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# Functional Integral and Effective Hamiltonian t-J-V Model of Strongly Correlated Electron System

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The functional integral representation for the generating functional of the t-J-V model is obtained. In the case close to half-filling this functional integral representation reduces the conventional Hamiltonian of the t-J-V model to the Hamiltonian of the system containing holes and spins 1/2 at each lattice size. This effective Hamiltonian coincides with that obtained by one of the authors by a different method. This Hamiltonian and its dynamical variables can be used for a description of different magnetic phases of the t-J-V model.

**KEY WORDS:** Strongly correlated electrons; Hubbard model; t-J model; electron hopping Hamiltonian; Heisenberg Hamiltonian; superconductivity; kinematic interaction.

## 1. INTRODUCTION

The problem of the theoretical description of high-temperature superconductivity (HTSC) that arose some years ago is still open.[1,2] The t-J Hubbard model of strongly correlated electrons[3,4] is one of the most popular models for the explanation of HTSC. This model reflects correctly some properties of HTSC compounds: the phase diagram, the close connection of the magnetic and transport properties, etc. The Hamiltonian of the t-J-V model can be expressed in terms of the Hubbard operators, which exclude double occupancy, $X_n^{ab} = |a, n\rangle\langle n, b|$, where $n$ is the lattice site and $|a, n\rangle = |0, n\rangle, |\uparrow, n\rangle, |\downarrow, n\rangle$:

$$H_{\mathrm{tJV}} = \sum_{n \neq m} [t_{nm} X_n^{\sigma,0} X_m^{0,\sigma} + \tfrac{1}{2} J_{nm} \mathbf{S}_n \mathbf{S}_m + \tfrac{1}{2} V_{nm} N_n N_m] - \sum_n \mu_\sigma X_n^{\sigma\sigma}$$
$$\mu_\sigma = \mu - \boldsymbol{\sigma} w_0, \qquad T \ll \mu \tag{1}$$

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where $N_n = X_n^{\uparrow\uparrow} + X_n^{\downarrow\downarrow}$ is the operator of the electron number; $\mathbf{S}$ is the spin operator, $\mathbf{S}_{nx} = (X_n^{\uparrow\downarrow} + X_n^{\downarrow\uparrow})/2$, $\mathbf{S}_{ny} = (X_n^{\uparrow\downarrow} - X_n^{\downarrow\uparrow})/2i$, $\mathbf{S}_{nz} = (X_n^{\uparrow\uparrow} - X_n^{\downarrow\downarrow})/2$; $\sigma = \pm 1/2$, $\uparrow$, $\downarrow$ is the spin projection; $t_{nm} = t_{mn}$ is the electron hopping integral from lattice site $n$ to lattice site $m$; $J_{nm}$ is the spin exchange integral; $V_{nm}$ describes the Coulomb interaction of electrons on different lattice sites; $\mu_\sigma$ is the chemical potential depending on the spin projection $\sigma$; $w_0$ is the precession frequency of the electron spin in an external magnetic field; and $T$ is a temperature which is supposed to be much less than the usual chemical potential $\mu$. This Hamiltonian follows[1,2] from the usual Hubbard Hamiltonian in the limit $u \gg t$ (where $u$ is the constant of Coulomb repulsion on a lattice site at a filling $n$ close to one electron per lattice site, $0 < 1 - n \equiv p \ll 1$.[4,5] In that case $J_{nm} = 8(t_{nm})^2/u$.

Belinicher[6] obtained the following representation for the Hubbard operators $X^{ab}$ in terms of Fermi hole operators $h_{n\sigma}^+$ and $h_{n\sigma}$ and local spins $\mathbf{s}$:

$$X^{0\sigma} = h^+(1/2 - (\boldsymbol{\sigma}\mathbf{s}) + (h^+h))_{\sigma'}\tau_{\sigma'\sigma}, \qquad X^{\sigma 0} = -\tau_{\sigma\sigma'}h_{\sigma'}$$
$$N_h = X^{\uparrow\uparrow} + X^{\downarrow\downarrow} = 1 - N, \qquad X^{00} = N, \qquad \mathbf{S} = \mathbf{s} + (1/2)(h^+\boldsymbol{\sigma}h) \tag{2}$$
$$\tau = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$$

This representation makes it possible to reduce the Hamiltonian (1), $H_{\mathrm{tJV}}$, to the Hamiltonian of the Fermi hole operators and spins 1/2,

$$H_{\mathrm{tJV}} = H_0 + H_{\mathrm{int}}, \qquad H_0 = \sum_{n\sigma} \mu_{-\sigma} h_{n\sigma}^+ h_{n\sigma} + \sum_n s_n^z$$
$$H_{\mathrm{int}} = \sum_{n \neq m} [t_{nm} h_n^+ (-1/2 + (\mathbf{s}_n\boldsymbol{\sigma}) - (h_n^+ h_n)) + \tfrac{1}{2} V_{nm}(h_n^+ h_n)(h_m^+ h_m) \tag{3}$$
$$+ \tfrac{1}{2} J_{nm}(\mathbf{s}_n + \tfrac{1}{2}(h_n^+\boldsymbol{\sigma}h_n))(\mathbf{s}_m + \tfrac{1}{2}(h_m^+\boldsymbol{\sigma}h_m))]$$

The representation (2) and the effective Hamiltonian (3) were obtained in the framework of the Wick theorem for Hubbard operators. The representation (2) and the Hamiltonian (3) do not represent direct operator identities. Some isomorphism of the form $A \to VAV^{-1}$ must exist which transforms the relation (2) and (3) into identities. In this point this representation differs from known slave boson representations.[7-9] In the present form the Hamiltonian (3) can be used for the calculation of the Green function of the Hubbard operators in the framework of the temperature diagram technique. Such a calculation was performed for the simplest magnetic states, ferromagnetic, paramagnetic, and antiferromagnetic, in ref. 6 and the properties of the hole transport and the hole interaction

were determined on the basis of two small parameters: the hole number per lattice site $p \ll 1$ and the inverse number of neighbors $1/z \ll 1$.

