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STRONG COUPLING APPROACH FOR STRONGLY CORRELATED ELECTRON SYSTEMS

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Підхід сильного зв'язку до розгляду електронних систем з сильними кореляціями

А. М. Швайка

Анотація. Запропонована схема в термінах теорії збурень за електронним переносом, яка ґрунтується на теоремі Віка для операторів Хаббарда. Діаґрамні ряди містять одновузлові вершини з'єднані лініями переносу. Показано, що для кожної вершини задача розпадається на підпростори з "вакуумними станами", які визначаються діаґональними операторами Хаббарда і дозволеними є тільки збудження відносно цих "вакуумних станів". Запропоновані правила побудови діаґрам. У границі безмежної розмірності простору повна допоміжна одновузлова задача точно розпадається на підпростори, що дозволяє побудувати аналітичний термодинамічно самоузгоджений підхід для моделі Хаббарда. Приведені деякі аналітичні результати для простих наближень коли отримується 2-х і 4-х полюсна структура для функцій Ґріна.

Strong Coupling Approach for Strongly Correlated Electron Systems

A. M. Shvaika

Abstract. A perturbation theory scheme in terms of electron hopping which is based on the Wick's theorem for Hubbard operators is developed. Diagrammatic series contain single-site vertices connected by hopping lines and it is shown that for each vertice the problem splits into the subspaces with "vacuum states" determined by the diagonal Hubbard operators and only excitations around these "vacuum states" are allowed. The rules to construct diagrams are proposed. In the limit of infinite spatial dimensions the total auxiliary single-site problem exactly splits into subspaces which allows to build an analytical thermodynamically consistent approach for Hubbard model. Some analytical results are given for simple approximations when 2-pole and 4-pole structure for Green's function is obtained.

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1. Introduction

Many unconventional properties (e.g. metal-insulator transition, electronic (anti)ferromagnetism) of the narrow band systems (transition metals and their compounds, some organic systems, high–T_c superconductors, etc.) can be explained only by proper treatment of the strong local electron correlations. The simplest models allowing for the electron correlations are a single-band Hubbard model with on-site repulsion U and hopping energy t and its strong coupling limit ($U \gg t$): $t-J$ model. Resent studies of the Hubbard type models connected mainly with the theory of high–T_c superconductivity and performed in the weak ($U \leq 4t$) and strong ($U \gg t$) coupling limits elucidate some important features of these models [1]. But still a lot of problems remains, especially for the $U \gg t$ case where there are no rigorous approaches.

Such approaches can be built using systematic perturbation expansion in terms of the electron hopping [2] using diagrammatic technique for Hubbard operators [3,4]. One of them was proposed in for the Hubbard ($U = \infty$ limit) and $t - J$ models [5,6]. The lack of such approach is connected with the concept of "hierarchy" system for Hubbard operators when the form of the diagrammatic series and final results strongly depend on the system of the pairing priority for Hubbard operators. On the other hand it is difficult to generalize it on the case of arbitrary U.

In last decade the essential achievements of the theory of the strongly correlated electron systems are connected with the development of the dynamical mean field theory (DMFT) proposed by Metzner and Vollhardt [7] for Hubbard model (see also Ref. [8] and references there in). DMFT is a nonperturbative scheme which allows to project Hubbard model on the single impurity Anderson model and is exact in the limit of infinite space dimensions ($d = \infty$). There are no restrictions on the U value within this theory and it turns out to be useful for intermediate coupling ($U \sim t$) for which it ensures the correct description of the metal-insulator phase transition and determines the region of the Fermi liquid behaviour of the electron subsystem. Moreover, some class of the binary alloy type models (e.g. Falicov-Kimball model) can be studied almost analytically within DMFT [9]. But in the case of Hubbard model, the treatment of the effective single impurity Anderson model is very complicated and mainly computer simulations (exact diagonalization of the finite sized systems or quantum Monte Carlo) are used which calls for the development of analytical approaches.

