: \( a^\dagger a + b^\dagger b = 1 \), the restricted Hilbert space is spanned by \( \{|a = 1, b = 0, \alpha = 0, b = 1 \} \), in which the slave-spin Hamiltonian (C6) has the form

\[
H_{S}^{MF} = \epsilon \langle \langle \hat{z}^\dagger \rangle \langle \hat{z} \rangle \rangle + \frac{\lambda}{2} \langle \hat{n}^a - \hat{n}^b \rangle = \left( \frac{\lambda}{2} \right) \epsilon \langle \hat{R} \rangle \langle \hat{z} \rangle \, . \tag{C7} \]
with $R = \langle P^+_a \rangle \langle P^-_a \rangle$, which has the ground state and energy as

$$|\Psi_\lambda\rangle = \left(\frac{-\epsilon R(\lambda)}{N}, \frac{\lambda R_0}{N}\right),$$  \hspace{1cm} (C8)

$$E_\lambda = -\sqrt{\frac{\lambda^2}{2} + \epsilon^2 R^4} |\langle \hat{z} \rangle|^2,$$  \hspace{1cm} (C9)

where $R_0 = \sqrt{\frac{\lambda^2}{2} + \epsilon^2 R^2}$, $N = \sqrt{2R_0(\frac{\lambda}{2} + R_0)}$.

Accordingly, the expectation value of $\hat{n}_a - \hat{n}_b$ and $\hat{z}$ can be calculated as

$$\langle \hat{n}_a - \hat{n}_b \rangle = -\frac{\lambda}{2R_0}, \hspace{1cm} \langle \hat{z} \rangle = -\frac{\epsilon R^2 |\langle \hat{z} \rangle|}{2R_0}.$$  \hspace{1cm} (C10)

Because of the constraints $n_a - n_b = 2n_f - 1$ and $|\langle \hat{z} \rangle|^2 = 1$ in the noninteracting case, we have

$$|\langle \hat{z} \rangle|^2 = \frac{\epsilon^2 R^4}{4R_0^4} = 1$$  \hspace{1cm} (C11)

with $R = \frac{1}{\sqrt{n_f(1-n_f)}}$. Then, we finally arrive at

$$\lambda = -2R_0(2n_f - 1) = -\epsilon \frac{2n_f - 1}{n_f(1-n_f)},$$  \hspace{1cm} (C12)

$$\mu = 4\epsilon \eta = \frac{4\epsilon(2n_f - 1)}{4n_f(1-n_f)} = \epsilon \frac{(2n_f - 1)}{n_f(1-n_f)},$$  \hspace{1cm} (C13)

where $\epsilon$ is negative. Thus, $\lambda = \mu$ in the noninteracting case ($Z=1$) for the single orbital system, and it is straightforward to generalize the conclusion to the multiorbital systems.

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