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The Hubbard model, spin degeneracy and Ising spins

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ABSTRACT

The Hubbard model is used as a starting point for a study of an electronic system with spin $\frac{1}{2}$. Using a functional integral representation at half-filling it is demonstrated that the spin degeneracy is equivalent to dynamic Ising spins coupled to the fermions. A magnetic phase transition of the model is related to a transition of the Ising spins from a paramagnetic to an antiferromagnetic phase. A metal–insulator transition in the paramagnetic phase can be described within this approach by the Green’s function of non-interacting fermions, coupled to Ising spins. This picture is compared with the earlier Ising spin representation of the Hubbard model by Hirsch and discussed in terms of a small hopping amplitude.

§ 1. INTRODUCTION

The Hubbard model was originally constructed to describe a metal–insulator transition for spin-dependent fermions (Hubbard 1959, Fradkin 1991, Rasetti 1991, Fulde 1993, Gebhard 1997). This transition reflects the competition between interaction and kinetic energy. The model is defined on a lattice, where the potential energy consists of a chemical potential and an on-site repulsion of fermions with opposite spin. The kinetic energy is given by a nearest-neighbour hopping. It turned out from a number of calculations that this model has a rich structure because of the complicated interplay of charge and spin degrees of freedom. For instance, mean-field calculations for a magnetic order parameter indicate paramagnetic, ferromagnetic and antiferromagnetic states for the half-filled system (Fradkin 1991). Thus, the magnetic properties of the model became a central subject of investigations in solid-state physics.

The metal–insulator transition was discussed originally by Hubbard (1959) using self-consistent approximations, later in terms of a variational approach (Gutzwiller 1965, Brinkman and Rice 1970) and in the limit of an infinite-dimensional lattice (Metzner and Vollhardt 1993, Gebhard 1997). Very interesting investigations were obtained from computer simulations which indicate an insulating phase at half-filling for sufficiently strong fermion interaction (Hirsch 1987, Scalettar *et al.* 1989, Assaad and Imada 1996, Staudt *et al.* 2000).

To study the metal–insulator transition, one can, in principle, start either from the metallic or from the insulating side. As the simplest approximations, one could use non-interacting fermions on the metallic side or the local limit on the insulating side, where the hopping rate is zero. Unfortunately, neither of these starting points is very useful in order to understand the interacting Hubbard model; non-interacting

fermions are unstable against an arbitrarily weak interaction (Fradkin 1991), and the local limit of the half-filled states are completely degenerate with respect to the spin, that is the spins represent a paramagnetic state. Therefore, an arbitrarily weak hopping rate would lift the degeneracy, leading to a new state that might be magnetically ordered (Tasaki 1998). The main idea of this work is to start from the extreme insulating state at low temperatures and to study the degeneracy with respect to the spin. The most interesting is the case of a grand canonical ensemble, described by the partition function $Z = \text{Tr} [\exp (-\beta H)]$, where on average one fermion per site (half-filled system) is considered. Static fermions (i.e. fermions without a hopping term) have a 2^M degeneracy (M is the number of lattice sites) because each site can accommodate a fermion with spin up or a fermion with spin down. Consequently, a perturbation theory around one of these limiting states is plagued by degeneracies. For instance, a spontaneous hop of a fermion from a site to one of its nearest-neighbour sites in a half-filled state creates spontaneously a doubly occupied site and an empty site. The doubly occupied site may decay again into two singly occupied sites. The resulting state is twofold degenerate because of the possible two spin orientations (figure 1). If the unperturbed state is an antiferromagnetic (Néel) state, a hopping process at a time t_1 in terms of the expansion of Z can exchange two neighbouring fermions that leads to two pairs of neighbouring fermions with parallel spins. At time t_2 the inverse hopping process can recreate the original antiferromagnetic state. Therefore, the two hopping processes are not independent. Since the intermediate state between time t_1 and t_2 has the same energy as the antiferromagnetic state, there is a constant interaction in time. Consequently, the linked cluster theorem cannot be applied, since it works only for independent clusters or clusters which interact with a decaying interaction (Brydges 1986, Glimm and Jaffe 1987). The central point of this work is the development of a method that deals with the degeneracy.

In order to control the exponential spin degeneracy it is natural to eliminate one spin orientation. This can be achieved formally by integrating out one of the spin orientations, for example \uparrow , in the functional integral representation of the Hubbard

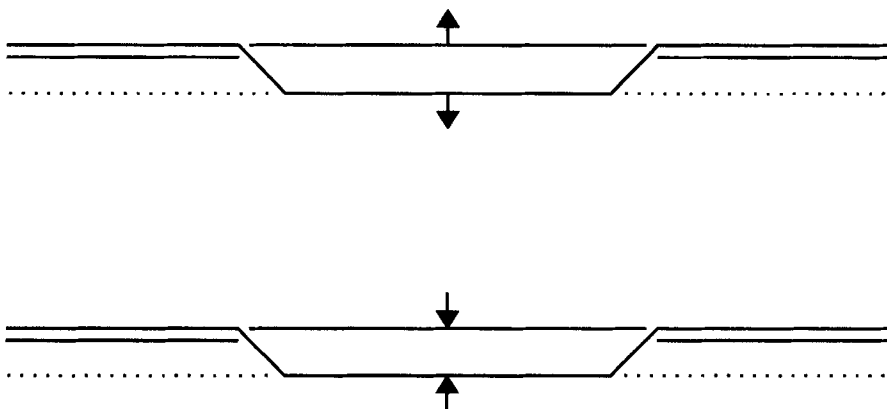


Figure 1. Decay of a doubly occupied site in two electrons with spin \uparrow and \downarrow has a twofold degeneracy. The re-creation of the doubly occupied site connects the two related hopping events by a degenerate interaction.

model. The resulting fermion determinant of spin \uparrow can be decomposed by a space–time lattice partition. The result of this operation reveals an important structure of the effective spinless fermion model which is formally an expansion of the model in terms of the degeneracy; the partitions are not degenerated, and the hopping expansion can be applied independently to each of them. It turns out that the expansion is equivalent to the summation over the 2^M states of Ising spins at each time step. After an approximation which is applicable to the regime of a small hopping amplitude in the Hubbard model, the remaining fermionic degrees of freedom can be integrated out. Thus, the physics are described by the Ising spins, where the strongly interacting regime is characterized by an antiferromagnetic Ising structure.

