The Hubbard Model, Spinless Fermions, and Ising Spins

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Abstract

The Hubbard model is used to study an electronic system at half filling. Starting from a functional integral representation the spin-up Grassmann field is integrated out. It is shown that the resulting spinless fermion theory has an instantaneous cluster interaction, and that the spinless fermions are coupled to thermally fluctuating Ising spins. The coupling parameter of the spinless fermion interaction is a product of the Hubbard interaction and the hopping rate. As an example the strongly metallic as well as the strongly insulating regime are investigated in terms of the effective Ising statistics.

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I. INTRODUCTION

The Hubbard model was originally constructed to describe a metal-insulator transition for spin-dependent fermions in a simple way [1–5]. This transition reflects the competition between potential (static) energy 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 neighbor 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 para-, ferro- and antiferromagnetic states for the half-filled system [2]. 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 using self-consistent approximations [1], later in terms of a variational approach [6,7], and in the limit of an infinite dimensional lattice [8,9,5]. Very interesting investigations were obtained from computer simulations which indicate an insulating phase at half filling for sufficiently strong fermion interaction [10,11]. However, the detailed mechanism and the properties of the transition are not entirely clear.

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 [2], and the local limit is completely degenerate with respect to the spin. Therefore, an arbitrarily weak hopping rate would lift the degeneracy leading to a new state which might be magnetically ordered [12]. The basic idea of the present work is to start from the extreme insulating as well as from the extreme metallic state at low temperatures and to construct a perturbation theory without analyzing its magnetic order. The latter is a restriction which simplifies the calculations significantly because the spin degree of freedom can be ignored.

In this work a grand canonical ensemble is considered, where on average one fermion per site (half-filled system) is assumed. The non-interacting fermions as well as the 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 accomodate a fermion with spin-up or one with spin-down. Consequently, a perturbation theory around one of these limiting states is plagued by the degeneracies. For instance, a perturbation around the static state is a spontaneous hop of a fermion from any site to its nearest neighbor site. As a consequence, the fermion spontaneously creates a doubly occupied site and an empty site. The doubly occupied site may decay after some time again into two singly occupied sites. The resulting state is two-fold degenerate because of the possible two spin orientations. The unperturbed state can be an antiferromagnetic (Néel) state. A hopping process at a time t_1 can exchange two neighboring fermions which leads to two pairs of neighboring fermions with parallel spins. At time t_2 the inverse hopping process can re-create the original antiferromagnetic state. Therefore, the two hopping processes are not independent.

Moreover, the intermediate state between time t_1 and t_2 has the same energy as the antiferromagnetic state. This implies 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 [13,14]. The central point of the present work is a concept which deals with this degeneracy.

In order to control this exponential degeneracy it is natural to eliminate one spin orientation. This can be achieved formally by integrating out one of the spin orientation in the functional integral representation of the Hubbard model. 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 expansion terms are not degenerate and the perturbation 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 thermal Ising spins which are coupled to the spinless fermions. After an approximation which is applicable for the strongly metallic and the strongly insulating regime of the Hubbard model, the fermionic degrees of freedom can be integrated out. Thus, the physics is described by the Ising spins: The strongly metallic regime is characterized by a ferromagnetic Ising structure in which the fermions can freely move at low temperatures. On the contrary, the strongly insulating regime is characterized by an antiferromagnetic Ising structure which creates a gap for the fermions, in formal analogy to a Peierls instability.

The article is organized as follows: In Sect. II the Hubbard model is defined in a coherent state representation for a grand canonical ensemble of fermions. The static limit (no hopping) of the Hubbard is briefly discussed in Sect. III. Then in Sect. IV the integration over the spin-up component of the model is performed. The resulting model of spinless fermions, which has a complicated but instantaneous cluster interaction, is analyzed in Sect. IV.A. In Sect. V the Ising spin representation of the spinless fermion model is introduced and discussed. Finally, in Sect. V.A the weak-coupling limit and in Sect. V.B the weak hopping limit are studied. Appendices A, B, and C give details of the calculations.

