IC/90/250

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

FUNCTIONAL INTEGRAL AND EFFECTIVE HAMILTONIAN t-J-V MODEL OF STRONGLY CORRELATED ELECTRON SYSTEM

V.I. Belinicher

and

M.V. Chertkov

INTERNATIONAL ATOMIC ENERGY AGENCY

UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

1990 MIRAMARE - TRIESTE

IC/90/250

International Atomic Energy Agency

and

United Nations Educational Scientific and Cultural Organization

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

FUNCTIONAL INTEGRAL AND EFFECTIVE HAMILTONIAN t-J-V MODEL OF STRONGLY CORRELATED ELECTRON SYSTEM *

V.I. Belinicher**

International Centre for Theoretical Physics, Trieste, Italy

and

M.V. Chertkov

Institute of Nuclear Physics, 630090 Novosibirsk, USSR.

ABSTRACT

The functional integral representation for the generating functional of t-J-V model is obtained. In the case close to half filling this functional integral representation reduces the conventional Hamiltonian of 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 one obtained one of the authors by different method. This Hamiltonian and its dynamical variables can be used for description of different magnetic phases of t-J-V model.

MIRAMARE – TRIESTE

September 1990

* To be submitted for publication.

** Permanent address: Institute of Semiconductor Physics, 630090 Novosibirsk, USSR.

1. INTRODUCTION

The problem of a theoretical description of the 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 the one of the most popular for HTSC explanation. 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 that exclude double occupancy $X_n^{ab} = |an\rangle\langle nb|$ where n is the lattice site and $|an\rangle = |0\,n\rangle, |\uparrow n\rangle, |\downarrow n\rangle$

$$H_{tJV} = \sum_{nn'}[t_{nn'} X_n^{\sigma 0} X_{n'}^{0\sigma} + (1/2) J_{nn'} \vec{S}_n \cdot \vec{S}_{n'} + (1/2) V_{nn'} N_n N_{n'}] - \\ - \sum_n \mu_\sigma X_n^{\sigma\sigma},\ \mu\sigma = \mu - \sigma\omega_0,\ T << \mu\ . \qquad (1)$$

where $N_n = X_{n\uparrow}^{\uparrow\uparrow} + X_n^{\downarrow\downarrow}$ is operator of the electron number; $\vec{S}_n$ is the spin operator $S_{nx} = (X_n^{\uparrow\downarrow} + X_n^{\downarrow\uparrow})/2$, $S_{ny} = (X_n^{\uparrow\downarrow} - X_n^{\downarrow\uparrow})/2i$, $S_{nz} = (X_n^{\uparrow\uparrow} - X_n^{\downarrow\downarrow})/2$; $\sigma = \pm 1/2 \equiv \uparrow, \downarrow$ is spin projection; $t_{nn'} = t_{n'n}$ is the electron hopping integral from lattice site n to the lattice site n'; $J_{nn'}$ is the spin exchange integral; $V_{nn'}$ describes Coulomb interaction of electrons on different lattice sites; μ_σ is the chemical potential depending on the spin projection σ and ω_0 is the precession frequency of electron spin in external magnetic field; T is a temperature which is supposed to be much less than usual chemical potential μ. That Hamiltonian follows [1],[2] from the usual Hubbard Hamiltonian in the limit $U >> t$ (where U is the constant of Coulomb repulsion on a lattice site) at the filling n close to one electron per lattice site $0 < 1 - n \equiv p << 1$ [4],[5]. In that case $J_{nn'} = 8|t_{nn'}|^2/U$.

In the paper [6] one of the authors (V.I.B.) has obtained the following representation for the Hubbard operators X^{ab} in terms of Fermi operators ψ_σ^+, ψ_σ and local spins $1/2\ \vec{s}$:

$$N = (\psi^+\psi) - 1,\ X^{00} = 1 - N,\ \vec{S} = \vec{s} + (\psi^+\vec{\sigma}\psi)/2\ , \\ X^{0\sigma} = \psi_\sigma,\ X^{\sigma 0} = [\psi^+(3/2 - (\psi^+\psi) + (\vec{s}\cdot\vec{\sigma}))]\sigma\ . \qquad (2)$$