But it is well known that superconductivity arises in the nontrivial state of the paramagnetic spin liquid and it is not obvious that the Hamiltonian (3) obtained in the framework of the perturbation theory can be applied to the nontrivial magnetic state, which must be investigated on the basis of some variational approach.[10]

The reason for doubt concerning the validity of the representation (2) is based on the example of the Heisenberg model, which was studied with the functional integral method by Kolokolov and Podivilov.[11,12] They showed that the spin operator representation[13]

$$s_z = a^+ a + \phi, \qquad s^- = a, \qquad s^+ = -a^+(a^+ a + 2\phi) \tag{4}$$

where $\phi$ is a random field with given statistical properties similar to the representation (2), is not precise and contains some corrections. The substitution (2) and Hamiltonian (3) are Hermitian. The latter does not allow one to examine (3) as a Hamiltonian of some correct quantum problem. But ref. 6 made the assumption that the Hamiltonian (3) is defined only for the calculation of various matrix elements. This assumption requires proof.

In the present paper we shall construct the functional integral representation for the generating functional of the Hubbard operator temperature Green functions for the Hamiltonian (1) t-J-V model of the strongly correlated electron system (Section 2). We shall show that the effective Hamiltonian (3) is the correct Hamiltonian for a filling of close to one electron per lattice site that is actual for HTSC compounds (Section 3). The functional integral method allows one to solve the problem of the calculation of matrix elements with respect to the Hamiltonian (3) in the case of a filling of close to one. It is possible to suggest a Hermitian variant of the substitution (3) and the Hamiltonian (4) (Section 4). We believe that the Hamiltonian (3) has some advantage in comparison with the usual t-J model[3,4] because it does not contain any constraint on double occupancy and can be used for the variational calculation of nontrivial magnetic states.

## 2. FUNCTIONAL INTEGRAL REPRESENTATION

The generating functional for the Hubbard temperature Green function may be represented in the form

$$Z(h) = \mathrm{Tr}\left(T_\tau\left(\exp\left(-\beta H_{\mathrm{tJV}} + \int_0^\beta h^{ab}\, d\tau + \beta F\right)\right)\right) \tag{5}$$

where $\beta$ is the inverse temperature; $T_\tau$ means the ordering product over temperature for time $\tau$; $h^{ab}(\tau)$ represents eight external fields conjugated to eight Hubbard operators $X^{ab}$ excluding $X^{00}=1-N$; the external fields conjugate to $X^{0\sigma}$, $X^{\sigma 0}$, are Grassmann variables; $F$ is the free energy; and $Z(0)=1$. Using the Hubbard–Stratanovich identity,[14,11] one can represent the generating functional (5) in the form

$$Z(h)=\int \prod_n D\pi_n^\alpha\, D\pi_n^\gamma\, D\pi_n^N \times \exp\left[\tfrac{1}{2}\int_0^\beta (\pi_n^\alpha A_{\alpha\eta}^{-1} t_{nm}^{-1}\pi_m^\eta - \pi_n^\gamma B_{\gamma\nu}^{-1} J_{nm}^{-1}\pi_m^\nu - \pi_n^N V_{nm}^{-1}\pi_m^N)\,d\tau\right] \times \mathrm{Tr}\left(T_\tau\left(\exp\left\{\int_0^\beta [\tilde\pi_n^\alpha(\tau)\, X_n^\alpha + \tilde\pi_n^\gamma(\tau)\, X_n^\gamma + \tilde\pi_n^N]\,d\tau\right\}\right)\right) \tag{6}$$

where $\pi^{\alpha,\eta}=(\pi^{0\uparrow}, \pi^{\uparrow 0}, \pi^{0\downarrow}, \pi^{\downarrow 0})$ are the Grassmann fields conjugate to the corresponding Hubbard Fermi operators; $\pi^{\gamma,\nu}=(\pi^{\uparrow\downarrow}, \pi^{\downarrow\uparrow}, \pi^z)$ are the complex fields conjugate to the spin Hubbard Bose operators; $\pi^N$ is conjugate to $N$; $\tilde\pi^a=\pi^a+h^a$ for $a=0\sigma$, $\sigma 0$, $\uparrow\downarrow$, $\downarrow\uparrow$; $\tilde\pi^z=\pi^z+h^z-w_0$; $\tilde\pi^N=\pi^N+h^N+\mu$. The numerical matrices $A_{\alpha\eta}$, $B_{\gamma\nu}$ as follow from the Hamiltonian (1) have the form

$$A_{\alpha\eta}=\begin{pmatrix} 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 1\\ 0 & 0 & -1 & 0\end{pmatrix}, \qquad B_{\gamma\nu}=\frac{1}{2}\begin{pmatrix} 0 & 1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 1\end{pmatrix} \tag{7}$$

Let us notice that the integration over variables $\pi^{\uparrow\downarrow}$, $\pi^{\downarrow\uparrow}$, $\pi^z$, $\pi^N$ can be understood as the integration over the surface in the complex space defined by the condition

$$\pi_n^{\uparrow\downarrow}(\tau)=-(\pi_n^{\downarrow\uparrow}(\tau))^*, \qquad \mathrm{Re}(\pi_n^z(\tau))=\mathrm{Re}(\pi_n^N(\tau))=0 \tag{8}$$

Correspondingly, the integration over Grassmann variables $\pi_n^{0\sigma}$, $\pi_n^{\sigma 0}$ can be understood as an integration over the four-dimensional Grassmann manifold determined by the condition

$$\pi_n^{0\sigma}(\tau)=-(\pi_n^{\sigma 0}(\tau))^* \tag{9}$$

The problem of the determination of the explicit form of the generating functional (6) is reduced to the determination of the $T$-ordered exponent

$$A(\tau)=T_\tau\left(\int_0^\tau \pi^c(\tilde\tau)\, X^c + \pi^0(\tilde\tau)\right)d\tilde\tau \tag{10}$$

where $c = 0\sigma$, $\sigma 0$, $\uparrow\downarrow$, $\downarrow\uparrow$, $z$, $n$ and the quantity $\pi(\tau)$ is introduced for convenience. The operator exponent $A(\tau)$ satisfies the obvious equation

