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PHASE DIAGRAM OF THE HUBBARD MODEL WITH ARBITRARY BAND FILLING: RENORMALIZATION GROUP APPROACH

by

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Abstract

The finite temperature phase diagram of the Hubbard model in d = 2 and d = 3 is calculated for arbitrary values of the parameter U/t and chemical potential μ using a quantum real space renormalization group. Evidence for a ferromagnetic phase at low temperatures is presented.

Keywords : Hubbard model,phase diagram, real space renormalization group, hierarchical lattice.

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The Hubbard model [1], as one of the simplest models of many-fermions systems, has attracted much attention over years in connection with itinerant magnetism [2,3,4] and more recently with high T_c superconductivity [5]. The dimensionless Hubbard Hamiltonian is defined by

$$\mathcal{H}_H \equiv -\beta \mathrm{H}_H = t \sum_{\langle i,j \rangle, \sigma} \left(c_{i,\sigma}^{\dagger} c_{j,\sigma} + c_{j,\sigma}^{\dagger} c_{i,\sigma} \right) + \frac{1}{2} U \sum_{i} (n_{i,\uparrow} - n_{i,\downarrow})^2 + \mu \sum_{i,\sigma} n_{i,\sigma} \qquad (1)$$

where $\beta \equiv 1/k_B T$, $c_{i,\sigma}^{\dagger}$ creates an electron with spin $\sigma = \uparrow, \downarrow$ in a Wannier state centered at the site i of the lattice and $n_{i,\sigma} \equiv c_{i,\sigma}^{\dagger} c_{i,\sigma}$; t, U and μ are respectively the dimensionless hopping constant, intra-site Coulomb interaction and chemical potential; $\langle i,j \rangle$ denotes first-neighboring lattice sites. We consider $t \geq 0$ (the $t < 0$ case is isomorphic to the $t > 0$ one whenever the lattice can be partitioned into two sublattices, such that all the first-neighboring sites of an arbitrary site of any sublattice belong to the other sublattice), $U > 0$ (*i.e.*, repulsive Coulomb interaction) and $\mu \leq 0$ ($\mu < 0$ correspopnds to less than half-filling; $\mu = 0$ corresponds to the half-filled band case; the $\mu > 0$ case is isomorphic to the $\mu < 0$ one).

Since only a few rigorous results for this model are available, several approaches have been applied in an attempt to understand its general properties, in particular its finite temperature phase diagram. However, there is no agreement on the general structure of the phase diagram obtained through different approximate methods; in particular, a controversy exists about the existence of a ferromagnetic state at either vanishing or finite temperatures. Self-consistent methods [4,6] predict, for the $d = 3$ model, the existence of a ferromagnetic phase at finite temperature for high values of U/t, at least close to near half-filling. On the other hand, high-temperature expansions [7] in the $d \to \infty$ limit exhibit no evidence of a ferromagnetic phase transition for any value of the electronic density.

Here we calculate the finite temperature phase diagram of the $d = 2$ and $d = 3$ Hubbard model by means of a quantum real space renormalization group (RG) method (see [9] and references therein). In the present approximation d-dimensional hipercubic Bravais lattices are replaced by diamond-like hierarchical lattices (whose fractal dimensionality equals d), namely, those generated through infinite iterations of two-terminal clusters like those shown in Fig. 1. The RG recurrence equations are obtained by computing the partial trace

$$\exp(\mathcal{H}'+\mathcal{C}) = \operatorname*{Tr}_{internal\ sites} \exp(\mathcal{H}) \tag{2}$$

where $\mathcal{H}$ denotes the Hamiltonian of the cluster under consideration and $\mathcal{H}'$ denotes the Hamiltonian of the renormalized two-site cluster (see Fig. 1). The partial trace is calculated by summing the matrix elements of $\exp(\mathcal{H})$ over the set of occupation numbers $\{n_{i,\sigma}\}$ associated with the internal sites of the cluster. This procedure neglects, at every RG iteration, the non-commutativity between the Hamiltonians associated with the neighboring clusters. This approximation is a high temperature one. In fact, it is asymptotically exact at infinite temperature and believed to be a good approximation even at low temperatures [9]. In particular the relation (2) does not preserve the form of the Hamiltonian (1), in other words, if $\mathcal{H}$ is the standard Hubbard Hamiltonian then the resulting $\mathcal{H}'$ contains terms that were not present in $\mathcal{H}$. In a previous work [8] we derived a generalized Hubbard Hamiltonian whose form is preserved by the RG transformation (2) and which contains the Hubbard model as a particular case. This generalized Hamiltonian is given by

