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Зарядові та магнітні стани моделі Хаббарда на тривузловому кластері

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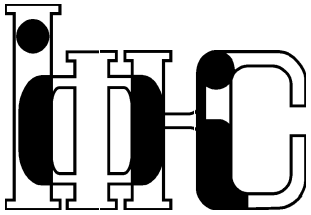

ІНСТИТУТ ФІЗИКИ КОНДЕНСОВАНИХ СИСТЕМ

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Charge and magnetic states for the Hubbard model on a three-site cluster

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Зарядові та магнітні стани моделі Хаббарда на тривузловому кластері

О.П. Матвєєв, А.М. Швайка

Анотація. Досліджується модель Хаббарда на кластерах малого розміру. Методом функцій Гріна розраховані електронна, магнітна і спінова сприйнятливості та досліджена їх поведінка при низьких температурах. Досліджена температурна поведінка сприйнятливостей для дво- та тривузлового кластерів на краю та в центрі зони Бріллюена. Отримано, що якщо при заданій концентрації основний стан є поляризований, то сприйнятливості розбігаються по закону Кюрі і система переходить у магнітовпорядкований стан при $T = 0$.

Charge and magnetic states for the Hubbard model on a three-site cluster

O.P. Matveev, A.M. Shvaika

Abstract. The Hubbard model for small size clusters is investigated. Using direct diagonalization of the small cluster Hamiltonian, an electronic, magnetic and spin susceptibilities are calculated and their behavior at low temperature is investigated. The temperature behavior of susceptibilities for two- and three-site clusters is investigated for both center and edge of the Brillouin zone. If at given concentration ground state is polarized, a susceptibilities diverge following the Courier law and system is transformed to the magnetically ordered state at $T = 0$.

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1. Introduction

Compounds with transition- and rare-earth metals (oxides, sulfides and other) possess an unique physical properties and attract great attention in the fields of practical applications and general-theoretical learning. Regarding the magnetic properties of such compounds, they are ferromagnetic, ferrimagnetic, antiferromagnetic. The peculiarity of some of them is in possibility of magnetic transitions which are followed by the change of magnetic-order type under the external influence. According to the electrical properties, transition- and rare-earth metal compounds may be divided into four groups: insulators, metals, compounds which possess a possibility of a metal-insulator transition (caused by external factors) with simultaneous change of the magnetic properties and a magnetic-disordered compounds in which a metal-insulator transition takes place too. But at the same time, mechanisms of the exchange interactions at the metal-insulator transition in such compounds are investigated insufficiently and that is connected with the according of strong electron correlation. In this connection there is a need for the investigation of physics of such phenomena as ferromagnetism, antiferromagnetism etc. by using the Hubbard model.

The Hubbard model [1–3] was originally proposed for the description of correlations in narrow-band materials on a three-dimensional lattice. It takes into account the main system characteristics namely electron hopping and Coulomb interaction. Its two-dimensional version is often considered as the minimal model for describing the copper oxide planes in high-T_c superconductors [4,5]. The one-dimensional Hubbard model has an exact solution in terms of the Bethe-Ansatz [6], displays Luttinger liquid and Mott insulator phases and has received much attention [7]. In infinite dimensions an another exact solutions for Hubbard model were obtained within Dynamical Mean Field Theory [8].

In other dimensions, for which there are no exact solutions, a great variety of approximate treatments have been proposed in order to accommodate a suitable theoretical framework. In this connection, much efforts were used to obtain exact ground states of few electrons for the Hubbard model on a finite size cluster (see, Ref. [9] and references therein) from which the ground state energy for the low-dimensional cases can be estimated using a concept of dimensional scaling [10].

The last period has provided new motivations for the further investigations of the systems containing small number of particles confined in a device or unit, as for example in the case of quantum dots, quantum well structures, mesoscopic systems, experimental entanglement, etc., for

which the knowledge of the ground state is not enough. Consideration of the excited states is much more complicated problem and at the moment it is studied in detail only for the two-site [11–13] and four-site [14] clusters. In Ref. [15] the linear chains and rings containing two to six atoms were studied numerically and it was found that with increase of the cluster size the thermodynamic properties of the model at half-filling approaches its one-dimensional limit whereas magnetic susceptibility shows clear even-odd effect in the very low temperature region.

As there is no direct interaction between spins in the Hubbard model, it is hard to predict a behavior of a spin system. Going out of the fact, that a susceptibility of spin system at zero temperature diverges following the Courier law [16], by means of calculating cluster susceptibilities and investigating their behavior at low temperatures, one can speculate about the system order. The problem is also interesting, because a phenomenon of the frustration (problem of spins mutual accommodation) is appearing in three-site case and it is worth investigating how it influences on a system ordering [17]. In particular, recently great attention was paid to the systems where the geometrical frustration exists, because an interesting phenomenon was discovered. Namely in compounds LiV_2O_4 with polychlorine ions structure a strong fermion behavior is observed [18]. Also another polychlorine compound Y(SC)Mn_2 [19] exhibits a quantum spin-liquid behavior at low temperature. The influence of frustration is investigated for the Hubbard model on triangular lattice, which is a net of a tetrahedron edges in which an interactions between the apexes (sites) are not the same: the hopping integral (t') between the sites of base of a tetrahedron is different then between the base site and the apex of a tetrahedron (t) [20]. It was shown that frustration due to non-local correlations suppresses short-range antiferromagnetic fluctuations and thereby assists the formation of heavy quasi-particles near half-filling. That is why a three-site cluster is investigated in presented work.

The aim of this work is investigation of Hubbard model on a three-site cluster, namely calculation of the energy of the many-electron states and one-electron transitions, the charge and longitudinal and transverse spin susceptibilities, which will contain the information about charge and magnetic states of a system.

2. Method

In this work the direct calculation of the relevant Green's functions is carried out for investigation of susceptibilities of small size clusters (two-

and three-site) by means of the direct diagonalization of the Hamiltonian of a system. In such approach the analytical expressions for magnetic and spin susceptibilities are determined in the case of two-site cluster. For tree-site cluster a numerical methods are used because the analytical expressions are too complicated. The theoretical derivation of a work formula is the same for both cases and is presented below.

By definition, the Green's function built on operators $\hat{A}_{i\sigma}$, $\hat{B}_{j\sigma'}$ is equal

$$\mathcal{G}_{ij\sigma\sigma'}(\tau) = -\langle T\hat{A}_{i\sigma}(\tau)\hat{B}_{j\sigma'}(0)\rangle, \tag{1}$$

where $\hat{A}_{i\sigma}, \hat{B}_{j\sigma'}$ are operators of the Bose or Fermi type, i and j are site indexes, and $\sigma, \sigma' = (\uparrow, \downarrow)$.

In general, all operators act in some complete basis of many particle states and can be represented by the Hubbard operators

$$\hat{A}_{i\sigma} = \sum_{pq} A^{pq}_{i\sigma} X^{pq}, \qquad \hat{B}_{j\sigma'} = \sum_{p'q'} B^{p'q'}_{j\sigma'} X^{p'q'}, \tag{2}$$

where p, q denote many particles states, then the Green's function can be expressed in terms of Green's functions constructed by the Hubbard operators

$$\mathcal{G}_{ij\sigma\sigma'}(\tau) = -\sum_{pqp'q'} A^{pq}_{i\sigma} B^{p'q'}_{j\sigma'} \langle T X^{pq}(\tau) X^{p'q'}(0)\rangle. \tag{3}$$

Now, let us introduce a certain unitary transformation $V^{p\tilde{p}}$ which transforms the Hamiltonian of system to a diagonal form. Then, Hubbard operators defined on initial basis $|p\rangle$ are connected with the Hubbard operators defined on eigenstates by

$$X^{pq} = |p\rangle\langle q| = \sum_{\tilde{p}\tilde{q}} V^{p\tilde{p}} (V^{q\tilde{q}})^\dagger |\tilde{p}\rangle\langle\tilde{q}| = \sum_{\tilde{p}\tilde{q}} V^{p\tilde{p}} (V^{q\tilde{q}})^\dagger X^{\tilde{p}\tilde{q}} \tag{4}$$

and, respectively, the Green's function is equal

$$\mathcal{G}_{ij\sigma\sigma'}(\tau) = -\sum_{\substack{pqp'q' \\ \tilde{p}\tilde{q}\tilde{p}'\tilde{q}'}} A^{pq}_{i\sigma} B^{p'q'}_{j\sigma'} V^{p\tilde{p}} (V^{q\tilde{q}})^\dagger V^{p'\tilde{p}'} (V^{q'\tilde{q}'})^\dagger \times \langle T X^{\tilde{p}\tilde{q}}(\tau) X^{\tilde{p}'\tilde{q}'}(0)\rangle. \tag{5}$$

By definition, the Heisenberg's representation for X-operators defined on eigenstates is reduced to [21]

$$X^{\tilde{p}\tilde{q}}(\tau) = e^{(\lambda_{\tilde{p}} - \lambda_{\tilde{q}})\tau} X^{\tilde{p}\tilde{q}} \tag{6}$$

and introducing notations

$$\tilde{A}^{\tilde{p}\tilde{q}}_{i\sigma} = \sum_{pq} V^{p\tilde{p}} (A^{pq}_{i\sigma} V^{q\tilde{q}})^{\dagger}, \tag{7}$$
$$\tilde{B}^{\tilde{p}'\tilde{q}'}_{j\sigma'} = \sum_{p'q'} V^{p'\tilde{p}'} (B^{p'q'}_{j\sigma'} V^{q'\tilde{q}'})^{\dagger}$$

an expression for the Green's function takes form

$$\mathcal{G}_{ij\sigma\sigma'}(\tau) = -\sum_{\tilde{p}\tilde{q}} \tilde{A}^{\tilde{p}\tilde{q}}_{i\sigma} \tilde{B}^{\tilde{q}\tilde{p}}_{j\sigma'} e^{(\lambda_{\tilde{p}} - \lambda_{\tilde{q}})\tau} \langle X^{\tilde{p}\tilde{p}} \rangle, \tag{8}$$
$$\langle X^{\tilde{p}\tilde{p}} \rangle = \frac{e^{-\beta\lambda_{\tilde{p}}}}{\sum_{\tilde{r}} e^{-\beta\lambda_{\tilde{r}}}}.$$

Now we will pass on to an energy representation, or in other words, we will carry out the Fourier transformation.

$$\mathcal{G}_{ij\sigma\sigma'}(\omega_n) = -\int_0^{\beta} e^{-i\omega_n\tau} \sum_{\tilde{p}\tilde{q}} \tilde{A}^{\tilde{p}\tilde{q}}_{i\sigma} \tilde{B}^{\tilde{q}\tilde{p}}_{j\sigma'} e^{(\lambda_{\tilde{p}} - \lambda_{\tilde{q}})\tau} \langle X^{\tilde{p}\tilde{p}} \rangle d\tau$$
$$= -\sum_{\tilde{p}\tilde{q}} \tilde{A}^{\tilde{p}\tilde{q}}_{i\sigma} \tilde{B}^{\tilde{q}\tilde{p}}_{j\sigma'} \langle X^{\tilde{p}\tilde{p}} \rangle \frac{1 - e^{\beta(\lambda_{\tilde{p}} - \lambda_{\tilde{q}} - i\omega_n)}}{i\omega_n - (\lambda_{\tilde{p}} - \lambda_{\tilde{q}})} \tag{9}$$

Taking into consideration that for the Bose particles $\omega_n = \frac{2\pi n}{\beta}$, while for the Fermi particles $\omega_n = \frac{\pi(2n+1)}{\beta}$, we will obtain:

$$\mathcal{G}_{ij\sigma\sigma'}(\omega_n) = \sum_{\tilde{p}\tilde{q}} \tilde{A}^{\tilde{p}\tilde{q}}_{i\sigma} \tilde{B}^{\tilde{q}\tilde{p}}_{j\acute{\sigma}} \frac{\langle X^{\tilde{p}\tilde{p}} \mp X^{\tilde{q}\tilde{q}} \rangle}{i\omega_n - (\lambda_{\tilde{p}} - \lambda_{\tilde{q}})}, \tag{10}$$

where plus is for the Fermi particles and minus is for the Bose particles.

Given expression is final in case of the Fermi particles, while for the Bose particles we should take into account a presence of diagonal components, namely that

$$\langle X^{\tilde{p}\tilde{p}} X^{\tilde{q}\tilde{q}} \rangle = \delta_{\tilde{p}\tilde{q}} \langle X^{\tilde{p}\tilde{p}} \rangle, \tag{11}$$
$$\frac{1 - e^{-i\omega_n\beta}}{i\omega_n} = \beta\delta(\omega_n) = \begin{cases} \frac{1}{T}, & \omega_n = 0 \\ 0, & \omega_n \neq 0 \end{cases}$$

then we will obtain final expression of a work formula for Bose particles:

$$\langle T\hat{A}_{i\sigma}(\tau)\hat{B}_{j\sigma'}(0)\rangle - \langle \hat{A}_{i\sigma}\rangle\langle \hat{B}_{j\sigma'}\rangle \tag{12}$$

$$\xrightarrow{FT} \sum_{\tilde{p}\tilde{q}} \tilde{A}^{\tilde{p}\tilde{q}}_{i\sigma} \tilde{B}^{\tilde{q}\tilde{p}}_{j\sigma'} \frac{\langle X^{\tilde{p}\tilde{p}} - X^{\tilde{q}\tilde{q}} \rangle}{i\omega_n - (\lambda_{\tilde{p}} - \lambda_{\tilde{q}})} + \frac{1}{T}\delta(\omega_n)$$
$$\times \left[\sum_{\tilde{p}} \tilde{A}^{\tilde{p}\tilde{p}}_{i\sigma} \tilde{B}^{\tilde{p}\tilde{p}}_{j\sigma'} \langle X^{\tilde{p}\tilde{p}} \rangle - \sum_{\tilde{p}} \tilde{A}^{\tilde{p}\tilde{p}}_{i\sigma} \langle X^{\tilde{p}\tilde{p}} \rangle \sum_{\tilde{q}} \tilde{B}^{\tilde{q}\tilde{q}}_{j\sigma'} \langle X^{\tilde{q}\tilde{q}} \rangle \right]$$

(FT denotes Fourier transformation).