The article is organized as follows. In §2 the Hubbard model is defined in a coherent state representation for a grand canonical ensemble of fermions. The static limit (no hopping) and the formal hopping expansion of the Hubbard model are discussed in §3. Then in §4.1 the decoupling of the electron–electron interaction by a Hubbard–Stratonovich transformation is briefly reviewed. In §4.2 the integration over the spin-up component of the model is performed. The resulting model is analysed in §4.3, using the lattice partition and the related Ising spin representation. In §5 the new effective Ising–fermion model is discussed in terms of a hopping expansion. Appendixes A and B give details of the calculations.

§ 2. THE HUBBARD MODEL

The Hubbard model describes fermions with spin $\sigma = \downarrow, \uparrow$ on lattice λ of dimensionality d . It is defined by the Hamiltonian (Fradkin 1991, Gebhard 1997)

$$H = -\bar{t} \sum_{\langle r, r' \rangle, \sigma} c_{\sigma, r}^\dagger c_{\sigma, r'} + \sum_r \left(\mu \sum_\sigma c_{\sigma, r}^\dagger c_{\sigma, r} + U c_{\uparrow, r}^\dagger c_{\uparrow, r} c_{\downarrow, r}^\dagger c_{\downarrow, r} \right), \quad (1)$$

where $c_{\sigma, r}^\dagger$ and $c_{\sigma, r}$ are fermion creation and annihilation operators respectively. $\bar{t} \geq 0$ is the hopping rate. $\langle r, r' \rangle$ means pairs of nearest-neighbour sites on the lattice and μ is the chemical potential.

Using this Hamiltonian a grand canonical ensemble of fermions at the inverse temperature β can be defined by the partition function, given in terms of a functional integral (coherent state representation) on a Grassmann algebra (Negele and Orland 1988). For the latter the integration over a complex Grassmann field $(\Psi_\sigma(r, t), \bar{\Psi}_\sigma(r, t))$ is given as a linear mapping from a Grassmann algebra to the complex numbers. At a space–time point (r, t) we have for integers $k, l \geq 0$

$$\int [\bar{\Psi}_\sigma(r, t)]^k [\Psi_\sigma(r, t)]^l d\Psi_\sigma(r, t) d\bar{\Psi}_\sigma(r, t) = \delta_{k, l} \delta_{l, 1}.$$

The partition function $\text{Tr}[\exp(-\beta H)]$ of the grand canonical ensemble of fermions then is

$$Z = \int \exp(-S) \mathcal{D}[\Psi_\uparrow, \Psi_\downarrow], \quad (2)$$

with the action

$$S = \sum_{r, t} \bar{\Psi}_\sigma(r, t) [\Psi_\sigma(r, t) - \Psi_\sigma(r, t - \Delta)] + \Delta \sum_t H[\bar{\Psi}_\sigma(r, t), \Psi_\sigma(r, t - \Delta)] \quad (3)$$

and the product measure

$$\mathcal{D}[\Psi_{\uparrow}, \Psi_{\downarrow}] = \prod_{r,t,\sigma} d\Psi_{\sigma}(r,t) d\bar{\Psi}_{\sigma}(r,t).$$

The discrete time is used with $t = \Delta, 2\Delta, \dots, \beta$, implying that the limit $\Delta \rightarrow 0$ has to be taken in the end. $\bar{\Psi}_{\sigma}(r,t)$ and $\Psi_{\sigma}(r,t)$ are independent Grassmann fields which satisfy antiperiodic boundary conditions in time $\Psi_{\sigma}(r, \beta + \Delta) = -\Psi_{\sigma}(r, \Delta)$ and $\bar{\Psi}_{\sigma}(r, \beta + \Delta) = -\bar{\Psi}_{\sigma}(r, \Delta)$. For the subsequent calculations it is convenient to rename $\Psi_{\sigma}(r,t) \rightarrow \Psi_{\sigma}(r, t + \Delta)$ because then the Grassmann field appears with the same time in the Hamiltonian of the action (3).

§ 3. THE LOCAL LIMIT

Neglecting the hopping term in the Hamiltonian (i.e. for $\bar{t} = 0$), the integration in the partition function factorizes in space, and the corresponding expression can be evaluated as

$$Z = \int \prod_{r,t} \exp[-S_d(r,t)] \mathcal{D}[\Psi_{\uparrow}, \Psi_{\downarrow}] = \prod_r \int \prod_t \exp[-S_d(r,t)] \mathcal{D}[\Psi_{\uparrow}, \Psi_{\downarrow}] = Z_0^M, \quad (4)$$

where

$$S_d = \bar{\Psi}_{\sigma}(r,t) \Psi_{\sigma}(r, t + \Delta) - \bar{\mu} \bar{\Psi}_{\sigma}(r,t) \Psi_{\sigma}(r,t) + \Delta U \bar{\Psi}_{\uparrow}(r,t) \Psi_{\uparrow}(r,t) \bar{\Psi}_{\downarrow}(r,t) \Psi_{\downarrow}(r,t),$$

with $\bar{\mu} = 1 - \Delta\mu$. Z_0 is the partition function of the Hubbard model with one lattice site (static, local or atomic limit):

$$Z_0 = 1 + 2\bar{\mu}^{\beta/\Delta} + (\bar{\mu}^2 - \Delta U)^{\beta/\Delta} \sim 1 + 2 \exp(-\beta\mu) + \exp[-\beta(2\mu + U)] \quad (5)$$

for $\Delta \sim 0$. Using the new parameters $U' = \Delta U$ and $\beta' = \beta/\Delta$, we can define the following weights, depending on the number of particles per site

$$\begin{aligned} w_0 &= \frac{1}{Z_0}, \\ w_1 &= \frac{2\bar{\mu}^{\beta'}}{Z_0}, \\ w_2 &= \frac{(\bar{\mu}^2 - U')^{\beta'}}{Z_0}. \end{aligned}$$

