

## Restricted path integral approach to the doped Hubbard model

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**Abstract.** – We present a restricted path integral approach to the 2D repulsive Hubbard model. It amounts to evaluating the partition function by restricting the summation over states to a small subclass and generalizes mean-field theory. Analyzing the simplest of these approximations, we find a mixed phase of fermions with local antiferromagnetic correlations coexisting with conventional metallic fermions. This mixed phase persists in a big parameter regime. We also discuss a refinement of our approximation which suggests simple explanations of several peculiar experimental features of HTSC.

The two-dimensional one-band Hubbard model has received much attention as a prototype model for high-temperature superconductors (HTSC). At half-filling, Hartree-Fock (HF) theory predicts a Néel state, which is a good starting point for describing the insulating parent compounds of HTSC. Much remains to be understood in the doped regime. HF theory for the doped Hubbard model does not lead to a simple picture [1], [2]. A variety of states has been suggested, including magnetic domain walls, polarons and vortices [1], spiral states [2], phase separation [3]. Systematic investigations have been done by numerical methods for small lattices [1]. Denoting (imaginary) time as  $\tau$  and lattice points as  $\mathbf{x}$ , one has to consider HF fields

$$\phi_0(x) = r(x), \quad \phi(x) = s(x)\mathbf{e}(x)(-)^{x_1+x_2} \quad (1)$$

(we write  $x = (\tau, \mathbf{x})$ , and  $\mathbf{x} = (x_1, x_2)$ ,  $x_i$  integers, are lattice points), where  $s$  is the magnitude of the *local* (LO) antiferromagnetic (AF) order parameter,  $\mathbf{e}$  its direction, and  $r$  is the charge degree of freedom. In the doped region, one finds a large number of solutions of the HF equations which correspond to metastable spin and charge configurations [1].

In this paper we present a novel analytic approach to antiferromagnetism in the doped Hubbard model which aims at extracting the main thermodynamic information by integrating over the important configurations in eq. (1). Starting from the exact path integral formula for the partition function

$$Z = \int \mathcal{D}\phi \exp[-\mathcal{F}(\phi)] \quad (2)$$

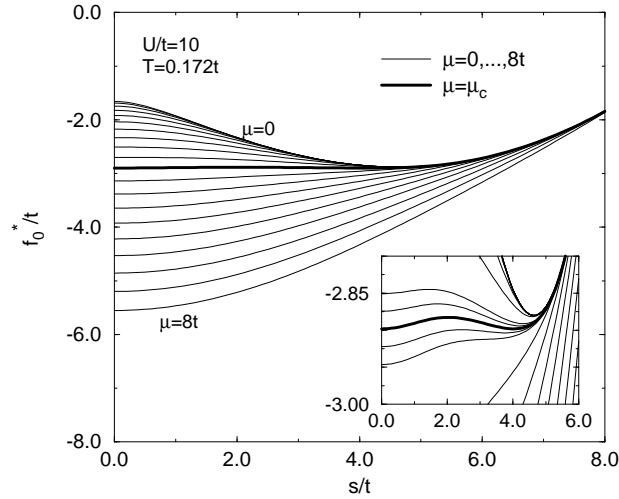


Fig. 1. – Dependence of effective action  $f_0^*$  on the magnitude of the antiferromagnetic order  $s$  for a sequence of different values of the chemical potential  $\mu$ . Note that there are sometimes two minima, and these become degenerate at a critical value  $\mu_c = 4.37645 t$  of the chemical potential (thick curve). Inset: zoom with additional curves for  $\mu = \mu_c(1 + i/100)$ ,  $i = 0, \pm 1, \pm 2$ .

the fields  $\phi(x) = (\phi_0(x), \phi(x))$  in eq. (1) naturally appear as Hubbard-Stratonovich bosons to be integrated over [4].  $\mathcal{F}(\phi)$  is the free energy of non-interacting fermions in the external field  $\phi(x)$ . Each boson configuration  $\phi(x)$  represents a state of the fermion system, especially the Néel state at half-filling corresponds to  $s(x) = s$ ,  $r(x) = r$  and  $\mathbf{e}(x)$  independent of  $x$ , where  $s$  and  $r$  are determined by the HF equations. This suggests the following approximation: restrict the exact path integral for  $Z$  by summing only over the Néel configurations. Then we obtain

$$e^{-\beta L^2 \Omega} = \int_0^\infty ds \int_{-\infty}^\infty dr \exp[-\beta L^2 f_0(r, s)], \quad (3)$$