II. THE HUBBARD MODEL

The Hubbard model describes fermions with spin $\sigma =\downarrow,\uparrow$ on a d-dimensional lattice λ. It is defined by the Hamiltonian [2,5]

$$H[c_\sigma^\dagger(r), c_\sigma(r)] = -\bar{t} \sum_{\langle r,r'\rangle,\sigma} c_\sigma^\dagger(r) c_\sigma(r') + \sum_r \Big[\mu \sum_\sigma c_\sigma^\dagger(r) c_\sigma(r) + U c_\uparrow^\dagger(r) c_\uparrow(r) c_\downarrow^\dagger(r) c_\downarrow(r)\Big],$$

where $c_\sigma^\dagger(r)$, $c_\sigma(r)$ are fermion creation and annihilation operators, respectively. $\bar{t} \geq 0$ is the hopping rate. $\langle r, r'\rangle$ means pairs of nearest neighbor sites on the lattice. 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 [15]. 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 $k, l \geq 0$

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

The partition function of the grand canonical ensemble of fermions then reads

$$Z = \int \exp(-S)\mathcal{D}[\Psi, \bar{\Psi}]$$

with the action

$$S = i\Delta \sum_{r,t} \frac{1}{i\Delta} \bar{\Psi}_\sigma(r,t)[\Psi_\sigma(r,t) - \Psi_\sigma(r,t-\Delta)] + i\Delta \sum_t \frac{1}{\hbar} H[\bar{\Psi}_\sigma(r,t), \Psi_\sigma(r,t-\Delta)] \tag{1}$$

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 $t = \Delta, 2\Delta, ..., \beta$. $\bar{\Psi}_\sigma(r,t)$ 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 $\Psi_\sigma(r,t) \to \Psi_\sigma(r,t+\Delta)$ because then the Grassmann field appears with the same time in the Hamiltonian of the action (1).

III. 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 evalueated as

$$Z = \int \prod_{r,t} \exp[-S_d(r,t)]\mathcal{D}[\Psi_\uparrow, \Psi_\downarrow] = \prod_r \int \prod_t \exp[-S_d(r,t)]\mathcal{D}[\Psi_\uparrow, \Psi_\downarrow] = Z_1^M, \tag{2}$$

where

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

with $\hbar = 1$ and $\bar{\mu} = 1 - i\Delta\mu$. Z_1 is the partition function of the Hubbard model with one lattice site (static, local or atomic limit):

$$Z_1 = \int \prod_t \exp[-S_d(r,t)] d\mu(r,t) = 1 + 2\bar{\mu}^{\beta/\Delta} + [\bar{\mu}^2 - i\Delta U]^{\beta/\Delta}.$$

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

$$\begin{aligned} w_0 &= 1/Z_1 \\ w_1 &= 2(1-\mu')^{\beta'}/Z_1 \\ w_2 &= [(1-\mu')^2 - U']^{\beta'}/Z_1. \end{aligned}$$

In the temperature formalism, where the time t is replaced by the imaginary time through a Wick rotation, the weights w_0, w_1 and w_2 are statistical weights. Then the average number of particles per site is

$$n = w_1 + 2w_2.$$

At zero temperature ($\beta' \to \infty$) this gives

$$n = \begin{cases} 0 & \text{if } 0 < \mu' < 1 + \sqrt{1+U'} \\ 1 & \text{if } \mu' < 0 \text{ and } \mu'(\mu'-1) < U' \\ 2 & \text{otherwise} \end{cases}.$$

The groundstate of the expansion around the local limit is degenerated because each singly occupied site can accomodate a fermion with either spin $\uparrow$ or with spin $\downarrow$. This degeneracy must be handled with care. In particular, to obtain a unique hopping expansion one has to separate the degenerate contributions. Therefore, one cannot directly work with the hopping term as a perturbation but have to set up a perturbation theory which works with non-degenerate groundstates. This means that one has to divide the degenerate groundstate such that the perturbations remain in their corresponding non-degenerate groundstates.

IV. INTEGRATION OVER THE SPIN-UP FIELD $\Psi_\uparrow$

The action S can be divided into three pieces as

$$S = S_\uparrow + S_\downarrow + S_I$$

with

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

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

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

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

$$\int e^{-S_\uparrow - S_I} \prod_{r,t} d\Psi_\uparrow(r,t) d\bar{\Psi}_\uparrow(r,t) = det[-\partial_t + \bar{\mu} + \hat{t} - U'\bar{\Psi}_\downarrow\Psi_\downarrow], \tag{3}$$

where ∂_t is the time-shift operator

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

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

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

We assume that the number of time slices β' is even such that $det(-\partial_t) = det(\partial_t) = 1$. The matrix $\hat{t}_{r,r'} = \tau$ if r, r' are nearest neighbors and 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 $\hat{t}$ is multiplied by the time-like unit matrix.