The first analitical approximation proposed for Hubbard model was a simple Hubbard-I approximation [10] (see Ref. [11] for its possible improvement) which is correct in the atomic ($t = 0$) and band ($U = 0$) limits but is inconsistent in the intermediate cases and can not describe metal-insulator transition. Hubbards alloy-analogy solution [12] (so-called Hubbard-III approximation) incorporates into the theory an electron scattering on the charge and spin fluctuations that allow to give qualitative description of the changes of the density of state at the metal-insulator transition point. Hubbard-I and Hubbard-III approximations introduces two types of particles (electrons moving between empty sites and electrons moving between sites occupied by an electrons of opposite spin) with the different energies which differ by U and form two Hubbard bands. Related schemes of the so-called 2-pole approximations [13,14] are also considered. However, in the recent QMC studies [15,16] it is clearly distinguished 4 bands in the spectral functions rather then the 2 bands predicted by the 2-pole approximations. Such 4-band structure is reproduced by the strong coupling expansion for the Hubbard model [16] in the one-dimensional case. Within other approches let us mention non-crossing approximation [17,18], Edwards-Hertz approach [19,20], iterative perturbation theory [21], alloy analogy based approaches [22–24] and linked cluster expansions [25,26] which are reliable in certain limits and the construction of the thermodynamically consistent theory still remains open.

The aim of this paper is to develop for Hubbard type models a rigorous perturbation theory scheme in terms of electron hopping which is based on the Wick's theorem for Hubbard operators [3,4] and is valid for arbitrary value of U ($U < \infty$) and does not depend on the "hierarchy" system for X operators. In the limit of infinite spatial dimensions these analytical scheme allows to build a self-consistent Kadanoff-Baym type theory [27] for Hubbard model and some analytical results are given for simple approximations. Falicov-Kimball model is also considered as an exactly soluble limit of Hubbard model.

2. Perturbation theory in terms of electron hopping

We consider lattice electronic system which can be described by the following statistical operator

$$\begin{aligned} \hat{\rho} &= e^{-\beta \hat{H}_0} \hat{\sigma}(\beta), \\ \hat{\sigma}(\beta) &= T \exp \left\{ - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{ij\sigma} t_{ij}^\sigma (\tau - \tau') a_{i\sigma}^\dagger(\tau) a_{j\sigma}(\tau') \right\}, \quad (1) \end{aligned}$$

where

$$\hat{H}_0 = \sum_i \hat{H}_i \tag{2}$$

is a sum of the single site contributions and for Hubbard model we must put

$$H_i = U n_{i\uparrow} n_{i\downarrow} - \mu(n_{i\uparrow} + n_{i\downarrow}) - h(n_{i\uparrow} - n_{i\downarrow}),$$
$$t_{ij}^{\sigma}(\tau - \tau') = t_{ij}\delta(\tau - \tau'). \tag{3}$$

In addition for Falicov-Kimball model we must also put

$$t_{ij}^{\sigma}(\tau - \tau') = \begin{cases} t_{ij}\delta(\tau - \tau') & \text{for } \sigma = \uparrow \\ 0 & \text{for } \sigma = \downarrow \end{cases}. \tag{4}$$

It is supposed that we know eigenvalues and eigenstates of the zero-order Hamiltonian (2)

$$H_i|i,p\rangle = \lambda_p|i,p\rangle$$

and one can introduce Hubbard operators

$$\hat{X}_i^{pq} = |i,p\rangle\langle i,q| \tag{5}$$

in terms of which zero-order Hamiltonian is diagonal

$$H_0 = \sum_i \sum_p \lambda_p \hat{X}_i^{pp}.$$

For Hubbard model we have four states $|i,p\rangle = |i, n_{i,\uparrow}, n_{i,\downarrow}\rangle$: $|i,0\rangle = |i,0,0\rangle$ (empty site), $|i,2\rangle = |i,1,1\rangle$ (double occupied site), $|i,\uparrow\rangle = |i,1,0\rangle$ and $|i,\downarrow\rangle = |i,0,1\rangle$ (sites with spin-up and spin-down electrons) with energies

$$\lambda_0 = 0, \quad \lambda_2 = U - 2\mu, \quad \lambda_\downarrow = h - \mu, \quad \lambda_\uparrow = -h - \mu. \tag{6}$$