*i.e.*  $Z = \exp[-\beta L^2 \Omega]$  is approximated by a 2-dimensional integral ( $\Omega$  is the free-energy density,  $L^2$  is the number of lattice sites, and  $f_0$  is given in eq. (5) below). This gives a simple way to understand why HF theory away from half-filling is complicated: In the limit  $L \rightarrow \infty$  the saddle point evaluation of this integral is exact. The saddle point equations are identical with the HF equations, and we recover standard HF theory restricted to Néel states *in case there is only one relevant saddle point*. However, this integral depends on the chemical potential  $\mu$  which is fixed by the particle number constraint:  $x = -\partial\Omega/\partial\mu$ . In a big parameter regime, this constraint can be fulfilled only if  $\mu$  is at a critical value  $\mu_c$  where two saddle points, one with  $s = 0$  and another with  $s = s^* > 0$ , are degenerate and both contribute to the integral (see fig. 1). The latter saddle point corresponds to fermions with local AF order (Phase I), and the former to metallic fermions without AF correlations (Phase II). Thus the degenerate saddle points give a simple description of a state where two kinds of fermions with different properties coexist (Mixed Phase).

To interpret our result, we note that eq. (3) is also obtained if one sums over all configurations eq. (1) with varying  $r(x)$ ,  $s(x)$ , and  $\mathbf{e}(x)$ , as long as the variations are “slow” or restricted to small fractions of the total space-time volume [5]. These states have only in common that they *locally* resemble a state with  $r(x)$ ,  $s(x)$ , and  $\mathbf{e}(x)$  independent of  $x$ , and including also their contribution to the partition functions leaves the result unchanged. Degenerate saddle points thus show that the dominating states have regions with *local* AF order coexisting with regions

of non-ordered fermions, similarly as in the critical region of a first-order phase transition: it is not possible to distribute holes in the AF ordered state homogeneously. However, since the effect of phase boundaries is not included, eq. (3) does not describe size, shape or distribution of these pure-phase regions: it is a simple mean-field description of a variety of possible inhomogeneous states [1]-[3]. Put differently: our approximation does not distinguish phase separation from the inhomogeneous states found in numeric HF calculations. A more detailed description of these states is obtained if more states are included: eq. (3) is the simplest in a sequence of increasingly refined approximations of the partition function by finite-dimensional integrals [5].

We now briefly review our formalism [5]. We write the partition function as a fermion path integral,  $Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp[-S]$ , where  $\bar{\psi}_\sigma(x)$ ,  $\psi_\sigma(x)$  are Grassmann fields carrying a spin index  $\sigma = \uparrow, \downarrow$ . We use square lattices with  $L^2$  sites, and we will eventually take the thermodynamic limit  $L \rightarrow \infty$ . The action is  $S = S_2 + S_4$  with  $S_2 = \sum_{x,y} \bar{\psi}(x)G_0^{-1}(x-y)\psi(y)$  and  $S_4 = U \sum_x [n(x)^2 - s_3(x)^2] / 4$  with  $n = n_\uparrow + n_\downarrow$  the particle density and  $s_3 = n_\uparrow - n_\downarrow$  the local spin along the 3-axis ( $n_\sigma \equiv \bar{\psi}_\sigma\psi_\sigma$  and  $\sum_x \equiv \int_0^\beta d\tau \sum_{\mathbf{x}}$ ).  $G_0^{-1}$  is the inverse one-particle propagator with the Fourier transform  $G_0^{-1}(\omega_n, \mathbf{k}) = [i\omega_n + \mu - \epsilon(\mathbf{k})] \mathbf{1}$ , where  $\epsilon(\mathbf{k}) = 2t [\cos(k_1) + \cos(k_2)]$  and  $\mathbf{1}$  the  $2 \times 2$  (spin) unit matrix. Here  $\omega_n = (2n+1)\pi/\beta$ ,  $n$  integer,  $\mathbf{k} = (k_1, k_2)$ ,  $-\pi \leq k_i \leq \pi$ , and  $U$  and  $t$  are the Hubbard parameters as usual.