3. Two-site cluster

It is appropriate to consider first a simpler case of the Hubbard model on a two-site cluster. Using the Green's function formalism, we shall calculate an electronic, magnetic and spin susceptibilities and investigate their behavior at $T \to 0$ case. It will allow us to estimate the possibilities of the ferromagnetic or antiferromagnetic ordered ground states. In case of a two-site cluster, the problem can be solved analytically without using a numerical calculations, what is practically impossible for a three-site cluster case.

3.1. Basic equations

Our aim is to calculate the Matsubara Green's functions $\langle T\hat{n}_i(\tau)\hat{n}_j(0)\rangle$, $\langle T\hat{m}_i(\tau)\hat{m}_j(0)\rangle$ and $\langle T\hat{S}^+_i(\tau)\hat{S}^-_j(0)\rangle$, where $\hat{n}_i = \hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}$, ($\hat{n}_{i\sigma} = \hat{a}^{\dagger}_{i\sigma}\hat{a}_{i\sigma}$) is particle number operator, $\hat{m}_i = \frac{1}{2}(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})$ is magnetic moment operator, $\hat{S}^+_i = \hat{a}^{\dagger}_{i\uparrow}\hat{a}_{i\downarrow}$, $\hat{S}^-_i = \hat{a}^{\dagger}_{i\downarrow}\hat{a}_{i\uparrow}$ are spin-flip operators.

The Hamiltonian of the Hubbard model on a two-site cluster is as follows

$$\mathcal{H} = \sum_{i=1,2} (U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu\sum_{\sigma} \hat{n}_{i\sigma}) + t\sum_{\sigma} (\hat{a}^{\dagger}_{1\sigma}\hat{a}_{2\sigma} + \hat{a}^{\dagger}_{2\sigma}\hat{a}_{1\sigma}), \tag{13}$$

where U denotes the single-site Coulomb interaction, μ is a chemical potential, and t is a hopping energy.

Solution of the problem in the case of two-site cluster (density of states is calculated and energy spectra is analyzed) is shown in Ref. [12], that is why here we will not present any details of derivations. We will apply only that results, which are needed for the calculation of susceptibilities.

The initial basis of states $|p\rangle = |n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}\rangle$ consists of sixteen states:

$$|1\rangle = |0,0,0,0\rangle,$$

$$
\begin{aligned}
|2\rangle &= |0,1,0,0\rangle = \hat{a}^\dagger_{1\downarrow}|1\rangle,\\
|3\rangle &= |0,0,0,1\rangle = \hat{a}^\dagger_{2\downarrow}|1\rangle,\\
|4\rangle &= |1,0,0,0\rangle = \hat{a}^\dagger_{1\uparrow}|1\rangle,\\
|5\rangle &= |0,0,1,0\rangle = \hat{a}^\dagger_{2\uparrow}|1\rangle,\\
|6\rangle &= |0,1,0,1\rangle = \hat{a}^\dagger_{2\downarrow}|2\rangle = -\hat{a}^\dagger_{1\downarrow}|3\rangle,\\
|7\rangle &= |1,0,1,0\rangle = \hat{a}^\dagger_{2\uparrow}|4\rangle = -\hat{a}^\dagger_{1\uparrow}|5\rangle,\\
|8\rangle &= |1,1,0,0\rangle = \hat{a}^\dagger_{1\uparrow}|2\rangle = -\hat{a}^\dagger_{1\downarrow}|4\rangle,\\
|9\rangle &= |1,0,0,1\rangle = \hat{a}^\dagger_{1\uparrow}\|3\rangle = -\hat{a}^\dagger_{2\downarrow}|4\rangle,\\
|10\rangle &= |0,1,1,0\rangle = \hat{a}^\dagger_{2\uparrow}|2\rangle = -\hat{a}^\dagger_{1\downarrow}|5\rangle,\\
|11\rangle &= |0,0,1,1\rangle = \hat{a}^\dagger_{2\uparrow}|3\rangle = -\hat{a}^\dagger_{2\downarrow}|5\rangle,\\
|12\rangle &= |1,1,0,1\rangle = \hat{a}^\dagger_{1\uparrow}|6\rangle = \hat{a}^\dagger_{1\downarrow}|9\rangle = -\hat{a}^\dagger_{2\downarrow}|8\rangle,\\
|13\rangle &= |0,1,1,1\rangle = \hat{a}^\dagger_{2\uparrow}|6\rangle = \hat{a}^\dagger_{1\downarrow}|11\rangle = -\hat{a}^\dagger_{2\downarrow}|10\rangle,\\
|14\rangle &= |1,1,1,0\rangle = \hat{a}^\dagger_{1\downarrow}|7\rangle = \hat{a}^\dagger_{2\uparrow}|8\rangle = -\hat{a}^\dagger_{1\uparrow}|10\rangle,\\
|15\rangle &= |1,0,1,1\rangle = \hat{a}^\dagger_{2\downarrow}|7\rangle = \hat{a}^\dagger_{2\uparrow}|9\rangle = -\hat{a}^\dagger_{1\uparrow}|11\rangle,\\
|16\rangle &= |1,1,1,1\rangle = \hat{a}^\dagger_{1\uparrow}|13\rangle = -\hat{a}^\dagger_{2\uparrow}|12\rangle\\
&\quad = \hat{a}^\dagger_{1\downarrow}|15\rangle = \hat{a}^\dagger_{2\downarrow}|14\rangle,
\end{aligned}
\tag{14}
$$

which, by transformation $|p\rangle = \sum_{\tilde{p}} V^{p\tilde{p}}|\tilde{p}\rangle$

$$
|\tilde{1}\rangle = |1\rangle, |\tilde{6}\rangle = |6\rangle, \qquad |\tilde{7}\rangle = |7\rangle, |\widetilde{16}\rangle = |16\rangle, \tag{15}
$$

$$
\begin{pmatrix} |2\rangle & |4\rangle & |12\rangle & |13\rangle \\ |3\rangle & |5\rangle & |14\rangle & |15\rangle \end{pmatrix}
= \begin{Vmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{Vmatrix}
\begin{pmatrix} |\tilde{2}\rangle & |\tilde{4}\rangle & |\widetilde{12}\rangle & |\widetilde{13}\rangle \\ |\tilde{3}\rangle & |\tilde{5}\rangle & |\widetilde{14}\rangle & |\widetilde{15}\rangle \end{pmatrix},
$$

$$
\begin{pmatrix} |8\rangle \\ |9\rangle \\ |10\rangle \\ |11\rangle \end{pmatrix}
= \begin{Vmatrix} \frac{1}{\sqrt{2}}\cos\phi & -\frac{1}{\sqrt{2}}\sin\phi & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}}\sin\phi & \frac{1}{\sqrt{2}}\cos\phi & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}}\sin\phi & \frac{1}{\sqrt{2}}\cos\phi & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}}\cos\phi & -\frac{1}{\sqrt{2}}\sin\phi & 0 & \frac{1}{\sqrt{2}} \end{Vmatrix}
\begin{pmatrix} |\tilde{8}\rangle \\ |\tilde{9}\rangle \\ |\widetilde{10}\rangle \\ |\widetilde{11}\rangle \end{pmatrix},
$$

where $\sin 2\phi(t) = \frac{2t}{\sqrt{\frac{U^2}{4}+4t^2}}$, create a new basis of eigenstates $|\tilde{p}\rangle$, where

the Hamiltonian has a diagonal form $\mathcal{H} = \sum_{\tilde{p}} \lambda_{\tilde{p}} X^{\tilde{p}\tilde{p}}$, with energy spectra:

$$
\begin{aligned}
\lambda_{\tilde{1}} &= 0,\\
\lambda_{\tilde{2}} &= \lambda_{\tilde{4}} = -\mu + t,\\
\lambda_{\tilde{3}} &= \lambda_{\tilde{5}} = -\mu - t,\\
\lambda_{\tilde{6}} &= \lambda_{\tilde{7}} = \lambda_{\widetilde{10}} = -2\mu,\\
\lambda_{\tilde{8}} &= U + J - 2\mu,\\
\lambda_{\tilde{9}} &= -J - 2\mu,\\
\lambda_{\widetilde{11}} &= U - 2\mu,\\
\lambda_{\widetilde{12}} &= \lambda_{\widetilde{14}} = U - 3\mu + t,\\
\lambda_{\widetilde{13}} &= \lambda_{\widetilde{15}} = U - 3\mu - t,\\
\lambda_{\widetilde{16}} &= 2U - 4\mu,
\end{aligned}
\tag{16}
$$

and $J = \frac{4t^2}{\sqrt{\frac{U^2}{4}+4t^2}+\frac{U}{2}}$.

3.2. Calculation of susceptibilities

For the chain with N=2 periodic boundary conditions we calculate charge and magnetic susceptibilities at the center ($q = 0$) and edges ($q = \pm\frac{\pi}{a}$) of the Brillouin zone. The charge and magnetic susceptibilities are constructed by the particle number operators which are represented by the Hubbard operators on a diagonalized basis as follow:

$$
\begin{aligned}
\hat{n}_{1\uparrow} &= \frac{1}{2}X^{\tilde{4},\tilde{4}} + \frac{1}{2}X^{\tilde{5},\tilde{5}} + X^{\tilde{7},\tilde{7}} + \frac{1}{2}X^{\tilde{8},\tilde{8}} + \frac{1}{2}X^{\tilde{9},\tilde{9}}\\
&+ \frac{1}{2}X^{\widetilde{10},\widetilde{10}} + \frac{1}{2}X^{\widetilde{11},\widetilde{11}} + \frac{1}{2}X^{\widetilde{12},\widetilde{12}} + \frac{1}{2}X^{\widetilde{13},\widetilde{13}}\\
&+ X^{\widetilde{14},\widetilde{14}} + X^{\widetilde{15},\widetilde{15}} + X^{\widetilde{16},\widetilde{16}}\\
&- \frac{1}{2}(X^{\tilde{4},\tilde{5}} + X^{\tilde{5},\tilde{4}}) - \frac{1}{2}(X^{\widetilde{12},\widetilde{13}} + X^{\widetilde{13},\widetilde{12}})\\
&- \frac{1}{2}\sin\phi\,(X^{\tilde{8},\widetilde{10}} + X^{\widetilde{10},\tilde{8}}) - \frac{1}{2}\cos\phi\,(X^{\tilde{9},\widetilde{10}} + X^{\widetilde{10},\tilde{9}})\\
&- \frac{1}{2}\cos\phi\,(X^{\tilde{8},\widetilde{11}} + X^{\widetilde{11},\tilde{8}}) + \frac{1}{2}\sin\phi\,(X^{\tilde{9},\widetilde{11}} + X^{\widetilde{11},\tilde{9}}),
\end{aligned}
\tag{17}
$$

$$
\begin{aligned}
\hat{n}_{1\downarrow} &= \frac{1}{2}X^{\tilde{2},\tilde{2}} + \frac{1}{2}X^{\tilde{3},\tilde{3}} + X^{\tilde{6},\tilde{6}} + \frac{1}{2}X^{\tilde{8},\tilde{8}} + \frac{1}{2}X^{\tilde{9},\tilde{9}}\\
&+ \frac{1}{2}X^{\widetilde{10},\widetilde{10}} + \frac{1}{2}X^{\widetilde{11},\widetilde{11}} + X^{\widetilde{12},\widetilde{12}} + X^{\widetilde{13},\widetilde{13}}
\end{aligned}
\tag{18}
$$

$$
\begin{aligned}
&+\frac{1}{2}X^{\widetilde{14},\widetilde{14}}+\frac{1}{2}X^{\widetilde{15},\widetilde{15}}+X^{\widetilde{16},\widetilde{16}}\\
&-\frac{1}{2}(X^{\tilde{2},\tilde{3}}+X^{\tilde{3},\tilde{2}})-\frac{1}{2}(X^{\widetilde{14},\widetilde{15}}+X^{\widetilde{15},\widetilde{14}})\\
&+\frac{1}{2}\sin\phi\,(X^{\tilde{8},\widetilde{10}}+X^{\widetilde{10},\tilde{8}})+\frac{1}{2}\cos\phi\,(X^{\tilde{9},\widetilde{10}}+X^{\widetilde{10},\tilde{9}})\\
&-\frac{1}{2}\cos\phi\,(X^{\tilde{8},\widetilde{11}}+X^{\widetilde{11},\tilde{8}})+\frac{1}{2}\sin\phi\,(X^{\tilde{9},\widetilde{11}}+X^{\widetilde{11},\tilde{9}}),
\end{aligned}
$$

$$
\begin{aligned}
\hat{n}_{2\uparrow} &= \frac{1}{2}X^{\tilde{4},\tilde{4}}+\frac{1}{2}X^{\tilde{5},\tilde{5}}+X^{\tilde{7},\tilde{7}}+\frac{1}{2}X^{\tilde{8},\tilde{8}}+\frac{1}{2}X^{\tilde{9},\tilde{9}} \qquad (19)\\
&+\frac{1}{2}X^{\widetilde{10},\widetilde{10}}+\frac{1}{2}X^{\widetilde{11},\widetilde{11}}+\frac{1}{2}X^{\widetilde{12},\widetilde{12}}+\frac{1}{2}X^{\widetilde{13},\widetilde{13}}\\
&+X^{\widetilde{14},\widetilde{14}}+X^{\widetilde{15},\widetilde{15}}+X^{\widetilde{16},\widetilde{16}}\\
&+\frac{1}{2}(X^{\tilde{4},\tilde{5}}+X^{\tilde{5},\tilde{4}})+\frac{1}{2}(X^{\widetilde{12},\widetilde{13}}+X^{\widetilde{13},\widetilde{12}})\\
&+\frac{1}{2}\sin\phi\,(X^{\tilde{8},\widetilde{10}}+X^{\widetilde{10},\tilde{8}})+\frac{1}{2}\cos\phi\,(X^{\tilde{9},\widetilde{10}}+X^{\widetilde{10},\tilde{9}})\\
&+\frac{1}{2}\cos\phi\,(X^{\tilde{8},\widetilde{11}}+X^{\widetilde{11},\tilde{8}})-\frac{1}{2}\sin\phi\,(X^{\tilde{9},\widetilde{11}}+X^{\widetilde{11},\tilde{9}}),
\end{aligned}
$$