Connection between the electron operators and Hubbard ones is following

$$n_{i\sigma} = X_i^{22} + X_i^{\sigma\sigma}; \quad a_{i\sigma} = X_i^{0\sigma} + \sigma X_i^{\bar{\sigma}2}. \tag{7}$$

Our aim is to calculate grand canonical potential functional

$$\Omega = -\frac{1}{\beta}\ln \mathrm{Sp}\,\hat{\rho} = \Omega_0 - \frac{1}{\beta}\ln\langle\hat{\sigma}(\beta)\rangle_0,$$
$$\Omega_0 = -\frac{1}{\beta}\ln \mathrm{Sp}\, e^{-\beta H_0}, \tag{8}$$

single-electron Green's functions

$$G_{ij\sigma}(\tau - \tau') = \langle T a_{i\sigma}^{\dagger}(\tau) a_{j\sigma}(\tau')\rangle = \frac{\delta\Omega}{\delta t_{ij}^{\sigma}(\tau - \tau')} \tag{9}$$

and mean values

$$n = \frac{1}{N}\sum_i \langle n_{i\uparrow} + n_{i\downarrow}\rangle = -\frac{1}{N}\frac{d\Omega}{d\mu},$$
$$m = \frac{1}{N}\sum_i \langle n_{i\uparrow} - n_{i\downarrow}\rangle = -\frac{1}{N}\frac{d\Omega}{dh}. \tag{10}$$

Here, $\langle\ldots\rangle = \frac{1}{Z}\mathrm{Sp}(\ldots\hat{\rho})$, $Z = \mathrm{Sp}\,\hat{\rho}$, or in interacting representation

$$\langle\ldots\rangle = \frac{1}{\langle\hat{\sigma}(\beta)\rangle_0}\langle\ldots\hat{\sigma}(\beta)\rangle_0 = \langle\ldots\hat{\sigma}(\beta)\rangle_{0c}, \tag{11}$$

where $\langle\ldots\rangle_0 = \frac{1}{Z}\mathrm{Sp}(\ldots e^{-\beta H_0})$; $Z_0 = \mathrm{Sp}\, e^{-\beta H_0}$.

We expand scattering matrix $\hat{\sigma}(\beta)$ in (1) into the series in terms of electron hopping and for $\langle\sigma(\beta)\rangle_0$ we obtain a series of terms which are products of the hopping integrals and averages of the electron creation and annihilation operators or, using (7), Hubbard operators which will be calculated with the use of the corresponding Wick's theorem.

Wick's theorem for Hubbard operators was formulated in Ref. [3] (see also Ref. [4] and references therein). For the Hubbard model we can define four diagonal Hubbard operators X^{pp} ($p = 0, 2, \downarrow, \uparrow$) which are of bosonic type, four annihilation $X^{0\downarrow}$, $X^{0\uparrow}$, $X^{\uparrow 2}$, $X^{\downarrow 2}$ and four conjugated creation fermionic operators, and two annihilation $X^{\downarrow\uparrow}$, X^{02} and two conjugated creation bosonic operators. The algebra of $\hat{X}$ operators is defined by the multiplication rule

$$X_i^{rs} X_i^{pq} = \delta_{sp} X_i^{rq}, \tag{12}$$

conserving condition

$$\sum_p X_i^{pp} = 1 \tag{13}$$

and commutation relations

$$[X_i^{rs}, X_j^{pq}]_{\pm} = \delta_{ij}(\delta_{sp} X_i^{rq} \pm \delta_{rq} X_i^{ps}), \tag{14}$$

where one must use anticommutator when both operators are of the fermionic type and commutator in all other cases. So, commutator or anticommutator of two Hubbard operators is not a $\mathbb{C}$ number but a new

