

## DIAGRAMMATIC ANALYSIS OF THE HUBBARD MODEL: STATIONARY PROPERTY OF THE THERMODYNAMIC POTENTIAL

*V. A. Moskalenko*<sup>1,2</sup>, *L. A. Dohotaru*<sup>3</sup>

<sup>1</sup>Institute of Applied Physics, Moldova Academy of Sciences, Chisinau, Moldova

<sup>2</sup>Joint Institute for Nuclear Research, Dubna

<sup>3</sup>Technical University, Chisinau, Moldova

Diagrammatic approach proposed many years ago for strong correlated Hubbard model is developed for analyzing of the thermodynamic potential properties. The new exact relation between such renormalized quantities as thermodynamic potential, one-particle propagator, and correlation function is established. This relation contains additional integration of the one-particle propagator by the auxiliary constant. The vacuum skeleton diagrams constructed from irreducible Green's functions and tunneling propagator lines are determined, and special functional is introduced. The properties of such functional are investigated and its relation to the thermodynamic potential is established. The stationary properties of this functional with respect to first-order changing of the correlation function is demonstrated, and as a consequence the stationary properties of the thermodynamic potential are proved.

PACS: 71.27.+a; 71.10.Fd

The Hubbard model [1] is one of the most important models for the electron of solids which describes quantum mechanical hopping of electron between lattice sites and their short-ranged repulsive Coulomb interaction.

The Hamiltonian of Hubbard model is a sum of the two terms

$$H = H^0 + H', \quad (1)$$

where  $H^0$  is the atomic contribution, which contains the Coulomb interaction term  $U$  and local electron energy  $\bar{\epsilon}$  on the atom

$$H^0 = \sum_{\mathbf{i}} H_{\mathbf{i}}^0, \quad H_{\mathbf{i}}^0 = \sum_{\sigma} \epsilon n_{\mathbf{i}\sigma} + U n_{\mathbf{i}\uparrow} n_{\mathbf{i}\downarrow}, \quad \epsilon = \bar{\epsilon} - \mu, \quad n_{\mathbf{i}\sigma} = C_{\mathbf{i}\sigma}^+ C_{\mathbf{i}\sigma} \quad (2)$$

and hopping Hamiltonian

$$H' = \sum_{\mathbf{ij}} \sum_{\sigma} t(\mathbf{i} - \mathbf{j}) C_{\mathbf{i}\sigma}^+ C_{\mathbf{j}\sigma}, \quad t(\mathbf{i} - \mathbf{j}) = t^*(\mathbf{j} - \mathbf{i}), \quad t(0) = 0. \quad (3)$$

Here  $C_{i\sigma}^+$  ( $C_{i\sigma}$ ) are the creation (annihilation) electron operators with local site  $\mathbf{i}$  and spin  $\sigma$ . Because in the thermodynamic perturbation theory we shall use thermal averages in a grand canonical ensemble, we have added to the Hamiltonian (1) the term  $-\mu\hat{N}_e$

$$\hat{N}_e = \sum_{i\sigma} n_{i\sigma}, \quad (4)$$

where  $\mu$  is the chemical potential and  $\hat{N}_e$  is electron number operator. The quantities  $U$  and  $\hat{N}_e$  are the fundamental parameters of the model and because of large value of the Coulomb repulsion it is taken into account in zero approximation of our theory. The operator  $H'$ , which describes hopping of the electrons between sites of the crystal lattice, is regarded as a perturbation.

For investigating this model, new physical and mathematical concepts and techniques have been elaborated. A short and comprehensive reviews of the methods can be found in papers and books [2–7].

The other diagrammatic approach around the atomic limit also has been proposed for Hubbard model both in normal [8, 9] and in superconducting state [10]. This theory introduces the Generalized Wick Theorem (GWT) that uses cumulant expansion of the statistical average values for the products of the Fermion operators. The GWT takes into account the fact that Hamiltonian  $H^0$  is nonquadratic in fermion operators due to Coulomb interaction. This last circumstance is responsible for the appearance of the nonvanishing site cumulants called irreducible Green's functions. These new Green's functions take into account all the spin, charge and pairing fluctuations of the system.