$$\dot{A}(\tau) = (\pi^c(\tau)\, X^c + \pi^0(\tau))\, A(\tau) \tag{11}$$

with the initial condition $A(0) = 1$. We are not able to solve Eq. (11) when the conditions (8) and (9) are fulfilled. However, following the method of ref. 11, we can deform the surface (8), (9) in a special manner and find the operator $A(\tau)$. To this end, we shall use the ansatz

$$\begin{aligned} A(\tau) &= B^+(\tau)\, B^0(\tau)\, B^-(\tau)[B^+(0)]^{-1} \\ B^+(\tau) &= \exp[\varphi^{\uparrow 0}(\tau)\, X^{\uparrow 0} + \varphi^{\downarrow 0}(\tau)\, X^{\downarrow 0} + \varphi^{\uparrow\downarrow}(\tau)\, X^{\uparrow\downarrow}] \\ B^0(\tau) &= \exp[\varphi^{\uparrow\uparrow}(\tau)\, X^{\uparrow\uparrow} + \varphi^{\downarrow\downarrow}(\tau)\, X^{\downarrow\downarrow}] \\ B^-(\tau) &= \exp[\varphi^{0\uparrow}(\tau)\, X^{0\uparrow} + \varphi^{0\downarrow}(\tau)\, X^{0\downarrow} + \varphi^{\downarrow\uparrow}(\tau)\, X^{\downarrow\uparrow}] \end{aligned} \tag{12}$$

In the formulas (10)–(12) and below the index of the lattice site $m$ is omitted for the sake of simplicity. The expression (12) for $A(\tau)$ satisfies the initial condition $A(0) = 1$. After differentiation with respect to $\tau$ and representation of the result in the form (11), we get the system of equations connecting $\pi^c(\tau)$ and $\varphi(\tau)$:

$$\begin{gathered} \pi^{\downarrow 0} = \dot{\psi}^{\downarrow 0} - \pi^{\downarrow\uparrow}\psi^{\uparrow 0} - (\pi^n - \tfrac{1}{2}\pi^z)\,\psi^{\downarrow 0} + \psi^{\downarrow 0}\psi^{0\uparrow}\psi^{\uparrow 0} \\ \pi^{\uparrow 0} = \dot{\psi}^{\uparrow 0} - \pi^{\uparrow\downarrow}\psi^{\downarrow 0} - (\pi^n + \tfrac{1}{2}\pi^z)\,\psi^{\uparrow 0} + \psi^{\uparrow 0}\psi^{0\downarrow}\psi^{\downarrow 0} \\ \pi^{0\uparrow} = \psi^{0\uparrow}, \qquad \pi^{0\downarrow} = \psi^{0\downarrow} \\ \pi^{\downarrow\uparrow} = \psi^{\downarrow\uparrow} + \psi^{\downarrow 0}\psi^{0\uparrow} \\ \pi^{\uparrow\downarrow} = \psi^{\uparrow\downarrow} - (\psi^z + \psi^{\uparrow\downarrow}\psi^{\downarrow\uparrow})\,\psi^{\uparrow\downarrow} + \psi^{\uparrow 0}\psi^{0\downarrow} \\ \pi^z \equiv \pi^{\uparrow\uparrow} - \pi^{\downarrow\downarrow} = \psi^z + 2\psi^{\downarrow\uparrow}\psi^{\uparrow\downarrow} + \psi^{\uparrow 0}\psi^{0\uparrow} - \psi^{\downarrow 0}\psi^{0\downarrow} \\ \pi^N \equiv \tfrac{1}{2}(\pi^{\uparrow\uparrow} + \pi^{\downarrow\downarrow}) = \psi^N + \tfrac{1}{2}\psi^{\sigma 0}\psi^{0\sigma} \\ \pi^0 = -\psi^{\sigma 0}\psi^{0\sigma} \end{gathered} \tag{13}$$

where the new field variables $\psi$ are expressed in terms of the initial variables $\varphi$ in the following way:

$$\begin{gathered} \psi^{0\uparrow} = (\dot{\varphi}^{0\uparrow} - \dot{\varphi}^{0\downarrow}\varphi^{\downarrow\uparrow})\exp(-\varphi^{\uparrow\uparrow}) \\ \psi^{0\downarrow} = \dot{\varphi}^{0\downarrow}\exp(-\varphi^{\downarrow\downarrow}) - (\varphi^{0\uparrow} - \varphi^{0\downarrow}\varphi^{\downarrow\uparrow}) > \varphi^{\uparrow\downarrow}\exp(-\varphi^{\uparrow\uparrow}) \\ \psi^{\uparrow 0} = \varphi^{\uparrow 0}, \qquad \psi^{\downarrow 0} = \varphi^{\downarrow 0}, \qquad \psi^{\uparrow\downarrow} = \varphi^{\uparrow\downarrow} \\ \psi^{\downarrow\uparrow} = \dot{\varphi}^{\downarrow\uparrow}\exp(-\varphi^z), \qquad \varphi^z \equiv \varphi^{\uparrow\uparrow} - \varphi^{\downarrow\downarrow} \\ \psi^z \equiv \psi^{\uparrow\uparrow} - \psi^{\downarrow\downarrow} = \dot{\varphi}^z \\ \psi^N \equiv \tfrac{1}{2}(\psi^{\uparrow\uparrow} + \psi^{\downarrow\downarrow}) = \dot{\varphi}^N \end{gathered} \tag{14}$$

The dependence of $\pi^0$ on $\psi$ represented separately in (13) can be considered as a definition. Performing the functional change of variables (13), one can calculate the exponent explicitly and obtain an explicit functional representation for the generating functional $Z(h)$.

