

Mean-field approach to antiferromagnetic domains in the doped Hubbard model

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We present a restricted path integral approach to the two-dimensional and three-dimensional repulsive Hubbard model. In this approach the partition function is approximated by restricting the summation over all states to a (small) subclass that is chosen so as to well represent the important states. This procedure generalizes mean-field theory and can be systematically improved by including more states or fluctuations. We analyze in detail the simplest of these approximations, which corresponds to summing over states with local antiferromagnetic (AF) order. If in the states considered the AF order changes sufficiently little in space and time, the path integral becomes a finite-dimensional integral for which the saddle point evaluation is exact. This leads to generalized mean-field equations allowing for the possibility of more than one relevant saddle point. In a big parameter regime (both in temperature and filling), we find that this integral has *two* relevant saddle points, one corresponding to finite AF order and the other without. These degenerate saddle points describe a phase of AF ordered fermions coexisting with free, metallic fermions. We argue that this mixed phase is a simple mean-field description of a variety of possible inhomogeneous states, appropriate on length scales where these states appear homogeneous. We sketch systematic refinements of this approximation, which can give more detailed descriptions of the system. [S0163-1829(97)01815-8]

I. INTRODUCTION

The two-dimensional (2D) one-band Hubbard model¹ has received much attention as a simple prototype model for high-temperature superconductors (HTSC).² It provides a good description of the insulating antiferromagnets, which, upon doping, become HTSC. Of central interest is the transition from the insulating antiferromagnetic (AF) state to the metal state at high doping. Experiments on HTSC show that AF correlations are also important away from half filling, but despite much effort a satisfactory theoretical understanding of HTSC based on the Hubbard model has not been achieved (for a recent review see Ref. 3).

Hartree-Fock (HF) theory is the basis of most successful theories in solid-state physics: “. . . *modern many-body theory has mostly just served to show us how, where, and when to use HF theory and how flexible and useful a technique it can be.*”⁴ One should thus expect that it is useful also for correlated electron systems. Indeed, HF theory seems to be a good starting point for describing the half-filled Hubbard model. For strong coupling, it predicts a ground state with AF long-range order (Néel state).⁵ This state is invariant by translations by two sites and thus allows a simple analytic treatment using Fourier transformation. Away from half filling, HF theory of the Hubbard model becomes very complicated. The reason for this is an apparent rigidity of the AF ordered electron system, which does not allow homogeneous doping. A variety of inhomogeneous HF ground states have been found, including magnetic domain walls,⁶ magnetic polarons, magnetic vortices,⁷ spiral states,⁸ and phase separation.⁹ Systematic investigations of these states have been done by numeric methods and were restricted to small dopings and finite lattices.¹⁰ In these calculations the HF equations for general space-dependent HF fields are analyzed. Denoting (imaginary) time as τ and lattice points as \mathbf{x} , these HF fields are

$$\phi_0(x) = r(x), \quad \boldsymbol{\phi}(x) = s(x) \mathbf{e}(x) e^{i\mathbf{Q} \cdot \mathbf{x}} \quad (1)$$

[we write $x = (\tau, \mathbf{x})$, and our lattice points are $\mathbf{x} = (x_1, \dots, x_d)$ with x_i integers], where s is the magnitude of the *local* AF order parameter, \mathbf{e} its direction, and r is a charge degree of freedom; $\mathbf{Q} = (\pi, \dots, \pi)$ is the AF vector as usual. In the doped region, one finds a large number of solutions of the HF equations that correspond to metastable spin and charge configurations.¹⁰

Such numeric calculations are important to learn what the essential features of the Hubbard model are. Ultimately, however, it would be desirable to develop analytic methods taking into account these essential features and allowing simple computations. In this paper we propose such a method, which corresponds to an averaging over highly degenerate HF solutions. This leads to a simple homogeneous mean-field description of AF in the doped Hubbard model, which makes manifest the physical expectation that, at large enough length scales, the system should appear homogeneous even if the HF solutions are not. The results of this paper are restricted to the simplest nontrivial ansatz for states describing AF order. We find that already this approximation allows one to systematically determine the parameter regime where no homogeneous AF solutions of the HF equations are possible, and it leads to a simple understanding of this phenomenon. Our approach can be interpreted as an approximation of the exact partition function by restricting the sum over the (huge) set of all states to a (small) subset that one chooses to represent the “most important states.” This approach is very general and can be systematically refined by increasing the subset of states taken into account. Thus one can obtain increasingly complicated approximations, which will give increasingly refined information about the dominating states of the system. Moreover, fluctuations can be naturally taken into account in this approach (this will be only outlined in this paper).

It is often believed that mean-field theory (based on HF equations) is not appropriate for correlated fermions systems. We propose that it is only mean-field theory *in its usual formulation* that fails. Our approach leads to a generalized mean-field theory that we believe is a reasonable starting point for a good theory of these systems also. Fluctuations are important, of course (especially in two dimensions), but are corrections to generalized mean-field theory, as discussed.

We now describe our method in more detail. We recall that the HF fields $\phi(x) = (\phi_0(x), \boldsymbol{\phi}(x))$ in Eq. (1) naturally appear if one writes the exact partition function of the Hubbard model as a boson path integral using a Hubbard-Stratonovitch transformation, $Z = \int \mathcal{D}\phi \exp[-\mathcal{F}(\phi)]$.¹¹ The boson action $\mathcal{F}(\phi)$ here has a simple physical interpretation: it is the free energy of noninteracting fermions in the *external* boson fields $\phi(x)$. HF theory amounts to a saddle point evaluation of this path integral.¹² Since $\mathcal{F}(\phi)$ is a complicated functional of ϕ , a search of the relevant saddle points among all possible spacetime-dependent boson field configurations $\phi(x)$ is not feasible. Thus usually a certain ansatz for $\phi(x)$ is made. We will refer to this procedure as *mean-field theory*: the search for saddle points of $\mathcal{F}(\phi)$ restricted to a (small) subset of boson configurations. Obviously one can expect this to give a good description of the system only if this subset is chosen so as to contain boson configurations that are sufficiently similar to the saddle points that actually dominate the exact path integral. We now propose the following: instead of analyzing the saddle point equations by restricting to some subset of boson fields, *approximate the HS path integral by summing over all boson configurations in this subset*. Parametrizing this subset by finitely many real parameters, we thus approximate Z by a finite-dimensional integral. In many interesting cases one finds that a saddle point evaluation of this integral is exact, and we recover standard mean-field theory *in case there is only one relevant saddle point*. In general, we obtain a generalized mean-field theory allowing for degenerate saddle points to contribute to the partition function. To be more specific, for the Hubbard model the simplest ansatz for boson fields Eq. (1) describing AF order is

$$\phi_0(x) = r, \quad \boldsymbol{\phi}(x) = s \mathbf{e} e^{i\mathbf{Q} \cdot \mathbf{x}}. \quad (2)$$

Equation (2) describes a Néel state, i.e., AF long-range order. This ansatz gives a reasonable description of the Hubbard model at half filling, thus it is natural to also attempt it in the doped regime. One can sum over all configurations of the form Eq. (2) and thus approximate Z by an integral over r , s , and \mathbf{e} . Since \mathcal{F} in this case is proportional to the spacetime volume, $\mathcal{F} = \beta L^d f_0(r, s)$ [L^d is the number of lattice sites, f_0 a function given in Eq. (19) below], and independent of \mathbf{e} , and the free energy per lattice site is $\Omega = -\ln(Z)/\beta L^d$, we obtain

$$e^{-\beta L^d \Omega} = \int_0^\infty ds \int_{-\infty}^\infty dr e^{-\beta L^d f_0(r, s)} \quad (3)$$

(the \mathbf{e} integration gives an irrelevant constant factor, which we drop). In the thermodynamic limit $L \rightarrow \infty$, the saddle point evaluation of this integral is exact.

We now discuss in more depth the nature of this approximation, which is necessary to correctly interpret our results described below (this paragraph is not essential for understanding these results, however). It is important to note that our Eq. (3) is not only obtained by summing over the Néel states Eq. (2), but in fact also by summing over a much larger class of configurations Eq. (1) where $r(x)$, $s(x)$, and $\mathbf{e}(x)$ are “slowly” varying functions with “fast” changes occurring only in a small fraction of the total spacetime volume: there are such configurations *without long-range order* but still so that they *locally* resemble a Néel configuration Eq. (2) so much that adding their contribution to the partition functions essentially leaves the result unchanged. These configurations describe states with *local* AF order (i.e., they have a finite correlation length). For these configurations, the boson action can be computed as $\mathcal{F} = \mathcal{F}_0 + \mathcal{F}_1$ with

$$\mathcal{F}_0(\phi) = \sum_x f_0(r(x), s(x)), \quad (4)$$

and \mathcal{F}_1 a correction involving gradient terms that are negligibly small if $r(x)$, $s(x)$, and $\mathbf{e}(x)$ change sufficiently little. This formula has a simple physical interpretation: for states with local AF order, each spacetime point x contributes a term $f_0(r(x), s(x))$ to the fermion free energy. This term depends only on the local s and r values (the local direction of the AF order is irrelevant), and thus is the same one would have in a Néel state, provided $r(x)$, $s(x)$, and $\mathbf{e}(x)$ have sufficiently little variation. This argument immediately shows that Eq. (3) is also obtained if we sum over all boson configurations Eq. (1) with $s(x) = s$ and $r(x) = r$ constant but $\mathbf{e}(x)$ varying not much as a function of x . More generally, we will show that also $s(x)$ and $r(x)$ are allowed to vary, provided the average correlation volume where $s(x)$ and $r(x)$ are constant is sufficiently large: if we sum over such configurations, we also obtain Eq. (3) but with βL^d replaced by this correlation volume. To avoid misunderstanding, we stress that this does not mean that the effect of fluctuations, domain walls, etc. is not important: this argument only shows that a nontrivial solution of HF equations (i.e., with $s \neq 0$) resulting from Eq. (3) should not be interpreted as Néel order but as the existence of *local* AF correlations. To decide whether there is long-range order or not one has to go beyond this simple approximation. For example, one can improve Eq. (3) by making a more general ansatz for the boson configurations $\phi(x)$ to be summed over (describing, e.g., domain walls, etc.), or one can include the effect of fluctuations. Only this will give more detailed information about the structure of the state.