It is important to write the partition function in a manner that makes  $SU(2)$  (spin rotation) invariance and the Pauli principle manifest [4]. Thus we replace, at each  $x$ ,  $s_3 = \bar{\psi}\sigma_3\psi$  in the interaction  $S_4$  by the spin density  $\mathbf{e} \cdot \mathbf{s}$  in an arbitrary direction  $\mathbf{e} = (e_1, e_2, e_3)$ , where  $\mathbf{s} = \bar{\psi}\boldsymbol{\sigma}\psi$ , and  $\boldsymbol{\sigma}$  are the Pauli spin matrices.  $S_4$  is independent of the directions  $\mathbf{e}(x)$ , thus we can average over these. A Hubbard-Stratonovitch transformation [4] leads to eq. (2) with boson fields  $\underline{\phi} = \phi_s \mathbf{e} = (\phi_1, \phi_2, \phi_3)$  corresponding to spin and  $\phi_0$  corresponding to charge, and the boson action is

$$\mathcal{F}(\phi) = \sum_{x,\alpha} \frac{1}{U} \phi_\alpha(x)^2 - \text{Tr} \log(G_0^{-1} - \underline{\phi}), \quad (4)$$

where  $\underline{\phi}(x) = i\phi_0(x)\mathbf{1} + \phi(x) \cdot \boldsymbol{\sigma}$ . The boson path integration  $\int \mathcal{D}\phi$  is  $\prod_x \int d\phi_0(x) \int d^3\phi(x) / \phi(x)^2$  [5]. Up to now everything is exact.

To derive eq. (3), we note that a Néel state is described by eq. (1) where  $r(x)$ ,  $s(x)$  and  $\mathbf{e}(x)$  all are independent of  $x$ . For such configurations we can calculate the boson action exactly using Fourier transformation,  $\mathcal{F} = \beta L^2 f_0$ . For  $L \rightarrow \infty$ ,

$$f_0(r, s) = \frac{r^2 + s^2}{U} - \iint \frac{d^2\mathbf{k}}{(2\pi)^2} (\text{Ln}_\beta(E_+) + \text{Ln}_\beta(E_-)), \quad (5)$$

where  $\beta \text{Ln}_\beta(E) = \log(2 \cosh(\beta E/2))$  and  $E_\pm = ir - \mu \pm \sqrt{\epsilon(\mathbf{k})^2 + s^2}$  are the AF bands. Summing only over these configurations reduces the path integral in eq. (2) to an integral over  $r$  and  $s$  and we obtain eq. (3). We now discuss how to evaluate this integral for  $L \rightarrow \infty$ . To parameterize filling we use the doping parameter  $-1 \leq x \leq 1$ , *i.e.* half-filling is  $x = 0$ . Particle-hole symmetry allows to restrict to  $0 \leq x \leq 1$ . At fixed  $s$ , there is a single, purely imaginary  $r^*$  obeying  $\partial f_0 / \partial r|_{r=r^*} = 0$ , and  $r^*$  dominates the  $r$ -integral,  $Z = \int_0^\infty ds \exp[-\beta L^2 f_0^*(s)]$ , with  $f_0^*(s) = f_0(r^*, s)$  real valued. This integral thus is dominated by the absolute minima of  $f_0^*(s)$ . Figure 1 shows  $f_0^*(s)$  from numeric integration, at fixed temperature  $T$  and for different values of  $\mu$ . The high  $T \approx 0.172t$  is chosen as a generic case. There are two regimes: for  $\mu$  from zero to a critical value  $\mu_c$ ,  $f_0^*(s)$  has its absolute minimum at a finite  $s = s^*$ , and for  $\mu$  larger than  $\mu_c$  at  $s = 0$ . In the former case,  $\Omega = f_0^*(s^*)$ , in the latter,  $\Omega = f_0^*(0)$ . Increasing  $\mu$  from zero has initially no effect on the minimum at  $s = s^*$ , whereas  $f_0^*(s)$  decreases significantly with

