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HIGH TEMPERATURE EFFECTS IN THE HUBBARD MODEL

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In this paper we investigate the Hubbard model at high temperatures. For this reason a simple algebraic method based on the Γ-representation of an original Hamiltonian is developed. The results thus obtained does imply no paradoxes as it is when doing some approximations starting from Lieb's and Wu's solutions. It is shown that a periodic behavior of observables can be predicted from high temperature perturbation theory. This periodicity is based on the Aharonov–Bohm-like effects on a lattice with the dimension $d > 1$. An explicit formula for the periodic part of magnetization is given for $d = 2$.

1. Introduction

Recently discovered high-T_c superconductivity has initiated the search for new mechanisms of this phenomenon which are not based on electron–phonon interactions as it is in the BCS theory. It is believed that the simplest Hamiltonian relevant for the superconducting transition at high temperatures is the Hubbard Hamiltonian[1] describing basic properties of fermionic systems with short-range repulsive interactions.

Originally proposed as a quantum mechanical model of the metal–insulator phase transiton, the Hubbard model serves as basic model for understanding superconducting properties of fermions in Cu–O lattices.[2] Despite its seeming simplicity basic properties of the model are exactly analyzed in the one-dimensional case only. The exact solution of the Hubbard model was given in 1968 by Lieb and Wu[3] and was used later for an analysis of magnetic properties of the model.[4–6] The Hubbard Hamiltonian has three free parameters t, U and $n = \frac{N_e}{N}$. Here t is the hopping energy between neighbor lattice sites, U is the coulomb repulsive energy of electrons in a site, N_e is the number of electrons and N is the number of lattice sites.

The magnetic susceptibility χ calculated from Lieb and Wu's solution is[5,6]

$$\chi = N\mu_0^2 \frac{U}{\pi^2 t^2} \left(1 - \frac{\sin 2\pi n}{2\pi n}\right)^{-1} \quad \text{for} \quad U \gg t \tag{1.1a}$$

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and

$$\chi = N\mu_0^2 \frac{1}{\pi t}\left(\sin\frac{\pi}{2}n\right)^{-1} \quad \text{for} \quad U \gg t \tag{1.1b}$$

where μ_0 is the Bohr magneton. These expressions however imply paradoxical behaviors. Both in the limiting case of an empty lattice ($n = 0$) and for a totally filled one the magnetic susceptibility has a nonzero value. Let us note that these contradictions are consequences of approximations based on the substitution of discrete sums by integrals and are not inherent in Lieb's and Wu's solution.

Still an open question remains the behavior of the model at finite temperatures and dimensions $d > 1$. As shown in Sec. 2, it is not possible to apply the standard perturbation technique in the original Hubbard Hamiltonian for the physically interesting case of strong coupling $U \gg t$. Noga and Franz[8] have shown that it is possible (at least in one dimension) to develop a regular perturbative theory based on a unitary transformation of the 1D Hubbard Hamiltonian.

In this paper we investigate the Hubbard model in the limit $U \gg t$ at high temperatures on a d-dimensional lattice with N sites. The original Hamiltonian is rewritten in terms of Γ-matrices which fulfil the Clifford algebra of $4^N \times 4^N$ matrices.[13,14] Thermodynamical quantities thus obtained are free of paradoxes and are in agreement with the causality and Pauli principles.

Interesting features of the model can be seen in the presence of an external magnetic field. At high temperatures this model describes normal metallic phase. Static properties of conductivity electrons in a normal metal lattice cause various macroscopic effects as the Landau diamagnetism or the de Haas–van Alphen effect. In the latter states there is a periodic part in the magnetization of a metallic lattice and it is observed (and theoretically explained) for low temperatures and strong magnetic fields.[9] This periodical dependence of magnetization on an external magnetic field is caused by quantization of an orbital motion of electrons.

As shown in the paper (see Sec. 3.3) similar oscillations of average magnetic quantities in the Hubbard model can occur also at high temperatures in dimensions $d > 1$. The reason is the appearance of the Aharonov–Bohm effect in normal metals. Macroscopic demonstrations of this topological effect in solids were measured at low temperatures.[10] At high temperatures it is assumed[11] that thermal noise causes a random distribution of wave phases of electrons at atomic level and the interference of conductivity electrons vanishes. A lattice structure of normal metal makes such interference possible also at high temperatures. In Sec. 3.3 we show that such macroscopic oscillations have a very large period ($\sim 10^4 T$) which is apparently the reason it is impossible to measure such an effect in normal metals. A qualitative approach however enables us to predict the presence of magnetic oscillations with smaller periods, depending on the temperature decrease. Because this is due to kinetic transitions of electrons in more-dimensional structures ($d > 1$) we have not a suitable method for treating this problem in a rigorous way.