A main result of this paper is that, in a big parameter regime, the integral in Eq. (3) has two relevant saddle points: one with $s = s^* > 0$ corresponding to (local) AF order, and another with $s = 0$ corresponding to no AF order. This means that no HF solution of the form Eq. (2) exists and, as discussed below, unusual physical behavior is to be expected. Physically this can be interpreted as follows: the homogeneous AF ordered electron system can only exist at half fillings, and the only way to achieve doping is to have the chemical potential such that the AF saddle point is degenerate with a trivial one, which serves as a particle reservoir. The analysis of the integral (3) provides a simple and sys-

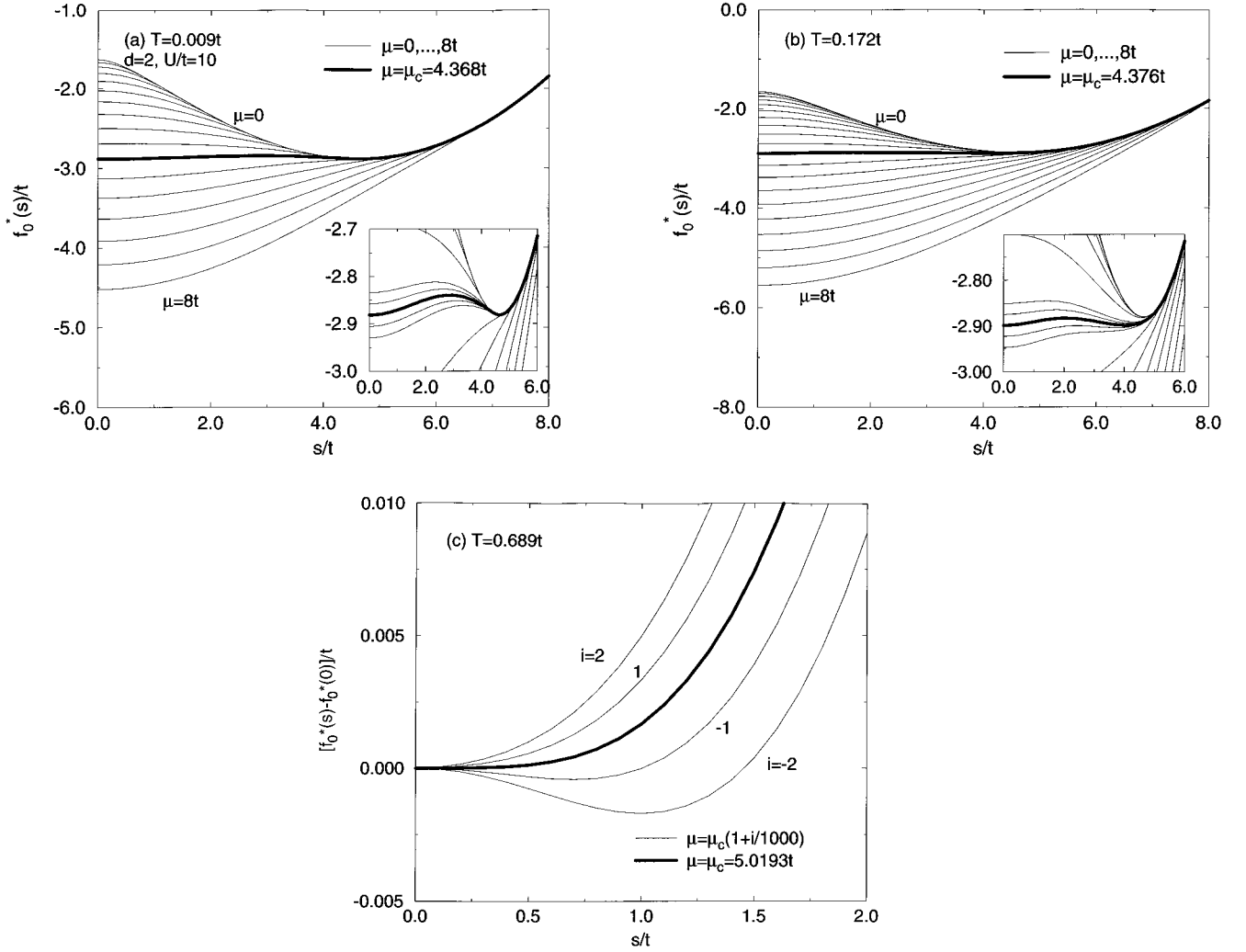


FIG. 1. Dependence of effective action f^* in Eq. (27) on the magnitude of the antiferromagnetic order s for a sequence of different values of the chemical potential and different temperatures T (Ref. 15). Parameters here are $U/t=10$ and $d=2$. (a) Temperature close to zero ($T=0.009t$). Note that there are sometimes two minima, and these become degenerate at a critical value of the chemical potential, $\mu = \mu_c$ (bold curve). Inset: Closeup with additional curves for $\mu = \mu_c(1+i/100)$, $i=0, \pm 1, \pm 2$. (b) Higher temperature but still below T^* . Otherwise the same as in (a). Note that the nontrivial minimum now becomes slightly μ dependent close to $\mu = \mu_c$. (c) Temperature above T^* . Note that there are no longer two minima possible at the same μ . We zoomed in close to $\mu = \mu_c$ where the nontrivial minimum merges with the trivial one and disappears.

tematic way to determine the parameter regime where this happens. The resulting phase diagrams for the Hubbard model and different parameter values are shown in Fig. 2. There are always three different regimes: an AF regime where the nontrivial saddle points $s=s^*>0$ dominates, a free regime with the only relevant saddle point $s=0$, and the mixed regime discussed above. The doping x_1 separating the AF regime from the mixed one increases with temperature as it approaches the doping x_2 separating the mixed and the free regime. At a characteristic temperature T^* , x_1 merges with x_2 and the mixed regime disappears. Note that since $x_2>0$, the free regime describes metallic fermions, i.e., there is a Fermi surface with a finite density of states (DOS). For low temperatures, $x_1 \approx 0$; i.e., the AF regime is insulating (no DOS at the Fermi surface).

It is known that, in various limits, holes in the t - J and Hubbard models accumulate in hole-rich regions separated from pure AF regions, and it has been conjectured that this

tendency to phase separation is a general feature of holes in an antiferromagnet.^{9,13} Our method can be regarded as a simple systematic way to check this conjecture, without any restriction of parameters: the occurrence of two degenerate saddle points shows that there is a frustration not allowing a homogeneous distribution of holes. However, since in Eq. (3) the effect of phase boundaries is not included, no information about the actual distribution of the holes is obtained that way. Previously it has been suggested that the size of pure-phase regions is limited only by long-range Coulomb forces.¹³ However, numeric results^{7,3} show that this happens also without long-range forces. Within our formalism, a more detailed understanding of the distribution of the two different phases can be obtained by summing over a larger class of boson configurations, e.g., configurations describing domain walls of variable size.

We finally note that our approach not only provides phase diagrams but also gives approximations for all observables in