In this paper, we shall develop the diagrammatic theory proposed before for Hubbard model [8, 9] with the aim to demonstrate the existence of the relation between renormalized quantities of thermodynamic potential and one-particle Green's function and also to prove the stationary properties of this potential.

Such a theorem was proved firstly by Luttinger and Ward [11] for uncorrelated systems by using the diagrammatic technique of weak coupling field theory.

The strong coupling diagram theory used by us needs new conceptions and new equations and they are used to prove stationary property of thermodynamic potential for strongly correlated systems. Such a proof has been already achieved for Anderson impurity model in paper [12].

We shall use the definition of the one-particle Matsubara Green's functions in interaction representation as in paper [8, 9]:

$$G(x|x') = - \langle TC_{\mathbf{x}\sigma}(\tau)\overline{C}_{\mathbf{x}'\sigma'}(\tau')U(\beta)\rangle_0^c, \quad (5)$$

where  $x$  stands for  $(\mathbf{x}, \sigma, \tau)$ , and index  $c$  for  $\langle \dots \rangle_0^c$  means the connected part of the diagrams which appear in the right-hand part of (5). We use the series expansion for the evolution operator  $U(\beta)$  with some generalization because we

introduce the auxiliary constant  $\lambda$  and use  $\lambda H'$  instead of  $H'$ :

$$U_\lambda(\beta) = T \exp \left( -\lambda \int_0^\beta H'(\tau) d\tau \right). \tag{6}$$

In the presence of this constant we shall use index  $\lambda$  as label for all dynamical quantities as  $G_\lambda(x|x')$  and so on. At the last stage of the calculations this constant will be put equal to one.

As has been proved in papers [8,9], propagator (5) has the diagrammatic representation depicted on Fig. 1. The irreducible Green's functions of order  $n$  are depicted with rectangles with  $2n$  vertices. The arrows which enter in the vertex point depict annihilation electrons, and those which go out — the created electrons.

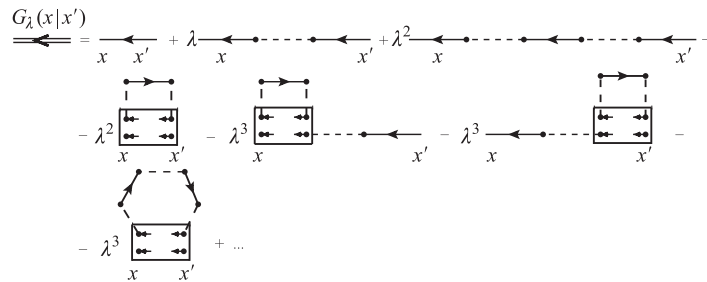


Fig. 1. First three orders of perturbation theory for one-particle propagator. The thin solid line depicts zero order propagator, thin dashed line depicts the tunneling matrix element. The rectangles depict irreducible two-particle Green's functions  $G_2^{(0)ir}$ , and points are the vertices of diagrams

In paper [8], we have introduced the notion of correlation function  $Z_\lambda(x|x')$  which is the sum of strongly connected diagrams containing irreducible Green's functions and related to a more convenient function  $\Lambda_\lambda(x|x') = G^0(x|x') + Z_\lambda(x|x')$ .

In Fig. 1, the fourth and seventh diagrams of the right-hand site belong to correlation function. Due to the fact that irreducible functions are local and tunneling matrix elements have the property  $t(\mathbf{x} - \mathbf{x}) = 0$ , in Fig.1 all the diagrams which contain self-locked tunneling elements are omitted.