Then the average number of particles per site is

$$n = w_1 + 2w_2.$$

At zero temperature ($\beta \rightarrow \infty$) and in the continuous-time limit $\Delta \rightarrow 0$ this gives the well-known result (Gebhard 1997)

$$n = \begin{cases} 0 & \text{if } 0 < \mu, \\ 1 & \text{if } -U < \mu < 0, \\ 2 & \text{if } \mu < -U. \end{cases}$$

3.1. Degenerate hopping expansion

If one assumes that $-U < \mu < 0$, the system has an average of one fermion per site. Then the projection on the singly occupied ground state yields for the partition function in the absence of hopping $Z_0 = 2\bar{\mu}^{\beta'}$. The factor 2 is the degeneracy of the (unperturbed) ground state because each singly occupied site can accommodate a fermion with either spin \uparrow or with spin \downarrow . This degeneracy must be handled with care. The expansion of $Z = \text{Tr}[\exp(-\beta H)]$ for $\mu = -U/2$ gives

$$Z = Z_0^M \left\{ 1 + \frac{dM\bar{t}^2}{\cosh^2(\beta U/4)} \left[\frac{\beta^2}{2} + \frac{\beta}{U} \sinh\left(\frac{\beta U}{2}\right) \right] + o(\bar{t}^3) \right\}$$

and for $\beta \approx \infty$

$$Z_0^M \left(1 + \frac{2dM\bar{t}^2\beta}{U} + o(\bar{t}^3) \right). \quad (6)$$

On the other hand, one can set up a non-degenerate perturbation theory expression

$$Z = \sum_{j=1}^{2^M} Z_j(\bar{t})$$

with

$$Z_j(\bar{t}) = Z_{0,j}^M [1 + \bar{t}^2 Z_j' + o(\bar{t}^3)]. \quad (7)$$

The unperturbed partition function is degenerate: $Z_{0,j} = \zeta$. For each of the non-degenerate states we can apply the linked cluster theorem (Glimm and Jaffe 1987) to write

$$Z_j(\bar{t}) = \zeta^M \exp[\bar{t}^2 Z_j' + o(\bar{t}^3)].$$

This gives eventually for the total partition function

$$Z = \zeta^M \sum_{j=1}^{2^M} \exp[\bar{t}^2 Z_j' + o(\bar{t}^3)]. \quad (8)$$

Naive exponentiation of equations (7) and (6) results in

$$Z = Z_0^M \exp\left(\frac{\bar{t}^2}{2^M} \sum_j Z_j' + o(\bar{t}^3)\right) = Z_0^M \exp\left(\frac{2dM\bar{t}^2\beta}{U} + o(\bar{t}^3)\right). \quad (9)$$

The exponent in equation (8) is a series of linked clusters due to the linked cluster theorem. In contrast, the exponent in equation (9) is a series of linked clusters averaged over the degenerate states. Subsequently, an expansion analogous to equation (8) will be derived.

§ 4. FERMIONS AND ISING SPINS

The aim of this section is to obtain a model for fermions coupled to Ising spins. As a first example, the decoupling of the electron-electron interaction by a Hubbard–Stratonovich transformation with dynamic Ising spins is briefly reviewed. Then a new approach is developed through the partition of the space–time lattice;

the summation over the lattice partitions is equivalent to the summation over the configurations of dynamic Ising spins. It turns out that this is also equivalent with the summation over degenerate states of the Hubbard model.

4.1. Hubbard–Stratonovich transformation: fermions coupled to Ising spins

It was observed some time ago that the fermion–fermion interaction of the Hubbard model can be represented by a dynamic Ising spin that couples to non-interacting electrons (Hirsch 1983). In terms of the functional integral (2) this fact is formally related to a Hubbard–Stratonovich transformation

$$\begin{aligned} & \exp[-\alpha \bar{\Psi}_{\uparrow}(r, t) \Psi_{\uparrow}(r, t) \bar{\Psi}_{\downarrow}(r, t) \Psi_{\downarrow}(r, t)] \\ &= \frac{1}{2} \sum_{S(r, t)=\pm 1} \exp\{-\alpha^{1/2} S(r, t) [\bar{\Psi}_{\uparrow}(r, t) \Psi_{\uparrow}(r, t) - \bar{\Psi}_{\downarrow}(r, t) \Psi_{\downarrow}(r, t)]\} \end{aligned}$$

with $\alpha = \Delta U$. In physical terms, the Ising spin $S(r, t)$ couples to the z component of the electron spin. Going back to the partition function Z , the latter becomes after integration over the Grassmann field

$$Z = \frac{1}{2^{M\beta/\Delta}} \sum_{\{S(r, t)=\pm 1\}} \det(G_0^{-1} - \alpha^{1/2} S) \det(G_0^{-1} + \alpha^{1/2} S), \quad (10)$$

with the Green's function G_0 of a free fermion (i.e. $U = 0$).

4.2. Integration over the spin-up field Ψ_{\uparrow}

An electron with spin \downarrow is considered in the ‘bath’ of the other electrons. For this purpose the Green's function $G(r, t; r', t') = \langle \Psi_{\downarrow}(r, t) \bar{\Psi}_{\downarrow}(r', t') \rangle$ can be studied under a systematic integration over the electrons with \uparrow . It will lead to an effective theory for the spin \downarrow electrons. In this case the action S can be divided into three pieces as

$$S = S_{\uparrow} + S_{\downarrow} + S_{\text{I}},$$

with

$$S_{\sigma} = \sum_t \left(\sum_r [\bar{\Psi}_{\sigma}(r, t) \Psi_{\sigma}(r, t + \Delta) - \bar{\mu} \bar{\Psi}_{\sigma}(r, t) \Psi_{\sigma}(r, t)] - \tau \sum_{\langle r, r' \rangle} \bar{\Psi}_{\sigma}(r, t) \Psi_{\sigma}(r', t) \right)$$

for $\sigma = \uparrow, \downarrow$ with $\tau = \Delta \bar{t}$. The interaction between the two spin orientations is given by

$$S_{\text{I}} = U' \sum_{r, t} \bar{\Psi}_{\uparrow}(r, t) \Psi_{\uparrow}(r, t) \bar{\Psi}_{\downarrow}(r, t) \Psi_{\downarrow}(r, t).$$