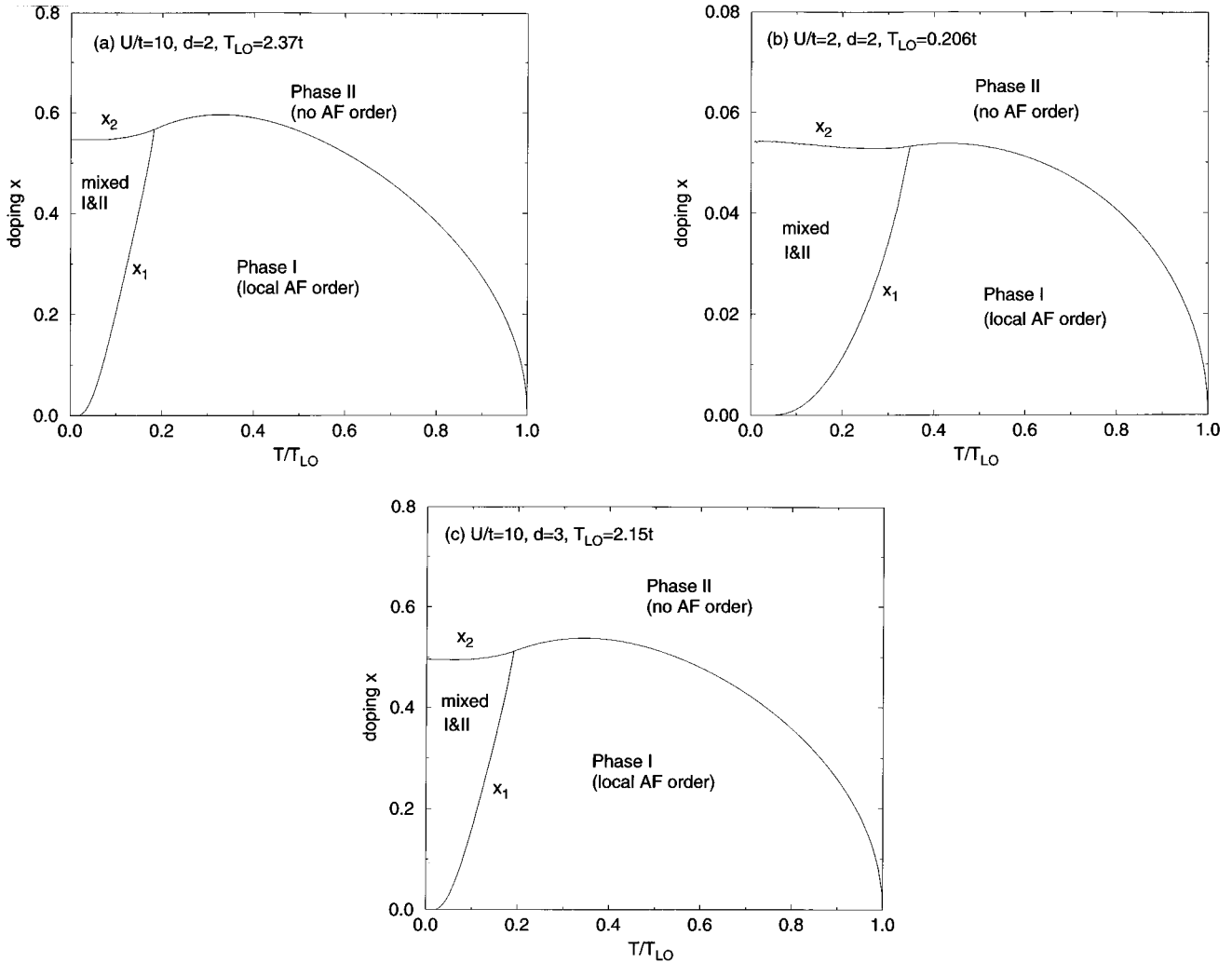


FIG. 2. Phase diagram for the 2D Hubbard model and different parameters. (a) $U/t=10$ and $d=2$, (b) $U/t=2$ and $d=2$, (c) $U/t=10$ and $d=3$. Note that the phase diagram is qualitatively the same in all three cases. At fixed low temperature T there is a homogeneous phase I with local AF order for doping less than x_1 , and a homogeneous metallic phase II without AF correlations for doping larger than x_2 . In the regime between x_1 and x_2 these two phases coexist. $x_1=0$ for low temperatures, and it increases with T until a characteristic temperature T^* , where it merges with x_2 and the mixed phase disappears. For higher T there is a smooth transition from phase I to phase II. T_{LO} is the highest temperature at which *local* AF order exists.

the system: An exact formula for all Green functions G of the Hubbard model is given by the path integral $G = \int \mathcal{D}\phi \exp[-\mathcal{F}(\phi)] G_0(\phi) / Z$, where $G_0(\phi)$ is the corresponding Green function of *noninteracting* fermions in the external boson field ϕ . Thus by our restricted path integral method we obtain approximations of G by finite-dimensional integrals. In the case where this integral is dominated only by one saddle point, we obtain $G = G_0(\phi_{\text{saddle}})$, i.e., Green functions of noninteracting fermions. This is a simple description of a Fermi liquid. For the mixed phase discussed above we get

$$G = (1-w)G_0(\phi_{\text{AF}}) + wG_0(\phi_{\text{triv}}), \quad (5)$$

with a weight factor w changing smoothly from $w=0$ at doping $x=x_1$ to $w=1$ at $x=x_2$. Here $G_0(\phi_{\text{AF}})$ [ϕ_{AF} the Néel state Eq. (2) with $s=s^*$] describes AF ordered fermions that are ‘‘heavy,’’ and $G_0(\phi_{\text{triv}})$ [ϕ_{triv} the configuration Eq. (2) with $s=0$] describes free, metallic fermions. Thus

Eq. (5) gives a simple description of a system where two different kinds of fermions coexist. This system does not resemble a conventional Fermi liquid. We stress, however, that Eq. (5) only gives a good quantitative description when the effect of phase boundaries can be neglected, and it only is appropriate on length scales where the two phases appear homogeneously mixed. Thus this description applies in the case of phase separation.¹³ If there is a doping regime of HTSC where this description is adequate, the physical properties there should be of two different coexisting kinds of fermions. There is some experimental evidence for this, as discussed in Ref. 13.

The plan of this paper is as follows. In the next section we describe our path integral formalism, stressing a few important technical details. In Sec. III our approximation Eq. (3) to the partition function is derived, and we outline how to obtain refinements to this approximation. In Sec. IV we analyze Eq. (3) and calculate the resulting phase diagram of the 2D and 3D Hubbard model for a few representative parameter

values. Section V contains an outline of how to include fluctuations. We end with conclusions in Sec. VI. Some technical details are deferred to the two Appendices.

II. PATH INTEGRAL FORMALISM

In this section we review the path integral formalism for the Hubbard model,^{12,14} concentrating on some important technical details in which we deviate from standard approaches.

Configuration space is labeled by $x=(\tau, \mathbf{x})$, where $0 \leq \tau \leq \beta$ is the usual imaginary time and \mathbf{x} are vectors in space Λ_L . Our space Λ_L is a subset of the d -dimensional cubic lattice \mathbf{Z}^d (i.e., we set the lattice constant equal to 1). In intermediate steps of our derivation we will implicitly assume that Λ_L is a finite cube [i.e., $\mathbf{x}=(x_1, \dots, x_d)$ with $-L/2 \leq x_i < L/2$, L an integer multiple of 4 and $< \infty$) with a finite number L^d of points, but we will eventually take the thermodynamic limit $L \rightarrow \infty$. We are mainly interested in $d=2$ and 3.

To define the Hubbard model in this setting, we introduce fields at every point $x=(\tau, \mathbf{x})$, which are Grassmann variables $\bar{\psi}_\sigma(x), \psi_\sigma(x)$ carrying a spin index $\sigma = \uparrow, \downarrow$. The action is $S = S_2 + S_4$, with the quadratic part $S_2 = -(\bar{\psi}, G_0^{-1} \psi)$; we use a matrix notation, i.e., $(f, g) = \sum_{x, \alpha} f_\alpha(x) g_\alpha(x)$, $\Sigma_x \equiv \int_0^\beta d\tau \Sigma_{\mathbf{x} \in \mathbf{Z}^d}$, and $G_0^{-1}(x-y)$ is the inverse of the free electron propagator with the Fourier transform

$$(G_0)^{-1}(k) = [i\omega_n + \mu - \epsilon(\mathbf{k})] \sigma_0, \quad (6)$$

where

$$\epsilon(\mathbf{k}) = -2t \sum_{i=1}^d \cos(k_i) \quad (7)$$

is the Hubbard band relation and σ_0 the 2×2 (spin) unit matrix. Here $\omega_n = (2n+1)\pi/\beta$ (with n an integer) are the usual electron Matsubara frequencies, $\mathbf{k}=(k_1, \dots, k_d)$, $-\pi \leq k_i \leq \pi$, are the pseudomomenta, and μ is the chemical potential. The Hubbard interaction term is $S_4 = U \Sigma_x \bar{\psi}_\uparrow(x) \psi_\uparrow(x) \bar{\psi}_\downarrow(x) \psi_\downarrow(x)$. With that we can write the partition function of the Hubbard model as $Z = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-S}$, where $\int \mathcal{D}\bar{\psi} \mathcal{D}\psi = \prod_{x, \sigma} \int d\bar{\psi}_\sigma d\psi_\sigma$ are the usual Grassmann integrals.¹⁴

We now come to an important technical point. We recall that there are many equivalent ways of writing the Hubbard interaction S_4 . This ambiguity corresponds to an ambiguity in how to introduce Hubbard-Stratonovitch (HS) fields, and it turns out that the saddle point equations one finally obtains depend on the choice of HS fields.¹² To obtain an appropriate form for the partition function, we use U(1) (gauge) and SU(2) (spin rotation) invariance of the Hubbard model. We note that these symmetries are manifest for the term S_2 , but S_4 as written above is not explicitly SU(2) invariant. To find a manifestly symmetric form for the partition function¹¹ we introduce

$$n = \sum_{\sigma} \bar{\psi}_\sigma \psi_\sigma, \quad \mathbf{s} = \sum_{\sigma, \sigma'} \bar{\psi}_\sigma(\boldsymbol{\sigma})_{\sigma\sigma'} \psi_{\sigma'}, \quad (8)$$

which are the density and spin of the electrons; $\boldsymbol{\sigma}=(\sigma_1, \sigma_2, \sigma_3)$ are the Pauli spin matrices as usual. Manifestly invariant forms for the interaction would be $S_4 = U \Sigma_x n(x)^2/2 = -\Sigma_x \mathbf{s}(x)^2/6$, but both of them do not make manifest the Pauli principle: they contain terms $n_\sigma(x)^2 = [\bar{\psi}_\sigma(x) \psi_\sigma(x)]^2$ that are zero only by the Grassmann nature of the fermion fields. It is well known that the latter is not preserved in mean-field theory. In our framework this corresponds to $n_\sigma(x)^2$ contributing nonzero terms to saddle point equations. This is why both aforementioned choices for the interaction lead to different saddle point equations, both different from the Hartree-Fock equations, and are not appropriate. We thus must make sure to have no such terms present. Writing $S_4 = U \Sigma_x [n(x)^2 - s_3(x)^2]/4$ as above does make the Pauli principle manifest [i.e., contains no terms $n_\sigma(x)^2$], but so does

$$S_4 = U \sum_x \frac{n(x)^2 - [\mathbf{e}(x) \cdot \mathbf{s}(x)]^2}{4} \quad (9)$$

with arbitrary unit vectors $\mathbf{e}(x) [\mathbf{e}=(e_1, e_2, e_3)]$. In these expressions, SU(2) invariance is not manifest. However, we can average over the directions $\mathbf{e}(x)$ thus make SU(2) invariance and the Pauli principle manifest at the same time. Our HS transformation therefore is

$$\begin{aligned} & \exp \left[-\frac{U}{4} [n^2 - (\mathbf{e} \cdot \mathbf{s})^2] \right] \\ &= \frac{1}{4\pi^2 U} \int_{\mathbb{R}} d\phi_0 \int_{\mathbb{R}} d\phi_s \int_{4\pi} d^2\mathbf{e} \\ & \quad \times \exp \left(-\frac{\phi_0^2 + \phi_s^2}{U} + i\phi_0 n + \phi_s \mathbf{e} \cdot \mathbf{s} \right). \end{aligned}$$