2. The Hubbard Hamiltonian

2.1. *The Hubbard model in the presence of an external magnetic field*

Let us consider the d-dimensional lattice with N sites. The Hubbard Hamiltonian can be written in the form

$$H = 4u\sum_j n_{j+}n_{j-} - t\sum_{\langle i,j\rangle}\sum_\sigma a_{i\sigma}^+ a_{j\sigma} - \sum_j (\eta + 2u)(n_{j+} + n_{j-})\,, \tag{2.1.1}$$

where $a_{i\sigma}(a_{i\sigma}^+)$ is the annihilation (creation) operator of electron with spin $\sigma = \pm 1$ at the ith site, $n_{i\sigma}$ is the corresponding operator of the number of electrons and $\langle i, j\rangle$ stands for summation over nearest neighbors. The Hamiltonian thus describes on-site interactions of electrons with the Hubbard energy $U = 4u$ as well as the hops of electrons over lattice links with the energy t. We choose the chemical potential in the form $\eta + 2u$ so the case $\eta = 0$ corresponds to the half-filled lattice ($N_e = N$).

By putting the system into an external magnetic field the Hamiltonian of the system is not any more translational invariant due to the minimal coupling

$$a_{i\sigma}^+ a_{j\sigma} \to a_{i\sigma}^+ a_{j\sigma} \exp\left(-i\frac{e}{\hbar}\int_i^j A\cdot dr\right)\,, \tag{2.1.2}$$

where A is the magnetic vector potential and e is the electron charge. The resulting Hamiltonian is

$$H = \sum_j [4un_{j+}n_{j-} - \mu_0 B(n_{j+} - n_{j-} - (\eta + 2u)(n_{j+} + n_{j-})] - t\sum_{\langle i,j\rangle}\sum_\sigma a_{i\sigma}^+ a_{j\sigma}\exp\left(-i\frac{e}{\hbar}\int_i^j A\cdot dr\right)\,, \tag{2.1.3}$$

we put the magnetic field **B** in the zth direction: $\mathbf{B} = (0, 0, \ldots, B)$.

We note that when computing macroscopic variables the translational non-invariant phase shifts (2.1.2) in the Hamiltonian (2.1.3) compensate each other so the result depends on the magnetic field B only. We also note that for strong-coupling it is not possible to apply the standard perturbation theory to (2.1.3). This is because the nonperturbative term in the Hamiltonian (2.1.3) is not a billinear one. However, interesting results can be obtained from high-temperature expansion of partition function for $d > 1$.

2.2. *The Γ-representation of the Hubbard Hamiltonian*

First we transform the Hamiltonian (2.1.3) by the unitary transformation

$$a_{j\sigma} \to c_{j\sigma}e^{i\frac{\pi}{2}j\nu}$$
$$a_{j\sigma}^+ \to (a_{j\sigma})^+\,, \tag{2.2.1}$$

where ν is the vector which has all components equal to unity. We obtain

$$H = H_0 + H_1 \,, \tag{2.2.2}$$

where

$$\begin{aligned} H_0 = -uN + \sum_j [&u(c_{j+}c_{j+}^{+} - c_{j+}^{+}c_{j+})(c_{j-}c_{j-}^{+} - c_{j-}^{+}c_{j-} \\ &- \mu_0 B(c_{j+}^{+}c_{j+} - c_{j-}^{+}c_{j-}) - \eta(c_{j+}^{+}c_{j+} + c_{j-}^{+}c_{j-})] \end{aligned}$$

$$H_1 = -t \sum_{\langle i,j\rangle} \sum_{\sigma} c_{i\sigma}^{+} c_{j\sigma} e^{-i\alpha_{ij}} \,.$$

Here we denoted

$$\alpha_{ij} = \frac{e}{\hbar} \int_i^j \left(A - \frac{\pi\hbar}{2e}\nu \right) \cdot \mathrm{dr} = -\alpha_{ji} \,. \tag{2.2.3}$$

Now we introduce self-adjoint components Γ_j^a, $a = 1, 2, 3, 4$ (Refs. 13 and 14)

$$\begin{aligned} c_{j+} &= \frac{1}{2}(\Gamma_j^3 + i\Gamma_j^4) \,, \quad c_{j+}^{+} = (c_{j+})^{+} \\ c_{j-} &= \frac{1}{2}(\Gamma_j^1 - i\Gamma_j^2) \,, \quad c_{j-}^{+} = (c_{j-})^{+} \,. \end{aligned} \tag{2.2.4}$$