Now it is possible to integrate out the spin-up field Ψ_{\uparrow} , since it appears in S only as a quadratic form. The integration over this Grassmann field gives a determinant

$$\int \exp(-S_{\uparrow} - S_{\text{I}}) \prod_{r, t} d\Psi_{\uparrow}(r, t) d\bar{\Psi}_{\uparrow}(r, t) = \det(-\partial_t + \bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_{\downarrow} \Psi_{\downarrow}), \quad (11)$$

where ∂_t is the time-shift operator

$$\partial_t \Psi(r, t) = \begin{cases} \Psi(r, t + \Delta) & \Delta \leq t < \beta \\ -\Psi(r, \Delta) & t = \beta. \end{cases}$$

The last equation is due to the antiperiodic boundary condition of the Grassmann field. This definition gives

$$(\partial_t)^{-1} = \partial_t^T, \quad \det(-\partial_t) = 1.$$

The hopping matrix $\hat{\mathbf{t}}$ has elements $\hat{\mathbf{t}}_{r,r'} = \tau$ if r, r' are nearest neighbours and is zero otherwise. Expressions in the determinant which do not have a specified matrix structure are implicitly multiplied by the corresponding unit matrix. For instance, $\bar{\mu}$ is multiplied by the space-time unit matrix whereas $\hat{\mathbf{t}}$ is multiplied by the time-like unit matrix.

In the following subsets of the space-time lattice $\mathcal{A} = \lambda \otimes \{\mathcal{A}, 2\mathcal{A}, \dots, \beta\}$ will be considered. For a subset $\mathcal{A}_k \subset \mathcal{A}$ the determinant of the projected matrix $\mathbf{P}_k \mathbf{A} \mathbf{P}_k$ is defined as

$$\det_{\mathcal{A}_k} \mathbf{A} \equiv \det_{\mathcal{A}_k} (\mathbf{P}_k \mathbf{A} \mathbf{P}_k),$$

where \mathbf{P}_k is the projector on to \mathcal{A}_k .

4.3. Lattice partitions

The partition function is now a functional integral of the spin-down Grassmann field

$$Z = \int \exp(-S_\downarrow) \det(-\partial_t + \bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) \mathcal{D}[\Psi_\downarrow].$$

As shown in appendix A, the determinant can be expanded in terms of the partitions $\mathcal{A}_k \subseteq \mathcal{A}$ of the space-time lattice \mathcal{A} as

$$\begin{aligned} \det(-\partial_t + \bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) &= \sum_{\mathcal{A}_k \subseteq \mathcal{A}} \det_{\mathcal{A}_k} [-(\bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) \partial_t^T]. \\ &= \sum_{\mathcal{A}_k \subseteq \mathcal{A}} \det[\mathbf{1} - I_k - I_k(\bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) \partial_t^T I_k]. \end{aligned}$$

The partitions \mathcal{A}_k include the empty set which gives $\det_\emptyset \mathcal{A} = 1$. It is possible to express the projector $I_k(r, t) = 0, 1$ as $\mathbf{I}(r, t) = [1 + S(r, t)]/2$ with the Ising spin

$$S(r, t) = \begin{cases} 1, & r, t \in \mathcal{A}_k, \\ -1, & r, t \notin \mathcal{A}_k, \end{cases}$$

and to consider $\mathbf{I}(\{S(r, t)\})$ as a new field that couples to the fermion fields. This expansion is the most important step for the treatment of the Hubbard model in this work. The immediate consequence is that the partition function Z is now given by a summation over configurations of Ising spins as

$$Z = \sum_{\{S(r, t) = \pm 1\}} Z(\{S(r, t)\}),$$

with

$$Z(\{S(r, t)\}) = \int \exp(-S_\downarrow) \det[\mathbf{1} - \mathbf{I} - \mathbf{I}(\bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) \partial_t^T \mathbf{I}] \mathcal{D}[\Psi_\downarrow]. \quad (12)$$

The determinant in the integrand can be rewritten with the help of the Grassmann field Ψ_\uparrow as

$$Z(\{S(r, t)\}) = \int \exp(-S_{\text{IM}}) \mathcal{D}[\Psi_{\downarrow}, \Psi_{\uparrow}], \quad (13)$$

where the action is

$$S_{\text{IM}} = S_{\downarrow} - \bar{\Psi}_{\uparrow} [\mathbf{1} - \mathbf{I} + \mathbf{I}(\bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_{\downarrow} \Psi_{\downarrow}) \partial_t^T \mathbf{I}] \Psi_{\uparrow} \equiv S_{\downarrow} + S_{\uparrow\downarrow}. \quad (14)$$

The scalar product refers to space and time. An interpretation of the new action can be given in terms of random walks (Glimm and Jaffe 1987); particles with \downarrow propagate with the propagator given in S_{\downarrow} . The second term $S_{\uparrow\downarrow}$ describes the propagation of the particles with \uparrow . It is crucial for the understanding of the absence of degeneracies that there is no term diagonal in time on A_k due to the factor ∂_t^T .

Equation (14) can be used as a starting point for a hopping expansion or an expansion in powers of U . For the latter one can expand S_{IM} and obtain in first order in the action

$$S_{\text{IM}} \approx S_{\downarrow} - \bar{\Psi}_{\uparrow} [\mathbf{1} - \mathbf{I} - \mathbf{I}(\bar{\mu} + \hat{\mathbf{t}} - U' g) \partial_t^T \mathbf{I}] \Psi_{\uparrow},$$

where $g = (-\partial_t + \bar{\mu} + \hat{\mathbf{t}})^{-1}(r, t, r, t)$. This can be evaluated in a self-consistent approach along the lines of the Hartree–Fock approximation (Fradkin 1991).