(Note that the left-hand side here is independent of \mathbf{e} .) We thus have, for each spacetime point x , four HS fields ϕ_0 and $\boldsymbol{\phi} = \phi_s \mathbf{e} = (\phi_1, \phi_2, \phi_3)$ corresponding to density (charge) n and spin \mathbf{s} . Since S_4 is invariant under $\mathbf{e}(x) \rightarrow -\mathbf{e}(x)$ we use $\int_{\mathbb{R}} d\phi_s \int_{4\pi} d^2\mathbf{e} = 2 \int_{\mathbb{R}^3} d^3\boldsymbol{\phi} / \boldsymbol{\phi}^2$ and write the interactions as

$$e^{-S_4} = \int \mathcal{D}\boldsymbol{\phi} e^{-(1/U)(\boldsymbol{\phi}, \boldsymbol{\phi}) - (\bar{\psi}, \boldsymbol{\phi} \psi)},$$

where (up to an irrelevant constant factor which we drop)

$$\int \mathcal{D}\boldsymbol{\phi} = \prod_x \int_{\mathbb{R}} d\phi_0(x) \int_{\mathbb{R}^3} \frac{d^3\boldsymbol{\phi}(x)}{\boldsymbol{\phi}(x)^2}. \quad (10)$$

Here and in the following we use a convenient matrix notation $(\boldsymbol{\phi}, \boldsymbol{\phi}) = \sum_{x, \alpha} \phi_\alpha(x)^2$ ($\alpha=0, 1, 2, 3$), and

$$\boldsymbol{\phi}(x) = i\sigma_0 \phi_0(x) + \boldsymbol{\sigma} \cdot \boldsymbol{\phi}(x). \quad (11)$$

With that the electron can be integrated out and the partition function becomes a path integral over the HS fields,

$$Z = \int \mathcal{D}\boldsymbol{\phi} e^{-\mathcal{F}(\boldsymbol{\phi})}. \quad (12)$$

The HS action is equal to

$$\mathcal{F}(\phi) = \frac{1}{U}(\phi, \phi) - \text{Tr} \ln(G_0^{-1} - \underline{\phi}). \quad (13)$$

The trace Tr formally is defined for operators $A = [A_{\sigma\sigma'}(x, y)]$ (acting on electron one-particle states) as $\text{Tr} A \equiv \sum_{x, \sigma} A_{\sigma\sigma}(x, x)$.

We note that all details of the form of this path integral are essential for the approximations introduced in the next section to work. For example, the presence of the variable $\mathbf{e}(x)$ allows to describe, in a natural way, the effect of changes in the direction of the AF order parameter.

The free energy density (or rather thermodynamic potential) is defined as

$$\Omega(\beta, \mu) = - \lim_{L \rightarrow \infty} \frac{1}{L^d \beta} \ln(Z), \quad (14)$$

and the electron density fixes the chemical potential via the equation

$$x = - \frac{\partial \Omega}{\partial \mu}. \quad (15)$$

We find it convenient to make particle-hole symmetry manifest in our formalism, and not use the electron density n (average particle number per site) but the doping parameter $x = n - 1$. Thus $-1 \leq x \leq 1$, and $x = 0$ corresponds to half filling. Then interchanging particles and holes simply amounts to changing $\mu \rightarrow -\mu$, $x \rightarrow -x$. Technically this is achieved by defining

$$\frac{1}{\beta} \sum_{\omega_n}^{(\text{reg})} \frac{1}{i\omega_n - E} = - \frac{1}{2} \tanh\left(\frac{\beta E}{2}\right) \equiv f_\beta(E). \quad (16)$$

Here ‘‘reg’’ indicates that this sum is only conditionally convergent and thus a certain summation prescription is used — this is what is defined by this formula. This definition amounts to choosing a particle-hole symmetric summation prescription for the conditionally converging Matsubara sum defining the Fermi distribution function $f_\beta(E)$ [i.e., the standard Fermi distribution function $(e^{\beta E} + 1)^{-1}$ is shifted by a constant so that it becomes odd under exchange $E \rightarrow -E$]. We stress that this choice is just a matter of convenience: of course, one could use the standard Fermi distribution function throughout at the cost of having more complicated formulas for the particle-hole transformation. We will also need the following Matsubara sum

$$\frac{1}{\beta} \sum_{\omega_n}^{(\text{reg})} \ln(i\omega_n - E) = \frac{1}{\beta} \ln 2 \cosh\left(\frac{\beta E}{2}\right) \equiv \text{Ln}_\beta(E) \quad (17)$$

formally obtained by integrating Eq. (16) [here the regularization ‘‘reg’’ also requires to drop an infinite but E -independent term; in the standard conventions the right-hand side here would be $\ln(1 + e^{-\beta E})/\beta$].

We finally give an exact formula for the two-point Green function $G = [G_{\sigma\sigma'}(x, y)]$ of the Hubbard model,

$$G = \frac{1}{Z} \int \mathcal{D}\phi e^{-\mathcal{F}(\phi)} G_0(\phi), \quad (18a)$$

where

$$G_0(\phi) = [G_0^{-1} - \underline{\phi}]^{-1} \quad (18b)$$

is the Green function of noninteracting fermions in an external field ϕ . (This formula is easily obtained from standard expressions for fermion Green functions in the path integral formalism.¹⁴) Similar formulas holds for all other Green functions.

III. RESTRICTED PATH INTEGRAL METHOD

In this section we present the restricted path integral method and derive our generalized mean-field equation (3). We first sum over the Néel states since this immediately leads to Eq. (3). To clarify the meaning of this equation, we then show that it is also obtained if one sums certain classes of states with local AF order but no long-range correlations. We finally outline how to systematically refine our approximation.

A. Summing over Néel states

For a boson configuration Eq. (2) describing AF long-range order, the HS action (13) can be evaluated exactly using Fourier transformation. We obtain $\mathcal{F} = \beta L^d f_0$ (i.e., the action is proportional to the spacetime volume). In the thermodynamic limit,

$$f_0(r, s) = \frac{r^2 + s^2}{U} - \int \mathcal{d}\mathbf{k} [\text{Ln}_\beta(E_+) + \text{Ln}_\beta(E_-)] \quad (19)$$

with the function $\text{Ln}_\beta(E)$ defined in Eq. (17), and

$$\int \mathcal{d}\mathbf{k} \equiv \int_{-\pi \leq k_i \leq \pi} \frac{d^d k}{(2\pi)^d} \quad (20)$$

means integration over the Brillouin zone. Moreover,

$$E_\pm = ir - \mu \pm \sqrt{\epsilon(\mathbf{k})^2 + s^2} \quad (21)$$

are the AF bands as usual. Note that f_0 does not depend on the direction \mathbf{e} of the AF order, as expected. A formal derivation of this result from Eq. (13) can be found in Appendix A. It has a simple physical interpretation: $-\int \mathcal{d}\mathbf{k} \text{Ln}_\beta(E_\pm)$ is the free energy density of non-interacting fermions with dispersion relations $E_\pm(\mathbf{k})$.

From this we get the doping of the fermions in the Néel background (2) as $x(r, s) = -\partial f_0(r, s)/\partial \mu$, i.e.,

$$x(r, s) = \int \mathcal{d}\mathbf{k} [f_\beta(E_+) + f_\beta(E_-)], \quad (22)$$

where with $f_\beta(E)$ Eq. (16) is our fermion distribution function.

We now approximate the path integral (12) by summing only over the Néel states Eq. (2). Since the integrand then depends only on r and s , the path integration $\int \mathcal{D}\phi$ Eq. (10) reduces to $\int_0^\infty ds \int_{-\infty}^\infty dr$ (up to an irrelevant constant; we introduced spherical coordinates, $\int_{\mathbb{R}^3} d^3 \boldsymbol{\phi} / \boldsymbol{\phi}^2 = \int_0^\infty ds \int_{4\pi} d^2 \mathbf{e}$). Thus we obtain

$$Z = \int_{-\infty}^\infty dr \int_0^\infty ds e^{-V f_0(r, s)}, \quad (23)$$

where $V = \beta L^d$. Using the definition $Z = \exp(-V\Omega)$ we get Eq. (3). With that, the particle number constraint (15) becomes

$$x = \frac{1}{Z} \int_{-\infty}^{\infty} dr \int_0^{\infty} ds e^{-Vf_0(r,s)} x(r,s) \quad (24)$$

with $x(r,s)$ defined in Eq. (22). We are interested in the thermodynamic limit $V \rightarrow \infty$, thus the saddle point evaluation of the integrals in Eqs. (23) and (24) is exact. When there is only one relevant saddle point, we recover Hartree-Fock theory restricted to the Néel states.

B. Summing over states with local AF order

We now show that Eq. (23) is also obtained if sum over configurations with only local AF order, i.e., configurations of the form (1) where $r(x)$, $s(x)$, and $\mathbf{e}(x)$ do not vary much in spacetime. In the following we restrict ourselves to configurations ϕ such that $\mathcal{F}(\phi) = \mathcal{F}_0(\phi) + \mathcal{F}_1(\phi)$ with \mathcal{F}_0 Eq. (4) and \mathcal{F}_1 negligible, i.e., $\lim_{L \rightarrow \infty} \mathcal{F}_1 / \beta L^d = 0$; in this case we write $\mathcal{F} \approx \mathcal{F}_0$. We do not attempt to further specify what these configurations are. The only point important for us is that there are such configurations without long-range order.