$$\begin{aligned}
\mathcal{H}_G^{\mu} = \quad & t\sum_{\langle i,j\rangle,\sigma}\left(c_{i,\sigma}^{\dagger}c_{j,\sigma}+c_{j,\sigma}^{\dagger}c_{i,\sigma}\right)+\tfrac{1}{2}U\sum_{i}(S_i^z)^2+\mu\sum_{i,\sigma}n_{i,\sigma} \\
- \; & J\sum_{\langle i,j\rangle}\vec{S}_i.\vec{S}_j-K\sum_{\langle i,j\rangle}(S_i^z)^2\left(S_j^z\right)^2+Y\sum_{\langle i,j\rangle}\vec{\rho}_i.\vec{\rho}_j \\
- \; & I\sum_{\langle i,j\rangle}\left[\rho_i^z\rho_j^z-\left(\rho_i^x\rho_j^x+\rho_i^y\rho_j^y\right)\right]+R\sum_{\langle i,j\rangle}\left[(\rho_i^z)^2\rho_j^z+\left(\rho_j^z\right)^2\rho_i^z\right] \\
+ \; & D\sum_{\langle i,j\rangle,\sigma}\left(c_{i,\sigma}^{\dagger}c_{j,\sigma}+c_{j,\sigma}^{\dagger}c_{i,\sigma}\right)\left(n_{i,-\sigma}-n_{j,-\sigma}\right)^2 \\
+ \; & E\sum_{\langle i,j\rangle,\sigma}\left(c_{i,\sigma}^{\dagger}c_{j,\sigma}+c_{j,\sigma}^{\dagger}c_{i,\sigma}\right)n_{i,-\sigma}n_{j,-\sigma}
\end{aligned} \tag{3}$$

where the spin operators are defined by $\vec{S}_i \equiv \sum_{\alpha,\beta} c_{i,\alpha}^{\dagger}\vec{\sigma}_{\alpha,\beta}\, c_{i,\beta}$ ($\vec{\sigma}$ are the Pauli matrices and $\alpha, \beta = \uparrow, \downarrow$) and the charge operators by

$$\begin{aligned}
\rho_i^z &\equiv n_{i,\uparrow} + n_{i,\downarrow} - 1 \\
\rho_i^x &\equiv c_{i,\uparrow}^{\dagger} c_{i,\downarrow}^{\dagger} + c_{i,\downarrow} c_{i,\uparrow} \\
\rho_i^y &\equiv -i \left(c_{i,\uparrow}^{\dagger} c_{i,\downarrow}^{\dagger} - c_{i,\downarrow} c_{i,\uparrow} \right)
\end{aligned}$$

The Hamiltonian (3) is the *minimal* one that simultaneously contains the Hubbard Hamiltonian as a particular case and remains invariant under the RG transformation.

We then construct the recurrence equations between the set of parameters of $\mathcal{H}_G^{\mu}$ and that of $\mathcal{H}_G^{\mu\prime}$ by explicitly computing the partial trace (2). Since the calculation of $\exp(\mathcal{H}_G^{\mu})$ involves the diagonalization of very large matrices, part of the calculations was done numerically. A detailed analysis of the RG procedure and of the structure of the Hamiltonian (3) is given in Ref. [9]; the RG flow in the $\mu = R = E = Y = 0$ invariant subspace of the parameter space $(\mu, K, J, U, I, Y, R, t, D, E)$ was analyzed for $d = 2$ and $d = 3$. The RG flow in the full parameter space provides a very complex phase diagram; we present here the $K = J = I = Y = R = D = E = 0$ section of it (*i.e.*, the phase diagram in the (μ, U, t) space). The results are presented in terms of the temperature-independent variables U/t, μ/t and the dimensionless temperature $1/t$. We only consider here the case of *less* or equal than half-filling, *i.e.*, $0 < n < 1$, where $n \equiv \sum_{i,\sigma} n_{i,\sigma}/\mathcal{N}$ and $\mathcal{N}$ is the number of lattice sites. As already mentioned, this case corresponds to $\mu \leq 0$. The phase diagram for $\mu > 0$ is obtained by reflection on the $\mu = 0$ axis through the standard particle-hole exchange transformation.