$$
\begin{aligned}
\hat{n}_{2\downarrow} &= \frac{1}{2}X^{\tilde{2},\tilde{2}}+\frac{1}{2}X^{\tilde{3},\tilde{3}}+X^{\tilde{6},\tilde{6}}+\frac{1}{2}X^{\tilde{8},\tilde{8}}+\frac{1}{2}X^{\tilde{9},\tilde{9}} \qquad (20)\\
&+\frac{1}{2}X^{\widetilde{10},\widetilde{10}}+\frac{1}{2}X^{\widetilde{11},\widetilde{11}}+X^{\widetilde{12},\widetilde{12}}+X^{\widetilde{13},\widetilde{13}}\\
&+\frac{1}{2}X^{\widetilde{14},\widetilde{14}}+\frac{1}{2}X^{\widetilde{15},\widetilde{15}}+X^{\widetilde{16},\widetilde{16}}\\
&+\frac{1}{2}(X^{\tilde{2},\tilde{3}}+X^{\tilde{3},\tilde{2}})+\frac{1}{2}(X^{\widetilde{14},\widetilde{15}}+X^{\widetilde{15},\widetilde{14}})\\
&-\frac{1}{2}\sin\phi\,(X^{\tilde{8},\widetilde{10}}+X^{\widetilde{10},\tilde{8}})-\frac{1}{2}\cos\phi\,(X^{\tilde{9},\widetilde{10}}+X^{\widetilde{10},\tilde{9}})\\
&+\frac{1}{2}\cos\phi\,(X^{\tilde{8},\widetilde{11}}+X^{\widetilde{11},\tilde{8}})-\frac{1}{2}\sin\phi\,(X^{\tilde{9},\widetilde{11}}+X^{\widetilde{11},\tilde{9}}),
\end{aligned}
$$

Applying described in previous chapter method, the Green's functions constructed by the particle number operators, are calculated

$$
\begin{aligned}
&\langle T\hat{n}_1(\tau)\hat{n}_1(0)\rangle = \langle T\hat{n}_2(\tau)\hat{n}_2(0)\rangle \qquad (21)\\
&\overset{FT}{=}\delta(\omega_n)\Big[\frac{1}{4}(w_{\tilde{2}}+w_{\tilde{3}}+w_{\tilde{4}}+w_{\tilde{5}})+w_{\tilde{6}}+w_{\tilde{7}}+w_{\tilde{8}}+w_{\tilde{9}}\\
&+w_{\widetilde{10}}+w_{\widetilde{11}}+\frac{9}{4}(w_{\widetilde{12}}+w_{\widetilde{13}}+w_{\widetilde{14}}+w_{\widetilde{15}})+4w_{\widetilde{16}}\Big]
\end{aligned}
$$

$$
\begin{aligned}
&+\frac{1}{4}(g_{\tilde{2},\tilde{3}}+g_{\tilde{3},\tilde{2}}+g_{\tilde{4},\tilde{5}}+g_{\tilde{5},\tilde{4}}+g_{\widetilde{12},\widetilde{13}}+g_{\widetilde{13},\widetilde{12}}+g_{\widetilde{14},\widetilde{15}}+g_{\widetilde{15},\widetilde{14}})\\
&+\sin^2\phi\,(g_{\tilde{9},\widetilde{11}}+g_{\widetilde{11},\tilde{9}})+\cos^2\phi\,(g_{\tilde{8},\widetilde{11}}+g_{\widetilde{11},\tilde{8}})
\end{aligned}
$$

$$
\begin{aligned}
&\langle T\hat{n}_1(\tau)\hat{n}_2(0)\rangle = \langle T\hat{n}_2(\tau)\hat{n}_1(0)\rangle \qquad (22)\\
&\overset{FT}{=}\delta(\omega_n)\Big[\frac{1}{4}(w_{\tilde{2}}+w_{\tilde{3}}+w_{\tilde{4}}+w_{\tilde{5}})+w_{\tilde{6}}+w_{\tilde{7}}+w_{\tilde{8}}+w_{\tilde{9}}\\
&+w_{\widetilde{10}}+w_{\widetilde{11}}+\frac{9}{4}(w_{\widetilde{12}}+w_{\widetilde{13}}+w_{\widetilde{14}}+w_{\widetilde{15}})+4w_{\widetilde{16}}\Big]\\
&+\frac{1}{4}(g_{\tilde{2},\tilde{3}}+g_{\tilde{3},\tilde{2}}+g_{\tilde{4},\tilde{5}}+g_{\tilde{5},\tilde{4}}+g_{\widetilde{12},\widetilde{13}}+g_{\widetilde{13},\widetilde{12}}+g_{\widetilde{14},\widetilde{15}}+g_{\widetilde{15},\widetilde{14}})\\
&-\sin^2\phi\,(g_{\tilde{9},\widetilde{11}}-g_{\widetilde{11},\tilde{9}})+\cos^2\phi\,(g_{\tilde{8},\widetilde{11}}+g_{\widetilde{11},\tilde{8}})
\end{aligned}
$$

where we introduce notations $w_{\tilde{p}} = \langle X^{\tilde{p},\tilde{p}}\rangle = \frac{e^{-\beta\lambda_{\tilde{p}}}}{\sum\limits_{\tilde{q}} e^{-\beta\lambda_{\tilde{q}}}}$,

$$
g_{\tilde{p},\tilde{q}} = \frac{\langle X^{\tilde{p},\tilde{p}} - X^{\tilde{q},\tilde{q}}\rangle}{i\omega_n - (\lambda_{\tilde{p}} - \lambda_{\tilde{q}})} \qquad (23)
$$

and account that $\langle\hat{n}_i\hat{n}_j\rangle = \langle\hat{n}_{i\uparrow}\hat{n}_{j\uparrow}\rangle + \langle\hat{n}_{i\downarrow}\hat{n}_{j\downarrow}\rangle + \langle\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}\rangle + \langle\hat{n}_{i\downarrow}\hat{n}_{j\uparrow}\rangle$.

By definition, the electronic susceptibility for different values of the wave vector, is equal

$$
\chi_q = \sum_{i-j}\mathcal{G}_{ij}e^{-iq(R_i-R_j)}, \qquad (24)
$$

where $q = 0, \pm\frac{\pi}{a}$ (a is a lattice constant). Then for the homogeneous ($q = 0$) electronic susceptibility we will obtain only static ($\omega_n = 0$) contribution:

$$
\begin{aligned}
\chi_c &= \sum_{i-j}\Big\{\langle T\hat{n}_i(\tau)\hat{n}_j(0)\rangle - \langle\hat{n}_i\rangle\langle\hat{n}_j\rangle\Big\} \qquad (25)\\
&\overset{FT}{=}\frac{2}{T}\delta(\omega_n)\Big[w_{\tilde{1}}\Big(\frac{1}{4}w_{\tilde{2}}+\frac{1}{4}w_{\tilde{3}}+\frac{1}{4}w_{\tilde{4}}+\frac{1}{4}w_{\tilde{5}}+w_{\tilde{6}}+w_{\tilde{7}}+w_{\tilde{8}}\\
&+w_{\tilde{9}}+w_{\widetilde{10}}+w_{\widetilde{11}}+\frac{9}{4}w_{\widetilde{12}}+\frac{9}{4}w_{\widetilde{13}}+\frac{9}{4}w_{\widetilde{14}}+\frac{9}{4}w_{\widetilde{15}}\Big)\\
&+w_{\widetilde{16}}\Big(\frac{9}{4}w_{\tilde{2}}+\frac{9}{4}w_{\tilde{3}}+\frac{9}{4}w_{\tilde{4}}+\frac{9}{4}w_{\tilde{5}}+w_{\tilde{6}}+w_{\tilde{7}}+w_{\tilde{8}}\\
&+w_{\tilde{9}}+w_{\widetilde{10}}+w_{\widetilde{11}}+\frac{1}{4}w_{\widetilde{12}}+\frac{1}{4}w_{\widetilde{13}}+\frac{1}{4}w_{\widetilde{14}}+\frac{1}{4}w_{\widetilde{15}}\Big)
\end{aligned}
$$

$$+ (w_{\tilde{6}} + w_{\tilde{7}})\Big(\frac{1}{4}w_{\tilde{2}} + \frac{1}{4}w_{\tilde{3}} + \frac{1}{4}w_{\tilde{4}} + \frac{1}{4}w_{\tilde{5}}$$
$$+ \frac{1}{4}w_{\widetilde{12}} + \frac{1}{4}w_{\widetilde{13}} + \frac{1}{4}w_{\widetilde{14}} + \frac{1}{4}w_{\widetilde{15}}\Big)$$
$$+ (w_{\tilde{4}} + w_{\tilde{5}})\Big(\frac{1}{4}w_{\tilde{8}}+\frac{1}{4}w_{\tilde{9}}+\frac{1}{4}w_{\widetilde{10}}+\frac{1}{4}w_{\widetilde{11}}+\frac{1}{2}w_{\widetilde{14}}+\frac{1}{2}w_{\widetilde{15}}\Big)$$
$$+ (w_{\widetilde{12}} + w_{\widetilde{13}})\Big(\frac{1}{2}w_{\tilde{2}}+\frac{1}{2}w_{\tilde{3}}+\frac{1}{4}w_{\tilde{8}}+\frac{1}{4}w_{\tilde{9}}+\frac{1}{4}w_{\widetilde{10}}+\frac{1}{4}w_{\widetilde{11}}\Big)$$
$$+ 4w_{\tilde{1}}w_{\widetilde{16}}+(w_{\widetilde{12}}+w_{\widetilde{13}})(w_{\tilde{4}}+w_{\tilde{5}})+(w_{\widetilde{14}}+w_{\widetilde{15}})(w_{\tilde{2}}+w_{\tilde{3}})\Big].$$

In order to investigate a susceptibility behavior at $T \to 0$, we should consider limits:

$$\lim_{\lambda_{\tilde{p}}-\lambda_{\tilde{q}}\to 0} \frac{\langle X^{\tilde{p},\tilde{p}} - X^{\tilde{q},\tilde{q}}\rangle}{i\omega_n - \lambda_{\tilde{p}} + \lambda_{\tilde{q}}} = \begin{cases} 0, & i\omega_n \neq 0 \\ \beta\langle X^{\tilde{q},\tilde{q}}\rangle, & i\omega_n = 0 \end{cases}, \tag{26}$$

$$\lim_{\beta\to\infty} \beta\langle X^{\tilde{q},\tilde{q}}\rangle = \begin{cases} 0, & \lambda_{\tilde{q}} > \lambda_{min} \\ \infty, & \lambda_{\tilde{q}} = \lambda_{min} \end{cases}. \tag{27}$$

When electron concentration is equal $n = 1$: $\lambda_{min} = \lambda_{\tilde{3}} = \lambda_{\tilde{5}} = -\mu - t$; for $n = 2$: $\lambda_{min} = \lambda_{\tilde{9}} = -J - 2\mu$; for $n = 3$: $\lambda_{min} = \lambda_{\widetilde{13}} = \lambda_{\widetilde{15}} = U - 3\mu - t$, and analyzing an expression and taking into account corresponding limits, one can see that at temperatures close to zero the charge susceptibility follows to zero, since the lowest energy states do not give a contribution. At the edges of the Brillouin zone ($q = \pm\frac{\pi}{a}$), the electronic susceptibility is pure dynamical ($\omega_n \neq 0$):

$$\chi_c = \sum_{i-j} e^{\mp i\pi(i-j)}\Big\{\langle T\hat{n}_i(\tau)\hat{n}_j(0)\rangle - \langle\hat{n}_i\rangle\langle\hat{n}_j\rangle\Big\} \tag{28}$$
$$\overset{FT}{=} \Big(g_{\tilde{2},\tilde{3}}+g_{\tilde{3},\tilde{2}}+g_{\tilde{4},\tilde{5}}+g_{\tilde{5},\tilde{4}}+g_{\widetilde{12},\widetilde{13}}+g_{\widetilde{13},\widetilde{12}}+g_{\widetilde{14},\widetilde{15}}+g_{\widetilde{15},\widetilde{14}}\Big)$$
$$+ 4\Big[(g_{\tilde{8},\tilde{10}} + g_{\tilde{10},\tilde{8}})\sin^2\phi + (g_{\tilde{9},\widetilde{10}} + g_{\widetilde{10},\tilde{9}})\cos^2\phi\Big]$$

and do not diverge when $T \to 0$ also.

In order to determine magnetic (longitudinal) susceptibility, we should find expressions for the Green's functions constructed by the operators $\hat{m}_i = 2\hat{\sigma}_i^z = \hat{n}_{i\uparrow} - \hat{n}_{i\downarrow}$. They can be represented by the electronic functions, because of $\langle\hat{m}_i\hat{m}_j\rangle = \langle\hat{n}_{i\uparrow}\hat{n}_{j\uparrow}\rangle + \langle\hat{n}_{i\downarrow}\hat{n}_{j\downarrow}\rangle - \langle\hat{n}_{i\uparrow}\hat{n}_{j\downarrow}\rangle - \langle\hat{n}_{i\downarrow}\hat{n}_{j\uparrow}\rangle$.