That representation permits to reduce the Hamiltonian (1) H_{tJV} to the Hamiltonian of the Fermi hole operators

$$\mathcal{H}_{tJV} = \mathcal{H}_0 + \mathcal{H}_{int},\ \mathcal{H}_0 = \sum_{n\sigma} \mu^{-\sigma} h_{n\sigma}^+ h_{n\sigma} + \omega_0 \sum_n s_n^0\ , \\ \mathcal{H}_{int} = \sum_{nn'}[t_{nn'} h_{n'}^+(-1/2 - (h_n^+ h_n) + (\vec{s}_n\vec{\sigma}))h_n + (1/2) V_{nn'}(h_n^+ h_n)(h_{n'}^+ h_{n'}) + \\ + (1/2) J_{nn'}(\vec{s}_n + (1/2)(h_n^+\vec{\sigma}h_n))(\vec{s}_{n'} + (1/2)(h_{n'}^+\vec{\sigma}h_{n'}))\ , \\ h_n^+ = \tau\psi_n,\ h_n = \psi_n^+\tau,\ \tau = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\ . \qquad (3)$$

The representation (2) and the effective Hamiltonian (3) were obtained in the framework of the Wick's theorem for Hubbard operators. The representation (2) and the Hamiltonian (3) do not

represent direct operator identities. Some isomorphism of the form $A \rightarrow VAV^{-1}$ must exist which transforms the relation (2) and (3) in identities. In this point this representation differs from known slave bosons representation [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 calculation was produced for the simplest magnetic states: ferromagnetic, paramagnetic and antiferromagnetic in [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 $\rho << 1$ and the inverse number of neighbours $1/z << 1$.

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

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

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

where ϕ is random field with given statistical properties similar to representation (2) by its sense is not precise and contains some corrections.

In the present paper we shall construct the functional integral representation for the generating functional of the Hubbard operator temperture Green functions for the Hamiltonian (1) t-J-V model of the strongly correlated electron system. We shall show that the effective Hamiltonian (3) is the correct Hamiltonian for the filling closed to one electron per lattice site that is actual for HTSC compounds. We believe that 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 variational calculation nontrivial magnetic states.

2. FUNCTIONAL INTEGRAL REPRESENTATION

The generating functional fur the Hubbard temperture Green function may be represented in the form

$$Z(h) = T\tau[T\tau(\exp(-\beta H_{tJV} + \int_0^\beta h^{ab}(\tau) X^{ab} d\tau + \beta F))] \, , \tag{5}$$

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

functional (5) in the form

$$\begin{aligned} Z(h) = \iint \prod_{n\alpha\beta} \mathcal{D}\pi_n^\alpha \mathcal{D}\pi_n^\beta \mathcal{D}\pi_n^N \exp[(1/2)\int_0^\beta [\pi_n^\alpha A^{-1}_{\alpha\alpha'} t^{-1}_{nn'}, \pi^{\alpha'}_{n'} - \\ - \pi_n^\beta B^{-1}_{\beta\beta'} J^{-1}_{nn'} \pi^{\beta'}_{n'} - \pi_n^N V^{-1}_{nn'} \pi^N_{n'}] d\tau] \times \\ \times T\tau[T_\tau \exp \int_0^\beta (\bar{\pi}_n^\alpha(\tau) X_n^\alpha + \bar{\pi}_n^\beta(\tau) X_n^\beta + \bar{\pi}_n^N N_n) d\tau] \, , \end{aligned} \tag{6}$$

where $\pi_n^\alpha = (\pi_n^{0\uparrow}, \pi_n^{\uparrow 0}, \pi_n^{0\downarrow}, \pi_n^{\downarrow 0})$ are the Grassmann fields conjugated to corresponding Hubbard Fermi operators: $\pi_n^\beta = (\pi_n^{\downarrow\uparrow}, \pi_n^{\uparrow\downarrow}, \pi_n^z)$ are the complex fields conjugated to spin Hubbard Bose operators, π_n^N is conjugated to N_n; $\bar{\pi}_n^\alpha = \pi_n^\alpha + h_n^\alpha$ for $\alpha = 0\sigma, \sigma 0, \uparrow\downarrow, \downarrow\uparrow$, $\bar{\pi}_n^z = \pi^z + h_n^z - \omega_0$; $\bar{\pi}_n^N = \pi_n^N + h_n^N + \mu$. The numerical matrices $A_{\alpha\alpha'}, B_{\beta\beta'}$ as it follows from Hamiltonan (1) have form

$$A_{\alpha\alpha'} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad B_{\beta\beta'} = \frac{1}{2}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} . \tag{7}$$