After the change of variables (13) it is natural to deform the initial surface of integration (8), (9) into the surface

$$\begin{gathered}\psi^{\uparrow\downarrow}(\tau) = -(\psi^{\downarrow\uparrow}(\tau))^*, \qquad \mathrm{Re}(\psi^z(\tau)) = \mathrm{Re}(\psi^N(\tau)) = 0 \\ \psi^{0\sigma}(\tau) = -(\psi^{\sigma 0}(\tau))^*\end{gathered} \tag{15}$$

Notice that after such a deformation the conditions (8), (9) for $\pi^{\uparrow\downarrow}(\tau)$, $\pi^{\downarrow\uparrow}(\tau)$, $\pi^{0\sigma}(\tau)$, $\pi^{\sigma 0}(\tau)$ are not valid. For the correctness of such a deformation the density of the generating functional must be regular with respect to the variables of the integration and the integral must exist for every surface of the integration in the process of deformation. The last condition is essential for the numerical variables $\pi^{\uparrow\downarrow}(\tau)$, $\pi^{\downarrow\uparrow}(\tau)$ because an integral over a finite number of Grassmann variables always exists. The discussion of the convergence of the integral over the variables $\pi^{\uparrow\downarrow}(\tau)$, $\pi^{\downarrow\uparrow}(\tau)$ can be performed in a manner similar to ref. 11.

The substitution of variables (13) contains the time derivatives in the right side because it is necessary to fix the initial or boundary conditions. For complex $\psi^{\uparrow\downarrow}(\tau)$ the standard boundary condition $\psi^{\uparrow\downarrow}(\beta) = \psi^{\uparrow\downarrow}(0)$ makes the transformation nonreversible. We shall use the initial condition for the $\psi^{\uparrow\downarrow}(\tau)$,[12]

$$\psi^{\uparrow\downarrow}(0) = 0 \tag{16}$$

For the Grassmann variables $\psi^{\sigma 0}(\tau)$ one can use the standard antiperiodic boundary condition

$$\psi^{\sigma 0}(0) = -\psi^{\sigma 0}(\beta) \tag{17}$$

When we perform the substitution of variables in the generating functional (6) we must calculate the Jacobian or more precisely the Berezinian of the transformation

$$D\pi^{\sigma 0}\, D\pi^{\uparrow\downarrow}\, D\pi^{\downarrow\uparrow}\, D\pi^z\, D\pi^N = \mathrm{Ber}[J(\psi)]\, D\psi^{\sigma 0}\, D\psi^{\uparrow\downarrow}\, D\psi^{\downarrow\uparrow}\, D\psi^z\, D\psi^N \tag{18}$$

where the matrix $J(\psi)$ may be represented in the block form

$$J \equiv \frac{\partial \pi}{\partial \psi} = \begin{pmatrix} J^{ab} & J^{al} \\ J^{kb} & J^{kl} \end{pmatrix}; \qquad a, b = \uparrow 0, \downarrow 0; \qquad k, l = \uparrow\downarrow, \downarrow\uparrow, z, N \tag{19}$$

here $J^{ab}$ is the Fermi part of the $J$ matrix; $J^{kl}$ is the Bose part; and $J^{al}$, $J^{kb}$ are the mixed parts of the $J$ matrix. When the derivatives over the Grassmann variables in (19) are computed they are taken as the right derivatives.

The Berezinian of the $J$ matrix is calculated according to the following rule[15]:

$$\mathrm{Ber}[J] = \mathrm{Det}[J^{kl} - J^{ka}(J^{ab})^{-1} J^{bl}](\mathrm{Det}[J^{ab}])^{-1} \tag{20}$$

The explicit form of the Berezinian (20) depends on the method of regularization of the time derivatives in (13). Because the Bose part of the $J$ matrix $J^{kl}$ practically coincides with the corresponding spin matrix of ref. 11, we shall use the same regularization,

$$\begin{aligned}
\pi_p^{\uparrow\downarrow} &= \psi_p^{\uparrow\downarrow} + (\psi^{\downarrow 0} - \psi^{\uparrow 0})_p \\
\pi_p^{\uparrow\downarrow} &= \Delta^{-1}(\psi_p^{\uparrow\downarrow} - \psi_{p-1}^{\uparrow\downarrow}) - \tfrac{1}{2}\psi_p^z(\psi_p^{\uparrow\downarrow} + \psi_{p-1}^{\uparrow\downarrow}) \\
&\quad - \tfrac{1}{4}(\psi_p^{\uparrow\downarrow} + \psi_{p-1}^{\uparrow\downarrow})^2 \psi_p^{\downarrow\uparrow} + (\psi^{\uparrow 0}\psi^{0\downarrow})_p \\
\pi_p^z &= \psi_p^z + \psi_p^{\downarrow\uparrow}(\psi_p^{\uparrow\downarrow} + \psi_{p-1}^{\uparrow\downarrow})
\end{aligned} \tag{21}$$

where the quantities $\psi_p$, $\pi_p$ are defined by the relations

$$\psi_p \equiv \psi(\tau_p), \qquad \pi_p \equiv \pi(\tau_p), \qquad \tau_p = \frac{p\beta}{L}, \qquad \Delta = \frac{\beta}{L}, \qquad L \to \infty \tag{22}$$

Here $1 \leqslant p \leqslant L$ and $p$, $L$ are integers. The $\mathrm{Det}[J^{kl}]$ can be easily calculated:

$$\mathrm{Det}[J^{kl}] = \lim \prod_{p=1}^{L} \left(\frac{1}{\Delta} - \frac{1}{2}\psi^z\right) = \mathrm{const} \cdot \exp\left(-\frac{1}{2}\int_0^\beta \psi_\tau^z \, d\tau\right) \tag{23}$$

For the computation of $\mathrm{Det}[J^{ab}]$ let us perform the regularization $\pi^{0\sigma}(\tau)$ in the following way:

$$\begin{aligned}
\pi_p^{\sigma 0} &= \Delta^{-1}(\psi_p^{\sigma 0} - \psi_{p-1}^{\sigma 0}) - A_p^\sigma((1+k)\,\psi_{p-1}^{\sigma 0} - k\psi_p^{\sigma 0}) \\
A_p^\sigma &= [\psi_p^N + \sigma\psi_p^z + 2\sigma\psi_p^{\uparrow\downarrow}\psi_p^{\downarrow\uparrow} + \psi_p^{\sigma 0}\psi_p^{0\sigma}]
\end{aligned} \tag{24}$$