Thus in center of the Brillouin zone, a longitudinal susceptibility is following

$$\chi_m = \sum_{i-j}\Big\{\langle T\hat{m}_i(\tau)\hat{m}_j(0)\rangle - \langle\hat{m}_i\rangle\langle\hat{m}_j\rangle\Big\} \tag{29}$$
$$\overset{FT}{=} \frac{2}{T}\delta(\omega_n)\Big[w_{\tilde{1}}\Big(\frac{1}{4}w_{\tilde{2}} + \frac{1}{4}w_{\tilde{3}} + \frac{1}{4}w_{\tilde{4}} + \frac{1}{4}w_{\tilde{5}} + w_{\tilde{6}} + w_{\tilde{7}}$$
$$+ \frac{1}{2}w_{\widetilde{12}}+\frac{1}{2}w_{\widetilde{13}}+\frac{1}{2}w_{\widetilde{14}}+\frac{1}{2}w_{\widetilde{15}}\Big)+(w_{\tilde{2}} + w_{\tilde{3}})\Big(\frac{1}{2}w_{\tilde{4}}+\frac{1}{2}w_{\tilde{5}}$$
$$+ \frac{1}{4}w_{\tilde{8}} + \frac{1}{4}w_{\tilde{9}} + \frac{1}{4}w_{\widetilde{10}} + \frac{1}{4}w_{\widetilde{11}} + w_{\widetilde{14}} + w_{\widetilde{15}} + \frac{1}{4}w_{\widetilde{16}}\Big)$$
$$+ (w_{\tilde{4}} + w_{\tilde{5}})\Big(\frac{1}{2}w_{\tilde{2}} + \frac{1}{2}w_{\tilde{3}} + \frac{1}{4}w_{\tilde{8}} + \frac{1}{4}w_{\tilde{9}}+\frac{1}{4}w_{\widetilde{10}}+\frac{1}{4}w_{\widetilde{11}}$$
$$+ w_{\widetilde{12}} + w_{\widetilde{13}} + \frac{1}{4}w_{\widetilde{16}}\Big)+w_{\tilde{6}}\Big(\frac{1}{4}w_{\tilde{2}} + \frac{1}{4}w_{\tilde{3}} + \frac{9}{4}w_{\tilde{4}} + \frac{9}{4}w_{\tilde{5}}$$
$$+ 2w_{\tilde{7}} + w_{\tilde{8}} + w_{\tilde{9}} + w_{\widetilde{10}} + w_{\widetilde{11}} + \frac{1}{4}w_{\widetilde{12}} + \frac{1}{4}w_{\widetilde{13}} + \frac{9}{4}w_{\widetilde{14}}$$
$$+ \frac{9}{4}w_{\widetilde{15}} + w_{\widetilde{16}}\Big)+w_{\tilde{7}}\Big(\frac{9}{4}w_{\tilde{2}} + \frac{9}{4}w_{\tilde{3}} + \frac{1}{4}w_{\tilde{4}} + \frac{1}{4}w_{\tilde{5}} + 2w_{\tilde{6}}$$
$$+ w_{\tilde{8}} + w_{\tilde{9}} + w_{\widetilde{10}} + w_{\widetilde{11}} + \frac{9}{4}w_{\widetilde{12}} + \frac{9}{4}w_{\widetilde{13}} + \frac{1}{4}w_{\widetilde{14}} + \frac{1}{4}w_{\widetilde{15}}$$
$$+ w_{\widetilde{16}}\Big)+(w_{\widetilde{12}} + w_{\widetilde{13}})\Big(+\frac{1}{4}w_{\tilde{8}} + \frac{1}{4}w_{\tilde{9}} + \frac{1}{4}w_{\widetilde{10}} + \frac{1}{4}w_{\widetilde{11}}$$
$$+ \frac{1}{2}w_{\widetilde{14}} + \frac{1}{2}w_{\widetilde{15}} + \frac{1}{4}w_{\widetilde{16}}\Big)+(w_{\widetilde{14}} + w_{\widetilde{15}})\Big(+\frac{1}{4}w_{\tilde{8}} + \frac{1}{4}w_{\tilde{9}}$$
$$+ \frac{1}{4}w_{\widetilde{10}} + \frac{1}{4}w_{\widetilde{11}} + \frac{1}{2}w_{\widetilde{12}} + \frac{1}{2}w_{\widetilde{13}} + \frac{1}{4}w_{\widetilde{16}}\Big)\Big].$$

An analysis of an expression shows, that for concentration $n = 1$: $\chi_m\big|_{T\to 0} \to \infty$, and the ground state is symmetric one:

$$|\tilde{3}\rangle = \frac{1}{\sqrt{2}}(|3\rangle - |2\rangle) = \frac{1}{\sqrt{2}}($$ $$), \tag{30}$$

$$|\tilde{5}\rangle = \frac{1}{\sqrt{2}}(|5\rangle - |4\rangle) = \frac{1}{\sqrt{2}}($$ $$).$$

When $n = 2$: $\chi_m\big|_{T\to 0} \to 0$ and the ground state is a superposition of

the RVB and doublon states:

$$|\tilde{9}\rangle = \frac{1}{\sqrt{2}}\{\cos\phi\,(|9\rangle + |10\rangle) - \sin\phi\,(|8\rangle + |11\rangle)\} \tag{31}$$

$$= \frac{1}{\sqrt{2}}(\cos\phi\,(\;+\;) - \sin\phi\,(\;+\;))$$

In case of three electrons, as for one, the magnetic susceptibility diverge and the ground state is doubly degenerated (it is symmetric hole state):

$$|\widetilde{13}\rangle = \frac{1}{\sqrt{2}}(|13\rangle - |12\rangle) = \frac{1}{\sqrt{2}}(\;-\;) \tag{32}$$

$$|\widetilde{15}\rangle = \frac{1}{\sqrt{2}}(|15\rangle - |14\rangle) = \frac{1}{\sqrt{2}}(\;-\;)$$

At the edges of the Brillouin zone ($q = \pm\frac{\pi}{a}$) susceptibility contains dynamic components only and does not diverge in limit $T \to 0$.

$$\begin{aligned}\chi_m &= \sum_{i-j} e^{\mp i\pi(i-j)}\left\{\langle T\hat{m}_i(\tau)\hat{m}_j(0)\rangle - \langle\hat{m}_i\rangle\langle\hat{m}_j\rangle\right\} \\ &\overset{FT}{=} \Big(g_{\tilde{2},\tilde{3}} + g_{\tilde{3},\tilde{2}} + g_{\tilde{4},\tilde{5}} + g_{\tilde{5},\tilde{4}} + g_{\widetilde{12},\widetilde{13}} \\ &+ g_{\widetilde{13},\widetilde{12}} + g_{\widetilde{14},\widetilde{15}} + g_{\widetilde{15},\widetilde{14}}\Big) \\ &+ 2\Big[\Big(g_{\tilde{8},\widetilde{10}} + g_{\widetilde{10},\tilde{8}} + g_{\tilde{9},\widetilde{11}} + g_{\widetilde{11},\tilde{9}}\Big)\sin^2\phi \\ &+ \Big(g_{\tilde{9},\widetilde{10}} + g_{\widetilde{10},\tilde{9}} + g_{\tilde{8},\widetilde{11}} + g_{\widetilde{11},\tilde{8}}\Big)\cos^2\phi\Big]\end{aligned}$$

The spin-flip operators represented by means of the Hubbard operators on a diagonalized basis are as follow:

$$\begin{aligned}\hat{S}_1^+ &= \frac{1}{2}X^{\tilde{4},\tilde{2}} - \frac{1}{2}X^{\tilde{4},\tilde{3}} - \frac{1}{2}X^{\tilde{5},\tilde{2}} + \frac{1}{2}X^{\tilde{5},\tilde{3}} \\ &- \frac{1}{2}X^{\widetilde{14},\widetilde{12}} - \frac{1}{2}X^{\widetilde{14},\widetilde{13}} - \frac{1}{2}X^{\widetilde{15},\widetilde{12}} + \frac{1}{2}X^{\widetilde{15},\widetilde{13}} \\ &+ \frac{1}{\sqrt{2}}\sin\phi\,X^{\tilde{7},\tilde{8}} + \frac{1}{\sqrt{2}}\cos\phi\,X^{\tilde{7},\tilde{9}} \\ &- \frac{1}{\sqrt{2}}\sin\phi\,X^{\tilde{8},\tilde{6}} - \frac{1}{\sqrt{2}}\cos\phi\,X^{\tilde{9},\tilde{6}} \\ &+ \frac{1}{\sqrt{2}}X^{\tilde{7},\widetilde{10}} + \frac{1}{\sqrt{2}}X^{\widetilde{10},\tilde{6}},\end{aligned} \tag{33}$$

$$\begin{aligned}\hat{S}_2^+ &= \frac{1}{2}X^{\tilde{4},\tilde{2}} + \frac{1}{2}X^{\tilde{4},\tilde{3}} + \frac{1}{2}X^{\tilde{5},\tilde{2}} + \frac{1}{2}X^{\tilde{5},\tilde{3}} \\ &- \frac{1}{2}X^{\widetilde{14},\widetilde{12}} + \frac{1}{2}X^{\widetilde{14},\widetilde{13}} + \frac{1}{2}X^{\widetilde{15},\widetilde{12}} - \frac{1}{2}X^{\widetilde{15},\widetilde{13}} \\ &- \frac{1}{\sqrt{2}}\sin\phi X^{\tilde{7},\tilde{8}} - \frac{1}{\sqrt{2}}\cos\phi\,X^{\tilde{7},\tilde{9}} \\ &+ \frac{1}{\sqrt{2}}\sin\phi\,X^{\tilde{8},\tilde{6}} + \frac{1}{\sqrt{2}}\cos\phi\,X^{\tilde{9},\tilde{6}} \\ &+ \frac{1}{\sqrt{2}}X^{\tilde{7},\widetilde{10}} + \frac{1}{\sqrt{2}}X^{\widetilde{10},\tilde{6}}\end{aligned} \tag{34}$$

and operator $\hat{S}_i^-$ is Hermitian conjugated to $\hat{S}_i^+$.

Similarly, a transversal susceptibility is determined at the center of the Brillouin zone by static contributions:

$$\begin{aligned}\chi_s &= \sum_{i-j}\langle T\hat{S}_i^+(\tau)\hat{S}_j^-(0)\rangle \\ &\overset{FT}{=} \frac{1}{4T}\Big[w_{\tilde{2}} + w_{\tilde{3}} + 2w_{\tilde{6}} + 2w_{\widetilde{10}} + w_{\widetilde{12}} + w_{\widetilde{13}}\Big]\delta(\omega_n),\end{aligned} \tag{35}$$

that, like a longitudinal susceptibility, diverges when electron concentration is $n = 1$ and $n = 3$.

At the edge of the Brillouin zone, a transversal susceptibility contains dynamic contributions and in limit $T \to 0$ approaches to certain constant value, what one can see from an expression:

$$\begin{aligned}\chi_s &= \langle T\hat{S}_1^+(\tau)\hat{S}_1^-(0)\rangle - \langle T\hat{S}_1^+(\tau)\hat{S}_2^-(0)\rangle \\ &\overset{FT}{=} g_{\tilde{4},\tilde{3}} + g_{\tilde{5},\tilde{2}} + g_{\widetilde{14},\widetilde{13}} + g_{\widetilde{15},\widetilde{12}} \\ &+ 2\cos^2\phi\left(g_{\tilde{7},\tilde{9}} + g_{\tilde{9},\tilde{6}}\right) + 2\sin^2\phi\left(g_{\tilde{7},\tilde{8}} + g_{\tilde{8},\tilde{6}}\right).\end{aligned} \tag{36}$$

In summary, we have calculated an electronic, magnetic and spin susceptibilities and investigated their behavior in limit $T \to 0$. At the center of the Brillouin zone, the magnetic and spin susceptibilities diverge when electron concentration is $n = 1$ and $n = 3$, while the charge susceptibility approaches to zero at any electron concentrations. At the edge of the Brillouin zone, all susceptibilities approach to constant value for any filling of cluster.

4. The Hubbard model on a three-site cluster

It is seen from the consideration of a two-site cluster, that the ferromagnetism can appear in the case of odd number of electrons in system. Such result is in good agreement with Nagaoke solution [22], which has shown that if in system, described by the Hubbard model, a number of electrons is $n_e = n \pm 1$ (n- number of sites) and $U \to \infty$, the ground state will be ferromagnetic for the simple lattices.

Now, let us investigate the Hubbard model on a three-site cluster. In this case, the frustration phenomenon can appear and it is interesting to research how it affects on the result.

4.1. Basic set of equations

We will start from the Hubbard Hamiltonian for the three-site cluster:

$$\mathcal{H} = \sum_i (U\hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_\sigma \hat{n}_{i\sigma}) + t \sum_{i\neq j} \sum_\sigma (\hat{a}^\dagger_{i\sigma}\hat{a}_{j\sigma} + \hat{a}^\dagger_{j\sigma}\hat{a}_{i\sigma}), \qquad (37)$$

where $\sigma = \uparrow, \downarrow$ and $[i, j] = (1, 2, 3)$.