As is seen from Fig. 1, the process of propagator renormalization is accompanied by the analogous process for tunneling matrix elements renormalization, and replacing of the instant quantity  $\lambda t(x - x') = \lambda t(\mathbf{x} - \mathbf{x}')\delta(\tau - \tau' - 0^+)$  by

dynamical one  $\tilde{T}_\lambda(x|x')$  is equal to

$$\tilde{T}_\lambda(x|x') = \lambda t(\mathbf{x} - \mathbf{x}') \delta(\tau - \tau' - 0^+) + \sum_{12} \lambda t(x-1) G_\lambda(1|2) \lambda t(2-x'), \quad (7)$$

which in the Fourier representation

$$\begin{aligned} t(\mathbf{x}) &= \frac{1}{N} \sum_{\mathbf{k}} \epsilon(\mathbf{k}) \exp(-i\mathbf{k}\mathbf{x}), \quad G_\lambda(x|x') = \\ &= \frac{1}{N} \sum_{\mathbf{k}} \frac{1}{\beta} \sum_{\omega_n} G_\lambda(\mathbf{k}|i\omega_n) \exp[-i\mathbf{k}(\mathbf{x} - \mathbf{x}') - i\omega_n(\tau - \tau')] \end{aligned}$$

has the form:

$$\tilde{T}_\lambda(\mathbf{k}|i\omega_n) \equiv \lambda T_\lambda(\mathbf{k}|i\omega_n) = \lambda \epsilon(\mathbf{k}) (1 + \lambda \epsilon(\mathbf{k}) G_\lambda(\mathbf{k}|i\omega_n)). \quad (8)$$

The renormalized tunneling matrix element  $T_\lambda$  really is tunneling Green's function and will be depicted as double dashed line.  $\tilde{T}_\lambda$  is represented by such double dashed line multiplied by  $\lambda$ .

Now we introduce the skeleton diagrams which contain only irreducible Green's functions and simple dashed lines without any renormalization. In such skeleton diagrams the thin dashed lines are replaced by double dashed lines with realizing the complete renormalization of dynamical quantities.

The skeleton diagrams for correlation  $\Lambda_\lambda$  function are depicted on Fig. 2.

$$\begin{aligned} \Lambda_\lambda(x|x') &= \overline{x \leftarrow x'} - \lambda \begin{array}{c} \overline{\leftarrow} \\ \boxed{\leftarrow \leftarrow} \\ \overline{\leftarrow} \end{array} - \frac{\lambda^2}{2} \begin{array}{c} \overline{\leftarrow \leftarrow} \\ \boxed{\leftarrow \leftarrow \leftarrow \leftarrow} \\ \overline{\leftarrow \leftarrow} \end{array} - \\ &- \frac{\lambda^3}{2} \begin{array}{c} \overline{\leftarrow \leftarrow \leftarrow} \\ \boxed{\leftarrow \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow} \\ \overline{\leftarrow \leftarrow \leftarrow} \end{array} - \frac{\lambda^3}{2} \begin{array}{c} \overline{\leftarrow \leftarrow \leftarrow \leftarrow} \\ \boxed{\leftarrow \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow \leftarrow} \\ \overline{\leftarrow \leftarrow \leftarrow \leftarrow} \end{array} + \dots \end{aligned}$$

Fig. 2. The skeleton diagrams for correlation function  $\Lambda_\lambda$ . Double-dashed lines depict the tunneling Green's functions  $T_\lambda$  and the rectangles depict the irreducible Green's functions

As was proved in papers [8, 9], the knowledge of function  $\Lambda_\lambda$  permits one to formulate the following Dyson-type equation for one-particle Green's function:

$$G_\lambda(k) = \frac{\Lambda_\lambda(k)}{1 - \lambda \epsilon(\mathbf{k}) \Lambda_\lambda(k)}. \quad (9)$$