The crossing terms $J^{\sigma 0}$, $J^{-\sigma 0}$ give small contributions at $\Delta \to 0$ in Det $(J^{ab})$ and can be omitted. Thus

$$\mathrm{Det}(J^{ab}) = \mathrm{Det}\left(\frac{\partial \pi^{\uparrow 0}}{\partial \psi^{\uparrow 0}}\right) \mathrm{Det}\left(\frac{\partial \pi^{\downarrow 0}}{\partial \psi^{\downarrow 0}}\right) \tag{25}$$

and taking into account (16) and (17), we get

$$\begin{pmatrix} \mathcal{A}^{-1}+A_1^\sigma k & 0 & \cdots & \mathcal{A}^{-1}+A_1^\sigma(1+k) \\ \mathcal{A}^{-1}-A_2^\sigma(1+k) & \mathcal{A}^{-1}+A_2^\sigma k & 0 & \cdots \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \cdots & 0 \\ 0 & \cdots & -\mathcal{A}^{-1}-A_p^\sigma(1+k) & \mathcal{A}^{-1}+A_1^\sigma k \end{pmatrix} = \frac{\partial \pi^{\sigma 0}}{\partial \psi^{\sigma 0}} \tag{26}$$

where $A_p^\sigma$ is defined in (24) and

$$\begin{aligned} \mathrm{Det}\left[\frac{\partial \pi_p^{\sigma 0}}{\partial \psi_p^{\sigma 0}}\right] &= \lim\left(\prod_{p=1}(\mathcal{A}^{-1}+kA_p^\sigma)+\prod_{p=1}^{L}(\mathcal{A}^{-1}+(1+k)\,A_p^\sigma)\right) \\ &= \mathrm{const}\cdot\left\{\exp\left(k\int_0^\beta A_\tau^\sigma\,d\tau\right)\right. \\ &\quad \left.+\exp\left[(1+k)\int_0^\beta A_\tau^\sigma\,d\tau\right]\right\} \end{aligned} \tag{27}$$

The $\mathrm{Det}[(J^{ab})^{-1}]$ is not equal to zero on the surface of integration and one can conclude that the initial and boundary conditions (16) and (17) are correct. The regularization constant $k$ can be determined if we compare our result with the case of small filling (see below) where all results can be obtained in the gas approximation: $k=0$. The computation of the trace $A(\tau)$ can be easily performed. The general trace can be split into the product of the single-sites traces, and taking into account initial and boundary conditions (16) and (17), we get

$$\begin{aligned} &\mathrm{Tr}\left(T\exp\left\{\int_0^\tau [\pi^c(\tau)\,X^c+\pi^0(\tau)]\,d\tau\right\}\right) \\ &\quad = 1+\exp[\varphi^{\uparrow\uparrow}(\beta)]+[1+\varphi^{\uparrow\downarrow}(\beta)\,\varphi^{\downarrow\uparrow}(\beta)]\exp[\varphi^{\downarrow\downarrow}(\beta)] \\ &\quad = 1+\exp\left\{\int_0^\beta [\tilde{\psi}^N(\tau)+\tfrac{1}{2}\tilde{\psi}^z(\tau)]\,d\tau\right\} \\ &\qquad +\exp\left\{\int_0^\beta [\tilde{\psi}^N(\tau)-\tfrac{1}{2}\tilde{\psi}^z(\tau)]\,d\tau\right\} \\ &\qquad +\exp\left\{\int_0^\beta [\tilde{\psi}^N(\tau)-\tfrac{1}{2}\tilde{\psi}^z(\tau)]\,d\tau\right\}\psi^{\downarrow\uparrow}(\beta) \\ &\qquad \times\int_0^\beta \psi^{\uparrow\downarrow}(\tau)\exp\left[\int_0^\tau \tilde{\psi}^z(\tilde{\tau})\,d\tilde{\tau}\right]d\tau \end{aligned} \tag{28}$$

where $\tilde{\psi}^N(\tau)=\psi^N(\tau)-\mu$ and $\tilde{\psi}^z(\tau)=\psi^z(\tau)+w_0$.

In conclusion of this part of this paper, we shall get an explicit form of the generating functional in the case of small filling when the J and V contributions are absent and the Hubbard–Stratanovich transformation is produced for the t member only. In that case we have the expression for the generating functional

$$Z(h)=\int \prod_{n,\tau} D\pi_n^{0\sigma}\, D\pi_n^{\sigma 0}\, \mathrm{Tr}\left( T\exp\left\{ \int_0^\beta [\pi^c(\tau)\, X^c + \pi^0(\tau)]\, d\tau \right\}\right)$$
$$\times \exp\left[ \int_0^\beta \left( t_{nm}^{-1}\pi^{\sigma 0}\pi^{0\sigma} + \sum_n \pi_n^0 \right) d\tau \right] \tag{29}$$

Let us set $\pi^{\uparrow\downarrow}$, $\pi^{\downarrow\uparrow}$, $\pi^z$, $\pi^N$ equal to zero in (13) and (14) and perform the corresponding functional change of variables. Equation (13) can be considered in that case as the definition of $\psi^{\uparrow\downarrow}$, $\psi^{\downarrow\uparrow}$, $\psi^z$, $\psi^N$. Supposing $|\mu| \gg T$, $w_0$ and $\mu < 0$, we get that in this limit the trace (28) becomes unity. From (20), (23), and (27) it follows that for $k=0$ and $\beta\mu \to -\infty$, the Berezinian equal to $\mathrm{Det}[(J^{ab})^{-1}]$ becomes constant. Substituting in (29) the expression for $\pi$ in (13) and making the linear change of the integration variables

$$\psi_n^{0\sigma} \to t_{nm}\psi_m^{0\sigma}, \tag{30}$$

we get the following representation for the generating functional:

$$Z(h)=\int \prod_{n,\tau} D\pi_n^{0\sigma}(\tau)\, D\pi_n^{\sigma 0}(\tau) \exp(-\Gamma)$$
$$\Gamma=\int_0^\beta [\dot{\psi}_n^{\sigma 0}\psi_n^{0\sigma} - \mu_\sigma \psi_n^{\sigma 0}\psi_n^{0\sigma} + t_{nm}\psi_n^{\sigma 0}(1-\psi_n^{\tilde{\sigma}0}\psi_n^{0\tilde{\sigma}})\,\psi_m^{0\sigma} \tag{31}$$
$$+ h_n^{0\sigma}\psi_n^{0\sigma} + h_n^{\sigma 0}\psi_n^{\sigma 0}(1-\psi_n^{\tilde{\sigma}0}\psi_n^{0\tilde{\sigma}})]\, d\tau$$

This generating functional leads to an effective Hamiltonian that coincides with the Hamiltonian obtained[6] by the operator method. The mass renormalization, damping, and electron scattering amplitudes that follow from the generating functional (31) coincide with results of the gas approximation obtained from the initial Hubbard Hamiltonian.[16] Such a coincidence of the results may be obtained only for the regularization we have used and this in fact fixes it.