First of all, we observe that for $U > 0$, all points in the (μ, U, t) parameter space are driven (after a few RG steps) towards the region $U \to \infty$, whereas $\mu + U/2$ as well as $K, J, I, Y, R/t, D$ and E remain finite. In this limit, the states of the configuration space with at least one doubly occupied site, (*i.e.*, which satisfy $n_{i,\uparrow} n_{i,\downarrow} = 1$), do not contribute to the energy. In fact, in this $U \to \infty$ limit we obtain that: *(i)* the only remaining hopping processes will be those which only connect sites with zero or single occupancy; *(ii)* the non-diagonal charge operators ρ_i^x, ρ_i^y will not contribute at all. It can be seen that these two conditions yield, through the RG iterations,

$$D = E = -t \tag{4}$$

$$I = -Y \tag{5}$$

Finally, $n_{i,\uparrow} n_{i,\downarrow} = 0$ for all sites i implies

$$(\rho_i^z)^2 = -\rho_i^z = 1 - (S_i^z)^2 \tag{6}$$

$$(S_i^z)^2 = n_{i,\uparrow} + n_{i,\downarrow} \tag{7}$$

Applying the conditions (4)-(7) to the Hamiltonian (3) in the $U \to \infty$ limit (with fixed $\mu + U/2$) we find that the RG flow is governed by the following effective Hamiltonian (which acts on the configuration space with no doubly occupied sites):

$$\begin{aligned}\mathcal{H} \approx \quad & t \sum_{\langle i,j\rangle,\sigma} (1 - n_{i,-\sigma}) \left(c_{i,\sigma}^\dagger c_{j,\sigma} + c_{j,\sigma}^\dagger c_{i,\sigma}\right) (1 - n_{j,-\sigma}) \\ - \; & J \sum_{\langle i,j\rangle} \vec{S}_i.\vec{S}_j - \bar{K} \sum_{\langle i,j\rangle} (S_i^z)^2 \left(S_j^z\right)^2 + \overline{\mu} \sum_{i,\sigma} n_{i,\sigma}\end{aligned} \tag{8}$$

where, for the hierarchical lattices we are using here,

$$\overline{K} \equiv K + 2\,R + I \tag{9}$$

$$\overline{\mu} \equiv 2\,I + 4\,R + \tfrac{1}{2} U + \mu \tag{10}$$

The Hamiltonian (8) is a generalization of the tJ model, which in turn constitutes a strong coupling version of the Hubbard model (1) [10,11]. Consequently, all the critical properties of the Hubbard model will be determined by the RG flow in the $(\overline{\mu}, \overline{K}, J, t)$ parameter space. We have recently performed [12] the RG analysis of the full phase diagram corresponding to the Hamiltonian (8). So, we will not discuss here the general fixed point structure of the associated phase diagram (which in turn determines the structure of the phase diagram of the Hubbard model): see [12] for details.

We now discuss the $d = 2$ phase diagram. No long-range magnetic order exists in $d = 2$, because of the continuous symmetry of the magnetic interactions present in the Hamiltonian (8). We find that most of the points in the (μ, U, t) parameter space are attracted by one or the other of the following fully-stable fixed points: $(\overline{\mu}, \overline{K}, J, t) = (-\infty, 0, 0, 0)$ and $(+\infty, 0, 0, 0)$. The first fixed point is associated with a *paramagnetic hole-rich* (Ph) region, *i.e.*, low density of electrons ($n \ll 1$), while the second fixed point is associated with a *paramagnetic electron-rich* (Pe) region, *i.e.*, high density of electrons ($n \approx 1$). All points located at the frontier of these two sets of points are attracted by the semi-stable fixed point $(\overline{\mu}, \overline{K}, J, t) = (0, 0, 0, 0)$ [12]. The linearized recurrence equations at this fixed point provide eigenvalues which are smaller than unity, excepting one which equals l^d ($l = 3$ for the present case). Therefore, no real phase transition exists between the Ph and Pe regimes; in fact both describe one and the same paramagnetic phase. Indeed, passing through the above described frontier corresponds to an abrupt, but continuous, change in the electronic density n. We performed several calculations for a wide range of the U/t parameter, finding no evidence for a phase transition. The same result was encountered for the tJ model at low values of J/t [12], where such model is equivalent to the $U/t \gg 1$ Hubbard one. The present results suggest that the same behavior occurs for arbitrary values of U/t. Monte Carlo calculations [13] also support this assumption.