Using Eq. (1), the path integration $\int \mathcal{D}\phi$ Eq. (10) becomes

$$\prod_x \int_{-\infty}^{\infty} dr(x) \int_0^{\infty} ds(x) \int_{4\pi} d^2 \mathbf{e}(x).$$

We see that if we sum over configurations ϕ for which $\mathcal{F} \approx \mathcal{F}_0$ [Eq. (4)], the integration over the $\mathbf{e}(x)$ is irrelevant (it contributes only a constant factor to Z [Eq. (12)], which can be dropped).

We first sum over all such configurations with $r(x) = r$ and $s(x) = s$ independent of x but $\mathbf{e}(x)$ changing (i.e., the magnitude of the AF order parameter is constant but not its direction). For all these configurations we again obtain $\mathcal{F} \approx \beta L^d f_0(r,s)$, thus summing over these configurations we obtain Eq. (23) as before.

We now sum over even larger classes of configurations allowing also for spacetime-dependent $r(x)$ and $s(x)$, which have sufficiently large spatial and temporal correlation lengths ℓ_{space} and ℓ_{time} , respectively. One can regard ℓ_{space} and ℓ_{time} as variation parameters: calculate Z [Eq. (12)] by summing over a class of configurations characterized by these two parameters and determine them so as to minimize the free energy Ω . In this case we also obtain, to a good approximation, Eq. (23) but now with $V \approx (\ell_{\text{space}})^d \ell_{\text{time}}$ the correlation volume (note that these correlations only refer to the magnitude of the AF order but not to its direction). To illustrate that the precise structure of the boson configurations summed over does not affect the final result, we consider two different classes of configurations. The first class contains configurations $\phi(x)$ so that most points x belong to a sufficiently large region so that $\phi(x)$ restricted to this region equals a Néel configuration, Eq. (2). For configurations in the second class, the Fourier modes of $r(x)$, $s(x)$, and $\mathbf{e}(x)$ have support sufficiently close to $k=0$ but otherwise are arbitrary.

A configuration in the first class can be characterized as follows: set $x = X + \xi$ where ξ is a coordinate in a block [i.e., $s(X + \xi)$, $r(X + \xi)$ are (approximately) independent of ξ],

and X labels different blocks. For these configurations $\mathcal{F}(\phi) \approx \sum_x f_0(r(X), s(X))$, which equals $\sum_X V_X f_0(r(X), s(X))$, and this defines the correlation volumes V_X . The correction \mathcal{F}_1 to this should be proportional to the number of points that belong to the boundaries of different blocks (whatever their form is); thus it can be made negligibly small by choosing V_X sufficiently big. We now sum over these configurations. Since $\int \mathcal{D}\phi = \prod_X [\prod_{\xi} \int d\phi_0(X + \xi) d^3 \phi(X + \xi) / \phi(X + \xi)^2]$, the path integral in Eq. (12) restricted to these configurations gives

$$Z = \prod_X \int d\phi_0(X) \int \frac{d^3 \phi(X)}{\phi(X)^2} e^{-V_X f_0(r(X), s(X))},$$

which we can write as $Z = \prod_X \exp(-V_X \Omega_X)$, where $\Omega_X = \Omega(V_X)$ is defined by Eq. (23) with V replaced by V_X . We thus get $\Omega = \sum_X V_X \Omega_X / \sum_X V_X$. If we assume the configurations summed over such that $V_X = V$ is independent of X , we immediately obtain Eq. (23). More generally, we also obtain Eq. (23) if V_X is allowed to depend on X ; V in this case is to be interpreted as an average correlation volume.

We now turn to configurations in the second class. Let $s(k)$ and $r(k)$ be the Fourier transforms of $s(x)$ and $r(x)$ in Eq. (1). We consider boson configurations where these are different from zero only for ‘‘small’’ k , i.e., $|\omega_n| < 1/\ell_{\text{time}}$ and $|\mathbf{k}| < 1/\ell_{\text{space}}$. For these we can use the approximation $\mathcal{F}(\phi) \approx \sum'_k V'_k f_0(r(k), s(k))$ (which defines V) where the prime indicates summation (or integration) over ‘‘small’’ momenta only. If we restrict the path integration in Eq. (12) to these configurations, $\int \mathcal{D}\phi$ becomes $\prod'_k \int d\phi_0(k) d^3 \phi(k) / \phi(k)^2$, and we again obtain Eq. (23).

C. Refinements: An outline

As discussed, Eq. (3) is one simple approximation of many possible approximations of the partition function Z by finite-dimensional integrals. The simplest way to obtain Eq. (3) is by summing over the Néel states, Eq. (2). The strategy for refining this approximation is by the following natural generalization: make an ansatz for a set of boson configurations [Eq. (1)] parametrized by N real parameters α_i so that with one such configuration all others related to it by symmetry transformations are also in this set. If all these configurations are periodic (the period can be large), the HS action configuration will be proportional to the total spacetime volume βL^d , and it depends on the α_i . Restricting the path integral in Eq. (12) to these configurations we get an approximation of Z by a finite-dimensional integral over the α_i , and the saddle point evaluation for this integral is exact.

The nontrivial task is to find a useful ansatz for the boson configurations. We suggest using numeric studies of HF theory^{6,7,10} as a guide. One other criterion for a ‘‘good’’ ansatz is, of course, that one can easily (the best would be analytically) evaluate the HS action for the configurations considered.

IV. NUMERIC RESULTS

In this section we present numeric results for the solution of our mean-field theory, Eq. (3). We discuss in detail the calculation for the two-dimensional Hubbard model ($d=2$)

and the parameters $U/t=10$ motivated by HTSC.³ To demonstrate that the phase diagram in this approximation is qualitatively always the same, we also present results for three dimensions ($d=3$ and $U/t=10$) and weaker coupling ($U/t=2$, $d=2$).

Standard integration routines were used to numerically evaluate the \mathbf{k} integrals defining the functions in Eqs. (19) and (22), solve Eq. (26) below, etc. In all our calculations we ensured that numeric errors are negligible.

A. Saddle point evaluation

We now describe in detail how to evaluate the integral in Eq. (3) in the limit $L \rightarrow \infty$ under the constraint Eq. (24). We first perform the r integral (μ dependence suppressed):

$$e^{-Vf^*(s)} \simeq \int_{-\infty}^{\infty} dr e^{-Vf_0(r,s)} \quad (V \rightarrow \infty), \quad (25)$$

where $V = \beta L^d$ and $A \simeq B$ here means that $\lim_{V \rightarrow \infty} [\ln(A) - \ln(B)]/V = 0$. The saddle point equation for this integral is $\partial f_0 / \partial r = 0$, i.e.,

$$r = -\frac{i}{2} U x(r, s) \quad (26)$$

[we used Eq. (22)]. This equation has a unique purely imaginary solution $r = r^*(s)$, and one can show that this saddle point dominates the integral in Eq. (25), and a standard saddle point evaluation gives

$$f^*(s) = f_0(r^*(s), s). \quad (27)$$

The complete justification of this result is somewhat technical and deferred to Appendix B 1.

With that we get from Eq. (23),

$$Z = e^{-V\Omega} \simeq \int_0^{\infty} ds e^{-Vf^*(s)} \quad (V \rightarrow \infty). \quad (28)$$

Note that $r^*(s)$ enters here only in the combination $\tilde{\mu} = \mu - ir^*(s) = \mu - Ux(r^*(s), s)/2$. Physically this can be naturally interpreted as renormalization of the chemical potential by the Coulomb energy. Since $f^*(s)$ is real valued, this integral is determined by the absolute minimum (minima) of this function. Plotting the function $f^*(s)$ for different values of the chemical potentials μ is thus a simple way to understand why degenerate saddle points occur.

Figure 1(a) shows such a plot at a fixed temperature close to zero.¹⁵ We see that for $\mu=0$ up to some critical value $\mu = \mu_c$, the absolute minimum of $f^*(s)$ is at a finite value $s = s^*$, which thus dominates the integral in Eq. (28), $\Omega = f^*(s^*)$. For $\mu > \mu_c$ the minimum at $s=0$ takes over, and $\Omega = f^*(0)$. We refer to $s = s^*$ and $s=0$ as the nontrivial and trivial minima (or saddle points), respectively. We see from Fig. 1(a) that the nontrivial minimum is always at the same value $s = s^*$ (independent of $\mu < \mu_c$), and also $f^*(s^*)$ does not change with μ . Thus $x = -\partial f^*(s^*) / \partial \mu$ is always 0, and the nontrivial minimum can only account for half filling. The physical interpretation of this is that for $s = s^* > 0$, we have AF bands with a gap, and as long as μ is in this gap it cannot affect the doping. For $\mu > \mu_c$, we see that $x = -\partial f^*(0) / \partial \mu$ is always larger than

$x_2 = -\partial f^*(0) / \partial \mu|_{\mu=\mu_c}$ (which is larger than 0.5 here; note that x is monotonically increasing with μ). Thus the only doping that can be obtained with the nontrivial minimum $s = s^*$ is $x=0$, and for the trivial minimum $s=0$ only dopings $x > x_2$ are possible. A finite doping regime $x_1 < x < x_2$ is left out by this ($x_1=0$ here but will be nonzero for higher temperatures; see below). *The only way to get doping in this regime is to have μ so close to μ_c that both saddle points can contribute to the integral Eq. (28).* Indeed, for $\mu = \mu_c + \delta\mu$ we have $f^*(s^*) - f^*(0) = -(x_1 - x_2)\delta\mu + O(\delta\mu^2)$ [$x_{1,2} = -\partial f^*(s) / \partial \mu|_{\mu=\mu_c}$ at $s = s^*$ and 0, respectively], which suggests that we can adjust $\delta\mu = O(1/V)$ such that the saddle points $s = s^*$ and $s=0$ contribute with relative weight w and $(1-w)$ to the partition function Eq. (28) and dopings x between x_1 and x_2 are possible,

$$x = wx_1 + (1-w)x_2. \quad (29)$$

(We give a more careful argument in Appendix B 2.) This equation fixes w by doping, and one can now forget about $\delta\mu$, which, for $V \rightarrow \infty$, becomes zero.