In the following subsets of the space-time lattice $\Lambda = \lambda \otimes \{\Delta, 2\Delta, ..., \beta\}$ will be considered. For a subset $\Lambda_k \subset \Lambda$ we define the determinant of the the projected matrix $P_k A P_k$ as

$$det_{\Lambda_k} A \equiv det_{\Lambda_k}(P_k A P_k),$$

where P_k is the projector onto Λ_k.

A. Effective Cluster Action of Spinless Fermions

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

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

Formally, the determinant could be expressed as part of the action by using the identity $detA = \exp[Tr(\log A)]$. However, this would be too naive because the term

$$Tr\Big[\log\Big(-\partial_t + \bar{\mu} + \hat{t} - U'\bar{\Psi}_\downarrow \Psi_\downarrow\Big)\Big]$$

has a complicated interaction of the Grassmann field in space *and* time. Moreover, at least for $\bar{t} = 0$ the interaction has a long-range part in time which reflects the degeneracy of the unperturbed system. Fortunately, there is a way to avoid these difficulties: As shown in Appendix A, the determinant can be expanded in terms of the partitions $\Lambda_k \subseteq \Lambda$ of the space-time lattice Λ as

$$det[-\partial_t + \bar{\mu} + \hat{t} - U'\bar{\Psi}_\downarrow \Psi_\downarrow] = \sum_{\Lambda_k \subseteq \Lambda} det_{\Lambda_k}[-(\bar{\mu} + \hat{t})\partial_t^T] \exp\Big[Tr_{\Lambda_k} \log\Big(\mathbf{1} - (\hat{t} + \bar{\mu})^{-1} U' \bar{\Psi}_\downarrow \Psi_\downarrow\Big)\Big].$$

The partitions include the empty set which gives $det_\emptyset A = 1$. This expansion is the most important step for the treatment of the Hubbard model in this work. The first consequence is that the partition function Z is now given by an expansion in terms of Λ_k as $Z = \sum_{\Lambda_k} Z_{\Lambda_k}$ with

$$Z_{\Lambda_k} = det_{\Lambda_k}[-(\bar{\mu} + \hat{t})\partial_t^T] \int \exp(-S_{\Lambda_k}) \mathcal{D}[\Psi_\downarrow] \tag{4}$$

and the action

$$S_{\Lambda_k} = \bar{\Psi}_\downarrow \cdot (\partial_t - \bar{\mu} - \hat{t}) \Psi_\downarrow - Tr_{\Lambda_k} \log\Big(\mathbf{1} - (\hat{t} + \bar{\mu})^{-1} U' \bar{\Psi}_\downarrow \Psi_\downarrow\Big).$$

The second term of S_{Λ_k} can be expanded in powers of the Grassmann field. This yields an *instantaneous* cluster interaction

$$S_i = \sum_{l\geq 1} \frac{U'^l}{l} \sum_{(r,t)\in\Lambda_k} \sum_{r_1,\ldots,r_{l-1}} (\hat{t}+\bar{\mu})^{-1}_{r,r_1} \bar{\Psi}_\downarrow(r_1,t)\Psi_\downarrow(r_1,t)...(\hat{t}+\bar{\mu})^{-1}_{r_{l-1},r} \bar{\Psi}_\downarrow(r,t)\Psi_\downarrow(r,t).$$

Due to the identity

$$(\hat{t}+\bar{\mu})^{-1} = \frac{1}{\bar{\mu}} - \frac{\hat{t}}{\bar{\mu}}(\hat{t}+\bar{\mu})^{-1}$$

the action S_i can also be written with $u = U'(\hat{t}+\bar{\mu})^{-1}_{rr}$ as

$$S_i = u \sum_{(r,t)\in\Lambda_k} \bar{\Psi}_\downarrow(r,t)\Psi_\downarrow(r,t)$$

$$+\sum_{l\geq 2} \frac{U'^l}{l} \sum_{(r,t)\in\Lambda_k} \sum_{r_1,\ldots,r_{l-1}} \Big(\frac{-\hat{t}}{\bar{\mu}}(\hat{t}+\bar{\mu})^{-1}\Big)_{r,r_1} \bar{\Psi}_\downarrow(r_1,t)\Psi_\downarrow(r_1,t)$$

$$...\Big(\frac{-\hat{t}}{\bar{\mu}}(\hat{t}+\bar{\mu})^{-1}\Big)_{r_{l-1},r} \bar{\Psi}_\downarrow(r,t)\Psi_\downarrow(r,t).$$