Hubbard operator. Then the average of a T products of X operators can be evaluated by the consecutive pairing, with taking into account standard permutation rules for bosonic and fermionic operators, of all off-diagonal Hubbard operators X^{pq} according to the rule (Wick's theorem)

$$\overleftarrow{X_i^{rs}(\tau_1)X_0^{pq}}\ (\tau) = -\delta_{0i}g_{pq}(\tau-\tau_1)[X_i^{rs}(\tau_1), X_i^{pq}(\tau_1)]_{\pm} \qquad (15)$$

until we get the product of the diagonal Hubbard operators only. Here we introduce zero-order Green's function

$$g_{pq}(\tau-\tau_1) = e^{(\tau-\tau_1)\lambda_{pq}} \begin{cases} \pm n_{\pm}(\lambda_{pq}) & \tau > \tau_1 \\ \pm n_{\pm}(\lambda_{pq}) - 1 & \tau < \tau_1 \end{cases}, \qquad (16)$$

where $\lambda_{pq} = \lambda_p - \lambda_q$ and $n_{\pm}(\lambda) = \frac{1}{e^{\beta\lambda}\pm 1}$, and its Fourier transform is equal

$$g_{pq}(\omega_n) = \frac{1}{i\omega_n - \lambda_{pq}}. \qquad (17)$$

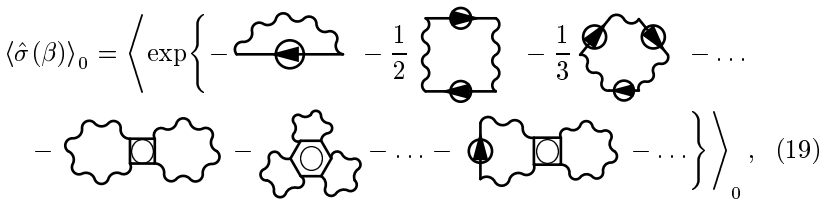
In particular, for Hubbard model one can introduce following pairings:

$$\begin{aligned}
\overleftarrow{a_{i\sigma}(\tau_1)a_{j\sigma}^{\dagger}}\ (\tau) &= -\delta_{ij}\{g_{\sigma 0}(\tau-\tau_1)(X_i^{00}(\tau_1) + X_i^{\sigma\sigma}(\tau_1)) \\
&\quad + g_{2\bar\sigma}(\tau-\tau_1)(X_i^{22}(\tau_1) + X_i^{\bar\sigma\bar\sigma}(\tau_1))\}, \\
\overleftarrow{a_{i\bar\sigma}(\tau_1)a_{j\sigma}^{\dagger}}\ (\tau) &= -\delta_{ij}f_{\sigma}(\tau-\tau_1)X_i^{\sigma\bar\sigma}(\tau_1), \\
\overleftarrow{a_{i\bar\sigma}^{\dagger}(\tau_1)a_{j\sigma}^{\dagger}}\ (\tau) &= \delta_{ij}f_{\sigma}(\tau-\tau_1)\cdot\sigma\cdot X_i^{20}(\tau_1), \\
\overleftarrow{a_{i\bar\sigma}^{\dagger}(\tau_1)X_j^{\sigma\bar\sigma}}\ (\tau) &= \delta_{ij}g_{\sigma\bar\sigma}(\tau-\tau_1)a_{i\sigma}^{\dagger}(\tau_1), \\
\overleftarrow{a_{i\sigma}(\tau_1)X_j^{\sigma\bar\sigma}}\ (\tau) &= -\delta_{ij}g_{\sigma\bar\sigma}(\tau-\tau_1)a_{i\bar\sigma}(\tau_1), \\
\overleftarrow{a_{i\sigma}(\tau_1)X_j^{20}}\ (\tau) &= -\delta_{ij}g_{20}(\tau-\tau_1)\cdot\sigma\cdot a_{i\bar\sigma}^{\dagger}(\tau_1),
\end{aligned} \qquad (18)$$

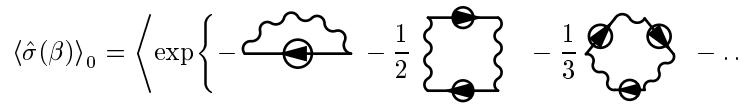
where

$$f_{\sigma}(\omega_n) \equiv g_{\sigma 0}(\omega_n) - g_{2\bar\sigma}(\omega_n) = -Ug_{\sigma 0}(\omega_n)g_{2\bar\sigma}(\omega_n).$$