Here  $k$  stands for  $(\mathbf{k}, i\omega_n)$  with odd Matsubara frequencies. Equations (8) and (9) give us the results

$$\tilde{T}_\lambda(k) = \lambda T_\lambda(k), \quad T_\lambda(k) = \frac{\epsilon(\mathbf{k})}{1 - \lambda \epsilon(\mathbf{k}) \Lambda_\lambda(k)}. \tag{10}$$

Equation (10) has the form of Dyson equation for tunneling Green's function, and the role of mass operator  $\Sigma_\lambda$  is carried out by correlation function multiplied by auxiliary constant  $\lambda$ :

$$\Sigma_\lambda(k) = \lambda \Lambda_\lambda(k). \tag{11}$$

The thermodynamic potential of the system is determined by the connected part of the mean value of the evolution operator [8, 9]

$$F = F_0 - \frac{1}{\beta} \langle U(\beta) \rangle_0^c. \tag{12}$$

Let us consider from the beginning a more general quantity

$$F(\lambda) = F_0 - \frac{1}{\beta} \langle U_\lambda(\beta) \rangle_0^c, \tag{13}$$

and put at the final stage  $\lambda = 1$ .

By using the perturbation theory we have obtained the first orders of diagrams for  $\langle U_\lambda(\beta) \rangle_0^c$ , depicted in Fig. 3.

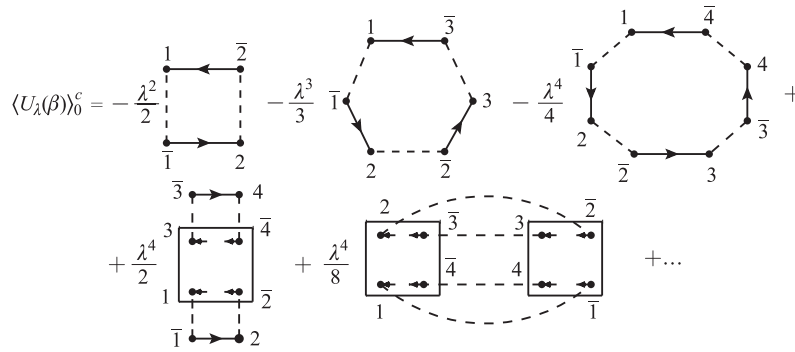


Fig. 3. The first four orders of perturbation theory for  $\langle U_\lambda(\beta) \rangle_0^c$

In order to obtain the better understanding of these diagrammatic contributions we examine the expression

$$\sum_{xx'} G_\lambda(x|x') \lambda t(\mathbf{x}' - \mathbf{x}) \delta(\tau - \tau' - 0^+) \delta_{\sigma\sigma'}, \tag{14}$$

where double repeated indices suppose summation and integration. Consequently (14) is equal to

$$\begin{aligned}
 -\beta \sum_{\mathbf{x}\mathbf{x}'} \sum_{\sigma} G_{\lambda\sigma}(\mathbf{x} - \mathbf{x}' | -0^+) \lambda t(\mathbf{x}' - \mathbf{x}) &= \\
 &= -\lambda \sum_{\mathbf{k}\sigma} \sum_{\omega_n} \epsilon(\mathbf{k}) G_{\lambda\sigma}(\mathbf{k} | i\omega_n) \exp(i\omega_n 0^+). \quad (15)
 \end{aligned}$$

Here we have carried out the integration by time.

In expression (15), the coefficients  $1/n$  before each diagram are absent, where  $n$  is the order of perturbation theory. These coefficients are present in Fig. 3. In order to restore these  $1/n$  coefficients in (15) and obtain the coincidence with  $\langle U_{\lambda}(\beta) \rangle_0^c$  series it is enough to integrate by  $\lambda$  in this expression and obtain:

$$-\sum_{\mathbf{x}\mathbf{x}'} \sum_{\sigma} \beta \int d\lambda t(\mathbf{x}' - \mathbf{x}) G_{\lambda\sigma}(\mathbf{x} - \mathbf{x}' | -0^+). \quad (16)$$