Thus, the summation over lattice partitions A_k is equivalent to a summation over configurations of Ising spins $\{S(r, t)\}$. Unfortunately, the Grassmann field Ψ_{\downarrow} couples to Ψ_{\uparrow} such that the integration over the Grassmann field in $Z(\{S(r, t)\})$ cannot be performed directly. From this point of view the Ising spin model introduced by Hirsch is simpler because the Grassmann field can be integrated out, as shown in equation (10). On the other hand, the advantage of the Ising spin from the lattice partition is the control of the degeneracy in terms of the hopping expansion.

§ 5. HOPPING EXPANSION

An advantage of the absence of degeneracies for a given realization of the Ising spins $\{S(r, t)\}$ is the possibility to apply the Linked Cluster Theorem (Glimm and Jaffe 1987) to $Z(\{S(r, t)\})$. This allows us to write

$$Z(\{S(r, t)\}) = \exp \left(\sum_{r, t} \sum_{\mathcal{C}(r, t)} f_{\mathcal{C}(r, t)}(\{S(r, t)\}) \right), \quad (15)$$

where $\mathcal{C}(r, t)$ is a connected cluster centred at r, t , $f_{\mathcal{C}(r, t)}$ is a function of all Ising spins on these clusters. It can be shown (Glimm and Jaffe 1987) that this function grows exponentially with the cluster size $|\mathcal{C}(r, t)|$ and is proportional to $\bar{t}^{|\mathcal{C}(r, t)|}$. Therefore, the function can be controlled if \bar{t} is sufficiently small. Equation (15) represents an Ising model with cluster interaction in space and time. The leading term is of order \bar{t}^2 , including two hoppings. Using the expression $Z(\{S(r, t)\})$ in equation (13), we begin with the Ψ_{\uparrow} integral

$$\int \exp(-S_{\uparrow\downarrow}) \mathcal{D}[\Psi_{\uparrow}]. \quad (16)$$

$S_{\uparrow\downarrow}$ is diagonal in time if $\Psi_{\uparrow}(r, t - \Delta)$ is renamed as $\Psi_{\uparrow}(r, t)$ on A_k :

$$\begin{aligned} S_{\uparrow\downarrow} = & - \sum_{r, t} [1 - \mathbf{I}(r, t)] \bar{\Psi}_{\uparrow}(r, t) \Psi_{\uparrow}(r, t) \\ & - \sum_{r, r', t} \bar{\Psi}_{\uparrow}(r, t) \mathbf{I}(r, t) \{ [\bar{\mu} - U' \bar{\Psi}_{\downarrow}(r, t) \Psi_{\downarrow}(r, t)] \delta_{r, r'} + \hat{t}_{r, r'} \} \mathbf{I}(r', t - \Delta) \Psi_{\uparrow}(r', t). \end{aligned}$$

Equation (16) can be expanded in terms of the hopping matrix $\hat{\mathbf{t}}$, and then the integration over Ψ_{\uparrow} can be performed, leading to

$$I_1 \left(1 + \sum_{t,t',r,r'} \mathbf{I}(r,t) \mathbf{I}(r',t) \langle \bar{\Psi}_{\uparrow}(r,t) \hat{\mathbf{t}}_{r,r'} \Psi_{\uparrow}(r',t) \bar{\Psi}_{\uparrow}(r',t') \hat{\mathbf{t}}_{r',r} \Psi_{\uparrow}(r,t') \rangle_0 \right) + o(\bar{t}^3), \quad (17)$$

with

$$I_1 = \prod_{r,t \in A_k} [\bar{\mu} - U' \bar{\Psi}_{\downarrow}(r,t) \Psi_{\downarrow}(r,t)] = \prod_{r,t \in A_k} \bar{\mu} \exp \left(- \frac{U' \bar{\Psi}_{\downarrow}(r,t) \Psi_{\downarrow}(r,t)}{\bar{\mu}} \right).$$

Here it has been used that, for a given site r , $\mathbf{I}(r,t) \neq 0$ for all t , otherwise the expectation value

$$I_1 \langle \dots \rangle_0 = \int \dots \exp \left(\sum_{r,r',t} \bar{\Psi}_{\uparrow}(r,t) \mathbf{I}(r,t) [\bar{\mu} - U' \bar{\Psi}_{\downarrow}(r,t) \Psi_{\downarrow}(r,t)] \mathbf{I}(r',t - \Delta) \Psi_{\uparrow}(r',t) \right) \mathcal{D}[\Psi_{\uparrow}]$$

would vanish. Thus, $\mathbf{I}(r,t)$ depends in this approximation only on r and can be replaced by $\mathbf{I}(r)$. The expression in (17) can also be written as

$$I_1 \left(1 - \sum_{t,t',r,r'} \mathbf{I}(r) \mathbf{I}(r') \hat{\mathbf{t}}_{r,r'} \hat{\mathbf{t}}_{r',r} \langle \bar{\Psi}_{\uparrow}(r,t) \Psi_{\uparrow}(r,t') \rangle_0 \langle \bar{\Psi}_{\uparrow}(r',t') \Psi_{\uparrow}(r',t) \rangle_0 \right). \quad (18)$$

Since $\langle \bar{\Psi}_{\uparrow}(r,t) \Psi_{\uparrow}(r,t') \rangle_0 \propto \delta_{t,t'}$ because the quadratic form in Ψ_{\uparrow} is diagonal in time, one of the summations over time drops out. Consequently, the remaining summation provides a factor β/Δ but the two hopping factors are proportional to Δ^2 . Therefore, equation (18) is of the order of Δ . As will be seen later (appendix B), the corresponding hopping term from the Ψ_{\downarrow} integration is of the order of Δ^0 . Thus, we have

$$\int \exp(-S_{\uparrow\downarrow}) \mathcal{D}[\Psi_{\uparrow}] \sim I_1 \quad (19)$$

or

$$Z \approx \sum_{\{S_r\}} \bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_1) \mathcal{D}[\Psi_{\downarrow}], \quad (20)$$

where the factor I_1 has been absorbed in the effective action of electrons with \downarrow :

$$S'_1 = S_{\downarrow} + \frac{U'}{\bar{\mu}} \sum_{r,t} \mathbf{I}(r) \bar{\Psi}_{\downarrow}(r,t) \Psi_{\downarrow}(r,t) \equiv \bar{\Psi}_{\downarrow} \left(\partial_t - \bar{\mu} - \hat{\mathbf{t}} + \frac{U'}{\bar{\mu}} \mathbf{I} \right) \Psi_{\downarrow}.$$

After performing the Ψ_{\downarrow} integration in the local limit $\bar{t} = 0$ of equation (20) the result agrees with equation (5).