A basis of states consist of 64 states which are grouped into sets of the states with the same number of electrons. In matrix representation, the Hamiltonian has a block structure. As in the previous case, a basis of states is created by functions in a particle number representation $|p\rangle = |n_{1\uparrow}, n_{1\downarrow}, n_{2\uparrow}, n_{2\downarrow}, n_{3\uparrow}, n_{3\downarrow}\rangle$:
we have one empty state

$$|1\rangle = |0,0,0,0,0,0\rangle, \qquad \mathcal{H}|1\rangle = 0, \qquad (38)$$

six states with one electron

$$\begin{aligned}
|2\rangle &= |1,0,0,0,0,0\rangle = \hat{a}^\dagger_{1\uparrow}|1\rangle,\\
|3\rangle &= |0,0,1,0,0,0\rangle = \hat{a}^\dagger_{2\uparrow}|1\rangle,\\
|4\rangle &= |0,0,0,0,1,0\rangle = \hat{a}^\dagger_{3\uparrow}|1\rangle,\\
|5\rangle &= |0,1,0,0,0,0\rangle = \hat{a}^\dagger_{1\downarrow}|1\rangle,\\
|6\rangle &= |0,0,0,1,0,0\rangle = \hat{a}^\dagger_{2\downarrow}|1\rangle,\\
|7\rangle &= |0,0,0,0,0,1\rangle = \hat{a}^\dagger_{3\downarrow}|1\rangle,
\end{aligned} \qquad (39)$$

$$\mathcal{H} = \begin{pmatrix}
-\mu & t & t & 0 & 0 & 0\\
t & -\mu & t & 0 & 0 & 0\\
t & t & -\mu & 0 & 0 & 0\\
0 & 0 & 0 & -\mu & t & t\\
0 & 0 & 0 & t & -\mu & t\\
0 & 0 & 0 & t & t & -\mu
\end{pmatrix}, \qquad (40)$$

nine states with two electrons with opposite spins

$$\begin{aligned}
|8\rangle &= |1,1,0,0,0,0\rangle = -\hat{a}^\dagger_{1\downarrow}|2\rangle = \hat{a}^\dagger_{1\uparrow}|5\rangle,\\
|9\rangle &= |1,0,0,1,0,0\rangle = -\hat{a}^\dagger_{2\downarrow}\|2\rangle = \hat{a}^\dagger_{1\uparrow}|6\rangle,\\
|10\rangle &= |1,0,0,0,0,1\rangle = -\hat{a}^\dagger_{3\downarrow}|2\rangle = \hat{a}^\dagger_{1\uparrow}|7\rangle,\\
|11\rangle &= |0,1,1,0,0,0\rangle = \hat{a}^\dagger_{1\downarrow}|3\rangle = -\hat{a}^\dagger_{2\uparrow}|5\rangle,\\
|12\rangle &= |0,1,0,0,1,0\rangle = \hat{a}^\dagger_{1\downarrow}|4\rangle = -\hat{a}^\dagger_{3\uparrow}|5\rangle,\\
|13\rangle &= |0,0,1,1,0,0\rangle = -\hat{a}^\dagger_{2\downarrow}|3\rangle = \hat{a}^\dagger_{2\uparrow}|6\rangle,\\
|14\rangle &= |0,0,1,0,0,1\rangle = -\hat{a}^\dagger_{3\downarrow}|3\rangle = \hat{a}^\dagger_{2\uparrow}|7\rangle,\\
|15\rangle &= |0,0,0,1,1,0\rangle = \hat{a}^\dagger_{2\downarrow}|4\rangle = -\hat{a}^\dagger_{3\uparrow}|6\rangle,\\
|16\rangle &= |0,0,0,0,1,1\rangle = -\hat{a}^\dagger_{3\downarrow}|4\rangle = \hat{a}^\dagger_{3\uparrow}|7\rangle,
\end{aligned} \qquad (41)$$

$$\mathcal{H} = \begin{pmatrix}
U-2\mu & t & t & -t & -t & 0 & 0 & 0 & 0\\
t & -2\mu & t & 0 & 0 & t & 0 & -t & 0\\
t & t & -2\mu & 0 & 0 & 0 & t & 0 & t\\
-t & 0 & 0 & -2\mu & t & -t & -t & 0 & 0\\
-t & 0 & 0 & t & -2\mu & 0 & 0 & t & -t\\
0 & t & 0 & -t & 0 & U-2\mu & t & -t & 0\\
0 & 0 & t & -t & 0 & t & -2\mu & 0 & t\\
0 & -t & 0 & 0 & t & -t & 0 & -2\mu & -t\\
0 & 0 & t & 0 & -t & 0 & t & -t & U-2\mu
\end{pmatrix} \qquad (42)$$

and six states with two electrons with the same spins

$$\begin{aligned}
|17\rangle &= |1,0,1,0,0,0\rangle = -\hat{a}^\dagger_{2\uparrow}|2\rangle = \hat{a}^\dagger_{1\uparrow}|3\rangle,\\
|18\rangle &= |1,0,0,0,1,0\rangle = -\hat{a}^\dagger_{3\uparrow}|2\rangle = \hat{a}^\dagger_{1\uparrow}|4\rangle,\\
|19\rangle &= |0,0,1,0,1,0\rangle = -\hat{a}^\dagger_{3\uparrow}|3\rangle = \hat{a}^\dagger_{2\uparrow}|4\rangle,\\
|20\rangle &= |0,1,0,1,0,0\rangle = -\hat{a}^\dagger_{2\downarrow}|5\rangle = \hat{a}^\dagger_{1\downarrow}|6\rangle,\\
|21\rangle &= |0,1,0,0,0,1\rangle = -\hat{a}^\dagger_{3\downarrow}|5\rangle = \hat{a}^\dagger_{1\downarrow}|7\rangle,\\
|22\rangle &= |0,1,0,1,0,0\rangle = -\hat{a}^\dagger_{3\downarrow}|6\rangle = \hat{a}^\dagger_{2\downarrow}|7\rangle,
\end{aligned} \qquad (43)$$

$$\mathcal{H} = \begin{pmatrix} -2\mu & t & -t & 0 & 0 & 0 \\ t & -2\mu & t & 0 & 0 & 0 \\ -t & t & -2\mu & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\mu & t & -t \\ 0 & 0 & 0 & t & -2\mu & t \\ 0 & 0 & 0 & -t & t & -2\mu \end{pmatrix}. \tag{44}$$

Nine states with three electrons and with total spin $\frac{1}{2}$

$$\begin{aligned}
|23\rangle &= |1,1,1,0,0,0\rangle = \hat{a}^\dagger_{2\uparrow}|8\rangle = \hat{a}^\dagger_{1\uparrow}|11\rangle = -\hat{a}^\dagger_{1\downarrow}|17\rangle, \\
|24\rangle &= |1,1,0,0,1,0\rangle = \hat{a}^\dagger_{3\uparrow}|8\rangle = \hat{a}^\dagger_{1\uparrow}|12\rangle = -\hat{a}^\dagger_{1\downarrow}|18\rangle, \\
|25\rangle &= |1,0,1,1,0,0\rangle = -\hat{a}^\dagger_{2\uparrow}|9\rangle = \hat{a}^\dagger_{1\uparrow}|13\rangle = \hat{a}^\dagger_{2\downarrow}|17\rangle, \\
|26\rangle &= |1,0,1,0,0,1\rangle = -\hat{a}^\dagger_{2\uparrow}|10\rangle = \hat{a}^\dagger_{1\uparrow}|14\rangle = \hat{a}^\dagger_{3\downarrow}|17\rangle, \\
|27\rangle &= |1,0,0,1,1,0\rangle = \hat{a}^\dagger_{3\uparrow}|9\rangle = \hat{a}^\dagger_{1\uparrow}|15\rangle = -\hat{a}^\dagger_{2\downarrow}|18\rangle, \\
|28\rangle &= |1,0,0,0,1,1\rangle = -\hat{a}^\dagger_{3\uparrow}|10\rangle = \hat{a}^\dagger_{1\uparrow}|16\rangle = \hat{a}^\dagger_{3\downarrow}|18\rangle, \\
|29\rangle &= |0,1,1,0,1,0\rangle = \hat{a}^\dagger_{3\uparrow}|11\rangle = -\hat{a}^\dagger_{2\uparrow}|12\rangle = \hat{a}^\dagger_{1\downarrow}|19\rangle, \\
|30\rangle &= |0,0,1,1,1,0\rangle = \hat{a}^\dagger_{3\uparrow}|13\rangle = \hat{a}^\dagger_{2\uparrow}|15\rangle = -\hat{a}^\dagger_{2\downarrow}|19\rangle, \\
|31\rangle &= |0,0,1,0,1,1\rangle = -\hat{a}^\dagger_{3\uparrow}|14\rangle = \hat{a}^\dagger_{2\uparrow}|16\rangle = \hat{a}^\dagger_{3\downarrow}|19\rangle,
\end{aligned} \tag{45}$$

$$\mathcal{H} = \tag{46}$$
$$\begin{pmatrix}
U{-}3\mu & t & -t & -t & 0 & 0 & t & 0 & 0 \\
t & U{-}3\mu & 0 & 0 & t & -t & -t & 0 & 0 \\
-t & 0 & U{-}3\mu & t & -t & 0 & 0 & t & 0 \\
-t & 0 & t & -3\mu & 0 & t & 0 & 0 & -t \\
0 & t & -t & 0 & -3\mu & -t & 0 & t & 0 \\
0 & -t & 0 & t & -t & U{-}3\mu & 0 & 0 & t \\
t & -t & 0 & 0 & 0 & 0 & -3\mu & -t & t \\
0 & 0 & t & 0 & t & 0 & -t & U{-}3\mu & -t \\
0 & 0 & 0 & -t & 0 & t & t & -t & U{-}3\mu
\end{pmatrix},$$

one state with three electrons and total spin $\frac{3}{2}$

$$|32\rangle = |1,0,1,0,1,0\rangle = \hat{a}^\dagger_{3\uparrow}|17\rangle = \hat{a}^\dagger_{2\uparrow}|18\rangle = \hat{a}^\dagger_{1\uparrow}|19\rangle, \tag{47}$$

$$\mathcal{H}|32\rangle = -3\mu|32\rangle. \tag{48}$$

Similarly for the states with total spin $-\frac{1}{2}$

$$|33\rangle = |1,1,0,1,0,0\rangle = \hat{a}^\dagger_{2\downarrow}|8\rangle = -\hat{a}^\dagger_{1\downarrow}|9\rangle = \hat{a}^\dagger_{1\uparrow}|20\rangle,$$

$$\begin{aligned}
|34\rangle &= |1,1,0,0,0,1\rangle = \hat{a}^\dagger_{3\downarrow}|8\rangle = -\hat{a}^\dagger_{1\downarrow}|10\rangle = \hat{a}^\dagger_{1\uparrow}|21\rangle, \\
|35\rangle &= |1,0,0,1,0,1\rangle = \hat{a}^\dagger_{3\downarrow}|9\rangle = -\hat{a}^\dagger_{2\downarrow}|10\rangle = \hat{a}^\dagger_{1\uparrow}|22\rangle, \\
|36\rangle &= |0,1,1,1,0,0\rangle = \hat{a}^\dagger_{2\downarrow}|11\rangle = \hat{a}^\dagger_{1\downarrow}|13\rangle = -\hat{a}^\dagger_{2\uparrow}|20\rangle, \\
|37\rangle &= |0,1,1,0,0,1\rangle = \hat{a}^\dagger_{3\downarrow}|11\rangle = \hat{a}^\dagger_{1\downarrow}|14\rangle = -\hat{a}^\dagger_{2\uparrow}|21\rangle, \\
|38\rangle &= |0,1,0,1,1,0\rangle = -\hat{a}^\dagger_{2\downarrow}|12\rangle = \hat{a}^\dagger_{1\downarrow}|15\rangle = \hat{a}^\dagger_{3\uparrow}|20\rangle, \\
|39\rangle &= |0,1,0,0,1,1\rangle = \hat{a}^\dagger_{3\downarrow}|12\rangle = \hat{a}^\dagger_{1\downarrow}|16\rangle = -\hat{a}^\dagger_{3\uparrow}|21\rangle, \\
|40\rangle &= |0,0,1,1,0,1\rangle = \hat{a}^\dagger_{3\downarrow}|13\rangle = -\hat{a}^\dagger_{2\downarrow}|14\rangle = \hat{a}^\dagger_{2\uparrow}|22\rangle, \\
|41\rangle &= |0,0,0,1,1,1,\rangle = \hat{a}^\dagger_{3\downarrow}|15\rangle = \hat{a}^\dagger_{2\downarrow}|16\rangle = -\hat{a}^\dagger_{3\uparrow}|22\rangle,
\end{aligned} \tag{49}$$

$$\mathcal{H} = \tag{50}$$
$$\begin{pmatrix}
U{-}3\mu & t & -t & -t & 0 & t & 0 & 0 & 0 \\
t & U{-}3\mu & t & 0 & -t & 0 & -t & 0 & 0 \\
-t & t & U{-}3\mu & 0 & 0 & 0 & 0 & t & -t \\
-t & 0 & 0 & -3\mu & t & -t & 0 & t & 0 \\
0 & -t & 0 & t & -3\mu & 0 & t & -t & 0 \\
t & 0 & 0 & -t & 0 & U{-}3\mu & -t & 0 & t \\
0 & -t & 0 & 0 & t & -t & -3\mu & 0 & t \\
0 & 0 & t & t & -t & 0 & 0 & U{-}3\mu & -t \\
0 & 0 & -t & 0 & 0 & t & t & -t & U{-}3\mu
\end{pmatrix}$$

and $-\frac{3}{2}$

$$|42\rangle = |0,1,0,1,0,1\rangle = \hat{a}^\dagger_{3\downarrow}|20\rangle = -\hat{a}^\dagger_{2\downarrow}|21\rangle = \hat{a}^\dagger_{1\downarrow}|22\rangle, \tag{51}$$