The expression (16) displayed in a diagrammatic representation coincides exactly with the mean value of the evolution operator:

$$\langle U_{\lambda}(\beta) \rangle_0^c = -\sum_{\mathbf{x}\mathbf{x}'} \beta t(\mathbf{x}' - \mathbf{x}) \int_0^{\lambda} d\lambda' G_{\lambda'\sigma}(\mathbf{x} - \mathbf{x}' | -0^+). \quad (17)$$

In Fourier representation we have

$$\langle U_{\lambda}(\beta) \rangle_0^c = -\int_0^{\lambda} d\lambda' \sum_{\mathbf{k}\sigma\omega_n} \epsilon(\mathbf{k}) G_{\lambda'\sigma}(\mathbf{k} | i\omega_n) \exp(i\omega_n 0^+). \quad (18)$$

From (13) and (18) we obtain

$$F(\lambda) = F_0 + \int_0^{\lambda} d\lambda' \sum_{\mathbf{k}\sigma} \frac{1}{\beta} \sum_{\omega_n} \epsilon(\mathbf{k}) G_{\lambda'\sigma}(\mathbf{k} | i\omega_n) \exp(i\omega_n 0^+). \quad (19)$$

Using the definition (12), the equation (19) can be written in the form:

$$F(\lambda) = F_0 + \int_0^{\lambda} \frac{d\lambda'}{\lambda'} \sum_{\mathbf{k}\sigma} \frac{1}{\beta} \sum_{\omega_n} T_{\lambda'}(k) \Sigma_{\lambda'}(k) \exp(i\omega_n 0^+). \quad (20)$$

From (20) we have

$$\lambda \frac{F(\lambda)}{d\lambda} = \sum_{\mathbf{k}\sigma} \frac{1}{\beta} \sum_{\omega_n} T_{\lambda}(k) \Sigma_{\lambda}(k) \exp(i\omega_n 0^+) = \frac{1}{\beta} \text{Tr}(T_{\lambda} \Sigma_{\lambda}). \quad (21)$$

In order to have a full system of equations we add to (20) the definition of the chemical potential of the system

$$N_e = \sum_{\mathbf{k}\sigma} \frac{1}{\beta} \sum_{\omega_n} G_{\sigma}(\mathbf{k}|i\omega_n) \exp(i\omega_n 0^+), \quad (22)$$

where  $N_e$  is the electron number.

Equation (19) establishes the relation between thermodynamic potential and renormalized one-particle propagator. This last quantity depends on the auxiliary parameter  $\lambda$ , and (19) contains an additional integration over it and is awkward because of that.

We shall obtain a more convenient equation for thermodynamic potential without such integration by  $\lambda$ . To do this, we shall introduce a special functional

$$Y(\lambda) = Y_1(\lambda) + Y'(\lambda), \quad (23)$$

where

$$Y_1(\lambda) = -\frac{1}{\beta} \sum_{\mathbf{k}, \sigma, \omega_n} [\ln(\epsilon(\mathbf{k}))\lambda\Lambda_{\lambda}(k) - 1 + T_{\lambda}(k)\lambda\Lambda_{\lambda}(k)] \exp(i\omega_n 0^+), \quad (24)$$

and  $Y'(\lambda)$  is constructed from skeleton diagrams without external lines and is depicted on Fig. 4.

$$Y'(\lambda) = -\frac{1}{\beta} \sum_{\mathbf{k}, \sigma} \sum_{\omega_n} \left\{ \lambda \left[ \text{diagram 1} \right] - \frac{\lambda^2}{2} \left[ \text{diagram 2} \right] - \frac{\lambda^3}{6} \left[ \text{diagram 3} \right] - \right. \\ \left. - \frac{\lambda^4}{24} \left[ \text{diagram 4} \right] - \frac{\lambda^4}{8} \left[ \text{diagram 5} \right] + \dots \right\}$$