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

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

Correspondingly the integration over Grassmann variables $\pi^{0\sigma}$, $\pi^{\sigma 0}$ can be understood as the integration over the four-dimensional Grassmann manifold determined in the eight-dimensional complex Grassmann manifold

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

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

$$A(\tau) = T\tau[\exp(\int_0^\tau (\pi^c(\tau') X^c + \pi^0(\tau')) d\tau')] \, , \tag{10}$$

where $c = 0\sigma, \sigma 0, \uparrow\downarrow, \downarrow\uparrow, z, n$ and the quantity $\pi^0(\tau)$ is introduced for convenience. The operator exponent $A(\tau)$ satisfied the following 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 the equation (11) when the conditions (8), (9) for $\pi^{\downarrow\uparrow}(\tau), \pi^{\uparrow\downarrow}(\tau), \pi^{0\sigma}(\tau), \pi^{\sigma 0}(\tau)$ are fulfilled. However, following the method of the papers [11] we can deform the surface (8) and (9) in a special manner and find the operator $A(\tau)$. To this end we shall use the following Ansatz for

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

In the formulae (10)-(12) and below the index of the lattice site n is omitted for the sake of simplicity of the expression. The expression (12) for $A(\tau)$ satisfies the initial condition $A(0) = 1$. After differentiation of $A(\tau)$ with respect τ and representation of the result in the form (11) one can get the system of equations connecting $\pi^c(\tau)$ and $\varphi^c(\tau)$

$$
\begin{aligned}
&\pi^{\uparrow 0} = \dot{\psi}^{\uparrow 0} - \pi^{\uparrow\downarrow}\psi^{\downarrow 0} - (\pi^n + \pi^z/2)\psi^{\uparrow 0} + \psi^{\uparrow 0}\psi^{0\downarrow}\psi^{\downarrow 0}\\
&\pi^{\downarrow 0} = \dot{\psi}^{\downarrow 0} - \pi^{\downarrow\uparrow}\psi^{\uparrow 0} - (\pi^n - \pi^z/2)\psi^{\downarrow 0} + \psi^{\downarrow 0}\psi^{0\uparrow}\psi^{\uparrow 0}\,,\\
&\pi^{0\uparrow} = \dot{\psi}^{0\uparrow}\,, \pi^{0\downarrow} = \dot{\psi}^{0\downarrow}\,,\\
&\pi^{\downarrow\uparrow} = \dot{\psi}^{\downarrow\uparrow} + \psi^{\downarrow 0}\psi^{0\uparrow}\,,\\
&\pi^{\uparrow\downarrow} = \dot{\psi}^{\uparrow\downarrow} - (\psi^z + \psi^{\uparrow\downarrow}\psi^{\downarrow\uparrow})\psi^{\uparrow\downarrow} + \psi^{\uparrow 0}\psi^{0\downarrow}\,,\\
&\pi^z = \dot{\psi}^z + 2\psi^{\downarrow\uparrow}\psi^{\uparrow\downarrow} + \psi^{\uparrow 0}\psi^{0\uparrow} - \psi^{\downarrow 0}\psi^{0\downarrow} \equiv \pi^{\uparrow\uparrow} - \pi^{\downarrow\downarrow}\,,\\
&\pi^n = \dot{\psi}^n + (1/2)\psi^{\sigma 0}\psi^{0\sigma} = (1/2)(\pi^{\uparrow\uparrow} + \pi^{\downarrow\downarrow})\,,\\
&\pi^0 = -\psi^{\sigma 0}\psi^{0\sigma}\,,
\end{aligned}
\tag{13}
$$

where the new field variables ψ are expressed in terms of the initial variables φ in the following way

$$
\begin{aligned}
&\psi^{0\uparrow} = (\dot{\varphi}^{0\uparrow} - \dot{\varphi}^{0\downarrow}\varphi^{\downarrow\uparrow})e^{-\varphi^{\uparrow\uparrow}}\,,\\
&\psi^{0\downarrow} = \dot{\varphi}^{0\downarrow}e^{-\varphi^{\downarrow\downarrow}} - (\dot{\varphi}^{0\uparrow} - \dot{\varphi}^{0\downarrow}\varphi^{\downarrow\uparrow})\varphi^{\uparrow\downarrow}e^{-\varphi^{\uparrow\uparrow}}\,,\\
&\psi^{\uparrow 0} = \varphi^{\uparrow 0}\,,\ \psi^{\downarrow 0} = \varphi^{\downarrow 0}\,,\ \psi^{\uparrow\downarrow} = \varphi^{\uparrow\downarrow}\,,\\
&\psi^{\downarrow\uparrow} = \dot{\varphi}^{\downarrow\uparrow}e^{-\varphi^z}\,,\ \varphi^z = \varphi^{\uparrow\uparrow} - \varphi^{\downarrow\downarrow}\,,\\
&\psi^z = \dot{\varphi}^z = \psi^{\uparrow\uparrow} - \psi^{\downarrow\downarrow}\\
&\psi^n = \dot{\varphi}^n = (\psi^{\uparrow\uparrow} + \psi^{\downarrow\downarrow})/2
\end{aligned}
\tag{14}
$$