This shows that the interaction terms with $l \geq 2$ do not distinguish between weak interaction ($U' \sim 0$) and weak hopping ($\bar{t} \sim 0$) because the expansion parameter is $U'\bar{t}$.

The non-interacting limit $U' = 0$ as well as the local limit $\hat{t} = 0$ can be checked immediately because of a vanishing interaction. The former gives the product of two determinants (from both spin orientations)

$$Z_0 = det(-\partial_t + \bar{\mu} + \hat{t})^2$$

and the latter

$$Z = Z_1^M,$$

in agreement with Eq. (2).

V. ISING SPIN STATISTICS

It is interesting to notice that the determinant $det_{\Lambda_k}[-(\bar{\mu}+\hat{t})\partial_t^T]$ in Z_{Λ_k} determines which partition Λ_k contributes with non-zero weight. Since ∂_t is diagonal in space but off-diagonal in time, the determinant $det_{\Lambda_k}(\partial_t^T)$ is non-zero only if a site r is in Λ_k at all times. Therefore, the contributing partitions are of the form $\Lambda_k = \lambda_k \times \{\Delta, 2\Delta, ..., \beta\}$, where λ_k is a partition of the space lattice λ. The determinant then reads

$$det_{\Lambda_k}[-(\bar{\mu}+\hat{t})\partial_t^T] = [det_{\lambda_k}(\bar{\mu}+\hat{t})]^{\beta'}.$$

Now it is convenient to introduce the projector I_{λ_k} which projects on λ_k

$$(I_{\lambda_k})_r = \begin{cases} 1 & \text{if } r \in \lambda_k \\ 0 & \text{if } r \notin \lambda_k \end{cases}.$$

Consequently, the determinant can be expressed as

$$[det_{\lambda_k}(\bar{\mu}+\hat{t})]^{\beta'} = \Big[det_{\lambda}(\mathbf{1}+I_{\lambda_k}[\bar{\mu}+\hat{t}-\mathbf{1}]I_{\lambda_k})\Big]^{\beta'}. \tag{5}$$

The interaction can also be written in terms of the projection operator:

$$S_i = \sum_{l\geq 1}\frac{U'^l}{l}\sum_t \sum_{r,r_1,\ldots,r_{l-1}} (I_{\lambda_k})_r(\hat{t}+\bar{\mu})^{-1}_{r,r_1}\bar{\Psi}_\downarrow(r_1,t)\Psi_\downarrow(r_1,t)...(\hat{t}+\bar{\mu})^{-1}_{r_{l-1},r}\bar{\Psi}_\downarrow(r,t)\Psi_\downarrow(r,t)$$

The partitions λ_k enter Z only through the projection operator I_{λ_k}. Eqs. (4) and (5) imply

$$Z = \sum_{\lambda_k} Z_{\lambda_k} = \sum_{\lambda_k}\Big[det_\lambda(\mathbf{1}+I_{\lambda_k}[\bar{\mu}+\hat{t}-\mathbf{1}]I_{\lambda_k})\Big]^{\beta'}\int \exp(-S_{\Lambda_k})\mathcal{D}[\Psi_\downarrow]$$

with the action

$$S_{\lambda_k} = \bar{\Psi}_\downarrow\cdot(\partial_t-\hat{t}-\bar{\mu}+uI_{\lambda_k})\Psi_\downarrow + O((U'\bar{t}/\bar{\mu}^2)^2).$$

The projection operator I_{λ_k} can be expressed as $(I(\{S_r\}))_{rr'} = (1+S_r)\delta_{rr'}/2$ with the Ising spin

$$S_r = \begin{cases} 1 & r\in\lambda_k \\ -1 & r\notin\lambda_k \end{cases}.$$

The partitions λ_k enter Z only through the projection operator I_{λ_k}. Therefore, the sum over the randomly chosen partitions λ_k of the space lattice is equivalent to the sum over randomly chosen Ising spins. This is a thermal Ising model with complicated interaction spin interaction in a magnetic field. The latter is implied by the missing invariance under a global transformation $S_r \to -S_r$.