It is easily seen that Γ_j^a matrices fulfill the anticommutation rules

$$\{\Gamma_i^a, \Gamma_j^b\} = 2\delta^{ab}\delta_{ij} \qquad a, b = 1, 2, 3, 4 \tag{2.2.5}$$

of the Clifford algebra of $4^N \times 4^N$ matrices. (A general analysis of such matrices is given in Ref. 12). Next we introduce Γ_j^0 and J_j^{ab} matrices

$$\Gamma_j^0 = -\Gamma_j^1\Gamma_j^2\Gamma_j^3\Gamma_j^4 \tag{2.2.6}$$

$$J_j^{ab} = -\frac{i}{2}[\Gamma_j^a, \Gamma_j^b] \,, \quad a \neq b \,. \tag{2.2.7}$$

Let us list basic characteristics of the just-defined Γ-representation which will be used in our next analysis. We will use mainly the rules

$$\begin{aligned} &\{\Gamma_j^0, \Gamma_j^a\} = 0 \\ &[\Gamma_j^0, \Gamma_k^a] = 0 \,, \quad j \neq k \\ &[\Gamma_j^0, \Gamma_k^0] = 0 \,, \quad \forall j, k \end{aligned} \tag{2.2.8}$$

Matrices J_j^{ab} defined in (2.2.7) satisfy

$$[\Gamma_j^a, J_k^{bc}] = 2i\delta_{jk}(\delta^{ac}\Gamma_k^b - \delta^{ab}\Gamma_k^c) \tag{2.2.9}$$

$$[\Gamma_i^0, J_j^{ab}] = 0 \ \forall a, b \tag{2.2.10a}$$

$$[J_j^{ab}, J_k^{cd}] = 4i\delta_{jk}(\delta^{ac}J_k^{bd} - \delta^{ad}J_k^{bc} - \delta^{bc}J_k^{ad} + \delta^{bd}J_k^{ac}) \,. \tag{2.2.10b}$$

From the definitions we obtain

$$(\Gamma_j^a)^2 = (\Gamma_j^0)^2 = (J_j^{ab})^2 = \mathbb{J} \,. \tag{2.2.11}$$

Therefore we can write for a c-number λ

$$\begin{aligned} e^{\lambda\Gamma_j^a} &= ch\lambda + \Gamma_j^a sh\lambda \\ e^{\lambda\Gamma_j^0} &= ch\lambda + \Gamma_j^0 sh\lambda \\ e^{\lambda J_j^{ab}} &= ch\lambda + J_j^{ab} sh\lambda \,. \end{aligned} \tag{2.2.12}$$

From commutating rules we have

$$\begin{aligned} &\mathrm{Sp}\,(\Gamma_j^a) = 0 \\ &\mathrm{Sp}\,(\mathbb{J}) = 4^N \,, \end{aligned} \tag{2.2.13}$$

where $\mathbb{J} = \bigotimes_{j=1}^{N} \mathbb{J}_j$. The electrons' number operators in the Γ-realization have the form

$$n_{j+} = \frac{1}{2}(\mathbb{J} - J_j^{34}) \tag{2.2.14a}$$

$$n_{j-} = \frac{1}{2}(\mathbb{J} + J_j^{12}) \,. \tag{2.2.14b}$$

Thus we can write the Hubbard Hamiltonian in terms of Γ-matrices as

$$H_0 = -(\eta + u)N + \sum_j \left[u\Gamma_j^0 + \frac{1}{2}(\mu_0 B - \eta)J_j^{12} + \frac{1}{2}(\mu_0 B + \eta)J_j^{34} \right] \tag{2.2.15a}$$

$$H_1 = \frac{it}{2} \sum_{\langle i,j\rangle} \sum_a \left[\frac{1}{2}\Gamma_i^a\Gamma_j^a \sin\alpha_{ij} - (\Gamma_i^1\Gamma_j^2 - \Gamma_i^3\Gamma_j^4)\cos\alpha_{ij} \right] \tag{2.2.15b}$$

Let us note that the Γ-realization of the Hamiltonian does not depend on the dimensionality of the lattice.

3. High Temperature Effects

3.1. *High temperature diagrams — a qualitative approach*

A system is fully described by its density matrix

$$\rho = e^{-\beta H} \tag{3.1.1}$$

or, equivalently, by its partition function

$$Z = \mathrm{Sp}\,(\rho)\,. \tag{3.1.2}$$

To calculate the density matrix we divide the Hubbard Hamiltonian into a nonperturbed part H_0 and a perturbed one H_1. Thus we can write the Dyson expansion for (3.1.1)

$$\rho(\beta) = e^{-\beta H_0} T_\tau \exp\left\{ - \int_0^\beta V(\tau) d\tau \right\} \tag{3.1.3}$$