$$\mathcal{H}|42\rangle = -3\mu|42\rangle. \tag{52}$$

Nine states with four electrons and with total spin 0

$$\begin{aligned}
|43\rangle = |1,1,1,1,0,0\rangle &= -\hat{a}^\dagger_{2\downarrow}|23\rangle = -\hat{a}^\dagger_{1\downarrow}|25\rangle \\
&= \hat{a}^\dagger_{2\uparrow}|33\rangle = \hat{a}^\dagger_{1\uparrow}|36\rangle, \\
|44\rangle = |1,1,1,0,0,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|23\rangle = -\hat{a}^\dagger_{1\downarrow}|26\rangle \\
&= \hat{a}^\dagger_{2\uparrow}|34\rangle = \hat{a}^\dagger_{1\uparrow}|37\rangle, \\
|45\rangle = |1,1,0,1,1,0\rangle &= \hat{a}^\dagger_{2\downarrow}|24\rangle = -\hat{a}^\dagger_{1\downarrow}|27\rangle \\
&= -\hat{a}^\dagger_{3\uparrow}|33\rangle = \hat{a}^\dagger_{1\uparrow}|38\rangle, \\
|46\rangle = |1,1,0,0,1,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|24\rangle = -\hat{a}^\dagger_{1\downarrow}|28\rangle
\end{aligned}$$

$$
\begin{aligned}
&= \hat{a}^\dagger_{3\uparrow}|34\rangle = \hat{a}^\dagger_{1\uparrow}|39\rangle,\\
|47\rangle = |1,0,1,1,0,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|25\rangle = \hat{a}^\dagger_{2\downarrow}|26\rangle\\
&= -\hat{a}^\dagger_{2\uparrow}|35\rangle = \hat{a}^\dagger_{1\uparrow}|40\rangle,\\
|48\rangle = |1,0,0,1,1,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|27\rangle = -\hat{a}^\dagger_{2\downarrow}|28\rangle\\
&= \hat{a}^\dagger_{3\uparrow}|35\rangle = \hat{a}^\dagger_{1\uparrow}|41\rangle,\\
|49\rangle = |0,1,1,1,1,0\rangle &= \hat{a}^\dagger_{2\downarrow}|29\rangle = \hat{a}^\dagger_{1\downarrow}|30\rangle\\
&= -\hat{a}^\dagger_{3\uparrow}|36\rangle = -\hat{a}^\dagger_{2\uparrow}|38\rangle,\\
|50\rangle = |0,1,1,0,1,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|29\rangle = \hat{a}^\dagger_{1\downarrow}|31\rangle\\
&= \hat{a}^\dagger_{3\uparrow}|37\rangle = -\hat{a}^\dagger_{2\uparrow}|39\rangle,\\
|51\rangle = |0,0,1,1,1,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|30\rangle = -\hat{a}^\dagger_{2\downarrow}|31\rangle\\
&= \hat{a}^\dagger_{3\uparrow}|40\rangle = \hat{a}^\dagger_{2\uparrow}|41\rangle,
\end{aligned}
\tag{53}
$$

$$
\mathcal{H} = \begin{pmatrix}
2U & t & -t & 0 & t & 0 & -t & 0 & 0\\
t & U & 0 & t & -t & 0 & 0 & t & 0\\
-t & 0 & U & -t & 0 & t & -t & 0 & 0\\
0 & t & -t & 2U & 0 & t & 0 & -t & 0\\
t & -t & 0 & 0 & U & -t & 0 & 0 & t\\
0 & 0 & t & t & -t & U & 0 & 0 & t\\
-t & 0 & -t & 0 & 0 & 0 & U & -t & -t\\
0 & t & 0 & -t & 0 & 0 & -t & U & -t\\
0 & 0 & 0 & 0 & t & t & -t & -t & 2U
\end{pmatrix} - 4\mu\hat{I}
\tag{54}
$$

and six states with total spin ± 1

$$
\begin{aligned}
|52\rangle = |1,1,1,0,1,0\rangle &= -\hat{a}^\dagger_{3\uparrow}|23\rangle = \hat{a}^\dagger_{2\uparrow}|24\rangle\\
&= \hat{a}^\dagger_{1\uparrow}|29\rangle = -\hat{a}^\dagger_{1\downarrow}|32\rangle,\\
|53\rangle = |1,0,1,1,1,0\rangle &= -\hat{a}^\dagger_{3\uparrow}|25\rangle = -\hat{a}^\dagger_{2\uparrow}|27\rangle\\
&= \hat{a}^\dagger_{1\uparrow}|30\rangle = \hat{a}^\dagger_{1\downarrow}|32\rangle,\\
|54\rangle = |1,0,1,0,1,1\rangle &= \hat{a}^\dagger_{3\uparrow}|26\rangle = -\hat{a}^\dagger_{2\uparrow}|28\rangle\\
&= \hat{a}^\dagger_{1\uparrow}|31\rangle = -\hat{a}^\dagger_{3\downarrow}|32\rangle,\\
|55\rangle = |1,1,0,1,0,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|33\rangle = \hat{a}^\dagger_{2\downarrow}|34\rangle\\
&= -\hat{a}^\dagger_{1\downarrow}|35\rangle = \hat{a}^\dagger_{1\uparrow}|42\rangle,\\
|56\rangle = |0,1,1,1,0,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|36\rangle = \hat{a}^\dagger_{2\downarrow}|37\rangle
\end{aligned}
\tag{55}
$$

$$
\begin{aligned}
&= \hat{a}^\dagger_{1\downarrow}|40\rangle = -\hat{a}^\dagger_{2\uparrow}|42\rangle,\\
|57\rangle = |0,1,0,1,1,1\rangle &= -\hat{a}^\dagger_{3\downarrow}|38\rangle = -\hat{a}^\dagger_{2\downarrow}|39\rangle\\
&= \hat{a}^\dagger_{1\downarrow}|41\rangle = \hat{a}^\dagger_{3\uparrow}|42\rangle,
\end{aligned}
$$

$$
\mathcal{H} = \begin{pmatrix}
U-4\mu & -t & t & 0 & 0 & 0\\
-t & U-4\mu & -t & 0 & 0 & 0\\
t & -t & U-4\mu & 0 & 0 & 0\\
0 & 0 & 0 & U-4\mu & -t & t\\
0 & 0 & 0 & -t & U-4\mu & -t\\
0 & 0 & 0 & t & -t & U-4\mu
\end{pmatrix}.
\tag{56}
$$

Six states with five electrons

$$
\begin{aligned}
|58\rangle = |1,1,1,1,1,0\rangle &= \hat{a}^\dagger_{3\uparrow}|43\rangle = \hat{a}^\dagger_{2\uparrow}|45\rangle\\
&= \hat{a}^\dagger_{1\uparrow}|49\rangle = -\hat{a}^\dagger_{2\downarrow}|52\rangle = -\hat{a}^\dagger_{1\downarrow}|53\rangle,\\
|59\rangle = |1,1,1,0,1,1\rangle &= -\hat{a}^\dagger_{3\uparrow}|44\rangle = \hat{a}^\dagger_{2\uparrow}|46\rangle\\
&= \hat{a}^\dagger_{1\uparrow}|50\rangle = \hat{a}^\dagger_{3\downarrow}|52\rangle = -\hat{a}^\dagger_{1\downarrow}|54\rangle,\\
|60\rangle = |1,0,1,1,1,1\rangle &= -\hat{a}^\dagger_{3\uparrow}|47\rangle = -\hat{a}^\dagger_{2\uparrow}|48\rangle\\
&= \hat{a}^\dagger_{1\uparrow}|51\rangle = \hat{a}^\dagger_{3\downarrow}|53\rangle = \hat{a}^\dagger_{2\downarrow}|54\rangle,\\
|61\rangle = |1,1,1,1,0,1\rangle &= \hat{a}^\dagger_{3\downarrow}|43\rangle = -\hat{a}^\dagger_{2\downarrow}|44\rangle\\
&= -\hat{a}^\dagger_{1\downarrow}|47\rangle = \hat{a}^\dagger_{2\uparrow}|55\rangle = \hat{a}^\dagger_{1\uparrow}|56\rangle,\\
|62\rangle = |1,1,0,1,1,1\rangle &= \hat{a}^\dagger_{3\downarrow}|45\rangle = \hat{a}^\dagger_{2\downarrow}|46\rangle\\
&= -\hat{a}^\dagger_{1\downarrow}|48\rangle = -\hat{a}^\dagger_{3\uparrow}|55\rangle = \hat{a}^\dagger_{1\uparrow}|57\rangle,\\
|63\rangle = |0,1,1,1,1,1\rangle &= \hat{a}^\dagger_{3\downarrow}|49\rangle = \hat{a}^\dagger_{2\downarrow}|50\rangle\\
&= \hat{a}^\dagger_{1\downarrow}|51\rangle = -\hat{a}^\dagger_{3\uparrow}|56\rangle = -\hat{a}^\dagger_{2\uparrow}|57\rangle,
\end{aligned}
\tag{57}
$$

$$
\mathcal{H} = \begin{pmatrix}
2U-5\mu & -t & -t & 0 & 0 & 0\\
-t & 2U-5\mu & -t & 0 & 0 & 0\\
-t & -t & 2U-5\mu & 0 & 0 & 0\\
0 & 0 & 0 & 2U-5\mu & -t & -t\\
0 & 0 & 0 & -t & 2U-5\mu & -t\\
0 & 0 & 0 & -t & -t & 2U-5\mu
\end{pmatrix}.
\tag{58}
$$

Finally, we have one state with six electrons

$$
|64\rangle = |1,1,1,1,1,1\rangle = -\hat{a}^\dagger_{3\downarrow}|58\rangle = -\hat{a}^\dagger_{2\downarrow}|59\rangle
\tag{59}
$$

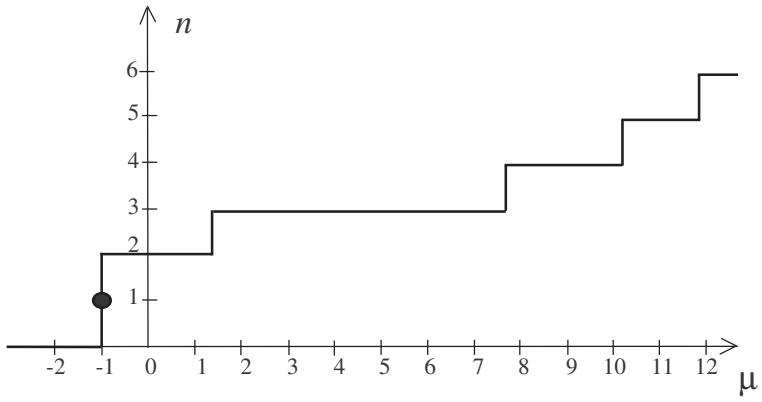


Figure 1. $n(\mu)$ plot for $t > 0$ and $T = 0$.

$$= -\hat{a}^{\dagger}_{1\downarrow}|60\rangle = \hat{a}^{\dagger}_{3\uparrow}|61\rangle = \hat{a}^{\dagger}_{2\uparrow}|62\rangle = \hat{a}^{\dagger}_{1\uparrow}|63\rangle,$$

$$\mathcal{H}|64\rangle = (3U - 6\mu)|64\rangle. \tag{60}$$

4.2. Diagonalization of the Hamiltonian

The unitary transformation, that diagonalize the Hamiltonian can be constructed by the eigenvectors of this Hamiltonian. The problem on eigenvectors and eigenvalues is solved numerically. We consider the case $U = 10t$ ($U \gg t$). The small fields $h_i \sim 10^{-5}$ at different sites, and to the chemical potential for different orientation of spins (of the same degree of smallness) with condition $\sum_\sigma \Delta\mu_\sigma = 0$, were introduced in the Hamiltonian for avoiding the degeneracy of eigenvalues.

Below all energetic quantities are given in units of t. For calculating the susceptibilities we use the same formula (12). It should be noticed that matrices of the unitary transformation $V^{p\tilde{p}}$ are calculated numerically and have dimension 64×64. In fig.1 we present dependence of the electron concentration on the chemical potential value at $T = 0$ and $t > 0$.

When $\mu = -1$, we have degeneracy and states with zero, one and two electrons have the lowest energy simultaneously, but if μ goes down then the state with "0" electrons is the lowest one and if μ goes up, the state with two electrons will be the ground state. In case of negative value of t, this dependence will be symmetric with regards to replacements $\mu \to (U/2 - \mu)$ and $n \to (6 - n)$.