The dependence π^0 on ψ represented separately in (13) can be considered as the definition. Producing the functional change of variables (13) one can calculate the T-exponent explicitly and obtained 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

$$
Re\psi_n^N(\tau) = Re\psi_n^z(\tau) = 0, \quad \psi^{\uparrow\downarrow}(\tau) = -(\psi^{\downarrow\uparrow}(\tau))^*, \quad \psi^{0\sigma} = (\psi^{\sigma 0}(\tau))^*\,. \tag{15}
$$

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 deformation the density of the generation 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 as integral over the finite number of Grassmann variables always exist. The discussion of convergence of the integral over the variables $\pi^{\uparrow\downarrow}(\tau), \pi^{\downarrow\uparrow})\tau)$ can be performed in the manner similar to [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 the complex field $\psi^{\uparrow\downarrow}(\tau)$ the standard boundary condition $\psi^{\uparrow\downarrow}(\beta) = \psi^{\uparrow\downarrow}(0)$ makes the transformation nonrevertible. We shall use the initial condition for the $\psi^{\uparrow\downarrow}(\tau)$ [12]:

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

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

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

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

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

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

$$
\hat{J} = \frac{\partial\pi}{\partial\psi} = \begin{pmatrix} J^{aa'} & J^{ak'} \\ J^{ka'} & J^{kk'} \end{pmatrix}, \quad \begin{matrix} a, a' = \uparrow 0\,, \downarrow 0\,, \\ k, k' = \uparrow\downarrow, \downarrow\uparrow, z, n, \end{matrix} \tag{19}
$$

here $J^{aa'}$ is the Fermi part of $\hat{J}$ matrix; $J^{kk'}$ is the Bose part and $J^{ak'}$ $J^{ka'}$ are the mixed parts of the $\hat{J}$ matrix. When the derivatives over Grassmann variables in (19) are computed they are as the right derivatives. Berezinian of the $\hat{J}$ matrix is calculated according to the following rule [15]

$$
Ber[\,j] = \det[\,J^{kk'} - J^{ka}(J^{aa'})^{-1}J^{a'k'}]\det(J^{aa'})^{-1}\,. \tag{20}
$$

The explicit form of Berzinian (20) depends on the method of regularization of the time derivatives in (13). Because the Bose part of $\hat{J}$ matrix $J^{kk'}$ practically coincides with the corresponding spin matrix of the paper [12] we shall use the same regularization

$$
\begin{aligned}
&\pi_\ell^{\downarrow\uparrow} = \psi_\ell^{\downarrow\uparrow} + (\psi^{\downarrow 0}\psi^{0\uparrow})_\ell\,,\\
&\pi_\ell^{\uparrow\downarrow} = \Delta_\ell^{-1} - (\psi_\ell^{\uparrow\downarrow} - \psi_{\ell-1}^{\uparrow\downarrow}) - (1/2)\psi_\ell^z(\psi_\ell^{\uparrow\downarrow} + \psi_{\ell-1}^{\uparrow\downarrow}) - (1/4)(\psi_\ell^{\uparrow\downarrow} + \psi_{\ell-1}^{\uparrow\downarrow})^2\psi_\ell^{\downarrow\uparrow} + (\psi^{\uparrow 0}\psi^{0\downarrow})_\ell\,,\\
&\pi_\ell^z = \psi_\ell^z + \psi_\ell^{\downarrow\uparrow}(\psi_\ell^{\uparrow\downarrow} + \psi_{\ell-1}^{\uparrow\downarrow})\,,
\end{aligned}
\tag{21}
$$