Neglecting the interaction S_i, which is weak for the metallic as well as for the insulating regime, one gets

$$Z \approx Z_I = \sum_{\{S_r=\pm 1\}}\Big[det_\lambda(\mathbf{1}+I[\bar{\mu}+\hat{t}-\mathbf{1}]I)\Big]^{\beta'} det(-\partial_t+\bar{\mu}-uI+\hat{t}). \tag{6}$$

The partition function Z_I can be used as a starting point for an approximative treatment of the Hubbard model. In the rest of this work the favoured spin structures will be analyzed, i.e., the spin configurations with maximal Boltzmann weight. Details of the calculations are given in App. B and C.

A. Weak Interaction: $U' \approx 0$

A metallic behavior is expected in this regime. Since

$$[det_{\lambda_k}(\bar{\mu}+\hat{t})]^{\beta'}$$

is independent of U', only the second determinant of Z_I must be expanded around $U'=0$. This yields in leading order

$$det(-\partial_t + \bar{\mu} - uI + \hat{t}) \approx \exp[\int \Theta(|\kappa| - 1) \log(\kappa) d^d k] \exp[\beta' h \sum_r (1 + S_r)].$$

with the effective magnetic field

$$h = \frac{u}{2} \int \frac{\Theta(|\kappa| - 1)}{\kappa} d^d k \quad \text{with} \quad \kappa = \bar{\mu} + 2\hat{t} \sum_{j=1}^{d} \cos k_j.$$

Thus, the weakly interacting regime prefers a ferromagnetic state in terms of the Ising spin $S_r = 1$. Knowing the Ising spin configuration with the highest weight, one can return to the partition function of Eq. (6) and obtains

$$Z_I \approx [det(\bar{\mu} + \hat{t})]^{\beta'} det(-\partial_t + \bar{\mu} - u + \hat{t}).$$

The argument of the determinant can be considered as an inverse Green's function

$$G = (-\partial_t + \bar{\mu} - u + \hat{t})^{-1}.$$

Thus, the effect of the ferromagnetic Ising spin structure is a constant shift of the chemical potential. Of course, the fluctuations of the Ising spins around the structure with maximal weight have to be taken into account as soon as $\beta' < \infty$.

B. Hopping Expansion: $\bar{t} \approx 0$

The expansion of the first determinant of Z_I in powers of τ is

$$\bar{\mu}^{\beta' |\lambda_k|} \exp[-\frac{\beta'}{2\bar{\mu}^2} \sum_{r, r \in \lambda_k} (\hat{t}_{r,r'})^2] \tag{7}$$

and the expansion of the second determinant is

$$det(-\partial_t + \bar{\mu} - uI + \hat{t}) \approx \bar{\mu}^{\beta'(M - |\lambda|)} \exp\Big[- \frac{\beta' \tau^2}{2} \sum_{\langle r,r \rangle} W(V_r, V_{r'}) \Big]. \tag{8}$$

Here the potential terms $V_r, V_{r'}$ are either $\bar{\mu}$ or $\bar{\mu} - u \approx \bar{\mu} - U'/\bar{\mu}$ with the function

$$W(V_r, V_{r'}) = \begin{cases} 0 & \text{for } V_r = V_{r'} = \bar{\mu} - u \\ -1/(u\bar{\mu}) & \text{for } V_r \neq V_{r'} \\ 1/\bar{\mu}^2 & \text{for } V_r = V_{r'} = \bar{\mu} \end{cases}.$$

For $\tau = 0$ all terms in the sum $\sum_\lambda Z_\lambda$ have the same weight. This reflects the fact that there is a degenerate perturbation theory for the hopping expansion in the half-filled system due to the spin degree of freedom. For $\tau \neq 0$ the second factor of (8) can be approximated for $\beta \approx \infty$ (β is now real) as

$$\exp\Big[\frac{\beta' \tau^2}{2} \sum_{\langle r,r \rangle} W(V_r, V_{r'}) \Big] \approx \exp\Big[- \beta \frac{\bar{t}^2}{2U} \sum_{\langle r,r \rangle} S_r S_{r'} \Big]. \tag{9}$$