4.3. Numerical results for susceptibilities

The particle number operators represented by Hubbard operators on the initial basis are:

$$\begin{aligned}\hat{n}_1 = \hat{n}_{1\uparrow} + \hat{n}_{1\downarrow} = {} & X^{2,2} + X^{5,5} + 2X^{8,8} + X^{9,9} \\ & + X^{10,10} + X^{11,11} + X^{12,12} + X^{17,17} + X^{18,18} \\ & + X^{20,20} + X^{21,21} + 2X^{23,23} + 2X^{24,24} + X^{25,25} \\ & + X^{26,26} + X^{27,27} + X^{28,28} + X^{29,29} + X^{32,32} \\ & + 2X^{33,33} + 2X^{34,34} + X^{35,35} + X^{36,36} + X^{37,37} \\ & + X^{38,38} + X^{39,39} + X^{42,42} + 2X^{43,43} + 2X^{44,44} \\ & + 2X^{45,45} + 2X^{46,46} + X^{47,47} + X^{48,48} + X^{49,49} \\ & + X^{50,50} + 2X^{52,52} + X^{53,53} + X^{54,54} + 2X^{55,55} \\ & + X^{56,56} + X^{57,57} + 2X^{58,58} + 2X^{59,59} + X^{60,60} \\ & + 2X^{61,61} + 2X^{62,62} + X^{63,63} + 2X^{64,64},\end{aligned} \tag{61}$$

$$\begin{aligned}\hat{n}_2 = \hat{n}_{2\uparrow} + \hat{n}_{2\downarrow} = {} & X^{3,3} + X^{6,6} + X^{9,9} + X^{11,11} \\ & + 2X^{13,13} + X^{14,14} + X^{15,15} + X^{17,17} + X^{19,19} \\ & + X^{20,20} + X^{22,22} + X^{23,23} + 2X^{25,25} + X^{26,26} \\ & + X^{27,27} + X^{29,29} + 2X^{30,30} + X^{31,31} + X^{32,32} \\ & + X^{33,33} + X^{35,35} + 2X^{36,36} + X^{37,37} + X^{38,38} \\ & + 2X^{40,40} + X^{41,41} + X^{42,42} + 2X^{43,43} + X^{44,44} \\ & + X^{45,45} + X^{47,47} + X^{48,48} + 2X^{49,49} + X^{50,50} \\ & + 2X^{51,51} + X^{52,52} + 2X^{53,53} + X^{54,54} + X^{55,55} \\ & + 2X^{56,56} + X^{57,57} + 2X^{58,58} + X^{59,59} + 2X^{60,60} \\ & + 2X^{61,61} + X^{62,62} + 2X^{63,63} + 2X^{64,64},\end{aligned} \tag{62}$$

$$\begin{aligned}\hat{n}_3 = \hat{n}_{3\uparrow} + \hat{n}_{3\downarrow} = {} & X^{4,4} + X^{7,7} + X^{10,10} \\ & + X^{12,12} + X^{14,14} + X^{15,15} + 2X^{16,16} + X^{18,18} \\ & + X^{19,19} + X^{21,21} + X^{22,22} + X^{24,24} + X^{26,26} \\ & + X^{27,27} + X^{28,28} + X^{29,29} + X^{30,30} + 2X^{31,31} \\ & + X^{32,32} + X^{34,34} + X^{35,35} + X^{37,37} + X^{38,38} \\ & + 2X^{39,39} + X^{40,40} + 2X^{41,41} + X^{42,42} + X^{44,44}\end{aligned} \tag{63}$$

$$
\begin{aligned}
&+ X^{45,45} + X^{46,46} + X^{47,47} + 2X^{48,48} + X^{49,49} \\
&+ 2X^{50,50} + 2X^{51,51} + X^{52,52} + X^{53,53} + 2X^{54,54} \\
&+ X^{55,55} + X^{56,56} + 2X^{57,57} + X^{58,58} + 2X^{59,59} \\
&+ 2X^{60,60} + X^{61,61} + 2X^{62,62} + 2X^{63,63} + 2X^{64,64},
\end{aligned}
$$

Now, let us find electronic susceptibility in the center and out of the center of the Brillouin zone ($q = 0, \pm\frac{2\pi}{3a}$). By means of numerical calculations we find the unitary transformation, which diagonalize Hamiltonian. Because we are interesting only in the low temperature behavior of the susceptibilities, we extract from the large number of terms in (12) only the one that involve the states with lowest energy. Then we have obtained that for $q = 0$ electronic susceptibility is equal to:

$$
\begin{aligned}
\chi_c &= \sum_{i-j}\Big\{\langle T\hat{n}_i(\tau)\hat{n}_j(0)\rangle - \langle\hat{n}_i\rangle\langle\hat{n}_j\rangle\Big\} \qquad (64)\\
&\stackrel{FT}{=} -0.1(g_{\widetilde{28},\widetilde{30}} + g_{\widetilde{30},\widetilde{28}}) + 0.12(g_{\widetilde{49},\widetilde{50}} + g_{\widetilde{50},\widetilde{49}}) \\
&+ 0.2(g_{\widetilde{43},\widetilde{45}} + g_{\widetilde{45},\widetilde{43}}) + 0.1(g_{\widetilde{45},\widetilde{47}} + g_{\widetilde{47},\widetilde{45}}) \\
&+ 0.1(g_{\widetilde{48},\widetilde{51}} + g_{\widetilde{51},\widetilde{48}}) + 0.1(g_{\widetilde{44},\widetilde{45}} + g_{\widetilde{45},\widetilde{44}}) \\
&+ 0.1(g_{\widetilde{47},\widetilde{49}} + g_{\widetilde{49},\widetilde{47}}) + \frac{1}{T}\Big[0.9w_{\tilde{3}}w_{\tilde{4}} + 0.9w_{\tilde{3}}w_{\tilde{7}} \\
&+ 0.9w_{\tilde{4}}w_{\tilde{6}} + 0.9w_{\tilde{6}}w_{\tilde{7}} + 0.2w_{\widetilde{14}}w_{\widetilde{17}} + 0.2w_{\widetilde{14}}w_{\widetilde{20}} \\
&+ 0.2w_{\widetilde{17}}w_{\widetilde{20}} - 0.2w_{\widetilde{58}}w_{\widetilde{61}} + n.s.\Big]\delta(\omega_n)
\end{aligned}
$$

(n.s. denote all other components, which do not contribute at $T \to 0$).

As is seen from the expression, the susceptibility has both dynamic and static components. Analyzing its behavior in limit $T \to 0$, one can see that for concentration $n = 1$, the ground states are $\lambda_{min} = \lambda_{\tilde{3}} = \lambda_{\tilde{4}} = \lambda_{\tilde{6}} = \lambda_{\tilde{7}}$ and susceptibility diverges at $T \to 0$, $\chi_n\big|_{T\to 0} \to \infty$.

For two electrons: $\lambda_{min} = \lambda_{\widetilde{14}} = \lambda_{\widetilde{17}} = \lambda_{\widetilde{20}}$, and therefore the susceptibility diverges in this case too.

In the case of three electrons, the states with lowest energy are $\lambda_{min} = \lambda_{\widetilde{23}} = \lambda_{\widetilde{24}} = \lambda_{\widetilde{33}} = \lambda_{\widetilde{34}}$ and as a result susceptibility goes to zero.

When we have four electrons $\lambda_{min} = \lambda_{\widetilde{44}}$ and at $T \to 0$, the susceptibility approaches constant value.

For five electrons $\lambda_{min} = \lambda_{\widetilde{58}} = \lambda_{\widetilde{61}}$, and the susceptibility diverges for such cluster filling.

Out of the center of the Brillouin zone $q = \pm\frac{2\pi}{3a}$, the electronic susceptibility is equal

$$
\begin{aligned}
\chi_c &= \sum_{i-j} e^{\mp i\frac{2\pi}{3}(i-j)}\Big\{\langle T\hat{n}_i(\tau)\hat{n}_j(0)\rangle - \langle\hat{n}_i\rangle\langle\hat{n}_j\rangle\Big\} \qquad (65)\\
&\stackrel{FT}{=} 2(g_{\tilde{2},\tilde{3}} + g_{\tilde{3},\tilde{2}}) + 3.7(g_{\tilde{8},\tilde{9}} + g_{\tilde{9},\tilde{8}}) \\
&+ 0.2(g_{\tilde{9},\widetilde{11}} + g_{\widetilde{11},\tilde{9}}) + 0.1(g_{\tilde{9},\widetilde{12}} + g_{\widetilde{12},\tilde{9}}) \\
&+ 0.2(g_{\widetilde{23},\widetilde{28}} + g_{\widetilde{28},\widetilde{23}}) + 0.3(g_{\widetilde{23},\widetilde{31}} + g_{\widetilde{31},\widetilde{23}}) \\
&+ 0.2(g_{\widetilde{26},\widetilde{28}} + g_{\widetilde{28},\widetilde{26}}) + 5.9(g_{\widetilde{26},\widetilde{30}} + g_{\widetilde{30},\widetilde{26}}) \\
&+ 5.8(g_{\widetilde{28},\widetilde{30}} + g_{\widetilde{30},\widetilde{28}}) + (g_{\widetilde{12},\widetilde{12}} + g_{\widetilde{12},\widetilde{11}}) \\
&+ 3(g_{\widetilde{14},\widetilde{15}} + g_{\widetilde{15},\widetilde{14}}) + 0.2(g_{\widetilde{46},\widetilde{47}} + g_{\widetilde{47},\widetilde{46}}) \\
&+ 2.7(g_{\widetilde{49},\widetilde{50}} + g_{\widetilde{50},\widetilde{49}}) + 0.1(g_{\widetilde{44},\widetilde{50}} + g_{\widetilde{50},\widetilde{44}}) \\
&+ 0.8(g_{\widetilde{44},\widetilde{47}} + g_{\widetilde{47},\widetilde{44}}) + 3.4(g_{\widetilde{43},\widetilde{45}} + g_{\widetilde{45},\widetilde{43}}) \\
&+ 0.1(g_{\widetilde{44},\widetilde{45}} + g_{\widetilde{45},\widetilde{44}}) + 0.1(g_{\widetilde{48},\widetilde{51}} + g_{\widetilde{51},\widetilde{48}}) \\
&+ 0.1(g_{\widetilde{47},\widetilde{49}} + g_{\widetilde{49},\widetilde{47}}) + 2(g_{\widetilde{58},\widetilde{59}} + g_{\widetilde{59},\widetilde{58}}) \\
&+ \frac{2}{T}\big[0.5w_{\tilde{3}} + w_{\tilde{9}} + 0.2w_{\widetilde{12}} + 0.7w_{\widetilde{15}} + 1.4w_{\widetilde{26}} \\
&+ 1.3w_{\widetilde{28}} + 1.1w_{\widetilde{45}} + 0.1w_{\widetilde{47}} + 0.7w_{\widetilde{50}} + 0.5w_{\widetilde{59}}\big]\delta(\omega_n)
\end{aligned}
$$

and in this case, the susceptibility will diverge if there is one electron in a system. In another cases ($n = 2, 3, 4, 5, 6$), the susceptibility is a finite quantity.

The longitudinal susceptibility is built on the magnetic moment operators, which are expressed through the particle number operators and by means of the Hubbard operators on initial basis and are as follow:

$$
\begin{aligned}
\hat{m}_1 &= \hat{n}_{1\uparrow} - \hat{n}_{1\downarrow} = X^{2,2} - X^{5,5} + X^{9,9} + X^{10,10} \qquad (66)\\
&- X^{11,11} - X^{12,12} + X^{17,17} + X^{18,18} - X^{20,20} - X^{21,21} \\
&+ X^{25,25} + X^{26,26} + X^{27,27} + X^{28,28} - X^{29,29} + X^{32,32} \\
&+ X^{35,35} - X^{36,36} - X^{37,37} - X^{38,38} - X^{39,39} - X^{42,42} \\
&+ X^{47,47} + X^{48,48} - X^{49,49} - X^{50,50} + X^{53,53} + X^{54,54} \\
&- X^{56,56} - X^{57,57} + X^{60,60} - X^{63,63},
\end{aligned}
$$

$$
\begin{aligned}
\hat{m}_2 &= \hat{n}_{2\uparrow} - \hat{n}_{2\downarrow} = X^{3,3} - X^{6,6} - X^{9,9} + X^{11,11} \qquad (67)\\
&+ X^{14,14} - X^{15,15} + X^{17,17} + X^{19,19} - X^{20,20} - X^{22,22}
\end{aligned}
$$

$$+ X^{23,23} + X^{26,26} - X^{27,27} + X^{29,29} + X^{31,31} + X^{32,32}$$
$$- X^{33,33} - X^{35,35} + X^{37,37} - X^{38,38} - X^{41,41} - X^{42,42}$$
$$+ X^{44,44} - X^{45,45} - X^{48,48} + X^{50,50} + X^{52,52} + X^{54,54}$$
$$- X^{55,55} - X^{57,57} + X^{59,59} - X^{62,62},$$

$$\hat{m}_3 = \hat{n}_{3\uparrow} - \hat{n}_{3\downarrow} = X^{4,4} - X^{7,7} - X^{10,10} + X^{12,12} \tag{68}$$
$$- X^{14,14} + X^{15,15} + X^{18,18} + X^{19,19} - X^{21,21} - X^{22,22}$$
$$+ X^{24,24} - X^{26,26} + X^{27,27} + X^{29,29} + X^{30,30} + X^{32,32}$$
$$- X^{34,34} - X^{35,35} - X^{37,37} + X^{38,38} - X^{40,40} - X^{42,42}$$
$$- X^{44,44} + X^{45,45} - X^{47,47} + X^{49,49} + X^{52,52} + X^{53,53}$$
$$- X^{55,55} - X^{56,56} + X^{58,58} - X^{61,61}.$$

At the center of the Brillouin zone ($q = 0$) the susceptibility contains the static components only:

$$\chi_m = \sum_{i-j} \Big\{ \langle T\hat{m}_i(\tau)\hat{m}_j(0)\rangle - \langle \hat{m}_i\rangle\langle \hat{m}_j\rangle \Big\} \tag{69}$$
$$\stackrel{FT}{=} \frac{1}{T}\big[4w_{\tilde{3}}w_{\tilde{7}} + 4w_{\tilde{4}}w_{\tilde{7}} + 3w_{\tilde{3}}w_{\tilde{6}} + 3w_{\tilde{4}}w_{\tilde{6}} + 16w_{\widetilde{17}}w_{\widetilde{20}}$$
$$+ 4w_{\widetilde{14}}w_{\widetilde{17}} + 4w_{\widetilde{14}}w_{\widetilde{20}} + 4w_{\widetilde{23}}w_{\widetilde{33}} + 4w_{\widetilde{24}}w_{\widetilde{33}}$$
$$+ 3w_{\widetilde{23}}w_{\widetilde{34}} + 3w_{\tilde{24}}w_{\tilde{34}} + 4w_{\tilde{58}}w_{\tilde{61}} + n.s.\big]\delta(\omega_n)$$

and diverges when electron concentration is $n = 2$, 3, 5.