Here we denoted

$$V(\tau) = e^{\tau H_0} H_1 e^{-\tau H_0} \tag{3.1.4}$$

the hopping Hamiltonian in the interaction picture and T_τ stands for the 'chronological' product. Let us first calculate the zeroth-order part of the density matrix

$$\rho_0 = e^{-\beta H_0} \tag{3.1.5}$$

Due to commuting properties of matrices contained in H_0 it is easy to derive this quantity

$$\rho_0 = e^{\beta(\eta+u)N} \prod_j (chx - \Gamma_j^0 shx)(cha - J_j^{12} sha)(chb - J_j^{34} shb) \tag{3.1.6}$$

where we use the notation

$$x = \beta u = x(\beta)$$

$$a = \frac{\beta}{2}(\mu_0 B - \eta) = a(\beta)$$

$$b = \frac{\beta}{2}(\mu_0 B + \eta) = b(\beta)$$

With this result we can write the interaction Hamiltonian in the form

$$V(\beta) = \frac{it}{2} \sum_{\substack{(i,j)\\ a}} (ch\,2x + \Gamma_i^0 sh\,2x)(ch\,2x + \Gamma_j^0 sh2x) \times \left[\frac{1}{2} \Gamma_i^a \Gamma_j^a \sin \alpha_{ij} - (\Gamma_i^1 \Gamma_j^2 - \Gamma_i^3 \Gamma_j^4) \cos \alpha_{ij} \right] \tag{3.1.7}$$

In order to calculate the partition function (3.1.2) it is sufficient to consider those terms in the high-temperature expansion which are proportional to the unity matrix only (see (2.2.13)).

To simplify our considerations let us turn back to the original Hubbard model formulated in terms of creation and annihilation operators. Here the relevant terms are those which contain particles number operators only. Therefore we consider only such operator products which result in operators of numbers of electrons. It is easy to find a graphical representation of relevant processes in the sense as explained above. We can draw the following graphs up to the fourth order.

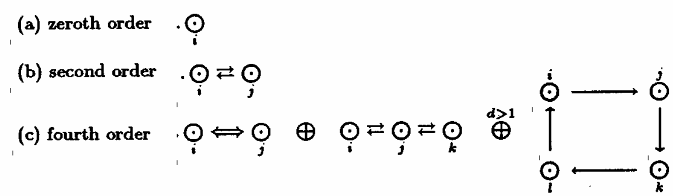


Fig. 1

Here $\underset{i}{\odot}$ represents the ith lattice site and '$\longrightarrow$' stands for the hopping process. We see that all relevant processes form closed graphs. Hence

$$Z(\beta, t, u) = Z(\beta, -t, u)\,. \tag{3.1.8}$$

This result can be obtained by considering symmetries in the Hubbard model (see Refs. 3 or 7).

In Sec. 2.1 we have shown that the Hubbard Hamiltonian does not exhibit an explicit translational symmetry due to nonperiodicity of the magnetic vector potential. A qualitative approach based on our diagramatic consideration shows that this symmetry braking disappears from averaging of measurables. We can divide our kinetic diagrams (every link represents hopping process of an electron between neighbor sites) into two parts. The first group consists of double links only and the second only of plaquettes. If we consider diagrams of higher orders we have clearly mixed diagrams consisting of double links as well as of plaquettes.

If we calculate contributions from double-links parts of a diagram we need not bother with phase shifts which compensate each other due to the relation

$$\alpha_{ij} = -\alpha_{ji} \,.$$

As for graphs with plaquettes we can assign to every plaquette the term

$$\exp \left(\frac{e}{\hbar} \oint_{\partial(\mathrm{pl})} A \cdot \mathrm{dr} \right) = \exp\left(\frac{e}{\hbar}\Phi_{\mathrm{pl}}\right) , \qquad (3.1.9)$$

where $\partial(\mathrm{pl})$ is the boundary of a given plaquette and Φ_{pl} is the magnetic flux through it. This term is apparently translational invariant. In Sec. 3.3 we will see that such plaquettes create magnetic oscillations at high temperatures.

Let us now consider correlation functions which are particularly relevant as they can indicate various interesting properties of a system (e.g. superconductivity, response to an external field, etc). We define the correlation function by the formula

$$\langle F(a^+, a)\rangle = Z^{-1}\mathrm{Sp}\,\{\rho F(a^+, a)\} , \qquad (3.1.10)$$

where $F(a^+, a)$ stands for a product of various creation and annihilation operators. Our diagramatic considerations lead to the fact that anomalous correlation functions defined as

$$\langle a^+_{i\sigma} a^+_{j\sigma}\rangle \,, \quad \langle a_{i\sigma} a_{j\sigma}\rangle$$

are zeros in the high temperature expansion (hopping energy of electrons makes impossible to create an electron in a lattice site without annihilation of another electron with the same spin in neighbor lattice site).