Standard mean-field theory corresponds to evaluating the integral (23) by insisting on having only one relevant saddle point. Then $\Omega = f_0(r, s)$, where r and s solve the saddle point equations $\partial f_0 / \partial r = \partial f_0 / \partial s = 0$, i.e., Eqs. (26) and

$$s = -sU \int d\mathbf{k} \left[\frac{f_{\beta}(E_+) - f_{\beta}(E_-)}{E_+ - E_-} \right]. \quad (30)$$

The doping constraint Eq. (15) becomes

$$x = x(r, s), \quad (31)$$

which makes Eq. (26) trivial, $r = -iUx/2$, and one needs to consider only Eqs. (30) and (31): for fixed s , Eq. (31) fixes the renormalized chemical potential $\tilde{\mu} = \mu - ir = \mu - Ux/2$, and Eq. (30) determines the possible s values. In general one gets more solutions. However, from our discussion above it is clear that in the doping regime $x_1 < x < x_2$ none of these solutions is appropriate: the trivial solution $s=0$ is not an absolute minimum of $f^*(s)$, and the nontrivial solution $s \neq 0$ corresponds to the maximum of $f^*(s)$. We conclude that *the correct mean-field theory corresponds to a saddle point evaluation of the integral (3) under the constraint (15) as described above: one can have two relevant saddle points of equal importance.*

Up to now our discussion has been restricted to low temperatures. At higher temperatures the situation is similar, only that the mixed phase occurs in a doping region $x_1 < x < x_2$, where $x_1 > 0$, and for dopings $0 \leq x \leq x_1$ one can have the nontrivial saddle point alone. This can be easily understood from the plot of $f^*(s)$ for different chemical potentials μ in Fig. 1(b): The nontrivial minimum $f^*(s^*)$ is completely independent of μ again, except in a tiny μ region close to the critical μ_c where the two minima become degenerate [inset of Fig. 1(b)]. The explanation for this is simple: as long as μ is in the AF gap, it has no effect on the doping, only when it comes close to the band edge the doping starts to depend on μ due to thermal effects (i.e., since Fermi distribution function no longer is a step function). Increasing μ further, the nontrivial minimum starts to move

but soon the trivial minimum takes over. The value $x_1 = -\partial f^*(s^*)/\partial \mu|_{\mu=\mu_c}$ is the upper limit for the doping, which can be obtained by the nontrivial minimum without superposing the trivial one.

The phase boundary x_1 of the pure AF phase increases with temperature and approaches the boundary x_2 of the free phase, which is quite temperature independent [see Fig. 2(a)]. At some temperature $T=T^*$, $x_1=x_2$, and the mixed phase disappears. For temperatures $T>T^*$, there is a direct second-order phase transition at the critical filling x_2 from the AF to the free phase with no mixed phase between. Figure 1(c) shows a typical plot of $f^*(s)-f^*(0)$ for different chemical potentials μ for such a high temperature case. We restricted ourselves to the interesting region close to the critical $\mu=\mu_c$ defining x_2 . One sees that for $\mu<\mu_c$, $f^*(s)$ has a nontrivial minimum $s^*(\mu)$ lower than the trivial one, but this minimum approaches the trivial minimum with increasing μ and merges with it at $\mu=\mu_c$ [i.e., $s^*(\mu_c)=0$]. The doping x_2 is equal to $-\partial f^*(0)/\partial \mu|_{\mu=\mu_c}$. The qualitative difference from Figs. 1(a) and 1(b) is that there exists no μ where the two minima are degenerate.

Our discussion above suggests that the occurrence of degenerate saddle points is a rather stable phenomenon and should survive corrections to mean-field theory, e.g., by fluctuations: a nontrivial saddle point can dominate the partition function only in a finite μ regime, and whenever not all doping values are realized in that regime degenerate saddle points occur. For the same reason we expect that degenerate saddle points are typical also for other interacting lattice fermion models.

B. Phase diagrams

In Sec. IV A we explained how our generalized mean-field theory allows one to determine the different regimes of the Hubbard model. In Fig. 2(a) we have plotted the resulting phase diagram. We see the three regions, the pure AF region with only the nontrivial saddle point, the free region with the trivial saddle point only, and the mixed region where both saddle points are relevant. The temperature T_{LO} is the largest temperature where a nontrivial saddle point can contribute, and the other characteristic temperature T^* is the upper limit for the mixed region to exist, as discussed. We note that T_{LO} is equal to the highest temperature where the HF equations restricted to Néel states [Eq. (2)] at half filling have a nontrivial solution. Usually this temperature is interpreted as the Néel temperature. However, from our derivations it is clear that we should interpret this temperature as the highest temperature where *local* AF correlations occur, and this is to be expected higher than the Néel temperature where long-range order disappears.

Our detailed discussion above was for the Hubbard parameters $U/t=10$ and $d=2$. However, the results obtained are representative. To illustrate this we give two further examples for phase diagrams in Fig. 2(b) ($U/t=2$, $d=3$) and Fig. 2(c) ($U/t=2$, $d=2$).

V. FLUCTUATIONS

In this section we discuss the effect of fluctuations. We first outline the general scheme of how to include fluctua-

tions in our formalism. As an illustration, we discuss in more detail the effect of fluctuations in the direction of the AF order using a simple approximation.

A. General formalism

Our derivation of mean-field theory in Sec. III suggests that a simple method to take into account fluctuations is as follows: We consider boson configurations of the form $\phi = \phi^{(0)} + \delta\phi$ where $\phi^{(0)}$ are the ‘‘little’’ varying ones leading to (generalized) mean-field theory, and $\delta\phi$ correspond to ‘‘fast’’ fluctuations. We assume the latter are such that we can expand

$$\begin{aligned} \mathcal{F}(\phi^{(0)} + \delta\phi) - \mathcal{F}(\phi^{(0)}) &\approx \sum_{x,\alpha} B_\alpha(x) \delta\phi_\alpha(x) \\ &+ \sum_{x,y,\alpha,\beta} C_{\alpha\beta}(x,y) \delta\phi_\alpha(x) \delta\phi_\beta(y) \end{aligned} \quad (32a)$$

and neglect the $O(\delta\phi^3)$ terms. The coefficients here are

$$\begin{aligned} B_\alpha(x) &= \left. \frac{\delta\mathcal{F}(\phi)}{\delta\phi_\alpha(x)} \right|_{\phi=\phi^{(0)}}, \\ C_{\alpha\beta}(x,y) &= \left. \frac{1}{2} \frac{\delta^2\mathcal{F}(\phi)}{\delta\phi_\alpha(x)\delta\phi_\beta(y)} \right|_{\phi=\phi^{(0)}}, \end{aligned} \quad (32b)$$

and depend only on $\phi^{(0)}$. We thus get a simple framework for taking into account AF and charge fluctuations $\delta\phi(x)$ and $\delta\phi_0(x)$ around mean-field theory: integrating over the fluctuations $\delta\phi_\alpha(x)$ gives a correction term $\delta\mathcal{F}(\phi^{(0)})$ to $\mathcal{F}(\phi^{(0)})$, which describes the effect of fluctuations. Summing then over the $\phi^{(0)}$ leads to a finite-dimensional integral as before. Symbolically we can summarize this procedure as follows:

$$\begin{aligned} e^{-\delta\mathcal{F}(\phi^{(0)})} &= \int_{\delta\phi(x)} e^{-\mathcal{F}(\phi^{(0)} + \delta\phi) + \mathcal{F}(\phi^{(0)})}, \\ Z &= \int_{\phi^{(0)}(x)} e^{-\mathcal{F}(\phi^{(0)}) - \delta\mathcal{F}(\phi^{(0)})}. \end{aligned} \quad (32c)$$

There is one important point to keep in mind: one can integrate only over fluctuations $\delta\phi$, where the second term in Eq. (32a) is positive definite, and this is an important restriction on which fluctuations can be taken into account in that way.¹⁶ Selecting appropriate ‘‘fast’’ fluctuations therefore is quite delicate. Also the summation over these fluctuations will be, in practice, a nontrivial task and require further approximations.

B. Example

As an illustration we consider fluctuations $\delta\mathbf{e}(x)$ around states $\phi^{(0)}$ defined in Eq. (1) with $r(x)=r$, $s(x)=s$ independent of x and $\mathbf{e}(x)=\mathbf{e}^{(0)}(x)$ varying ‘‘not much.’’ Then Eq. (32a) gives

$$\mathcal{F}(\phi) - \mathcal{F}(\phi^{(0)}) = \beta L^d \frac{\partial f_0(r,s)}{\partial s} s \mathbf{e}^{(0)}(x) \cdot \delta \mathbf{e}(x) + O(\delta \phi^2), \quad (33)$$

where we restrict ourselves to the lowest-order correction term for simplicity. In a simple approximation, integrating out such fluctuations amounts to replacing $\mathbf{e}^{(0)}(x) \cdot \delta \mathbf{e}(x)$ by its average, which should be an x -independent constant. Note that this constant depends on r, s, β, μ , and on the class of fluctuations considered. In any case, since $[\mathbf{e}^{(0)}(x) + \delta \mathbf{e}(x)]^2 = \mathbf{e}^{(0)}(x)^2 = 1$, this constant is equal to the average of $-\delta \mathbf{e}(x)^2/2$ and is thus negative. We get $\delta \mathcal{F} = \beta L^d f_1$ with

$$f_1(r,s) = \beta L^d \frac{\partial f_0(r,s)}{\partial s} s \alpha, \quad \alpha = -\frac{1}{2} \langle \delta \mathbf{e}(x)^2 \rangle \quad (34)$$

[the averaging $\langle \rangle$ of course defined through

$$e^{-\delta \mathcal{F}} = \int e^{-\mathcal{F}(\phi) + \mathcal{F}(\phi^{(0)})},$$

where \int here symbolizes integration (summation) over all configurations $\mathbf{e}^{(0)}(x)$ and $\delta \mathbf{e}(x)$ taken into account]. This then leads to Eq. (3) with f_0 replaced by $f_0 + f_1$.