Applying such pairing procedure to the expansion of $\langle\hat\sigma(\beta)\rangle_0$ we get the following diagrammatic representation:

$\langle\hat\sigma(\beta)\rangle_0 =$  (19)

where arrows denote zero order Green's functions (17), wavy lines denote hopping integrals and $\square, \ldots$ stay for some complicated "n-vertices" which for such type perturbation expansion are an irreducible many-particle single-site Green's functions calculated with single-site Hamiltonian (3). Each vertice (Green's function) is multiplied by a diagonal Hubbard operator denoted by a circle and one gets an expression with averages of a products of diagonal Hubbard operators. For Falicov-Kimball model expression (19) reduces and contains only single loop contributions

$\langle\hat\sigma(\beta)\rangle_0 =$  (20)

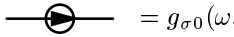
where $= \frac{\hat P_i^{\pm}}{i\omega_n + \mu^* \mp \frac{U}{2}}$; $\hat P_i^{+} = \hat n_{i\downarrow}$; $\hat P^{-} = 1 - \hat n_{i\downarrow}$ and by introducing pseudospin variables $S_i^z = \frac{1}{2}(\hat P_i^{+} - \hat P_i^{-})$ one can transform Falicov-Kimball model to an Ising type model with the effective multi-site retarded pseudospin interactions.

So, after applying Wick's theorem our problem splits into two ones:

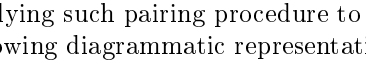
1. calculation of the irreducible many-particle Green's functions (vertices) in order to construct expression (19) and
2. calculation of the averages of the products of diagonal Hubbard operators and summing up of the resulting series.

3. Irreducible many-particle Green's functions

For Hubbard model by applying Wick's theorem for X operators one gets for 2-vertice

 $= g_{\sigma 0}(\omega_n)(\hat X_i^{\sigma\sigma} + \hat X_i^{00}) + g_{2\bar\sigma}(\omega_n)(\hat X_i^{22} + \hat X_i^{\bar\sigma\bar\sigma}),$ (21)

for 4-vertice

 $= \hat\Lambda_{i\sigma\bar\sigma}^{(4)}(\omega_n, \omega_{n+m}, \omega_{n'+m}, \omega_{n'})$ (22)

$$\begin{aligned}
&= \hat X_i^{00} g_{\sigma 0}(\omega_n)g_{\sigma 0}(\omega_{n+m})\left(U + U^2 g_{20}(\omega_{n+n'+m})\right) g_{\bar\sigma 0}(\omega_{n'})g_{\bar\sigma 0}(\omega_{n'+m}) \\
&+ \hat X_i^{22} g_{2\bar\sigma}(\omega_n)g_{2\bar\sigma}(\omega_{n+m})\left(U - U^2 g_{20}(\omega_{n+n'+m})\right) g_{2\sigma}(\omega_{n'})g_{2\sigma}(\omega_{n'+m}) \\
&+ \hat X_i^{\sigma\sigma} g_{\sigma 0}(\omega_n)g_{\sigma 0}(\omega_{n+m})\left(U + U^2 g_{\sigma\bar\sigma}(\omega_{n-n'})\right) g_{2\sigma}(\omega_{n'})g_{2\sigma}(\omega_{n'+m}) \\
&+ \hat X_i^{\bar\sigma\bar\sigma} g_{2\bar\sigma}(\omega_n)g_{2\bar\sigma}(\omega_{n+m})\left(U - U^2 g_{\sigma\bar\sigma}(\omega_{n-n'})\right) g_{\bar\sigma 0}(\omega_{n'})g_{\bar\sigma 0}(\omega_{n'+m}),
\end{aligned}$$

$$\hat\Lambda_{i\sigma\sigma}^{(4)}(\omega_n, \omega_{n+m}, \omega_{n'+m}, \omega_{n'}) \equiv 0$$