The Cooper pair on the lattice consists of two electrons with opposite spins placed in neighbor sites. High temperature expansion enables us to derive the correlation between two Cooper pairs placed at $\langle i, j\rangle$ and $\langle k, l\rangle$. The nonzero value of this function is due to transitions of electrons over lattice links. Thus we can write

$$\langle a^+_{i+} a^+_{j-} a_{k+} a_{l-}\rangle \sim O(t^{|k-i|+|l-j|})$$

We see that within our approximation $\beta t \ll 1$ that correlation is restricted to atomic distances. Nevertheless one can predict the importance of this function for processes which are important at low temperatures $\beta t \gg 1$, where existence of the superconducting phase is assumed.[2] Generally, only those groups can be correlated which are related by hops over lattice links.

3.2. Thermodynamical quantities in the second order of high temperature expansion

First we rewrite the zeroth-order density matrix (3.1.6) into the form

$$\rho_0(\beta) = e^{\beta(\eta+u)N} \prod_j (A + BJ_j^{12} + CJ_j^{34} + D\Gamma_j^0) \qquad (3.2.1)$$

where we use the notation

$$A = chx\, cha\, chb - shx\, sha\, shb = A(\beta)$$

$$B = shx\, cha\, shb - chx\, sha\, chb = B(\beta)$$

$$C = shx\, sha\, chb - chx\, cha\, shb = C(\beta)$$

$$D = chx\, sha\, shb - shx\, cha\, chb = D(\beta)$$

According to (2.2.13) we can calculate the partition function in zeroth-order

$$Z_0(\beta) = 2^N e^{\beta(\eta+u)N} q^N \qquad (3.2.2)$$

where

$$q \equiv 2A = (e^{\beta u} ch\beta\mu_0 B + e^{-\beta u} ch\beta\eta) \qquad (3.2.3)$$

The partition function $Z_0(\beta)$ characterizes a system of localized electrons on a lattice placed in a homogenous magnetic field B. In the case of half-filled lattice ($\eta = 0$) such a system stands for a Neel antiferromagnet.

Let us now calculate the second-order partition function according to

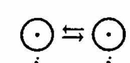
$$Z_2(\beta) = \int_0^\beta d\tau \int_0^\tau d\tau' \mathrm{Sp}\,[V(\tau')H_1 e^{-\beta H_0}] \,. \qquad (3.2.4)$$

As was shown in Sec. 3.1 we need not consider the gauge terms. Thus in the following we have

$$H_1 = \frac{it}{2} \sum_{\langle i,j\rangle} \sum_a \Gamma_i^a \Gamma_j^a \qquad (3.2.5)$$

$$V(\tau) = \frac{it}{2} \sum_{\langle i,j\rangle} \sum_a (ch2x + \Gamma_i^0 sh2x)(ch2x + \Gamma_j^0 sh2x)\Gamma_i^a \Gamma_j^a \qquad (3.2.6)$$

We compute the diagram



which has the analytical form

$$V(\tau)H_1e^{-\beta H_0} = e^{\beta(\eta+u)N}\left(\frac{it}{2}\right)^2 \sum_{(i,j)}\sum_a (ch2x' + \Gamma_i^0 sh2x') \times (ch2x' + \Gamma_j^0 sh2x')(\Gamma_i^a\Gamma_j^a)^2 \prod_m (A + BJ_m^{12} + CJ_m^{34} + D\Gamma_m^0)\,, \quad (3.2.7)$$

where $x' \equiv \tau' u$. Integrating the last expression in the sense of (3.2.4) we obtain

$$Z_2 = 2^N e^{\beta(\eta+u)N} q^{N-2} dN\beta t^2 \left[\frac{sh(2\beta u)}{2u} + \beta ch(\beta\mu_0 B)ch(\beta\eta)\right] \quad (3.2.8)$$

Here we performed the trace and used (2.2.13). Thus the partition function up to the second order has the form

$$Z = 2^N e^{\beta(\eta+u)N} q^N \left\{1 + \frac{dNt^2\beta}{q^2}\left[\frac{sh(2\beta u)}{2u} + \beta ch(\beta\mu_0 B)ch(\beta\eta)\right]\right\} \quad (3.2.9)$$

Magnetic properties of the model are characterized by magnetization and magnetic susceptibility stands for macroscopic response of the system to an external magnetic field. The magnetization M of our model is given as

$$M = \beta^{-1}\frac{\partial \ln Z}{\partial B} \quad (3.2.10)$$

Let us fix the average number of particles

$$N_e = \beta^{-1}\frac{\partial \ln Z}{\partial \eta} \quad (3.2.11)$$

Eliminating the chemical potential η from the last equation by iterations up to the relevant order in βt and substituting it to (3.2.10) we obtain

$$M = N(1 - |\delta|)\mu_0(th)(\beta\mu_0 B)\left[1 - \beta\frac{dt^2(1 - |\delta|)}{2uch^2(\beta\mu_0 B)}\right]. \quad (3.2.12)$$