According to (7) and (9) the maximal contribution to Z_I comes from $V_r \neq V_{r'}$ on nearest-neighbor sites. This corresponds with an antiferromagnet state of the Ising

spin $S_r = (-1)^{r_1+\cdots+r_d}$. The partition function in Eq. (6) reads with the staggered Ising spin structure

$$Z_I \approx 2\bar{\mu}^{\beta' M/2} det(-\partial_t + V_{AFM} + \hat{t}),$$

where V_{AFM} is the staggered antiferromagnetic potential

$$V_{AFM} = \bar{\mu} - \frac{u}{2}[1 + (-1)^{r_1+\cdots+r_d}].$$

As an effective Green's function of the fermions one can study

$$G = (-\partial_t + V_{AFM} + \hat{t})^{-1}.$$

The staggered potential creates a gap. This can be seen, for instance, in the special case of a two-dimensional lattice. Then the eigenvalues of G^{-1} are

$$\bar{\mu} - \frac{u}{2} \pm \sqrt{\frac{u^2}{4} + |\tau h_{12}|^2}$$

with $h_{12} = 1 + e^{ik_x} + e^{ik_y} + e^{ik_x+ik_y}$ $(-\pi \leq k_j < \pi)$. This result describes the physics of an insulator with a gap

$$U/2,$$

in contrast to the homogeneous potential of the ferromagnetic Ising structure for the weak interacting case.

There can be a phase transition from weak coupling (ferromagnetic Ising system) to weak hopping (*anti*ferromagnetic Ising system) even at finite β (i.e., non-zero temperature). It is not clear, however, whether this is a first or second order transition. Numerical (Monte Carlo) simulations may reveal more details of the transition.

VI. CONCLUSIONS

Considering quantities of the Hubbard model which depend only on one spin direction, e.g., 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 latter could have been extended to a generating function for spin-down Green's function without modification of the procedure. The result of this integration is a functional integral which has a representation in terms of thermal Ising spins. Moreover, the fermionic interaction of the effective model has a coupling parameter $U'\bar{t}$ which becomes small in the limit of weak Hubbard interaction U' as well as in the limit of low mobility of the particle (small hopping rate $\bar{t}$). Therefore, the effective fermionic interaction can be neglected if one is only interested in the strongly metallic and the strongly insulating regime at half filling. The advantage of this approach is that the degeneracy of the special cases $U' = 0$ and $\bar{t} = 0$, which are difficult to handle, are controlled by the coupling of U' and $\bar{t}$ to the Ising spins: a small Hubbard interaction U' creates an effective magnetic field $h \propto U'$ which couples linearly to the Ising spin. On the other hand, a small hopping term favours an

antiferromagnetic (staggered) Ising spin configuration because of the effective Ising spin interaction

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

The Boltzmann weights of the effective Ising spin system were used to extract the most relevant contributions to the sum over the spin configurations.

The introduction of Ising spins by a direct decoupling of the interaction term in Eq. (1) (Hubbard-Stratonovich transformation) is a well-known approach. It leads to a dynamic Ising spin [16]. The approach of the present work avoids the dynamics of the Ising spin. However, the price for this simplification is a cluster interaction of spinless fermions.

Although the approximations used in this work do not provide insight into the transition from the metallic to the insulating phase, a more accurate treatment of the partition function Z_I of (6) by including fluctuations of the Ising spins, e.g., using a Monte Carlo simulation, may allow to access the transition at not too low temperatures.