The Green's function

$$G_{\downarrow}(r,t;r',t') = \langle \Psi_{\downarrow}(r,t) \bar{\Psi}_{\downarrow}(r',t') \rangle$$

can be written in this approximation and the limit $\Delta \rightarrow 0$ as the matrix

$$\mathbf{G}_{\downarrow} = \frac{\sum_{\{S_r\}} (-\partial/\partial t - \mu + \bar{t}h - \mathbf{I}U)^{-1} \bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_1) \mathcal{D}[\Psi_{\downarrow}]}{\sum_{\{S_r\}} \bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_1) \mathcal{D}[\Psi_{\downarrow}]}$$

with the hopping matrix $h_{r,r'} = 1$ for nearest neighbours r, r' and $h_{r,r'} = 0$ otherwise. This expression can be understood as the averaged resolvent

$$\left\langle \left(-\frac{\partial}{\partial t} - \mu + \bar{t}\mathbf{h} - \mathbf{I}U \right)^{-1} \right\rangle_{\text{Ising}}, \quad (21)$$

where the average $\langle \dots \rangle_{\text{Ising}}$ is taken with respect to the distribution

$$P(\{S_r\}) = \frac{\bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_r) \mathcal{D}[\Psi_\downarrow]}{\sum_{\{S_r\}} \bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_r) \mathcal{D}[\Psi_\downarrow]}. \quad (22)$$

In a final step the integral over Ψ_\downarrow has to be performed. It is convenient to do that again in a hopping expansion. The result for $\mu = -U/2$ and large β is (see appendix B)

$$P(\{S_r\}) = \frac{\exp[-\beta(\bar{t}^2/2U) \sum_{\langle r,r' \rangle} S_r S_{r'} + o(\bar{t}^3)]}{\sum_{\{S_r\}} \exp[-\beta(\bar{t}^2/2U) \sum_{\langle r,r' \rangle} S_r S_{r'} + o(\bar{t}^3)]}. \quad (23)$$

5.1. The antiferromagnetic phase

The distribution (23) is the Boltzmann weight of a classical Ising model with nearest-neighbour antiferromagnetic coupling \bar{t}^2/U . This model has an antiferromagnetic phase in dimensions $d \geq 2$ if the temperature T is $T < T_c$. The critical temperature is

$$T_c \propto \frac{\bar{t}^2}{U}.$$

For $T > T_c$ the Ising spins are in a paramagnetic phase. The phase boundary is qualitatively the same as that obtained from the Heisenberg model (Fulde 1993, Gebhard 1997). It will be discussed subsequently that the antiferromagnetic phase creates a gap for the fermions, whereas the paramagnetic phase creates a (correlated) disorder potential for the fermions.

5.2. The metal-insulator transition

The metal-insulator transition in the paramagnetic regime (Hirsch 1987, Scalettar *et al.* 1989, Gebhard 1992, Staudt *et al.* 2000) can now be seen in the Green's function of free fermions, coupled to the fluctuating Ising spins, given in equation (21). Formally, it represents a criterion for insulating versus metallic behaviour of the Hubbard model in a form of an average Green's function; an exponential decay of \mathbf{G} corresponds with insulating and a non-exponential decay with metallic (i.e. diffusive) behaviour. Although this looks similar to the problem of Anderson localization, where non-interacting electrons live in a random potential, there are two major differences. Firstly, the criterion for metallic versus insulating behaviour in the case of the Hubbard model is given by the one-particle Green's function whereas the criterion for localization versus delocalization in the case of Anderson localization is the two-particle Green's function (Lee and Ramakrishnan 1985). Secondly, the distribution of the random variables is more complicated in the case of the Hubbard model because they (i.e. the Ising spins) are correlated and can form an antiferromagnetic state at low temperatures. These correlations do not exist

for the random potential in the models of Anderson localization. An important consequence is the generation of a gap at low temperatures ($\beta \bar{t}^2/U \gg 1$) when the Ising spins order antiferromagnetically. Then the maximal contribution to Z comes from $S_r = -S_{r'}$ on nearest-neighbour sites r, r' . This describes an antiferromagnet state of the Ising spins with $S_r = (-1)^{r_1 + \dots + r_d}$. If V_{AFM} is the staggered antiferromagnetic potential in the limit $\Delta \rightarrow 0$ given by

$$V_{\text{AFM}} = -\frac{U}{2}(-1)^{r_1 + \dots + r_d},$$

the Green's function (21) is in frequency representation

$$(\mathrm{i}\omega + \bar{t}\mathbf{h} + V_{\text{AFM}})^{-1}.$$

There is a gap due to the staggered potential, implying an exponential decay of the Green's function \mathbf{G} . This can be seen, for instance, in the special case of a two-dimensional lattice. Then the eigenvalues of \mathbf{G}^{-1} are

$$\pm \left(\frac{U^2}{4} + \bar{t}^2 |h_{12}|^2 \right)^{1/2}$$

with $h_{12} = 1 + \exp(\mathrm{i}k_x) + \exp(\mathrm{i}k_y) + \exp(\mathrm{i}k_x + \mathrm{i}k_y)$ ($-\pi \leq k_j < \pi$). This result is in agreement with the Hubbard I approximation (Gebhard 1997) and describes the physics of an insulator with a gap U . The antiferromagnetic state becomes less and less stable as the interaction U increases, since the Ising spin interaction $\bar{t}^2/2U$ decreases. This can result in a phase transition where the antiferromagnetic state is destroyed because the Ising spin fluctuations become too large. Inside the paramagnetic state, but near the phase boundary, the fermions still feel a 'fluctuating gap' of the antiferromagnetic state.