where the quantities ψ_ℓ^a, π_ℓ^a defined by the relation

$$
\psi_\ell^a \equiv \psi^a(\tau_\ell)\,,\ \pi_\ell^a \equiv \pi^a(\tau_\ell)\,,\ \tau_\ell = \ell\beta/L\,,\ \Delta = \beta/L\,,\ L \to \infty\,, \tag{22}
$$

here $1 \le \ell \le L$ and ℓ, $L$are integers. The $\det(J^{kk'})$ can be easily calculated:

$$
\det(J^{kk'}) = \lim_{\Delta\to 0}\pi_{\ell=1}^L\left(\frac{1}{\Delta} - \frac{1}{2}\psi_\ell^z\right) = \text{const}\,\exp\left(-\frac{1}{2}\int_0^\beta \psi^z(\tau)\,d\tau\right) \tag{23}
$$

For the computation $\det(J^{aa'})$ let us produce the regularization $\pi^{0\sigma}(\tau)$ in the following way

$$
\begin{aligned}
&\pi_\ell^{\sigma 0} = (\psi_\ell^{\sigma 0} - \psi^\sigma\psi_{\ell-1}^z)/\Delta - [\ ]_\ell^\sigma\cdot((1+K)\psi_{\ell-1}^{\sigma 0} - K\cdot\psi_\ell^{\sigma 0})\,,\\
&[\ ]_\ell^\sigma = [\psi_\ell^n + \sigma\psi_\ell^z + 2\sigma\psi_\ell^{\uparrow\downarrow}\psi_\ell^{\downarrow\uparrow} + \psi_\ell^{\sigma 0}\psi_\ell^{0\sigma}]
\end{aligned}
\tag{24}
$$

The crossing terms $J^{\sigma 0,-\sigma 0}$ gives small contribution at $\Delta \to 0$ in $\det(J^{\alpha\alpha'})$ and can be omitted. Thus

$$\det(J^{\alpha\alpha'}) = \det\left(\frac{\partial\pi^{\uparrow 0}}{\partial\psi^{\uparrow 0}}\right)\cdot\det\left(\frac{\partial\pi^{\downarrow 0}}{\partial\psi^{\downarrow 0}}\right) \tag{25}$$

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

$$\begin{pmatrix} \Delta^{-1}+[\ ]_1^\sigma K, & 0 & \cdot\cdot & 0 & \Delta^{-1}+[\ ]_1^\sigma(1+K) \\ -\Delta^{-1}-[\ ]_2^\sigma(1+K) & \Delta^{-1}+[\ ]_2^\sigma K & \cdot\cdot & 0 & 0 \\ \cdot & \cdot & \cdot\cdot & \cdot & 0 \\ \cdot & \cdot & \cdot\cdot & \cdot & \cdot \\ 0 & \cdot & \cdot\cdot & -\Delta^{-1}-[\ \ ]_L^\sigma(L+K) & \Delta^{-1}+[\ \ ]_L^\sigma K \end{pmatrix} \tag{26}$$

where $[\ \ ]_\ell^\sigma$ is defined in (24) and $\det(\partial\pi_\ell^{\sigma 0}/\partial\psi_\ell^{\sigma 0})$ is equal

$$\lim_{\Delta\to 0, L\to\infty}\left[\prod_{\ell=1}^{L}(\Delta^{-1}+K[\ ]_\ell^\sigma)+\prod_{\ell=1}^{L}(\Delta^{-1}+(1+K)[\ ]_\ell^\sigma)\right] =$$

$$= \text{const}\,(\exp(K\int_0^\beta[\ ]_\tau^\sigma d\tau)+\exp((1+K)\int_0^\beta[\ ]_\tau^\sigma d\tau))\ . \tag{27}$$

The $\det(J^{\alpha\alpha'})^{-1}$ is not equal to zero on the surface of integration and one can conclude that the initial and boundary conditions (16), (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), (17) we get

$$Tr[T\exp(\int_0^\beta(\pi^c(\tau)X^c+\pi^0(\tau))d\tau)] =$$

$$= 1+e^{\varphi^{\uparrow\uparrow}(\beta)}+(1+\varphi^{\uparrow\downarrow}(\beta)\varphi^{\downarrow\uparrow}(\beta))e^{\varphi^{\downarrow\downarrow}(\beta)} =$$

$$= 1+\exp(\int_0^\beta(\tilde\psi^n(\tau)+\frac{1}{2}\tilde\psi^s(\tau))d\tau)+\exp(\int_0^\beta(\tilde\psi^n(\tau)-\frac{1}{2}\tilde\psi^s(\tau))d\tau)+$$