At $d = 3$ we find two new phases. Besides the above described paramagnetic phase (Ph or Pe) two long-range magnetically ordered phases appear: an antiferromagnetic (AF) phase and a ferromagnetic (F) one, respectively governed by the fully stable fixed points $(+\infty, K_2^A, J_2^A, 0)$ and $(+\infty, +\infty, -\infty, 0)$, with $J_2^A = 2.475$; $K_2^A = -18.78$. Each of these two magnetic phases undergoes , at finite temperature, a *second* order phase transition (we recall that the corresponding phase transitions appearing in the tJ model can be *first* order ones [12]) to the paramagnetic phase (in fact, to the Pe region). The AF-P and F-P critical surfaces are respectively governed by the fixed points $(+\infty, K_c^A, J_c^A, 0)$ and $(+\infty, K_c^F, J_c^F, 0)$, with $J_c^A = 0.353$; $K_c^A = -0.001$; $J_c^F = -0.522$; $K_c^F = 0.328$; the corresponding correlation length critical exponents are $\nu_{AF} = 1.241$ and $\nu_F = 1.522$ [12].

As in the $d = 2$ case we find no evidence for a phase transition between the Pe and Ph regimes at finite temperatures. In Fig. 2 we show the phase diagram in the $(\mu/t, U/t)$ space for typical values of the temperature $1/t$; in Fig. 3 we show the phase diagram in the $(\mu/t, 1/t)$ space for typical values of U/t. Although strictly speaking no AF-Ph (or F-Ph) phase transitions exist, these two phases can be extremely close (see figures 2 and 3). Therefore, these phase transitiona can be followed through a fast decrease in the density n. In Fig. 2a we see that the F phase disappears for low values of U/t. This result agrees with the interpretation of ferromagnetism in terms of Nagaoka's ferromagnetic polarons [2,14]. Consistently, the phase diagram obtained by self-consistent methods like SDA ("spectral-density-aproach") [4] at zero temperature presents a critical value of U/t below which there is no ferromagnetism. Also our low temperature results (see Fig. 2a) exhibit a remarkable fact, namely, the existence of a paramagnetic region (Pe) between the F and AF phases. It cannot be excluded that the P region shrinks to zero for $1/t \to 0$, but we believe this is not the case. Unfortunately, numerical errors in the diagonalization procedure make extremely difficult to get accurate results at very low temperatures ($1/t < 0.1$), so we cannot fully check the $1/t \to 0$ limit. In addition to this, such low temperatures are outside the range where the present approach is reasonably reliable. On the other hand, the general characteristics of the fixed point associated to the Pe phase ($U = +\infty$, $\mu = +\infty$) are indicative of a high degree of localization. Then, such region could be due to the presence of disordered local moments in the ground state. Indeed, this assumption is supported by other approximate results [15].

Let us finally mention that the same RG equations we have used here for the $U > 0$ region are perfectly adequate for discussing the $U < 0$ one; the corresponding phase diagram is also expected to be a very rich one and deserves a study by itself.

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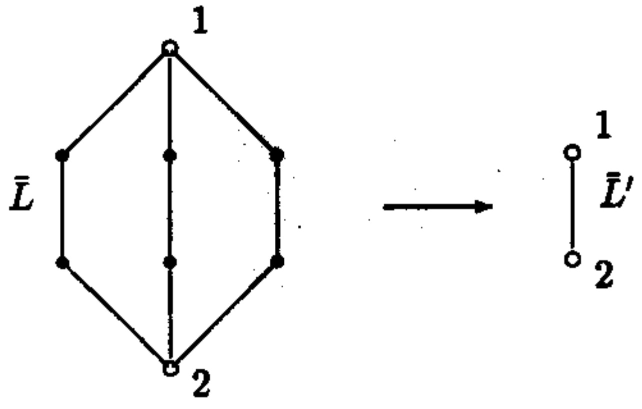
Figure Captions

Fig. 1: Renormalization group cell transformation. Every two-rooted cluster generates, through infinite iterations, an hierarchical lattice of intrinsic dimensionality d. $\bar{L}$ stands for the set of parameters of the Hamiltonian; ∘ and • respectively denote internal and terminal sites. (a) $d = 2$; (b) $d = 3$.

Fig. 2: Phase diagram of the $d = 3$ Hubbard model for constant $1/t$. Solid lines corresponds to second order phase transitions; dotted lines corresponds to a smooth continuation between the paramagnetic electron-rich (Pe) and hole-rich (Ph) regions; AF and F stand respectively for antiferromagnetic and ferromagnetic. (a) $1/t = 0.2$; (b) $1/t = 0.5$.