In a simple approximation, reasonable at high temperatures, one can ignore the correlation of the Ising spins and calculate the average Green's function (21) in a hopping expansion. The latter leads to a random walk between the two sites of the Green's function. The average over the local Ising spins can be performed at each site independently. Moreover, the average of multiple visited sites is approximated by the product of the averaged terms ($\mathrm{i}\omega \rightarrow z = E + \mathrm{i}\epsilon$):

$$\left\langle \frac{1}{(z + U/2 - U\mathbf{I}_r)^n} \right\rangle \approx \left(\left\langle \frac{1}{z + U/2 - U\mathbf{I}_r} \right\rangle \right)^n = \frac{1}{(z - U^2/(4z))^n}$$

This leads to

$$\left\langle \left(z + \frac{U}{2} + \bar{t}\mathbf{h} - \mathbf{I}U \right)^{-1} \right\rangle_{\text{Ising}} \approx \left(z - \frac{U^2}{4z} + \bar{t}\mathbf{h} \right)^{-1},$$

where $-U^2/4z$ is a self energy. This gives an opening of a gap at arbitrary small U . The band edges of this Green's function are shown in figure 2.

In more general terms, the Green's function (21) is characterized by the competition between the hopping term, parametrized by the hopping rate \bar{t} , and the spin term, parametrized by U . This leads to the following qualitative picture: if \bar{t}/U is larger than a certain value, the hopping term wins and creates a metallic state; on the other hand, if \bar{t}/U is smaller than a certain value, disorder due to the random Ising spin wins and creates an insulating state (figure 3).

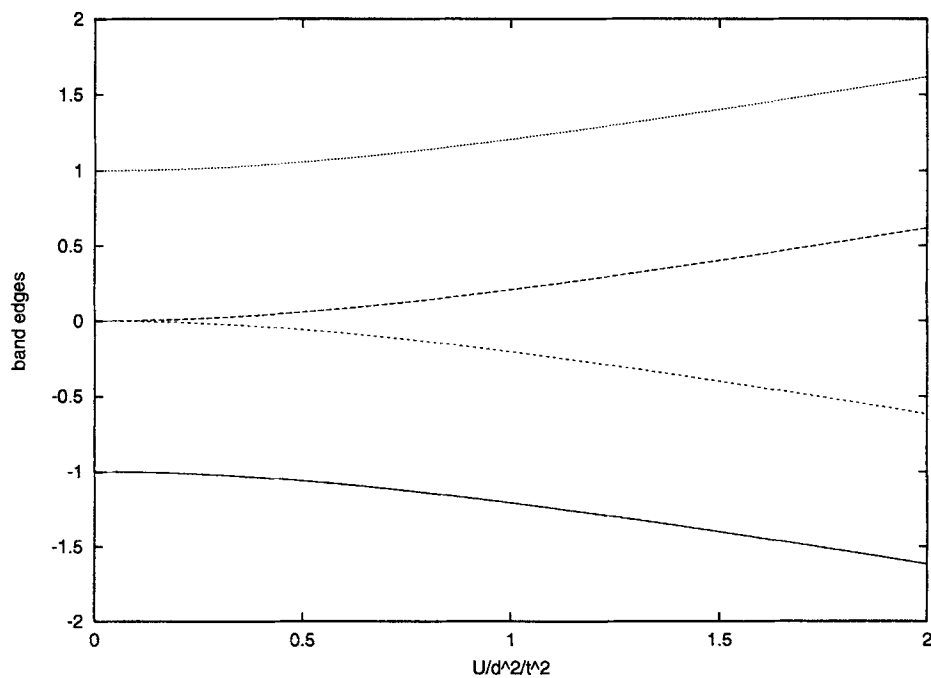


Figure 2. Band edges calculated from the self-consistent approximation. A gap is opening with interaction U around $E = 0$.

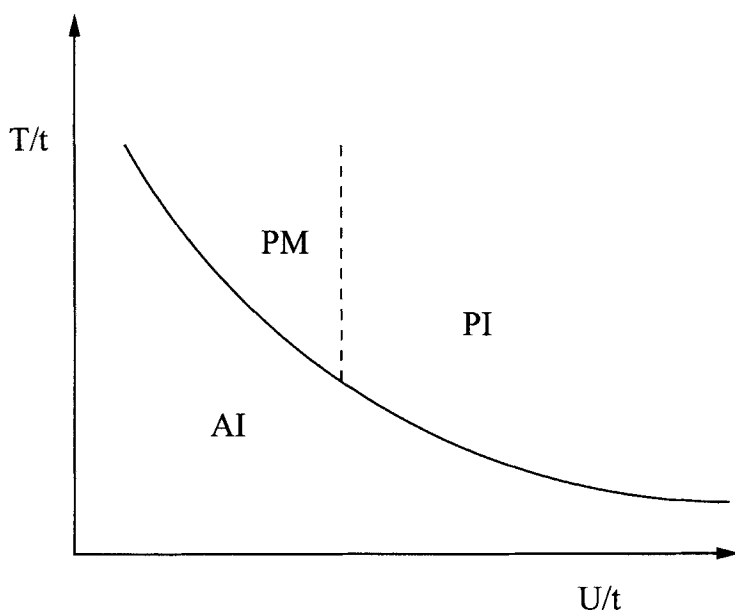


Figure 3. Sketch of the phase diagram of the antiferromagnetic insulator AI, the paramagnetic metal PM and the paramagnetic insulator PI. It is based on the interacting Ising spins ((AI-PM)-PI boundary (—)), and the coupling of the electrons to the Ising spins (PM-PI boundary (- - -)).