$$+\exp(\int_0^\beta(\tilde\psi^n(\tau)-\frac{1}{2}\tilde\psi^s(\tau)d\tau)\psi^{\downarrow\uparrow}(\beta)\int_0^\beta\psi^{\uparrow\downarrow}(\tau)(\exp(\int_0^\tau\tilde\psi^s(\tau')d\tau'))d\tau \tag{28}$$

where $\tilde\psi^n(\tau)=\psi^n(\tau)-\mu$, $\tilde\psi^s(\tau)=\psi^s(\tau)+\omega_0$.

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

$$Z(h)=\iint\prod_{n,\tau}\mathcal{D}\pi_n^{\sigma 0}(\tau)\mathcal{D}\pi_n^{0\sigma}(\tau)\exp(\int_0^\beta(t_{nn'}^{-1}\pi_n^{\sigma 0}\pi_{n'}^{0\sigma}+\sum_n\pi_n^0)d\tau\times$$

$$\times Tr[T\exp(\int_0^\beta(\bar\pi_n^c X_n^c+\sum_n\pi_n^0)d\tau)]\ . \tag{29}$$

Let us set $\pi^{\uparrow\downarrow}, \pi^{\downarrow\uparrow}, \pi^s, \pi^n$ equal to zero in (13), (14) and perform the corresponding functional change of variables. The equation (13) can be considered in that case as the definition of $\psi^{\uparrow\downarrow}, \psi^{\downarrow\uparrow}$, ψ^s, ψ^n. Supposing $|\mu| >> T, \omega_0$ and $\mu < 0$ we get (23), (27) it is followed that for $K = 0$ and $\beta\mu \to -\infty$ Berezinian equal $\det(J^{\alpha\alpha'})^{-1}$ turns to constant. Substituting in (29) the expression for π (13) and making the linear change of the integration variables

$$\psi_n^{0\sigma}\to t_{nn'}\psi_{n'}^{0\sigma},\quad \psi_n^{\sigma 0}\to\psi_n^{\sigma 0} \tag{30}$$

we get the following representation for the generating functional

$$Z(h)=\iint\prod_n\mathcal{D}\psi_n^{0\sigma}\mathcal{D}\psi_n^{\sigma 0}\exp(-S)\ ,$$

$$S=\int_0^\beta[\dot\psi_n^{\sigma 0}\psi_n^{0\sigma}-\mu_\sigma\psi_n^{\sigma 0}\psi_n^{0\sigma}+t_{nn'}\psi_n^{\sigma 0}(1-\psi_n^{\sigma' 0}\psi_n^{0\sigma'})\psi_{n'}^{\sigma}+$$

$$+h_n^{0\sigma}\psi_n^{0\sigma}+h_n^{\sigma 0}\psi_n^{\sigma 0}(1-\psi_n^{\sigma' 0}\psi_n^{0\sigma'})]d\tau\ . \tag{31}$$

This generating functional leads to the 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 initial Hubbard Hamiltonian [16]. Such coincidence of the results may be obtained only for the regularization we have used and this in fact fixes it.

3. THE FILLING CLOSED TO UNIT AND REDUCTION TO THE SPIN PARTITION FUNCTION

In the case considering in that part of paper $\mu > 0$, $\mu >> T, \omega_0$ and $\beta\mu \to \infty$. One can verify that $\det(J^{\alpha\alpha'})^{-1} \sim e^{-\mu}$ and

$$Ber(\hat J)=\det(J^{kk'})/\det(J^{\alpha\alpha'})=\text{const}\,\exp(-\int_0^\beta(2\psi^n+\frac{1}{2}\psi^s-\psi^{\sigma 0}\psi^{0\sigma})d\tau)\ . \tag{32}$$

Substituting (32) into (20) and (20), (28) into (6) at $\beta\mu\to\infty$ one can verify that the integral over $\psi^n(\tau)$ 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

$$Z(h)=\iint_{nd}\prod\psi_n^d\exp(-\Gamma_\phi-\Gamma_a)\prod_n[1+\exp(-\int_0^\beta\psi_n^s(\tau)d\tau))\times$$

$$\times(1+\psi_n^{\downarrow\uparrow}(\beta)\int_0^\beta(\psi_n^{\downarrow\uparrow}(\tau)\exp(\int_0^\tau\psi_n^s(\tau')d\tau'))d\tau)] \tag{33}$$