## 3. THE FILLING CLOSE TO UNITY AND REDUCTION TO THE SPIN PARTITION FUNCTION

Here we consider the case $\mu > 0$, $\mu \gg T$, $w_0$, and $\beta\mu \to \infty$. One can verify that $\mathrm{Det}[J^{ab}] \sim \exp(-\mu)$ and

$$\mathrm{Ber}[J]=\frac{\mathrm{Det}[J^{kl}]}{\mathrm{Det}[J^{ab}]}=\mathrm{const}\cdot\exp\left[ -\int_0^\beta (2\psi^N + \tfrac{1}{2}\psi^z - \psi^{\sigma 0}\psi^{0\sigma})\, d\tau \right] \tag{32}$$

Substituting (32) into (20), and (20) and (28) into (6) at $\beta\mu \to \infty$, one can verify that the integral over $\psi_\tau^N$ is Gaussian and thus it can be easily performed. As a result, we get the following functional integral over the seven field on the lattice

$$Z(h) = \int \prod_{n,\tau} D\psi_n^d(\tau) \exp(-\Gamma_f - \Gamma_s) \prod_n \left(1 + \exp\left[-\int_0^\beta \psi_n^z(\tau)\, d\tau\right] \times \left\{1 + \psi^{\downarrow\uparrow}(\beta)\left(\int_0^\beta \psi^{\uparrow\downarrow}(\tau) \exp\left[\int_0^\tau \psi^z(\tilde{\tau})\, d\tilde{\tau}\right]\right)\right\}\right) \tag{33}$$

where $d = (0\sigma, \sigma 0, \uparrow\downarrow, \downarrow\uparrow, z)$, and

$$\begin{aligned}
\Gamma_f = \int_0^\beta & (\dot{\psi}_n^{\sigma 0} t_{nm}^{-1} \psi_m^{0\sigma} - \mu_\sigma \psi_n^{\sigma 0} t_{nm}^{-1} \psi_n^{0\sigma} \\
& - \tfrac{1}{2}\psi_n^{\sigma 0}\psi_n^{0\sigma} - \tfrac{1}{2}\psi_n^{\sigma 0}\psi_n^{0\sigma}\psi_n^{\tilde{\sigma}0} t_{nm}^{-1}\psi_m^{0\tilde{\sigma}} \\
& - \tfrac{1}{2}\mathbf{h}_n \psi_n^{\sigma 0}\boldsymbol{\sigma} t_{nm}^{-1}\psi_m^{0\sigma} + \tfrac{1}{2}\psi_n^{\sigma 0}\boldsymbol{\sigma}\psi_n^{0\sigma}\psi_n^{\tilde{\sigma}0}\tilde{\boldsymbol{\sigma}} t_{nm}^{-1}\psi_m^{0\tilde{\sigma}} \\
& - \tfrac{1}{8} J_{nm}^{-1}(J_{kn} t_{kl}^{-1}\psi_k^{\sigma 0}\boldsymbol{\sigma}\psi_l^{0\sigma})(J_{pm} t_{pq}^{-1}\psi_p^{\tilde{\sigma}0}\tilde{\boldsymbol{\sigma}}\psi_q^{0\tilde{\sigma}}) \\
& - \tfrac{1}{2} t_{nl}^{-1} V_{nm} t_{mk}^{-1}\psi_n^{\sigma 0}\psi_l^{0\sigma}\psi_m^{\tilde{\sigma}0}\psi_k^{0\tilde{\sigma}}) + V_0 t_{nm}^{-1}\psi_n^{\sigma 0}\psi_m^{0\sigma})\, d\tau
\end{aligned} \tag{34}$$

$$\begin{aligned}
\Gamma_s = \int_0^\beta & \tfrac{1}{2} J_{nm}^{-1}(\boldsymbol{\eta}_n + \mathbf{g}_n + \psi_n^{\sigma 0}\boldsymbol{\sigma}\psi_n^{0\sigma} - \tfrac{1}{2} J_{kn} t_{kl}^{-1}\psi_k^{\sigma 0}\boldsymbol{\sigma}\psi_l^{0\sigma}) \\
& \times (\boldsymbol{\eta}_m + \mathbf{g}_m + \psi_m^{\tilde{\sigma}0}\tilde{\boldsymbol{\sigma}}\psi_m^{0\tilde{\sigma}} - \tfrac{1}{2} J_{pm} t_{pq}^{-1}\psi_p^{\tilde{\sigma}0}\tilde{\boldsymbol{\sigma}}\psi_q^{0\tilde{\sigma}})\, d\tau
\end{aligned}$$

where $\mathbf{g} = (h_x, h_y, h_z + w_0)$, $V_0 = \sum_n V_{nm}$, and the vector $\boldsymbol{\eta}$ has the following form:

$$\begin{aligned}
\eta^x = \eta^{\uparrow\downarrow} + \eta^{\downarrow\uparrow}, \qquad \eta^y = i(\eta^{\uparrow\downarrow} - \eta^{\downarrow\uparrow}) \\
\eta^z = \pi^z - \psi^{\uparrow 0}\psi^{0\uparrow} + \psi^{\downarrow 0}\psi^{0\downarrow} \\
\eta^{\downarrow\uparrow} = \pi^{\downarrow\uparrow} - \psi^{\downarrow 0}\psi^{0\uparrow}, \qquad \eta^{\uparrow\downarrow} = \pi^{\uparrow\downarrow} - \psi^{\uparrow 0}\psi^{0\downarrow}
\end{aligned} \tag{35}$$