and so on. Expressions (21), (22) and for the vertices of higher order possess one significant feature. They decompose into four terms with different diagonal Hubbard operators X^{pp}, which project our single site problem on certain "vacuum" states (subspaces), and zero-order Green's functions, which describe all possible excitations and scattering processes around these "vacuum" states (subspaces): i.e. creation and annihilation of single electrons and of the doublon (pair of electrons with opposite spins) for subspaces $p = 0$ and $p = 2$ and creation and annihilation of single electrons with appropriate spin orientation and of the magnon (spin flip) for subspaces $p =\uparrow$ and $p =\downarrow$.

In compact form expressions (21) and (22) can be written as

$$= \sum_p \hat{X}_i^{pp} g_{\sigma(p)}(\omega_n) \tag{23}$$

and

$$= \sum_p \hat{X}_i^{pp} \times g_{\sigma(p)}(\omega_n) g_{\sigma(p)}(\omega_{n+m}) \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_l|\omega_m) g_{\bar{\sigma}(p)}(\omega_l) g_{\bar{\sigma}(p)}(\omega_{l+m}), \tag{24}$$

where

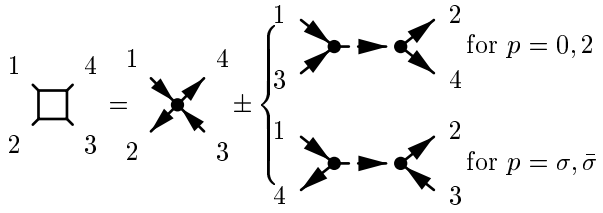
$$g_{\sigma(p)}(\omega_n) = \begin{cases} g_{\sigma 0}(\omega_n) & \text{for } p = 0, \sigma \\ g_{2\bar{\sigma}}(\omega_n) & \text{for } p = \bar{\sigma}, 2 \end{cases}. \tag{25}$$

Here

$$\widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_l|\omega_m) = \begin{cases} U(1 \pm U g_{20}(\omega_{n+l+m})) & \text{for } p = 0, 2 \\ U(1 \pm U g_{\sigma\bar{\sigma}}(\omega_{n-l})) & \text{for } p = \sigma, \bar{\sigma} \end{cases}, \tag{26}$$

$$\widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_l|\omega_m) = \widetilde{U}_{\bar{\sigma}\sigma(p)}(\omega_l, \omega_n|\omega_m)$$

is a renormalized Coulombic interaction in the subspaces, or in diagrammatic notations



, (27)

where dots denote Coulombic correlation energy $U = \lambda_2 + \lambda_0 - \lambda_\uparrow - \lambda_\downarrow$ and dashed arrows denote bosonic zero-order Green's functions: doublon $g_{20}(\omega_m)$ or magnon $g_{\sigma\bar{\sigma}}(\omega_m)$.

For 6-vertex one can get

$$\hat{\Lambda}^{(6)}_{i\sigma\sigma\sigma}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) \equiv 0,$$

$$\begin{aligned}
&\hat{\Lambda}^{(6)}_{i\sigma\bar{\sigma}\bar{\sigma}}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) = \delta(\omega_n - \omega_{n_1} + \omega_{n_2} - \omega_{n_3} + \omega_{n_4} - \omega_{n_5}) \\
&\times \sum_p \hat{X}_i^{pp} g_{\sigma(p)}(\omega_n) g_{\sigma(p)}(\omega_{n_1}) g_{\bar{\sigma}(p)}(\omega_{n_2}) g_{\bar{\sigma}(p)}(\omega_{n_3}) g_{\bar{\sigma}(p)}(\omega_{n_4}) g_{\bar{\sigma}(p)}(\omega_{n_5}) \\
&\times \Big\{ \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_3}|\omega_{n_2 - n_3}) g_{\bar{\sigma}(p)}(\omega_{n+n_2-n_3}) \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_4}|\omega_{n_5 - n_4}) \\
&- \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_5}|\omega_{n_2 - n_5}) g_{\bar{\sigma}(p)}(\omega_{n+n_2-n_5}) \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_4}|\omega_{n_3 - n_4}) \\
&- \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_3}|\omega_{n_4 - n_3}) g_{\bar{\sigma}(p)}(\omega_{n+n_4-n_3}) \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_2}|\omega_{n_5 - n_2}) \\
&+ \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n, \omega_{n_5}|\omega_{n_4 - n_5}) g_{\bar{\sigma}(p)}(\omega_{n+n_4-n_5}) \widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_{n_1}, \omega_{n_2}|\omega_{n_3 - n_2}) \\
&+ \Upsilon_{\sigma\bar{\sigma}\bar{\sigma}(p)}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) \Big\},
\end{aligned} \tag{28}$$