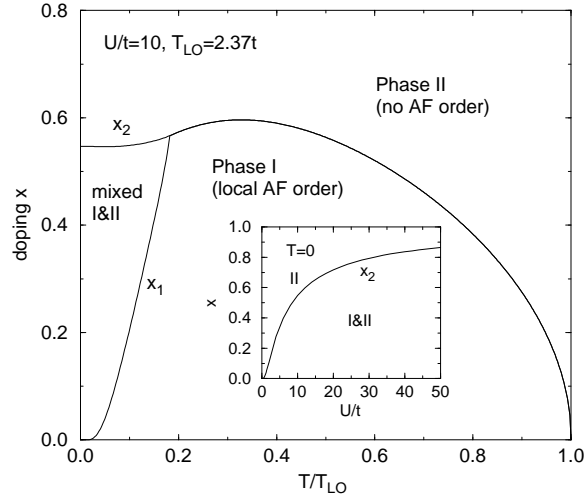


Fig. 2. – Phase diagram for the 2D Hubbard model. At fixed temperature  $T$  there is a homogeneous Phase I with local AF order for doping  $x \leq x_1$ , and a homogeneous metallic Phase II without AF correlations for  $x \geq x_2$ . For  $x_1 \leq x \leq x_2$  these two phases coexist.  $x_1 = 0$  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. Inset:  $x_2$  as a function of  $U/t$  at  $T = 0$ .

increasing  $\mu$  close to  $s = 0$ . For all these  $\mu$ -values,  $x = -\partial\Omega/\partial\mu = 0$ , *i.e.* half-filling. Physically this means that we have AF bands with a gap, and as long as  $\mu$  is in this gap it cannot affect the doping. Only when  $\mu$  reaches the AF band edge,  $s^*$  and  $\Omega = f_0^*(s^*)$  become slightly  $\mu$ -dependent and non-trivial  $x$  becomes possible. Close to this point, however, the minimum at  $s = 0$  takes over and LOAF is lost. The possible dopings which can be obtained in this way are:  $x_1 = -\partial f_0^*(s^*)/\partial\mu|_{\mu=\mu_c}$  is the maximum doping possible for the non-trivial saddle point  $s = s^*$ , and  $x_2 = -\partial f_0^*(0)/\partial\mu|_{\mu=\mu_c}$  is the minimum doping for the trivial saddle point  $s = 0$ . A finite regime  $x_1 < x < x_2$  is left out by this. *To get a doping in this regime,  $\mu$  must be so close to  $\mu_c$  that both saddle points contribute to the integral in eq. (3).* With  $\mu = \mu_c + \delta\mu$ ,  $f_0^*(s^*) - f_0^*(0) = -(x_1 - x_2)\delta\mu + \mathcal{O}(\delta\mu^2)$ , and one can adjust  $\delta\mu = \mathcal{O}(1/\beta L^2)$  such that both saddle points contribute with weights  $w_1 = w$  and  $w_2 = 1 - w$ :  $x = w x_1 + (1 - w) x_2$ . This fixes  $w$  through doping  $x$ , and one can now forget about  $\delta\mu$  which, for  $L \rightarrow \infty$ , becomes zero. Note that remarkably small energy differences are relevant here, *e.g.* the free-energy barrier separating the two minima of  $f_0^*(s)$  at  $s = 0$  and  $s = s^*$  is  $\approx 10^{-2}t$  (see fig. 1). Figure 2 shows the resulting phase diagram for parameters  $U/t = 10$  appropriate for HTSC [6]. The inset shows the  $U/t$  dependence of the mixed phase at  $T = 0$ . The phase diagram is similar also for other  $U/t$ -values and 3D [5].