To evaluate α is difficult. However, one can easily estimate the effect of these fluctuations by taking α as a fixed constant. Then one can determine the phase diagram as a function of α similarly to that described in Sec. IV. We do not present numeric results here and only note that, even though α has quite a *quantitative* effect on the phase diagram, the *qualitative* features of phase diagram are very stable.

VI. CONCLUSIONS

In this paper we presented a method for finding approximations for interacting fermions models. These approximations allow one to determine not only phase diagrams but also Green functions (i.e., observables) of the systems. Our discussion was for antiferromagnetic correlations and the Hubbard model but is straightforward to extend to other models. In simple cases our approximations correspond to generalized mean-field theory, which allows the possibility of degenerate saddle points. The occurrence of degenerate saddle points can be easily detected in our formulation and reveals a frustration usually referred to as phase separation. However, our interpretation of this phenomenon is somewhat more general: our approach allows one to clarify the meaning of the mean-field approximation and shows that degenerate saddle points only mean that no homogeneous mean-field solution exists. A more detailed description of the systems is then necessary, and this requires a refined approximation taking into account inhomogeneous states.

Our approach formalizes the simple and intuitive interpretation of mean-field theory as an approximation to the exact partition function by restricting the summation over the huge set of states to a (small) subset, which, on physical grounds, are expected to represent the ‘‘most important states.’’ This makes manifest that mean-field theory is not necessarily a weak-coupling approximation, and it also makes manifest that the simplest ansatz of translation invariant Hartree-Fock solutions not only describes long-range ordered states but

also states with only local correlation. Thus a nontrivial solution of HF equations restricted to long-range ordered states should not be interpreted as long-range order but only as the existence of *local* correlations. Moreover, our approach gives a systematic way to find increasingly refined (and increasingly complicated) mean-field theories, which give a homogeneous description of the system even if the HF solutions are not translation invariant. Our approach also allows one to include fluctuations in a natural way (the latter is only outlined in this paper).

Many successful theories in solid state physics are based on simple mean-field theory, i.e., HF equations and an ansatz allowing only for homogeneous solutions. If this latter ansatz is not appropriate, the system will be much more complicated and it will not resemble a free fermion system. This is the case for the Hubbard model and probably most correlated fermion models. This is one reason (and we believe the main reason) why our understanding of these systems is still rather poor. However, in such a situation a generalized mean-field theory as proposed in this paper is still possible, and we believe that this could be the starting point for a successful theory of correlated fermions systems.

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APPENDIX A: FREE ENERGY IN NÉEL STATE

In this appendix we evaluate the HS action Eq. (13) for the Néel configuration Eq. (2) and thus prove Eq. (19). The nontrivial step obviously is to evaluate $\text{Tr} \ln(G_0 - \phi)$ for $\phi = ir\sigma_0 + se \cdot \sigma e^{i\mathbf{Q} \cdot \mathbf{x}}$. We recall that our space Λ_L is a cube with points $\mathbf{x} = (x_1, \dots, x_d)$, x_i integers with $-L/2 \leq x_i < L/2$. We find it convenient to write points in Λ_L as $2\mathbf{x} + \mathbf{n}$ where $\mathbf{x} \in \Lambda_{L/2}$ and $\mathbf{n} = (n_1, \dots, n_d)$ with $n_j = 0, 1$. Then the Green function $G = (G_0^{-1} - \phi)^{-1}$ is represented by a translation invariant $2^{d+1} \times 2^{d+1}$ matrix,

$$(G)_{\sigma\sigma' m_1 n_1 \dots m_d n_d}(\tau - \tau', 2\mathbf{x} - 2\mathbf{y}) = G_{\sigma\sigma'}(\tau, 2\mathbf{x} + \mathbf{m}, \tau', 2\mathbf{y} + \mathbf{n}), \quad (A1)$$

and therefore,

$$\begin{aligned} \text{Tr} \ln G^{-1} &= \int_0^\beta d\tau \sum_{\mathbf{x} \in \Lambda_{L/2}} \text{tr}(\ln G^{-1})(\tau - \tau, 2\mathbf{x} - 2\mathbf{x}) \\ &= \sum_{\mathbf{k} \in \Lambda_{\pi/2}^*} \sum_{\omega_n}^{(\text{reg})} \text{tr} \ln G^{-1}(i\omega_n, \mathbf{k}), \end{aligned} \quad (A2)$$

where tr is the trace over the $2^{d+1} \times 2^{d+1}$ -matrix indices, $\Lambda_{\pi/2}^*$ is the set of all $\mathbf{k} = (k_1, \dots, k_d)$ with $k_i = 2\pi\nu_i/L$ with ν_i integer and such that $-\pi/2 \leq k_i < \pi/2$; the Fourier transform is defined as $G(\mathbf{k}) = \sum_{\mathbf{x} \in \Lambda_{L/2}} e^{-i\mathbf{k} \cdot 2\mathbf{x}} G(2\mathbf{x})$. To evaluate Eq. (A2), we first note that the matrix notation we use here comes from representing fermion field operators as

$$\psi_{\sigma n_1 \dots n_d}(\tau, 2\mathbf{x}) = \psi_\sigma(\tau, 2\mathbf{x} + \mathbf{n}).$$

From this we see that $\underline{\phi} = ir\sigma_0 + \mathbf{se} \cdot \boldsymbol{\sigma} e^{i\mathbf{Q} \cdot \mathbf{x}}$ is represented by

$$\underbrace{ir\sigma_0 \otimes \sigma_0 \otimes \dots \otimes \sigma_0}_{d \text{ times}} + \underbrace{\mathbf{se} \cdot \boldsymbol{\sigma} \otimes \sigma_3 \otimes \dots \otimes \sigma_3}_{d \text{ times}}$$

(we use an obvious tensor notation). We also need the hopping operators $(T_j \psi)_\sigma(\mathbf{x}) = -t[\psi_\sigma(\mathbf{x} + \mathbf{e}_j) + \psi_\sigma(\mathbf{x} - \mathbf{e}_j)]$ where \mathbf{e}_j is the lattice unit vector in the j direction [i.e., $\mathbf{e}_1 = (1, 0, \dots, 0)$, etc.]. It is easy to see that these are represented by

$$T_j = \underbrace{\sigma_0 \otimes \sigma_0 \otimes \dots \otimes \sigma_0}_{j-1 \text{ times}} \otimes T(k_j) \otimes \underbrace{\sigma_0 \otimes \dots \otimes \sigma_0}_{d-j \text{ times}} \quad (\text{A3})$$

with

$$T(k_j) = -2t \cos(k_j) \begin{pmatrix} 0 & e^{ik_j} \\ e^{-ik_j} & 0 \end{pmatrix} \quad (\text{A4})$$

$[\mathbf{k} = (k_1, \dots, k_d)]$. Thus

$$G^{-1}(k) = (i\omega_n + \mu - ir)\mathbf{1} - M, \quad (\text{A5a})$$

where $\mathbf{1} = \sigma_0 \otimes \dots \otimes \sigma_0$ is the $2^{d+1} \times 2^{d+1}$ unit matrix and

$$M = \mathbf{se} \cdot \boldsymbol{\sigma} \otimes \sigma_3 \otimes \dots \otimes \sigma_3 + \sum_{j=1}^d T_j. \quad (\text{A5b})$$

We now evaluate M^2 and obtain

$$M^2 = \left(s^2 + \sum_j \epsilon_j^2 \right) \mathbf{1} + \sum_{i < j} 2T_i T_j,$$

where $\epsilon_j = -2t \cos(k_j)$ [we used $\sigma_3 T(k_j) + T(k_j) \sigma_3 = 0$]. It is easy to diagonalize M^2 : let U_j be the 2×2 -matrix diagonalizing T_j , $U_j^{-1} T_j U_j = \epsilon_j \sigma_3$, then $U = \sigma_0 \otimes U_1 \otimes \dots \otimes U_d$ diagonalizes M^2 ,

$$\begin{aligned} (U^{-1} M^2 U)_{\sigma\sigma' m_1 n_1 \dots m_d n_d} \\ = \delta_{\sigma\sigma'} \delta_{m_1 n_1} \dots \delta_{m_d n_d} \left(s^2 + \sum_j \epsilon_j^2 \right. \\ \left. + 2 \sum_{i < j} \epsilon_i \epsilon_j (-)^{n_i + n_j} \right). \end{aligned} \quad (\text{A6})$$