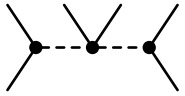
where

$$\begin{aligned}
&\Upsilon_{\sigma\bar{\sigma}\bar{\sigma}(p)}(\omega_n, \omega_{n_1}, \omega_{n_2}, \omega_{n_3}, \omega_{n_4}, \omega_{n_5}) \\
&= \begin{cases} \pm U^3 \left(g_{20}(\omega_{n+n_2}) - g_{20}(\omega_{n+n_4})\right) \left(g_{20}(\omega_{n_1+n_3}) - g_{20}(\omega_{n_1+n_5})\right) \\ \qquad\qquad \text{for } p = 0, 2 \\ \pm U^3 \left(g_{20}(\omega_{n-n_3}) - g_{20}(\omega_{n-n_5})\right) \left(g_{20}(\omega_{n_1-n_2}) - g_{20}(\omega_{n_1-n_4})\right) \\ \qquad\qquad \text{for } p = \sigma, \bar{\sigma} \end{cases}.
\end{aligned} \tag{29}$$

In expression (28) the contributions of the first four terms in braces can be presented by the following diagrams

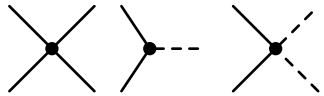
(30)

with the internal vertices of the same type as in (27), whereas the contribution of the last term can be presented diagrammatically as



(31)

So, we can introduce primitive vertices[1]



(32)

by which one can construct all n-vertices in expansion (19) according to the following rules:

1. n-vertices are constructed by the diagonal Hubbard operator X^{pp} and zero-order fermionic and bosonic lines connected by primitive vertices (32) specific for each subspace p.
2. External lines of n-vertices must be of the fermionic type.
3. Diagrams with the loops formed by zero-order fermionic and bosonic Green's functions are not allowed because they are already included into the formalism, e.g.

Diagrams (27), (30) and (31) topologically are truncated Bethe-lattices constructed by the primitive vertices (32) and can be treated as some generalization of the Hubbard stars [28,29] in the thermodynamical perturbation theory.

It should be noted that each n-vertice contains Coulombic interaction U as in primitive vertices (32) (denoted by dots) as in the denominators of zero-order Green's functions (17). In the $U \to \infty$ limit each term in expressions for n-vertices can diverge but total vertice possesses finite $U \to \infty$ limit when diagrammatic series of Ref. [5] are reproduced.

Second problem of calculation of the averages of diagonal X operators is more complicated. One of the ways to solve it is to use semi-invariant (cumulant) expansions as it was done in Refs. [5] and [6] for $U = \infty$ limit. Another way is to consider $d = \infty$ limit where new simplifications appear.

4. Dynamical mean-field theory

Within the frames of the considered perturbation theory in terms of electron hopping a single-electron Green's function (9) can be presented

[1] For n-vertices of higher order a new primitive vertices can appear but we do not check this due to the rapid increase of the algebraic calculations with the increase of n.