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APPENDIX A

The space-time determinant on the r.h.s. of Eq. (3) can also be written as

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

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

$$\sum_{\Lambda_k\subseteq\Lambda}\sum_\pi (-1)^\pi \Big[\prod_{(r,t)\in\Lambda_k} A_{r,t;\pi(r,t)}\Big]\Big[\prod_{(r,t)\in\Lambda_k'} \delta_{\pi(r,t),(r,t)}\Big].$$

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

$$det[-\partial_t + \bar{\mu} + \hat{t} - U'\bar{\Psi}_\downarrow\Psi_\downarrow] = \sum_{\Lambda_k\subseteq\Lambda} det_{\Lambda_k}(P_k A P_k) \equiv \sum_{\Lambda_k\subseteq\Lambda} det_{\Lambda_k} A \qquad (10)$$

with $det_\emptyset A = 1$ for an empty set Λ_k. The projected determinant is

$$det_{\Lambda_k}\Big(-(\bar{\mu}+\hat{t}-U'\bar{\Psi}_\downarrow\Psi_\downarrow)\partial_t^T\Big) = det_{\Lambda_k}[-(\bar{\mu}+\hat{t})\partial_t^T] det_{\Lambda_k}\Big(\mathbf{1} - (\bar{\mu}+\hat{t})^{-1}U'\bar{\Psi}_\downarrow\Psi_\downarrow\Big)\Big),$$

where the second second determinant reads

$$\exp\Big[Tr_{\Lambda_k}\log\Big(\mathbf{1} - (\hat{t}+\bar{\mu})^{-1}U'\bar{\Psi}_\downarrow\Psi_\downarrow\Big)\Big].$$

APPENDIX B

Expanding the second determinant of Z_I up to first order in $\delta\hat{V}$ yields

$$det(-\partial_t + \bar{\mu} + \delta\hat{V} + \hat{t}) \approx det(-\partial_t + \bar{\mu} + \hat{t}) \exp\Big(Tr[\delta\hat{V}(-\partial_t + \bar{\mu} + \hat{t})^{-1}]\Big).$$

The trace term can be written as

$$\beta' h \sum_r (1 + S_r),$$

where

$$h = \frac{u}{2} \int \frac{\Theta(|\kappa| - 1)}{\kappa} \frac{d^d k}{(2\pi)^d} \quad \text{with} \quad \kappa = \bar{\mu} + 2\tau \sum_{j=1}^{d} \cos k_j.$$

APPENDIX C

The first determinant of Z_I can be expanded up to second order in $\hat{t}$ as

$$[det_{\lambda_k}(\bar{\mu} + \hat{t})]^{\beta'} \approx \bar{\mu}^{\beta'|\lambda_k|} \exp[-\frac{\beta'}{2\bar{\mu}^2} \sum_{r,r' \in \lambda_k} (\hat{t}_{rr'})^2].$$

The second determinant of Z_I can be expanded in powers of $\hat{t}$ up to second order

$$det(-\partial_t + \bar{\mu} + \delta\hat{V} + \hat{t})$$

$$\approx det(-\partial_t + \bar{\mu} + \delta\hat{V}) \exp\Big(-\frac{1}{2} Tr[\hat{t}(-\partial_t + \bar{\mu} + \delta\hat{V})^{-1} \hat{t}(-\partial_t + \bar{\mu} + \delta\hat{V})^{-1}]\Big).$$

The trace term reads

$$Tr[\hat{t}(-\partial_t + \bar{\mu})^{-1} \hat{t}(-\partial_t + \bar{\mu})^{-1}] = \beta' \sum_{r,r'} (\hat{t}_{rr'})^2 \int_0^{2\pi} \frac{1}{V_r - e^{i\omega}} \frac{1}{V_{r'} - e^{i\omega}} \frac{d\omega}{2\pi},$$

where the integral gives

$$\int_0^{2\pi} \frac{1}{V_r - e^{i\omega}} \frac{1}{V_{r'} - e^{i\omega}} \frac{d\omega}{2\pi} = \begin{cases} 0 & \text{for } V_r = V_{r'} = \bar{\mu} - U'/\bar{\mu} \\ -1/(u\bar{\mu}) & \text{for } V_r \neq V_{r'} \\ 1/\bar{\mu}^2 & \text{for } V_r = V_{r'} = \bar{\mu} \end{cases}.$$

Due to $\tau \approx 0$, the approximation $u \approx U'/\bar{\mu}$ can be used. Then for $\beta' \approx \infty$ the determinant is

$$det(-\partial_t + \bar{\mu} + \delta\hat{V}) = \prod_r (1 + [\bar{\mu} + \delta\hat{V}_r]^{\beta'}) \approx \bar{\mu}^{\beta'(M - |\lambda_k|)},$$

since $|\bar{\mu}| > 1$ and $|\bar{\mu} - U'/\bar{\mu}| < 1$.