Out of the center of the Brillouin zone $q = \pm\frac{2\pi}{3a}$, the magnetic susceptibility contains both dynamic and static terms

$$\chi_m = \sum_{i-j} e^{\mp i\frac{2\pi}{3}(i-j)} \Big\{ \langle T\hat{m}_i(\tau)\hat{m}_j(0)\rangle - \langle \hat{m}_i\rangle\langle \hat{m}_j\rangle \Big\}$$
$$\stackrel{FT}{=} 2.02(g_{\tilde{2},\tilde{3}} + g_{\tilde{3},\tilde{2}}) + 2.01(g_{\widetilde{17},\widetilde{18}} + g_{\widetilde{18},\widetilde{17}}) \tag{70}$$
$$+ 2.96(g_{\widetilde{12},\widetilde{15}} + g_{\widetilde{15},\widetilde{12}}) + 2.73(g_{\widetilde{11},\widetilde{15}} + g_{\widetilde{15},\widetilde{11}})$$
$$+ 0.28(g_{\tilde{8},\widetilde{15}} + g_{\widetilde{15},\tilde{8}}) + 2.94(g_{\widetilde{12},\widetilde{14}} + g_{\widetilde{14},\widetilde{12}})$$
$$+ 0.04(g_{\tilde{9},\widetilde{14}} + g_{\widetilde{14},\tilde{9}}) + 0.01(g_{\tilde{9},\widetilde{16}} + g_{\widetilde{16},\tilde{9}})$$
$$+ 1.99(g_{\widetilde{26},\widetilde{28}} + g_{\widetilde{28},\widetilde{26}}) + 1.92(g_{\widetilde{26},\widetilde{30}} + g_{\widetilde{30},\widetilde{26}})$$
$$+ 1.92(g_{\widetilde{28},\widetilde{30}} + g_{\widetilde{30},\widetilde{28}}) + 7.56(g_{\widetilde{23},\widetilde{25}} + g_{\widetilde{25},\widetilde{23}})$$
$$+ 0.24(g_{\widetilde{25},\widetilde{28}} + g_{\widetilde{28},\widetilde{25}}) + 0.2(g_{\widetilde{25},\widetilde{26}} + g_{\widetilde{26},\widetilde{25}})$$

$$+ 0.11(g_{\widetilde{23},\widetilde{30}} + g_{\widetilde{30},\widetilde{23}}) + 0.08(g_{\widetilde{23},\widetilde{28}} + g_{\widetilde{28},\widetilde{23}})$$
$$+ 2.01(g_{\widetilde{52},\widetilde{53}} + g_{\widetilde{53},\widetilde{52}}) + 2.94(g_{\widetilde{47},\widetilde{50}} + g_{\widetilde{50},\widetilde{47}})$$
$$+ 2.85(g_{\widetilde{44},\widetilde{50}} + g_{\widetilde{50},\widetilde{44}}) + 0.14(g_{\widetilde{43},\widetilde{50}} + g_{\widetilde{50},\widetilde{43}})$$
$$+ 2.92(g_{\widetilde{47},\widetilde{49}} + g_{\widetilde{49},\widetilde{47}}) + 0.08(g_{\widetilde{45},\widetilde{49}} + g_{\widetilde{49},\widetilde{45}})$$
$$+ 0.06(g_{\widetilde{45},\widetilde{50}} + g_{\widetilde{50},\widetilde{45}}) + 2.02(g_{\widetilde{58},\widetilde{59}} + g_{\widetilde{59},\widetilde{58}})$$
$$+ \frac{2}{T}\big[0.49w_{\tilde{3}} + 0.49w_{\widetilde{18}} + 1.84w_{\widetilde{23}} + 0.49w_{\widetilde{53}}$$
$$+ 0.49w_{\widetilde{59}}\big]\delta(\omega_n)$$

Hence for $n = 3$, the static part of susceptibility diverges out of the center of the Brillouin zone. At temperatures close to zero, the dynamic part of susceptibility converges to positive constant for any filling of the cluster.

And at last the spin (transverse) susceptibility is built on the spin-flip operators. On the initial basis:

$$\hat{S}_1^+ = \hat{a}_{1\uparrow}^\dagger \hat{a}_{1\downarrow} = X^{2,5} + X^{9,20} + X^{10,21} + X^{17,11} \tag{71}$$
$$+ X^{18,12} + X^{25,36} + X^{26,37} + X^{27,38} + X^{28,39}$$
$$+ X^{32,29} + X^{35,42} + X^{47,56} + X^{48,57} + X^{53,49}$$
$$+ X^{54,50} + X^{60,63},$$

$$\hat{S}_2^+ = \hat{a}_{2\uparrow}^\dagger \hat{a}_{2\downarrow} = X^{3,6} + X^{11,20} + X^{14,22} + X^{17,9} \tag{72}$$
$$+ X^{19,15} + X^{23,33} + X^{26,35} + X^{29,38} + X^{31,41}$$
$$+ X^{32,27} + X^{37,42} + X^{44,55} + X^{50,57} + X^{52,45}$$
$$+ X^{54,48} + X^{59,62},$$

$$\hat{S}_3^+ = \hat{a}_{3\uparrow}^\dagger \hat{a}_{3\downarrow} = X^{4,7} + X^{12,21} + X^{15,22} + X^{18,10} \tag{73}$$
$$+ X^{19,14} + X^{24,34} + X^{27,35} + X^{29,37} + X^{30,40}$$
$$+ X^{32,26} + X^{38,42} + X^{45,55} + X^{49,56} + X^{52,44}$$
$$+ X^{53,47} + X^{58,61}.$$

If we switch to new basis and do all necessary operations, we will obtain that at the center of the Brillouin zone, the susceptibility is as follows:

$$\chi_s = \sum_{i-j} \langle T\hat{S}_i^+(\tau)\hat{S}_j^-(0)\rangle \tag{74}$$

$$\stackrel{FT}{=} \frac{2}{T}\Big[w_{\tilde{2}} + w_{\tilde{3}} + w_{\tilde{4}} + 4w_{\widetilde{14}} + 4w_{\widetilde{15}} + 4w_{\widetilde{16}} + 1.024w_{\widetilde{23}} + 1.024w_{\widetilde{24}} + 7w_{\widetilde{25}} + w_{\widetilde{26}} + w_{\widetilde{27}} + w_{\widetilde{28}} + w_{\widetilde{29}} + w_{\widetilde{30}} + w_{\widetilde{31}} + 3w_{\widetilde{35}} + 4w_{\widetilde{49}} + 4w_{\widetilde{50}} + 4w_{\widetilde{51}} + w_{\widetilde{58}} + w_{\widetilde{59}} + w_{\widetilde{60}}\Big]\delta(\omega_n)$$

At temperatures close to zero, it is obtained, that for concentration $n = 2$ $\lambda_{min} = \lambda_{\widetilde{14}} = \lambda_{\widetilde{17}} = \lambda_{\widetilde{20}}$ and the susceptibility follows to infinity. This states can be represented as a superposition of the initial states.

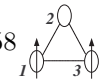
$$|\widetilde{14}\rangle = 10^{-7}|8\rangle - 0.4|9\rangle + 0.4|10\rangle - 0.4|11\rangle + 0.4|12\rangle + 10^{-6}|13\rangle - 0.4|14\rangle - 0.4|15\rangle - 10^{-7}|16\rangle \quad (75)$$

$$\approx -0.4$$  $$+ 0.4$$  $$- 0.4$$ 

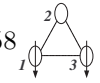
$$+ 0.4$$  $$- 0.4$$  $$- 0.4$$ 

is a superposition of the states with two opposite spins at different sites (something like an itinerant RVB bound) and

$$|\widetilde{17}\rangle = 0.58|17\rangle - 0.58|18\rangle + 0.58|19\rangle \quad (76)$$

$$= 0.58$$  $$- 0.58$$  $$+ 0.58$$ 

$$|\widetilde{20}\rangle = 0.58|20\rangle - 0.58|21\rangle + 0.58|22\rangle \quad (77)$$

$$= 0.58$$  $$- 0.58$$  $$+ 0.58$$ 

states with parallel spins.

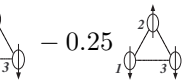
For $n = 3$, $\chi_{m,s}\big|_{T\to 0} \to \infty$ and the relative states reflect frustration

$$|\widetilde{23}\rangle = -0.1|23\rangle + 0.02|24\rangle + 0.1|25\rangle - 0.8|26\rangle + 0.37|27\rangle + 0.12|28\rangle + 0.42|29\rangle - 0.01|30\rangle - 0.13|31\rangle \quad (78)$$

$$\approx -0.8$$  $$+ 0.37$$  $$+ 0.42$$ 

$$|\widetilde{24}\rangle = 0.08|23\rangle - 0.1|24\rangle + 0.08|25\rangle - 0.03|26\rangle + 0.7|27\rangle + 0.05|28\rangle - 0.67|29\rangle - 0.13|30\rangle + 0.04|31\rangle \quad (79)$$

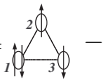
$$|\widetilde{33}\rangle = -0.1|33\rangle + 0.04|34\rangle - 0.5|35\rangle + 0.08|36\rangle - 0.25|37\rangle + 0.77|38\rangle + 0.1|39\rangle + 0.004|40\rangle - 0.13|41\rangle \quad (80)$$

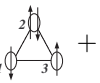
$$\approx -0.5$$  $$- 0.25$$  $$+ 0.77$$ 

$$|\widetilde{34}\rangle = 0.06|33\rangle - 0.12|34\rangle + 0.6|35\rangle + 0.1|36\rangle - 0.75|37\rangle + 0.15|38\rangle - 0.07|39\rangle - 0.1|40\rangle + 0.02|41\rangle \quad (81)$$

For electron concentration $n = 4$: $\lambda_{min} = \lambda_{\widetilde{43}}$, and ground state is

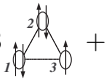
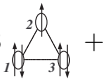
$$|\widetilde{43}\rangle = -0.12|43\rangle + 0.4|44\rangle - 0.4|45\rangle - 0.12|46\rangle + 0.4|47\rangle + 0.4|48\rangle - 0.4|49\rangle - 0.4|50\rangle + 0.12|51\rangle \quad (82)$$

$$\approx 0.4$$  $$- 0.4$$  $$+ 0.4$$ 

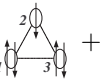
$$- 0.4$$  $$+ 0.4$$  $$- 0.4$$ 

When $n = 5, \lambda_{min} = \lambda_{\widetilde{58}} = \lambda_{\widetilde{61}}$, then $\chi_{m,s}\big|_{T\to 0} \to \infty$ and relative states are

$$|\widetilde{58}\rangle = 0.58|58\rangle + 0.58|59\rangle + 0.58|60\rangle \quad (83)$$

$$= 0.58$$  $$+ 0.58$$  $$+ 0.58$$ 

$$|\widetilde{61}\rangle = 0.58|61\rangle + 0.58|62\rangle + 0.58|63\rangle \quad (84)$$

$$= 0.58$$  $$+ 0.58$$  $$+ 0.58$$  .

Out of the center of the Brillouin zone $q = \pm\frac{2\pi}{3a}$ the susceptibility contains both static and dynamic components.

$$\chi_s = \sum_{i-j} e^{\mp i\frac{2\pi}{3}(i-j)}\langle T\hat{S}_i^-(\tau)\hat{S}_j^-(0)\rangle \quad (85)$$

$$\overset{FT}{=} \frac{1}{T}\left[0.3w_{\widetilde{3}}+0.3w_{\widetilde{15}}+1.25w_{\widetilde{23}}+0.3w_{\widetilde{51}}+0.3w_{\widetilde{59}}\right]\delta(\omega_n)$$
$$+ 0.3(g_{\widetilde{14},\widetilde{22}} + g_{\widetilde{22},\widetilde{14}}) + 0.5(g_{\widetilde{12},\widetilde{22}} + g_{\widetilde{22},\widetilde{12}})$$
$$+ 0.5(g_{\widetilde{12},\widetilde{17}} + g_{\widetilde{17},\widetilde{12}}) + 0.5(g_{\widetilde{11},\widetilde{22}} + g_{\widetilde{22},\widetilde{11}})$$
$$+ (g_{\widetilde{24},\widetilde{32}} + g_{\widetilde{32},\widetilde{24}}) + 0.3(g_{\widetilde{30},\widetilde{36}} + g_{\widetilde{36},\widetilde{30}})$$
$$+ 0.3(g_{\widetilde{27},\widetilde{38}} + g_{\widetilde{38},\widetilde{27}}) + 0.3(g_{\widetilde{30},\widetilde{38}} + g_{\widetilde{38},\widetilde{30}})$$
$$+ 0.3(g_{\widetilde{23},\widetilde{35}} + g_{\widetilde{35},\widetilde{23}}) + 0.3(g_{\widetilde{51},\widetilde{55}} + g_{\widetilde{55},\widetilde{51}})$$
$$+ 0.5(g_{\widetilde{44},\widetilde{56}} + g_{\widetilde{56},\widetilde{44}}) + 0.5(g_{\widetilde{47},\widetilde{56}} + g_{\widetilde{56},\widetilde{47}})$$
$$+ 0.5(g_{\widetilde{47},\widetilde{55}} + g_{\widetilde{55},\widetilde{47}}) + 0.3(g_{\widetilde{58},\widetilde{62}} + g_{\widetilde{62},\widetilde{58}})$$

Static contribution to the transverse susceptibility diverges out of the center of the Brillouin zone, only if there are three electrons in the system and dynamical contribution to the susceptibility approach to constant value for any filling of cluster.

5. Summary

The Hubbard model on a two- and three-site clusters is investigated. For the narrow conduction band ($U \gg t$), the susceptibilities are determined and their behavior is investigated in case of $T \to 0$. It is seen from the consideration of a two-site cluster, that the ferromagnetism can appear in the case of odd number of electrons in system and only at the center of the Brillouin zone. Such result is in good agreement with Nagaoke solution [22], which has shown that if in system, described by the Hubbard model, a number of electrons is $n_e = n \pm 1$ (n is number of sites) and $U \to \infty$, the ground state will be ferromagnetic for the simple lattices.

In case of a three-site cluster, at the center of the Brillouin zone, susceptibilities diverge in both cases of odd and even numbers of electrons in system. Out of the center of the Brillouin zone, modulated magnetic structure can appear at half-filling also. Such results shows that for the three site cluster, when the ferromagnetic state is destroyed by frustration, the Nagaoke solution is not more valid, and such behavior can be predicted for larger frustrated lattices.

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