Fig. 3: Phase diagram of the $d = 3$ Hubbard model for constant U/t (see caption of Fig. 2). (a) $U/t = 2.5$; (b) $U/t = 4.5$.

(a)



(b)

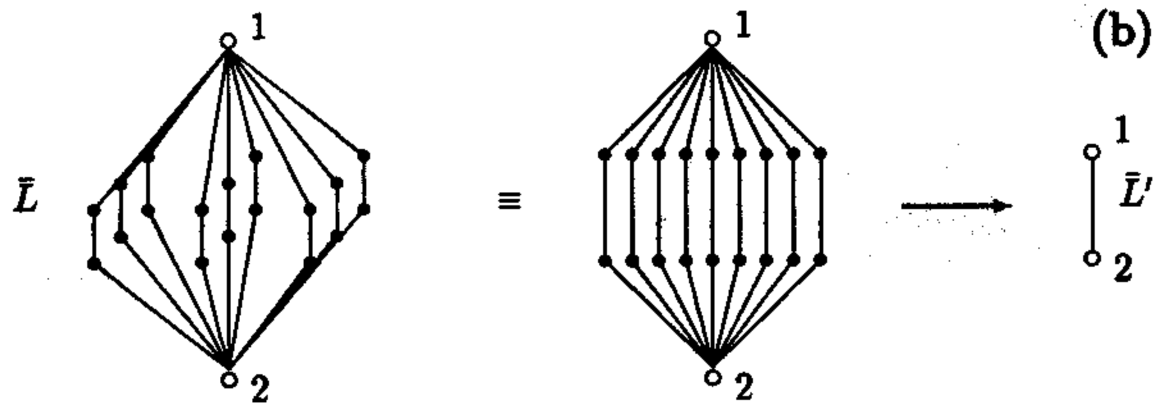


Figure 1

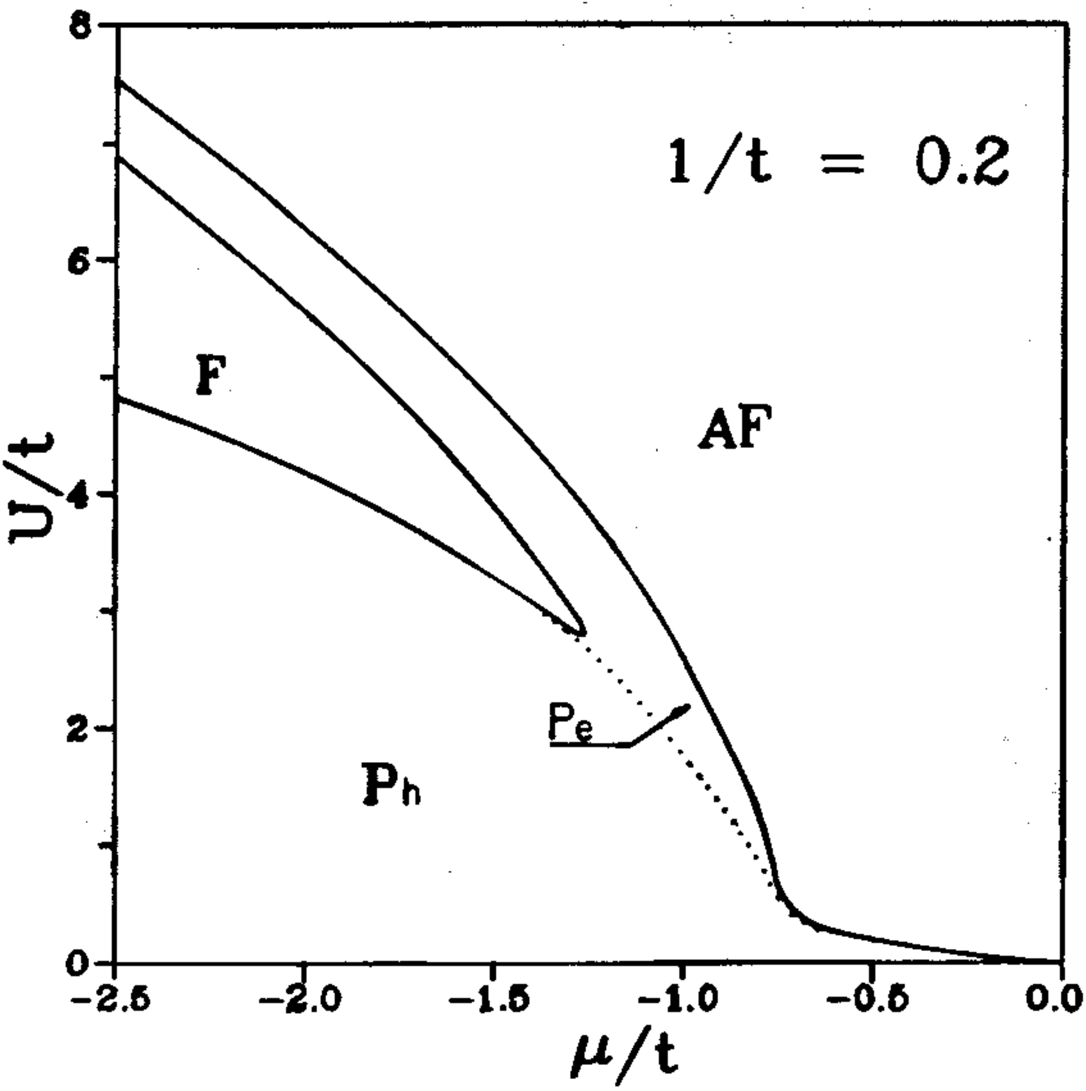