Our method not only gives approximations for  $Z$  but for all observables (*i.e.* Green functions) of the system: An exact formula for a Green function  $G$  is  $G = \int \mathcal{D}\phi \exp[-\mathcal{F}(\phi)] G_0(\phi) / Z$ , where  $G_0(\phi)$  is the corresponding Green function of *non-interacting* fermions in the external boson field  $\phi(x)$  [5]. Thus our restricted path integral method gives approximations of  $G$  by finite-dimensional integrals. In case there is only one saddle point, we obtain  $G = G_0(\phi_{\text{saddle}})$ , *i.e.* the Green function of non-interacting fermions. This is a simple description of a Fermi liquid. The mixed phase is different: we obtain  $G = w G_0(\phi_1) + (1 - w) G_0(\phi_2)$ , which should be adequate at large enough length scales [5]. The resulting physical properties are not those of a conventional Fermi liquid, but they are related in a simple way to that of two

distinct conventional systems described by  $G_0(\phi_{1,2})$ . This approximation gives a reasonable quantitative description if the average size of the pure-phase regions is large, for example in case of phase separation [3]. 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. Experiments suggest that this is the case in the overdoped regime, as discussed in [3].

It is obvious how to refine our approximation eq. (3): approximate  $Z$ , eq. (2), by summing over a class of boson configurations parametrized by a finite number of parameters. This leads to an approximation of  $Z$  by a (sum of) finite-dimensional integral(s) for which the saddle point evaluation is exact. We now describe one such specific refinement [5] which suggests a scenario that seems to account for several peculiar experimental features of HTSC [7]. Numeric studies show that, for small doping and  $U/t \approx 10$ , the boson action  $\mathcal{F}(\phi)$  (4) has minima corresponding to thin magnetic domain walls (DWs) [1], and there is convincing evidence that DWs are important for low-doped HTSC, see, *e.g.*, [8], [9]. This suggests that, to improve our eq. (3), one should sum also over such DW configurations [5], and the resulting equations seem to account already for several properties of HTSC: Firstly, holes localized in a DW freely move parallel to the DW and thus have 1D effective bands. If, at low doping, the chemical potential  $\mu$  crosses these 1D bands which are within the AF band gap, *i.e.* the LOAF fermions are insulating and the 1D fermions within the DWs metallic (this is formally seen by diagonalizing the Hamiltonian of fermions in an external-field configuration eq. (1) describing a DW [10]). This would be a simple mechanism leading to 1D metallic channels in the 2D Hubbard model, with no fermion hopping between the channels. It is plausible that the effective description of these is by Luttinger liquids. This would explain several unusual features of the transport properties of HTSC [11]. Secondly, at low doping, the DWs should be well-separated and nearly independent (this view is supported by numeric results [8]), thus the DW density should increase linearly with doping  $x$  and  $\mu$  be  $x$ -independent. This seems to explain the simple  $x$ -dependence of, *e.g.*, Hall coefficient and spin correlation length of underdoped HTSC [7]. Thirdly, we conjecture that, at certain doping, the mutual interactions of DWs become important so that further increase in doping is no longer by increasing the DW density but by increasing  $\mu$  towards the upper AF band. Recent numeric Monte Carlo calculations support this conjecture and show that  $\mu$ , at a certain doping, intersects the AF band [12], [6]. This would provide a simple explanation of superconductivity (SC) [13]: if the LOAF fermions are metallic, the DOS of the AF bands is so high that already a weak attractive nearest-neighbor interaction leads to SC with a high transition temperature  $T_c$ . Finally, we suggest that, by further increasing  $x$ , there are two degenerate saddle points and coexisting phases similarly as above, with Phase I the metallic LOAF fermion system with DWs, and Phase II the non-ordered metallic fermions. Since the latter carry no SC (the DOS is too small [13]), this would explain, *e.g.*, the decreases of  $T_c$  and the SC condensate density  $n_s$  with doping observed in the overdoped region of HTSC [7], [14].

To conclude, we presented a novel approach to the doped Hubbard model which gives a simple average description of a variety of degenerate states where regions with local AF order coexist with free, metallic ones. We also suggested a scenario for the doping dependence of antiferromagnetism which seems consistent with certain experimental features of HTSC.

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