Since $\epsilon_j (-)^{n_j} = -2t \cos(k_j + n_j \pi)$ for $n_j = 0, 1$ we see that the eigenvalues of M^2 are $s^2 + \epsilon(\mathbf{k} + \mathbf{n}\pi)^2$ where $\epsilon(\mathbf{k})$ is the Hubbard band relation Eq. (7). Moreover, for \mathbf{e}' a unit vector orthogonal to \mathbf{e} , the self-adjoint matrix $C = \mathbf{e}' \cdot \boldsymbol{\sigma} \otimes \sigma_3 \otimes \dots \otimes \sigma_3$ obeys $C^2 = \mathbf{1}$ and $CMC = -M$. We conclude that the eigenvalues of M are $\pm \sqrt{s^2 + \epsilon(\mathbf{k} + \mathbf{n}\pi)^2}$, thus the eigenvalues of $\ln G^{-1}(k)$ are $\ln[i\omega_n - E_\pm(\mathbf{k} + \mathbf{n}\pi)]$, $E_\pm = E_\pm(\mathbf{k})$ given in Eq. (21). With Eqs. (A2) and (16) we therefore obtain

$$\begin{aligned} \text{Tr} \ln G^{-1} &= \sum_{\mathbf{k} \in \Lambda_{\pi/2}^*} \sum_{\mathbf{n}} \sum_{\sigma = +, -} \beta \text{Ln}_\beta [E_\sigma(\mathbf{k} + \mathbf{n}\pi)] \\ &= \sum_{\mathbf{k} \in \Lambda_\pi^*} \sum_{\sigma = +, -} \beta \text{Ln}_\beta [E_\sigma(\mathbf{k})], \end{aligned} \quad (\text{A7})$$

where

$$\Lambda_\pi^* = \{ \mathbf{k} = (k_1, \dots, k_d) \mid -\pi \leq k_i < \pi, Lk_i/2\pi \in \mathbb{Z} \} \quad (\text{A8a})$$

is the Brillouin zone of the full lattice Λ_L . Thus $f_0^L = \mathcal{F}/\beta L^d$, \mathcal{F} [Eq. (13)], is

$$f_0^L = \frac{r^2 + s^2}{U} - \frac{1}{L^d} \sum_{\mathbf{k} \in \Lambda_\pi^*} [\text{Ln}_\beta(E_+) + \text{Ln}_\beta(E_-)]. \quad (\text{A8b})$$

Since $(1/L^d) \sum_{\mathbf{k} \in \Lambda_\pi^*}$ in the limit $L \rightarrow \infty$ becomes $\int d\mathbf{k}$, we obtain $f_0^\infty = f_0$ [Eq. (19)]. This concludes our proof.

APPENDIX B: SADDLE POINT EVALUATIONS

In this appendix we justify in detail the saddle point evaluation of our integral, Eq. (23). We first prove Eq. (25), and then evaluate $\mu(V)$ for $x_1 < x < x_2$.

1. The r integral

For finite L , the HS action Eq. (13) for the Néel configurations Eq. (2) equals $\mathcal{F} = \beta L^d f_0^L$ with f_0^L given in Eq. (A8b). We consider

$$\mathcal{I}^L(\mathcal{C}, V) = \int_{\mathcal{C}} dr e^{-V f_0^L(r, s)}, \quad (\text{B1})$$

with \mathcal{C} some integration path in the complex r plane. We are interested in this integral for $V \rightarrow \infty$ and the integration path along the real r line,

$$\mathcal{C}_{\text{real}} : r_{\text{real}}(\tau) = \tau, \quad -\infty \leq \tau \leq \infty. \quad (\text{B2})$$

For the saddle point evaluation of this integral below we need to show that one can deform $\mathcal{C}_{\text{real}}$ to a path of steepest descent \mathcal{C}_{std} through the dominating saddle point of f_0 . This is nontrivial since $\text{Ln}_\beta(z)$ has branch points in $z = i(2n+1)\pi\beta$, n integer. However, $e^{\beta \text{Ln}_\beta(z)} = 2 \cosh(\beta z/2)$, thus we see from Eq. (A8b) that $e^{-\beta L^d f_0^L(r, s)}$ is analytic for all $r \neq \infty$, and $\mathcal{I}^L(\mathcal{C}_{\text{real}}, \beta L^d) = \mathcal{I}^L(\mathcal{C}_{\text{std}}, \beta L^d)$ follows from Cauchy's theorem. Moreover, since $f_0^L = f_0^\infty + O(1/L)$, we get $\mathcal{I}^\infty(\mathcal{C}, V) = \mathcal{I}^L(\mathcal{C}, V) e^{O(V/L)}$. We thus conclude that

$$\mathcal{I}^\infty(\mathcal{C}_{\text{real}}, \beta L^d) = \mathcal{I}^\infty(\mathcal{C}_{\text{std}}, \beta L^d) e^{O(\beta L^{d-1})}. \quad (\text{B3})$$

In the following we consider $\mathcal{I}^\infty(\mathcal{C}_{\text{std}}, V)$. Introducing the DOS $N(E) = \int d\mathbf{k} [\delta(E-w) + \delta(E+w)]$ with $w = \sqrt{s^2 + \epsilon(\mathbf{k})^2}$ we write $f_0^\infty = f_0$ as

$$f_0(r) = \frac{s^2 + r^2}{U} - \int dE N(E) \text{Ln}_\beta(E + ir - \mu). \quad (\text{B4})$$

The saddle point equation $\partial f_0/\partial r=0$ has a single purely imaginary solution $r^*=iy^*$, y^* real, where

$$y^* = -\frac{U}{2} \int dEN(E) f_\beta(E - y^* - \mu). \quad (\text{B5})$$

To determine the path C_{std} we evaluate

$$f_0(r^* + \xi) = f_0(r^*) + a\xi^2 - ib\xi^3 + O(\xi^4), \quad (\text{B6a})$$

where

$$a = \frac{1}{U} + \int dEN(E) \frac{\beta}{8 \cosh^2[\beta(E - y^* - \mu)/2]},$$

$$b = \int dEN(E) \frac{\beta^2 \tanh[\beta(E - y^* - \mu)/2]}{12 \cosh^2[\beta(E - y^* - \mu)/2]}. \quad (\text{B6b})$$

From this we can determine the path of steepest descent $r^*(\tau) = \tau + iy^*(\tau)$ obeying $\text{Im}f_0[r^*(\tau)] = 0$,

$$y^*(\tau) = y^* + \frac{b}{2a} \tau^2 + O(\tau^4). \quad (\text{B7})$$

Note that $y^*(\tau) = y^*(-\tau)$. We now choose

$$C_{\text{std}}: r_{\text{std}}(\tau) = \begin{cases} \tau + iy^*(\tau) & \text{for } |\tau| \leq \varepsilon \\ \tau + iy^*(\varepsilon) & \text{for } |\tau| \geq \varepsilon \end{cases} \quad (\text{B8})$$

for some $\varepsilon > 0$. We obviously have $[r^* = r^*(0)]$

$$f_0(r^*(\tau)) = f_0(r^*) + a\tau^2 + O(\tau^4) \quad \text{for } |\tau| \leq \varepsilon.$$

Moreover, by a simple calculation

$$\begin{aligned} \text{Re}[f_0(x + iy) - f_0(iy)] \\ = \frac{x^2}{U} - \int dEN(E) \frac{1}{2\beta} \ln \left(1 - \frac{\sinh^2(\beta x/2)}{\cosh^2[\beta(E - y - \mu)/2]} \right) \\ \geq \frac{x^2}{U}, \end{aligned}$$

thus $a > 1/U$ gives the estimate (for ε sufficiently small)

$$\text{Re}[f_0(r_{\text{std}}(\tau)) - f_0(r^*)] \geq \frac{U}{2} \tau^2 \quad \forall \tau. \quad (\text{B9})$$

Thus $\mathcal{I}^\infty(C_{\text{std}}, V) = e^{-Vf_0(r^*)}(\dots)$ with $|\dots| \leq \int_{-\infty}^{\infty} d\tau e^{-VU\tau^2/2}$. Combining this with Eq. (B3) gives

$$-\lim_{V \rightarrow \infty} \frac{1}{V} \ln[\mathcal{I}^\infty(C_{\text{real}}, V)] = f_0(r^*), \quad (\text{B10})$$

equivalent to Eq. (25).

2. Degenerate saddle points

For large but finite V and μ close to μ_c the integral Eq. (23) equals

$$Z \simeq e^{-V\Omega_1} + e^{-V\Omega_2} \quad (\text{B11})$$

up to correction terms that are irrelevant for $V \rightarrow \infty$ and thus will be ignored. The first and second terms here are the contributions from the first and second saddle points $s_1^* = 0$ and $s_2^* = s^*$, respectively,

$$\Omega_i(\mu) = f_0^*(s_i^*, \mu) + c_V(s_i^*, \mu). \quad (\text{B12})$$

The contributions

$$c_V(s_i^*, \mu) \simeq \frac{1}{V} \ln[A_i(\mu)V] \quad (A_i > 0)$$

come from Gaussian integrations in the regions close to the saddle points. The precise form of the c_V actually is not important for us and we will only use that they vanish for $V \rightarrow \infty$. Using $Z = e^{-V\Omega}$ and $x = -\partial\Omega/\partial\mu$ we get

$$x \simeq \frac{e^{-V\Omega_1} x_1 + e^{-V\Omega_2} x_2}{e^{-V\Omega_1} + e^{-V\Omega_2}}, \quad (\text{B13})$$

where $x_i = -\partial\Omega_i/\partial\mu$. This is precisely of the form Eq. (29) if we choose

$$w/(1-w) = (x_2 - x)/(x - x_1) \simeq \exp[-V(\Omega_1 - \Omega_2)].$$

For $\mu = \mu_c + \delta\mu$ we have

$$\Omega_1 - \Omega_2 \simeq -(x_1 - x_2)\delta\mu + [c_V(s_1^*, \mu_c) - c_V(s_2^*, \mu_c)]$$

by definition of μ_c , thus we get

$$V\delta\mu \simeq -\frac{1}{(x_2 - x_1)} \ln \left(\frac{x_2 - x}{x - x_1} \right) \quad (\text{B14})$$

up to terms that vanish for $V \rightarrow \infty$. This shows that $\delta\mu = O(1/V)$ can be adjusted so as to produce arbitrary doping x between x_1 and x_2 , as claimed in the text.

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