Figure 2a

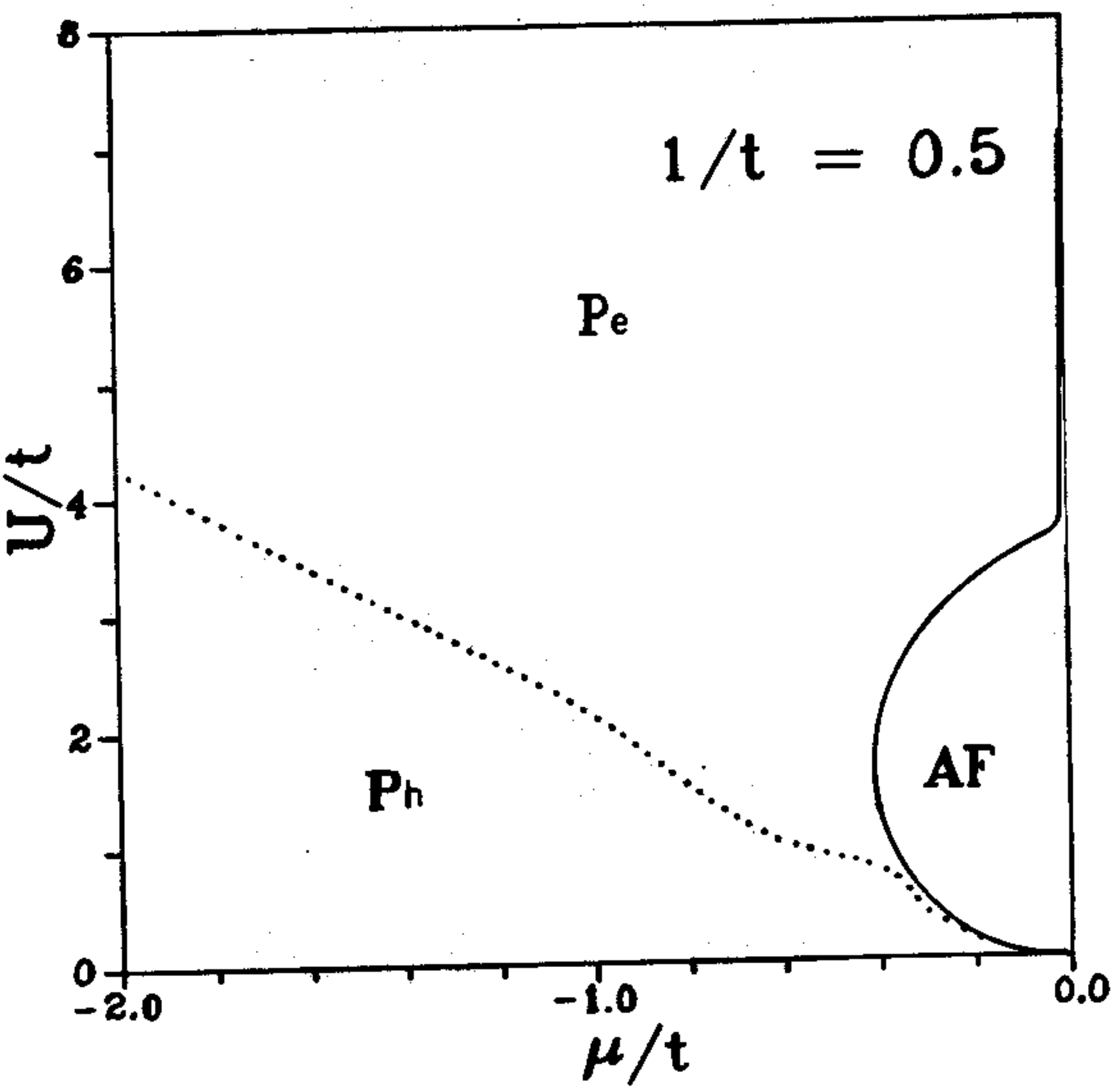


Figure 2b

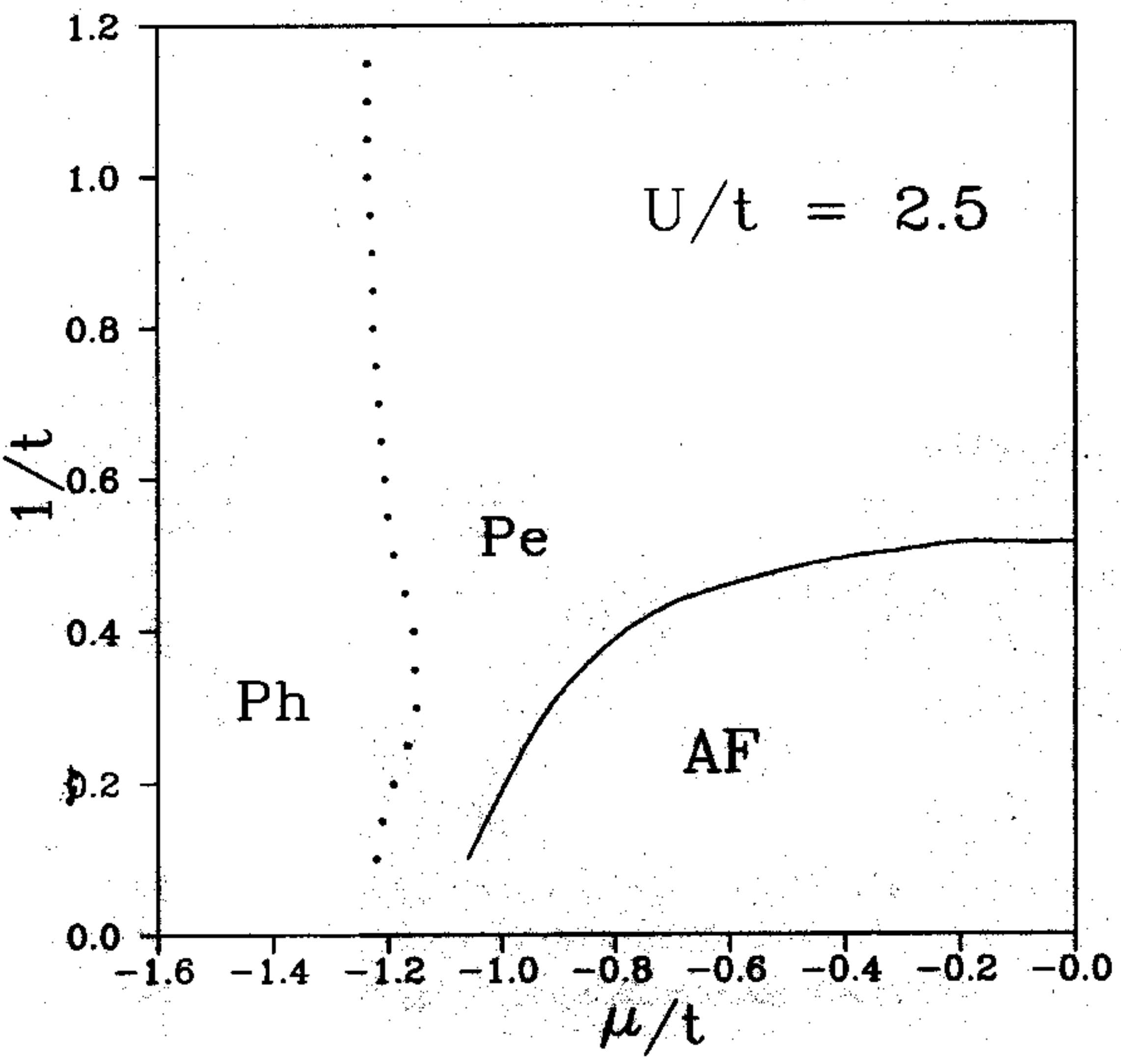