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

$$\Gamma_\phi = \int_0^\beta [\psi_n^{\sigma 0} t_{nn'}^{-1} \psi_{n'}^{0\sigma} - \mu \psi_n^{\sigma 0} t_{nn'}^{-1} \psi_{n'}^{0\sigma} - \frac{1}{2}\psi_n^{\sigma 0}\psi_n^{0\sigma} -$$
$$- \frac{1}{2}\psi_n^{\sigma 0}\psi_n^{0\sigma}\psi_n^{\sigma' 0} t_{nn'}^{-1}\psi_{n'}^{0\sigma'} - \frac{1}{2}\vec{h}_n \psi_n^{\alpha 0}\sigma_{\alpha\beta} t_{nn'}^{-1}\psi_{n'}^{0\beta} +$$
$$+ \frac{1}{2}\psi_n^{\alpha 0}\vec{\sigma}_{\alpha\beta}\psi_n^{0\beta}\psi_n^{\gamma 0} t_{nn'}^{-1}\vec{\sigma}_{\gamma\delta}\psi_{n'}^{0\delta} -$$
$$- \frac{1}{8} J_{nn'}^{-1}(J_{mn} t_{mm'}^{-1}\psi_m^{\alpha 0}\vec{\sigma}_{\alpha\beta}\psi_\ell^{0\beta})(J_{\ell' n'} t_{\ell\ell'}^{-1}\psi_{\ell'}^{\alpha' 0}\vec{\sigma}_{\alpha'\beta'}\psi_{\ell'}^{0\beta'}) -$$
$$- \frac{1}{2} t_{nn'}^{-1} V_{mn} t_{mm'}^{-1}\psi_m^{\sigma 0}\psi_n^{0\sigma}\psi_{m'}^{\sigma' 0}\psi_{n'}^{0\sigma'} + V_0 t_{nn'}^{-1}\psi_n^{\sigma 0}\psi_{n'}^{0\sigma}] d\tau$$
$$\Gamma_s = \frac{1}{2}\int_0^\beta J_{nn'}^{-1}(\vec{\eta}_n + \vec{g}_n + \psi_n^{\alpha 0}\vec{\sigma}_{\alpha\beta}\psi_n^{0\beta} - \frac{1}{2} J_{n'n} t_{mm'}^{-1}\psi_m^{\alpha 0}\vec{\sigma}_{\alpha\beta}\psi_{m'}^{0\beta}) \times$$
$$\times (\vec{\eta}_{n'} + \vec{g}_{n'} + \psi_{n'}^{\alpha' 0}\vec{\sigma}_{\alpha'\beta'}\psi_{n'}^{0\beta'} - \frac{1}{2} J_{\ell n'} t_{\ell\ell'}^{-1}\psi_{\ell'}^{\alpha' 0}\vec{\sigma}_{\alpha'\beta'}\psi_{\ell'}^{0\beta'}) ,$$

where $\vec{g} = (h_x, h_y, h_z + \omega_0)$, $V_0 = \sum_{n'} V_{nn'}$ and vector $\vec{\eta}_n$ has following form:

$$\eta_{nx} = \eta_n^{\uparrow\downarrow} + \eta_n^{\downarrow\uparrow}, \ \eta_{ny} = i(\eta_n^{\uparrow\downarrow} - \eta_n^{\downarrow\uparrow}) ,$$
$$\eta_{nz} = \pi_n^z - \psi_n^{\uparrow 0}\psi_n^{0\uparrow} + \psi_n^{\downarrow 0}\psi_n^{0\downarrow}$$
$$\eta_n^{\downarrow\uparrow} = \psi_n^{\downarrow\uparrow} - \psi_n^{\downarrow 0}\psi_n^{0\uparrow} , \eta_n^{\uparrow\downarrow} = \pi_n^{\uparrow\downarrow} - \psi_n^{\uparrow 0}\psi_n^{0\downarrow} .$$