Fig. 4. The simplest skeleton diagrams for functional  $Y'(\lambda)$ . Double-dashed lines are tunneling functions  $T_{\lambda}(k)$

We can prove the equations

$$\frac{\delta\beta Y_1(\lambda)}{\delta T_{\lambda}(k)} = -\lambda\Lambda_{\lambda}(k) = -\Sigma_{\lambda}(k), \quad \frac{\delta\beta Y'(\lambda)}{\delta T_{\lambda}(k)} = \lambda\Lambda_{\lambda}(k) = \Sigma_{\lambda}(k), \quad (25)$$

and, as a result, we obtain the stationary properties:

$$\frac{\delta \beta Y(\lambda)}{\delta T_\lambda(k)} = 0, \quad \frac{\delta Y(\lambda)}{\delta \Sigma_\lambda(k)} = 0. \quad (26)$$

We have established the equation

$$\lambda \frac{dF(\lambda)}{d\lambda} = \lambda \frac{dY(\lambda)}{d\lambda}, \quad (27)$$

and, as a consequence, we obtain

$$F(\lambda) = Y(\lambda) + \text{const.} \quad (28)$$

Because for  $\lambda = 0$  perturbation is absent and  $F(0) = F_0$ ,  $Y(0) = 0$ , we have

$$F(\lambda) = Y(\lambda) + F_0. \quad (29)$$

Now we can put  $\lambda = 1$  and obtain

$$F(1) = Y(1) + F_0 \quad (30)$$

with the stationary property

$$\frac{\delta F}{\delta \Sigma} = 0. \quad (31)$$

Two of us (V. A. M and L. A. D) would like to thank Professor N. M. Plakida and Dr. S. Cojocaru for a very helpful discussion.

#### REFERENCES

1. *Hubbard J.* // Proc. Roy. Soc. A. 1963. V. 276. P. 238; 1964. V. 277. P. 237; V. 281. P. 401.
2. *Fulde P.* Electron Correlations in Molecules and Solids. Berlin: Springer-Verlag, 1993.
3. *Hewson A. C.* The Kondo Problem to Heavy Fermions. Cambridge: Cambridge Univ. Press, 1993.
4. *Georges A. et al.* // Rev. Mod. Phys. 1996. V. 8. P. 13.
5. *Matsumoto H., Mancini F.* // Phys. Rev. B. 1997. V. 55. P. 2095.
6. *Avella A., Mancini F., Munzner R.* // Phys. Rev. B. 2001. V. 63. P. 245117.
7. *Kotliar G., Vollhardt D.* // Physics Today. 2004. V. 57. P. 53.
8. *Vladimir M. I., Moskalenko V. A.* // Teor. Mat. Fiz. 1990. V. 82. P. 428 (Theor. Math. Phys. 1990. V. 82. P. 301).



9. *Vakaru S. I., Vladimir M. I., Moskalenko V. A.* // Teor. Mat. Fiz. 1990. V. 85. P. 248 (Theor. Math. Phys. 1990. V. 85. P. 1185).
10. *Bogoliubov N. N., Moskalenko V. A.* // Teor. Mat. Fiz. 1991. V. 86. P. 16 (Theor. Math. Phys. 1991. V. 86. P. 10); Teor. Mat. Fiz. 1992. V. 92. P. 182 (Theor. Math. Phys. 1992. V. 92. P. 820); Dokl. AN SSSR. 1991. V. 316. P. 1107; JINR Rapid Commun. 1990. No. 44. P. 5.
11. *Luttinger J. M., Ward J. C.* // Phys. Rev. 1960. V. 118, No. 5. P. 1417.
12. *Moskalenko V. A. et al.* // Teor. Mat. Fiz. 2009. V. 159. P. 154 (Theor. Math. Phys. 2009. V. 159. P. 550); Cond. Mat. 2008. P. 914; arXiv:0804.1651.