Here we introduced the notation $\delta = n - 1$ for the deviation of number of electrons from the half-filled lattice. The magnetic susceptibility χ of the Hubbard system up to the second order is

$$\chi = \frac{\partial M}{\partial B} = \frac{N\beta\mu_0^2(1 - |\delta|)}{ch^2(\beta\mu_0 B)}\left[1 - \beta\frac{dt^2(1 - |\delta|)}{2uch^2(\beta\mu_0 B)}(1 - 2sh^2(\beta\mu_0 B))\right] \quad (3.2.13)$$

This result was obtained for $d = 1$ in Ref. 8. Clearly it does not imply any paradoxes as it was the case of solutions (1.1) and (1.2) which were derived from Lieb and Wu solutions. The magnetic susceptibility becomes zero for an empty lattice ($\delta = -1$) and for totally filled one ($\delta = 1$). Let us note that the zero-order part of magnetization

$$M(t = 0) = N(1 - |\delta|)\mu_0 th(\beta\mu_0 B)$$

represents its value for a system of localized electrons (solution (1.1) exhibits a divergency in that case).

3.3. *Aharonov–Bohm effect in the Hubbard model (calculation of the periodic part of magnetization)*

It has been verified by experiments[10] that the phase shift of electronic wavefunctions in metallic lattices can be observed at low temperatures. In this section we are going to show that oscillations of observables (magnetization, magnetic susceptibility) can arise due to the lattice structure at high temperatures as well but with a large period. For this purpose we need to apply the algebraic approach developed in previous chapters to the fourth-order of the perturbation theory, namely to the plaquette diagram in Fig. 1.3). In the following we restrict ourselves to $d = 2$ for simplicity. It is believed that namely this case is relevant for high-T_c superconductivity. Nevertheless generalization to higher dimensions presents no problems.

Thus we compute the trace of the expression

$$\rho_4^p(\beta) = e^{-\beta H}\int_0^\beta\int_0^\tau\int_0^{\tau_1}\int_0^{\tau_2} d\tau d\tau_1 d\tau_2 d\tau_3 [V(\tau)V(\tau_1)V(\tau_2)V(\tau_3)]_{\rm pl}\,. \quad (3.3.1)$$

Here 'p' denotes 'periodic part' of the density matrix. In the following we use the notation

$$V(\tau) = \frac{it}{2}\sum_{(i,j)} V_{ij}(\tau) \quad (3.3.2)$$

Hence

$$\rho_4^p(\beta) = \left(\frac{it}{2}\right)^4 e^{-\beta H_0}\int_0^\beta\int_0^\tau\int_0^{\tau_1}\int_0^{\tau_2} d\tau d\tau_1 d\tau_2 d\tau_3 \times \sum_{\substack{(i,j)\\ {\rm pl}(ijkl)}} V_{ij}(\tau)V_{jk}(\tau_1)V_{kl}(\tau_2)V_{li}(\tau_3) \quad (3.3.3)$$

After some calculations with the use of the commutating rules (2.2.8) we ge

$$\rho_4^p(\beta) = \left(\frac{it}{2}\right)^4 \sum_{\substack{i<j\\ \mathrm{pl}(ijkl)}} I(\beta)_{ijkl}(T_{ij}T_{jk}T_{kl}T_{li})e^{-\beta H_0} \qquad (3.3.4)$$

where

$$\begin{aligned} I(\beta)_{ijkl} = \int_0^\beta \int_0^\tau \int_0^{\tau_1} \int_0^{\tau_2} & d\tau d\tau_1 d\tau_2 d\tau_3 (ch2x + \Gamma_i^0 sh2x)(ch2x + \Gamma_j^0 sh2x) \\ & \times (ch2x_1 - \Gamma_j^0 sh2x_1)(ch2x_1 + \Gamma_k^0 sh2x_1) \\ & \times (ch2x_2 - \Gamma_k^0 sh2x_2)(ch2x_2 + \Gamma_l^0 sh2x_2) \\ & \times (ch2x_3 - \Gamma_l^0 sh2x_3)(ch2x_3 - \Gamma_i^0 sh2x_3) \end{aligned}$$

$$T_{ij} = \sum_a \Gamma_i^a\Gamma_j^a \sin\alpha_{ij} - (\Gamma_i^1\Gamma_j^2 + \Gamma_j^1\Gamma_i^2 - \Gamma_i^3\Gamma_j^4 - \Gamma_j^3\Gamma_i^4)\cos\alpha_{ij} \ .$$