For simplicity we omit fermion external fields $h^{\sigma 0}$, $h^{0\sigma}$. In the next step we shall distinguish the integral over the spin variables

$$\begin{aligned}
Z(h) = \int \prod_{n,\tau} & D\psi_n^{0\sigma}(\tau)\, D\psi_n^{\sigma 0}(\tau) \exp(-\Gamma_f) \left\{\prod_{n,\tau} D\psi_n^{\uparrow\downarrow}(\tau)\, D\psi_n^{\downarrow\uparrow}(\tau)\right. \\
& \times D\psi_n^z(\tau) \exp(-\Gamma_s) \prod_{n,\tau}\left[1 + \exp\left[-\int_0^\beta \psi_n^z(\tau)\, d\tau\right]\right. \\
& \left.\left. \times \left(1 + \psi^{\downarrow\uparrow}(\beta)\left\{\int_0^\beta \psi^{\uparrow\downarrow}(\tau) \exp\left[\int_0^\tau \psi^z(\tilde{\tau})\, d\tilde{\tau}\right] d\tau\right\}\right)\right]\right\}
\end{aligned} \tag{36}$$

It follows from formula (36) that the expression in curly brackets coincides explicitly with the generating functional of the Heisenberg model.[12] The external field with respect to the spin operators is

$$\tilde{\mathbf{h}}_n(\tau) = \mathbf{h}_n(\tau) + \psi_n^{\sigma 0}\boldsymbol{\sigma}\psi_n^{0\sigma} - \tfrac{1}{2}J_{kn}t_{kl}^{-1}\psi_k^{\sigma 0}\boldsymbol{\sigma}\psi_l^{0\sigma} \tag{37}$$

and the generating functional can be rewritten in the form

$$Z(h) = \int \prod_{n,\tau} D\psi_n^{0\sigma}(\tau)\, D\psi_n^{\sigma 0}(\tau) \exp(-\Gamma_f) \times \operatorname{Tr}\left( T\exp\left\{\left[ -\beta H_{\text{ex}} - \int_0^\beta \mathbf{h}_n(\tau)\,\mathbf{S}_n(\tau)\, d\tau \right]\right\}\right) s \tag{38}$$

where the trace is taken over spin variables and

$$H_{\text{ex}} = \tfrac{1}{2}\sum_{n,m} J_{nm}\mathbf{S}_n\mathbf{S}_m \tag{39}$$

is the usual Hamiltonian for quantum antiferromagnets (spin 1/2). The substitution (30) for the Grassmann fields reduces the generating functional (38) to the standard functional integral[15] with the Hamiltonian explicitly coinciding with the Hamiltonian (3).

Let us remark that in the general case of an arbitrary chemical potential the separation of the spin subsystem is not possible. Moreover, the universal polynomial substitution of the spin operators in terms of Bose and Fermi operators does not follow from the method of this paper. We think that further investigation of the Hamiltonian (3) must be based on the variational method[10] for the spin subsystem.

## 4. PHYSICAL INTERPRETATION OF EFFECTIVE HAMILTONIAN

First we recall the physical interpretation of the well-known non-Hermitian Dyson–Maleev representation,[17,18] which follows from (4) if we put $\phi = -s$. One can compare that representation with the Hermitian Holstein–Primakoff[19] representation for spin operators,

$$\begin{aligned} s_{\text{HP}}^- &= P(a^+a)(2s - a^+a)^{1/2}\, aP(a^+a) \\ s_{\text{HP}}^+ &= P(a^+a)\, a^+(2s - a^+a)^{1/2}\, P(a^+a) \\ s_{\text{HP}}^z &= P(a^+a)(-s + a^+a)\, P(a^+a) \end{aligned} \tag{40}$$

here $a^+$ and $a$ are creation and annihilation Bose operators, and $P(a^+a)$ is the projector operator on the lower $2s+1$ states: $|0\rangle$, $|1\rangle$,..., $|2s\rangle$. The

representation (40) is a direct operator identity which maps the algebra of the spin operators $\mathbf{s}$ into the Heisenberg algebra of the creation and annihilation operators $a^+$ and $a$.

One can check that there exists an operator $V(a^+a)$ with the property

$$\mathbf{s}_{\mathrm{HP}} = PV^{-1}\mathbf{s}_{\mathrm{DM}}VP \tag{41}$$

where $\mathbf{s}_{\mathrm{HP}}$ and $\mathbf{s}_{\mathrm{DM}}$ are the Holstein–Primakoff, (40), and Dyson–Maleev, (4), spin operators, respectively. The identity (41) means that matrix elements of both parts of Eq. (4.2) between any states $\langle n|$ and $|n'\rangle$ are equal to each other. If $n, n' > 2s$, these matrix elements are equal to zero. The explicit form of the matrix elements $V$ is

$$\langle n'|\, V\, |n\rangle = \delta_{n',n} \prod_{m=0}^{n} (2s+1-m)^{1/2}, \qquad n, n' \leqslant 2s \tag{42}$$

If we want to calculate the partition function

$$Z = \mathrm{Tr}\,(\exp[-\beta H(\mathbf{s})]) = \mathrm{Tr}(P\exp[-\beta H(\mathbf{s}_{\mathrm{HP}})]) \tag{43}$$

we can use the identity (41) and the commutation of the operators $V$ and $P$. As a result, we have for $Z$,

$$Z = \mathrm{Tr}(P\exp[-\beta H(\mathbf{s}_{\mathrm{DM}})]) \tag{44}$$

The relation (44) is valid because the action of $\mathbf{s}_{\mathrm{DM}}$ on the state $|n\rangle$ for $n = 0, 1, \ldots, 2s$ leads only to the same states, i.e., the lower $2s+1$ states form an invariant subspace with respect to Dyson–Maleev spin operators $\mathbf{s}_{\mathrm{DM}}$.

If we are interested in the properties of the partition function (43) at low temperatures in the ferromagnetic or antiferromagnetic state, we can omit the projector $P$ in formula (44) because the contribution to the higher states $|n\rangle$ with $n > 2s$ to the trace (44) is exponentially small over the parameter $\beta J$, where $J$ is an exchange integral.[20] This discussion explains the correctness of using the Dyson–Maleev representation for the description of low-energy processes at low temperatures in ferromagnetics and antiferromagnetics.