Figure 3a

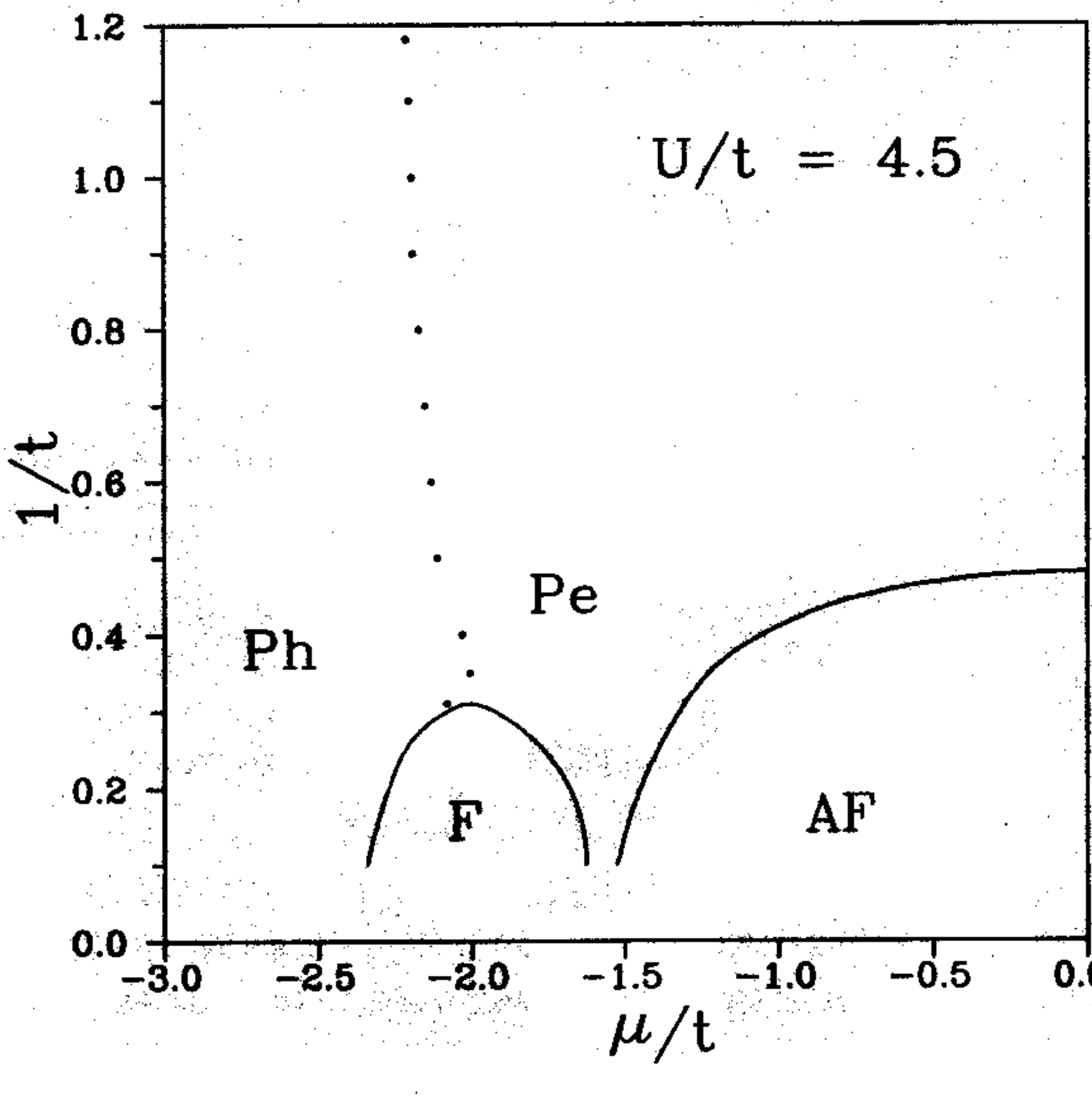


Figure 3b

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