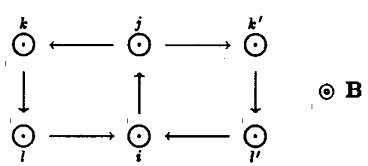
First we calculate the term $T_{ij}T_{jk}T_{kl}T_{li}$. We use the basic anticommutation rule (2.2.5) and relations (2.2.7) and (2.2.11). We write explicitly the relevant terms only (relevant for nonvanishing trace). Thus we get

$$\begin{aligned} T_{ij}T_{jk}T_{kl}T_{li} = 2\cos\alpha \Big[\frac{1}{2} & - J_i^{12}J_j^{12} - J_I^{12}J_k^{12} - J_i^{12}J_l^{12} + J_j^{12}J_l^{12} \\ & + J_j^{12}J_k^{12} + J_k^{12}J_l^{12} - J_i^{12}J_j^{12}J_k^{12}J_l^{12} + (12 \to 34)\Big] \\ & + 2i\sin\alpha \cdot f(J_r^{12}, J_s^{34}\ ; r, s = i, j, k, l)\ , \end{aligned} \qquad (3.3.5)$$

where f denotes a linear combination of matrix products and

$$\alpha = \alpha_{ij} + \alpha_{jk} + \alpha_{kl} + \alpha_{li} = \frac{e}{\hbar}\Phi_{\mathrm{pl}}\ .$$

At this step we add another diagram corresponding to our prior link (i, j) with its plaquette perpendicular to the direction of the magnetic field **B**. Thus we compute the diagram



To a given direction $i \to j$ there are two connected plaquettes with opposite orientations of electronic loops. Therefore the new 'prime' plaquette gives the same contribution as our original graph after substitution $\alpha \to -\alpha$. We see that the imaginary part in (3.3.5) vanishes and we get

$$\begin{aligned} T_{ij}T_{jk}T_{kl}T_{li} = 2\cos\alpha \Big[\frac{1}{2} & - J_i^{12}J_j^{12} - J_i^{12}J_k^{12} - J_i^{12}J_l^{12} + J_j^{12}J_l^{12} + J_j^{12}J_k^{12} \\ & + J_k^{12}J_l^{12} - J_i^{12}J_j^{12}J_k^{12}J_l^{12} + (12 \to 34)\Big]\ . \end{aligned}$$

Now let us calculate the integral $I(\beta)_{ijkl}$. All operators in this expression commute so the calculations are routine but rather lengthy. As a result we have

$$\begin{aligned} I(\beta)_{ijkl} = \frac{1}{2^3}[& I_1 + I_2(\Gamma_i^0\Gamma_j^0 + \Gamma_i^0\Gamma_l^0 + \Gamma_i^0\Gamma_k^0) + I_3(\Gamma_j^0\Gamma_k^0 + \Gamma_k^0\Gamma_l^0 + \Gamma_j^0\Gamma_l^0) \\ & + I_4\Gamma_i^0\Gamma_j^0\Gamma_k^0\Gamma_l^0 + I_5\Gamma_i^0 + I_6(\Gamma_j^0 + \Gamma_k^0 + \Gamma_l^0) + I_7\Gamma_j^0\Gamma_k^0\Gamma_l^0 \\ & + I_8(\Gamma_i^0\Gamma_j^0\Gamma_k^0 + \Gamma_i^0\Gamma_k^0\Gamma_l^0 + \Gamma_i^0\Gamma_j^0\Gamma_k^0)]\ , \end{aligned} \qquad (3.3.7)$$

where we denoted

$$I_1 = \frac{\beta^4}{24} + \frac{\beta^2 ch4u\beta}{2(4u)^2} + \frac{\beta sh4u\beta}{(4u)^3} - 3\frac{ch4u\beta - 1}{(4u)^4}$$

$$I_2 = -\frac{\beta^4}{24} + \frac{\beta^2}{(4u)^2}\left(1 + \frac{ch4u\beta}{2}\right) - \frac{\beta sh4u\beta}{(4u)^3} - \frac{ch4u\beta - 1}{(4u)^4}$$

$$I_3 = \frac{\beta^4}{24} + \frac{\beta^2 ch4u\beta}{2(4u)^2} - \frac{\beta sh4u\beta}{(4u)^3} + 5\frac{ch4u\beta - 1}{(4u)^4}$$

$$I_4 = -\frac{\beta^4}{24} - \frac{\beta^2}{(4u)^2}\left(3 - \frac{ch4u\beta}{2}\right) - 5\frac{\beta sh4u\beta}{(4u)^3} + 15\frac{ch4u\beta - 1}{(4u)^4}$$

$$I_5 = -\frac{\beta^3}{2(4u)} + \frac{\beta^2 sh4u\beta}{2(4u)^2} + \frac{\beta(2 + ch4u\beta)}{(4u)^3} - 3\frac{sh4u\beta}{(4u)^4}$$