§ 6. CONCLUSIONS

Considering quantities of the Hubbard model which depend only on one spin direction, for example spin down, it is possible to integrate out the other spin direction in the functional integral. This idea was carried out for the partition function Z . The result of this integration is a functional integral which has a representation in terms of Ising spins, coupled to fermions with spin $\frac{1}{2}$. The advantage of this approach is that the degeneracy of the special case without hopping, which is difficult to handle in the hopping expansion, is now controlled by the Ising spins. In other words, each Ising spin configuration leads to a non-degenerate hopping expansion. For small hopping rates \bar{t} the effective Ising spin interaction is

$$\frac{\bar{t}^2}{2U} \sum_{\langle r, r' \rangle} S_r S_{r'},$$

which favours an antiferromagnetic Ising spin configuration at low temperatures and a paramagnetic state at high temperatures. The Green's function of an electron with \downarrow is now a Green's function of non-interacting electrons coupled to the Ising spins. Apart from the magnetic transition of the Ising model the Green's function may also undergo a transition from a non-exponentially decaying behaviour at small Hubbard coupling U to an exponentially decaying behaviour with gap U at large U . This picture corresponds to a metal-insulator transition in the paramagnetic regime. The effective Ising model can be a useful starting point for further numerical investigations of this transition.

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APPENDIX A

The space-time determinant on the right-hand side of equation (11) can also be written as

$$\det(-\partial_t + \bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) = \det(\mathbf{1} + \mathbf{A}) \equiv \sum_{\pi} (-1)^{\pi} \prod_{(r,t) \in A} (\delta_{\pi(r,t), (r,t)} + A_{r,t; \pi(r,t)}),$$

with the matrix $\mathbf{A} = -(\bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) \partial_t^T$. The product over the lattice sites gives a sum over all subsets $A_k \subseteq A$ of the space A and their complements $A'_k = A \setminus A_k$

$$\sum_{A_k \subseteq A} \sum_{\pi} (-1)^{\pi} \left(\prod_{(r,t) \in A_k} A_{r,t; \pi(r,t)} \right) \left(\prod_{(r,t) \in A'_k} \delta_{\pi(r,t), (r,t)} \right).$$

The Kronecker delta $\delta_{\pi(r,t), (r,t)}$ on A'_k implies that $\pi(r,t) \in A_k$ for $(r,t) \in A_k$. Therefore, only that part of the matrix \mathbf{A} contributes which is projected on to A_k . This leads to an expansion of the determinant in terms of all partitions of the space-time lattice A as

$$\det(-\partial_t + \bar{\mu} + \hat{\mathbf{t}} - U' \bar{\Psi}_\downarrow \Psi_\downarrow) = \sum_{A_k \subseteq A} \det_{A_k} (\mathbf{P}_k \mathbf{A} \mathbf{P}_k) \equiv \sum_{A_k \subseteq A} \det_{A_k} \mathbf{A} \quad (\text{A } 1)$$

with $\det_{\emptyset} \mathbf{A} = 1$ for the empty set A_k .

APPENDIX B

The integral

$$\bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_1) \mathcal{D}[\Psi_1]$$

in the distribution (22) can be expanded in terms of the hopping as

$$\prod_r \bar{\mu}^{\beta' \mathbf{I}(r)} (1 + V_r^{\beta'}) \left(1 - \Delta^2 \sum_{t, t'; r, r'} \langle \bar{\Psi}_\downarrow(r, t) \Psi_\downarrow(r, t') \rangle_0 \langle \bar{\Psi}_\downarrow(r', t') \Psi_\downarrow(r', t) \rangle_0 \right) + o(\bar{t}^3)$$

with the expectation value

$$\begin{aligned} \Delta^2 \sum_{t, t'} \langle \bar{\Psi}_\downarrow(r, t) \Psi_\downarrow(r, t') \rangle_0 \langle \bar{\Psi}_\downarrow(r', t') \Psi_\downarrow(r', t) \rangle_0 &= \beta \Delta (V_r V_{r'})^{\beta'-1} \\ &- \frac{\Delta^2}{(1 + V_r^{\beta'})(1 + V_{r'}^{\beta'})} \left[\frac{V_r^{\beta'-1}}{V_r} \sum_{t=1}^{\beta'} \sum_{t'=1}^{t-1} \left(\frac{V_r}{V_{r'}} \right)^{t-t'} + \frac{V_r^{\beta'-1}}{V_{r'}} \sum_{t=1}^{\beta'} \sum_{t'=t+1}^{\beta'} \left(\frac{V_r}{V_{r'}} \right)^{t-t'} \right] \end{aligned}$$

and $V_r = \bar{\mu} - U' \mathbf{I}(r) / \bar{\mu}$. For $\mu = -U/2$ (half-filling) and $\Delta \rightarrow 0$ the expectation value is

$$\begin{aligned} &-\frac{\beta^2}{4 \cosh^2(\beta U/4)} \quad \text{for } V_r = V_{r'}, \\ &-\frac{\beta \sinh(\beta U/2)}{2U \cosh^2(\beta U/4)} \quad \text{for } V_r \neq V_{r'}. \end{aligned}$$

This can also be written as

$$\begin{aligned} &\Delta^2 \sum_{t, t'} \langle \bar{\Psi}_\downarrow(r, t) \Psi_\downarrow(r, t') \rangle_0 \langle \bar{\Psi}_\downarrow(r', t') \Psi_\downarrow(r', t) \rangle_0 \\ &= \frac{-1}{4 \cosh^2(\beta U/4)} \left\{ \frac{\beta^2}{2} + \frac{\beta}{U} \sinh \left(\frac{\beta U}{2} \right) + \left[\frac{\beta^2}{2} - \frac{\beta}{U} \sinh \left(\frac{\beta U}{2} \right) \right] S_r S_{r'} \right\}, \end{aligned}$$

which is approximated for large β by

$$-\frac{\beta}{2U} + \frac{\beta}{2U} S_r S_{r'}.$$

In this case the integral of equation (22) is

$$\begin{aligned} &\bar{\mu}^{\beta'} \sum_r \mathbf{I}(r) \int \exp(-S'_1) \mathcal{D}[\Psi_1] \sim \left[1 + \exp \left(\frac{\beta U}{2} \right) \right]^M \exp \left(\frac{\beta M d \bar{t}^2}{U} \right) \\ &\times \exp \left(-\beta \frac{\bar{t}^2}{2U} \sum_{\langle r, r' \rangle} S_r S_{r'} + o(\bar{t}^3) \right). \end{aligned}$$

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