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

$$Z(h) = \int\int \prod_{n\sigma\tau} \mathcal{D}\psi_n^{0\sigma}(\tau)\mathcal{D}\psi_n^{\sigma 0}(\tau)\exp(-\Gamma_\phi)\{\prod_{n\tau}\mathcal{D}\psi_n^{\uparrow\downarrow}(\tau)\mathcal{D}\psi_n^{\downarrow\uparrow}(\tau)\mathcal{D}_n^{\psi}(\tau)\times$$

$$(\exp(-\Gamma_s)\prod_n[1 + (\exp(-\int_0^\beta \psi_n^z(\tau)d\tau))(1 + \psi_n^{\downarrow\uparrow}(\beta)\int_0^\beta(\psi_n^{\downarrow\uparrow}(\tau)\exp(\int_0^\tau \psi_n^z(\tau')d\tau'))d\tau)]\} \tag{34}$$

It follows from the formula (34) 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

$$\vec{h}_n(\tau) = \vec{h}_n(\tau) + \psi_n^{\alpha 0}\vec{\sigma}_{\alpha\beta}\psi_n^{0\beta} - \frac{1}{2} J_{\ell n} t_{\ell m}^{-1}\psi_\ell^{\alpha 0}\vec{\sigma}_{\alpha\beta}\psi_m^\beta , \tag{35}$$

and the generating functional can be rewritten in the following form

$$Z(h) = \iint \prod_{n\sigma\tau}\mathcal{D}\psi_n^{\sigma 0}(\tau)\mathcal{D}\psi_n^{0\sigma}(\tau)(\exp(-\Gamma_\phi))\times$$

$$\times Tr[T\exp(-\beta\mathcal{H}_{ex} - \int_0^\beta \vec{h}'_n(\tau)\vec{s}_n(\tau)d\tau)]_s , \tag{36}$$

where trace is taken over spin variables and

$$\mathcal{H}_{ex} = \frac{1}{2}\sum_{nn'} J_{nn'}\vec{s}_n \cdot \vec{s}_{n'} , \tag{37}$$

is the usual antiferromagnet Heisenberg Hamiltonian for spin 1/2. The substitution (30) for the Grassmann fields $\psi_n^{\sigma 0}, \psi_n^{0\sigma}$ reduces the generating functional (36) to the standard functional integral [15] with Hamiltonian explicitly coinciding with the Hamiltonian (3),

In conclusion let us remark that in general case of an arbitrary chemical potential the separation of the spin subsystem is not possible. Beside that 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.

Acknowledgments

The authors are grateful to I.V. Kolokolov for stimulating discussion and suggestion of the Ansatz (12). One of the authors (V.I.B.) would like to thank Professor Abdus Salam, the International Atomic Energy Agency and UNESCO for hospitality at the International Centre for Theoretical Physics, Trieste. He would also like to thank Professors G. Bascaran and Yu Lu for helpful discussions.

REFERENCES

1) P.W. Anderson, Science **235**, 1196 (1987);
Frontiers and Borderlines in Many-Particle Physics, (E. Fermi School, Varenna) Eds. R.A. Broglia and J.R. Schriefer, p.1 (North Holland, 1988).

2) T.M. Rice, "*Theories of HTSC - What have we learned in 3 years?*" ETH-TH/90-17.

3) G. Baskaran and P.W. Anderson, Phys. Rev. **B37**, 580 (1988).

4) F.C. Zhang and T.M. Rice, Phys. Rev. **B37**, 3759 (1988).

5) P.B. Wiegman, Phys. Rev. Lett. **60**, 821 (1988).

6) V.I. Belinicher, Phys. Lett. **A12**, 523 (1989);
"*Method of strong coupling on lattice spin systems and electron systems with strong correlations*", preprint 42 IFP USSR, Novosibirsk (1989)

7) P. Coleman, Phys. Rev. **B29**, 3035 (1984).

8) G. Kotliar and A. Ruckenstein, Phys. Rev. Lett. **57**, 1362 (1986).

9) M. Grilli and G. Kotliar, Phys.Rev. Lett. **64**, 1170 (1990).

10) D. Vollhard, "*Variational wave function for correlated lattice fermions*", Proceedings of the NATO Advanced Research Workshop on Interacting Electrons in Reduced Dimenions, Eds. D. Baeriswyl and D. Campbel.

11) I.V. Kolokolov, Phys. Lett **A114**, 99 (1986).

12) I.V. Kolokolov and E.V. Podivilov, JETP **95**, 211 (1989).

13) V.I. Belinicher and V.S.L'vov, JETP **86**, 967 (1984).

14) J. Hubbard, Phys. Lett. **3**, 77 (1959).

15) F.A. Bereszin, *Method of Second Quantization*, (Moscow, Nauka,1986).

16) V.M. Galitski, JETP **34**, 151 (1958).