$$I_6 = \frac{\beta^3}{6(4u)} + \frac{\beta^2 sh4u\beta}{2(4u)^2} + \frac{\beta(2 - ch4u\beta)}{(4u)^3} - \frac{sh4u\beta}{(4u)^4}$$

$$I_7 = -\frac{\beta^3}{2(4u)} + \frac{\beta^2 sh4u\beta}{2(4u)^2} - \frac{5\beta(2 + ch4u\beta)}{(4u)^3} + 15\frac{sh4u\beta}{(4u)^4}$$

$$I_8 = \frac{\beta^3}{6(4u)} + \frac{\beta^2 sh4u\beta}{2(4u)^2} - \frac{\beta(2 + 3ch4u\beta)}{(4u)^3} + 5\frac{sh4u\beta}{(4u)^4}\ .$$

Substituting back to (3.3.4) and taking the relevant terms in tracing we get the result

$$Z_4^p = e^{\beta(u+\eta)N} t^4 2N 2^N q^{N-4} \frac{\cos\alpha}{2} \left\{ \frac{\beta^4}{24}(e^{-2\beta u} ch\beta\mu_0 B\, ch3\beta\eta + e^{2\beta u} ch3\beta\mu_0 B\, ch\beta\eta) - \frac{\beta^3}{8u}(ch2\beta\mu_0 B - ch2\beta\eta) + \frac{\beta^2}{(4u)^2}(3ch2\beta u\, ch\beta\mu_0 B\, ch\beta\eta - ch2\beta\mu_0 B - ch2\beta\eta) + \frac{\beta}{(4u)^3}\left[-(1-e^{4\beta u}) ch2\beta\mu_0 B + (1-e^{-4\beta u}) ch2\beta\eta - 6sh2\beta u\, ch\beta\mu_0 B\, ch\beta\eta\right] \right\}. \tag{3.3.8}$$

By the standard way we eliminate the chemical potential η by iterating according to (3.2.11). The periodic part of magnetization of the near half-filled lattice obtained by this procedure is

$$M^p = \frac{Nt^4}{(4u)^3} \frac{eS_{\rm pl}}{\hbar} \frac{1-|\delta|}{ch^4\beta\mu_0 B} \sin\left(\frac{e}{\hbar}S_{\rm pl}B\right) \left[\frac{4-9|\delta|}{2-2|\delta|} ch^2\beta\mu_0 B - 1\right] \tag{3.3.9}$$

where $S_{\rm pl}$ is the square of an elementary plaquette and we differentiated according to (3.2.10) only terms with the most rapid change in B (the terms with the cosine function). This function oscillates with the period

$$\Delta B = \frac{2\pi\hbar}{eS_{\rm pl}} \tag{3.3.10}$$

which is very large ($\sim 10^4 T$). Let us note that the period does not depend on temperature. Clearly such a basic period is contained in all higher-order parts of high-temperature expansion. Thus every next contribution of higher order to magnetization contains oscillating terms with periods equal to an integer fraction of our basic period (3.3.10). These integer fractions are given by corresponding order of the perturbation expansion. When temperature decreases oscillations with smaller periods become more relevant.

As can be seen from (3.3.10) a method how to decrease the period of oscillations at a given temperature is to increase the lattice parameter (or, equivalently, the square of an elementary lattice plaquette). An analogue of transmission of electrons over lattice links can be found in microelectronic devices of lattice-like structure. If the lattice parameter of such a structure is 1μm, our high-temperature effect should be measured in these materials. If it was the case the basic period of oscillations would be of order of 10^{-1} mT. Moreover at high temperatures the periodic part of magnetization has much larger magnitude comparing with other contributions. The relation is

$$M^p : M^n \sim \frac{e}{\hbar}S_{\rm pl} : \mu_0 B \gg 1$$

where M^n stands for nonperiodic contributions. Another way how to observe such oscillations is to use crystals made by method of epitaxy, when the lattice parameter could be of order of 10^{-7}m.

4. Conclusion

In this paper we have investigated magnetic properties of the Hubbard model at high temperatures in the strong-coupling limit. We have shown that the high temparature expansion of the density matrix does not imply any paradoxes which raise at zero temperature. These paradoxes are not inherent in Lieb and Wu solutions but are rather consequences of approximations done by Shiba and Uimin and Fomitchev.

We have calculated a periodic part of magnetization for $d = 2$ in the fourth order of high-temperature expansion. We have shown that the oscillations are due to Aharonov–Bohm-like effects and a lattice structure of normal metal. Corresponding period of such oscillations is very large for normal metals but there are materials where that high-temperature effect should raise.

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