A similar interpretation can be given for the representation (2) for the Hubbard operators $X^{ab}$. Let us consider the Gilbert space on every lattice site representing the direct product of a Gilbert space of a spin 1/2 and a fermion with a spin 1/2. The total number of states in that spin-hole Gilbert space is equal to eight: $|0, \sigma\rangle$, $|1, \sigma', \sigma\rangle$, $|2, \sigma\rangle$; here the first index represents the number of fermions, and $\sigma$, $\sigma' = \uparrow, \downarrow$ are spin projections. One can introduce the Fermi operators $h_\sigma^+$, $h_\sigma$,

$$|1, \sigma', \sigma\rangle = h_{\sigma'}^+ |0, \sigma\rangle, \qquad |0, \sigma\rangle = h_{\sigma'} |1, \sigma', \sigma\rangle \tag{45}$$

The singlet and triplet states can be formed from one-fermion states:

$$|s\rangle = (1/\sqrt{2})\,(|1\uparrow,\downarrow\rangle - |1\downarrow,\uparrow\rangle), \qquad |t1\rangle = |1\uparrow,\uparrow\rangle$$
$$|t0\rangle = (1/\sqrt{2}))\,|1\uparrow,\downarrow\rangle + |1\downarrow,\uparrow\rangle), \qquad |t-1\rangle = |1\downarrow,\downarrow\rangle \tag{46}$$

We can map the initial Gilbert space of the Hubbard model without two-fermion states into the spin-hole Gilbert space:

$$|0\rangle_h \Rightarrow |s\rangle, \qquad |1,\sigma\rangle_h \Rightarrow |0,\sigma\rangle \tag{47}$$

and obtain the following representation of the Hubbard operators $X^{ab}$ in terms of the holes $h_\sigma^+$, $h_\sigma$ and the spin-1/2 operators **s**:

$$X^{0\sigma} = (1/2\sqrt{2})[h^+(1-2\sigma\mathbf{s})]_{\sigma'}\,(1-N)\,\tau_{\sigma'\sigma}$$
$$X^{\sigma 0} = -(1/2\sqrt{2})\,\tau_{\sigma\sigma'}(1-N)_{\sigma'}\,[(1-2\sigma\mathbf{s})h]$$
$$N_h = X^{\uparrow\uparrow} + X^{\downarrow\downarrow} = 1 - N + D \tag{48}$$
$$X^{00} = (1/4)[N - 2D - 2(h^+\boldsymbol{\sigma}h)\mathbf{s}]$$
$$\mathbf{S} = \mathbf{s}(1-N+D)$$

Here

$$N = (h^+h), \qquad D = h_\uparrow^+ h_\uparrow h_\downarrow^+ h_\downarrow$$
$$\tau = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{49}$$

This representation is the direct operator identity: (1) the matrix elements, $X^{ab}$ operators (48), between physical states $|s\rangle$, $|0\sigma\rangle$ are the same as for the initial Hubbard operators $X^{ab}$; (2) the matrix elements between the unphysical states $|tm\rangle$, $|2\sigma\rangle$ are equal to zero; (3) the matrix elements between the physical states $|s\rangle$, $|0\sigma\rangle$ and the unphysical states $|tm\rangle$, $|2\sigma\rangle$ are equal to zero. The representation (48) for $X^{ab}$ certainly is Hermitian and does not require any constraints. If we compare the representation (48) with the initial expression of the Hubbard operators $X^{ab}$ in terms of the physical Fermi operators of electrons, we see that the number of electrons is close to unity, while the number of Fermi holes is small at a filling close to unity. The empty space without electrons can be imagined as the bound state of the Fermi hole and the spin 1/2 with the total spin equal to zero.

What is the connection between the non-Hermitian representation (2) and the Hermitian (48) for the Hubbard operators? One can check that if we perform a canonical transformation of the hole Fermi operators in (2),

$h_\sigma \to \sqrt{2}\, h_\sigma$, $h_\sigma^+ \to (1/\sqrt{2})\, h_\sigma^+$, then the matrix elements of the Hubbard operators in the representations (2) and (48) are the same between the physical states $|s\rangle$, $|0\sigma\rangle$. Moreover, the action of the Hubbard operators in the form (2) on the physical states $|s\rangle$, $|0\sigma\rangle$ does not lead to the unphysical states $|tm\rangle$, $|2\sigma\rangle$, i.e., the physical states form an invariant subspace over the algebra (2). The relation between the Hubbard operators $X_{\mathrm{H}}^{ab}$ of (48) and $X_{\mathrm{NH}}^{ab}$ of (2) can be represented in a form similar to (41):

$$X_{\mathrm{H}}^{ab} = PV^{-1}X_{\mathrm{NH}}^{ab}VP \tag{50}$$

Here $V$ is the generator of the canonical transformation determined in the physical subspace

$$V_{ss} = \sqrt{2}, \qquad V_{\sigma,\sigma'} = \delta_{\sigma,\sigma'}, \qquad V_{s,\sigma} = V_{\sigma,s} = 0 \tag{51}$$

and $P$ is the projector on the physical subspace

$$P = (1/4)(2-N)[2-N-2N(h^+\boldsymbol{\sigma}h)\mathbf{s}] \tag{52}$$

Naturally the operators $P$ and $V$ commute. The partition function of the Hubbard model can be represented a form similar to (43),

$$Z = \mathrm{Tr}(P\exp[-\beta H(X_{\mathrm{H}}^{ab})]) \tag{53}$$

and it can be transformed into a form similar to (44),

$$Z = \mathrm{Tr}(P\exp[-\beta H(X_{\mathrm{NH}}^{ab})]) \tag{54}$$

As the energies of the two-hole states and triplet states are essentially higher in the framework of the Hamiltonian (3), we can omit the projector $P$ in (53) at low temperatures and work with the Hamiltonian (3). This approximation is valid for a small number of holes insofar as the energy of the two-hole states at the lattice site and the triplet state are situated approximately at the center of the singlet hole bands.

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