in a form

$$G_\sigma(\omega_n, \boldsymbol{k}) = \frac{1}{\Xi_\sigma^{-1}(\omega_n, \boldsymbol{k}) - t_{\boldsymbol{k}}}, \tag{33}$$

where we introduce an irreducible part $\Xi_\sigma(\omega_n, \boldsymbol{k})$ of Green's function which, in general, is not local. In the case of infinite dimensions $d \to \infty$ one should scale hopping integral according to

$$t_{ij} \to \frac{t_{ij}}{\sqrt{d}}$$

in order to obtain finite density of states and it was shown by Metzner in his pioneer work [25] that in this limit the irreducible part become local

$$\Xi_{ij\sigma}(\tau - \tau') = \delta_{ij}\Xi_\sigma(\tau - \tau') \quad \text{or} \quad \Xi_\sigma(\omega_n, \boldsymbol{k}) = \Xi_\sigma(\omega_n) \tag{34}$$

and such site-diagonal function, as it was shown by Brandt and Mielsch [9], can be calculated by mapping the infinite-dimensional lattice problem (1) with $t_{ij}^\sigma(\tau - \tau') = \frac{1}{\sqrt{d}} t_{ij}$ on the atomic model with auxiliary Kadanoff-Baym field

$$t_{ij}^\sigma(\tau - \tau') = \delta_{ij} J_\sigma(\tau - \tau'), \tag{35}$$

which has to be self-consistently determined from the condition that the same function $\Xi_\sigma(\omega_n)$ defines Green's functions for the lattice and atomic limit. The self-consistent set of equations for $\Xi_\sigma(\omega_n)$ and $J_\sigma(\omega_n)$ (e.g. see Ref. [8] and references therein) is following

$$\frac{1}{N}\sum_{\boldsymbol{k}} \frac{1}{\Xi_\sigma^{-1}(\omega_n) - t_{\boldsymbol{k}}} = \frac{1}{\Xi_\sigma^{-1}(\omega_n) - J_\sigma(\omega_n)} = G_\sigma^{(a)}(\omega_n, \{J_\sigma(\omega_n)\}), \tag{36}$$

where $G_\sigma^{(a)}(\omega_n, \{J_\sigma(\omega_n)\})$ is Green's function for atomic limit (35).

Grand canonical potential for lattice is connected with the one for atomic limit by expression [9]

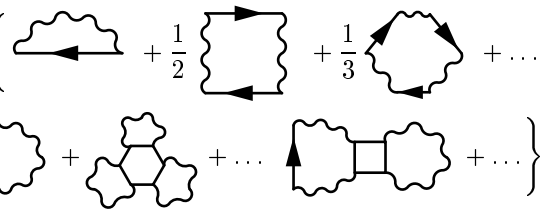
$$\frac{\Omega}{N} = \Omega_a - \frac{1}{\beta}\sum_{n\sigma}\left\{\ln G_\sigma^{(a)}(\omega_n) - \frac{1}{N}\sum_{\boldsymbol{k}} \ln G_\sigma(\omega_n, \boldsymbol{k})\right\}. \tag{37}$$

On the other hand, we can write for the grand canonical potential for atomic limit Ω_a the same expansion as in (19) but now we have averages of the products of diagonal X operators at the same site. According to (12) we can multiply them and reduce their product to a single X operator which can be taken outside of the brackets and exponent in

(19) and its average is equal $\langle X^{pp}\rangle_0 = \frac{e^{-\beta\lambda_p}}{\sum_q e^{-\beta\lambda_q}}$. Finally, for the grand canonical potential for atomic limit we get

$$\Omega_a = -\frac{1}{\beta}\ln\sum_p e^{-\beta\Omega_{(p)}}, \tag{38}$$

where $\Omega_{(p)}$ are "grand canonical potentials" for subspaces

$\Omega_{(p)} = \lambda_p +$  (39)

Now we can find single-electron Green's function for atomic limit by

$$G^{(a)}_\sigma(\tau-\tau') = \frac{\delta\Omega_a}{\delta J_\sigma(\tau-\tau')} = \sum_p w_p G_{\sigma(p)}(\tau-\tau'), \tag{40}$$

where

$$G_{\sigma(p)}(\tau-\tau') = \frac{\delta\Omega_{(p)}}{\delta J_\sigma(\tau-\tau')} \tag{41}$$

are single-electron Green's functions for the subspaces characterized by "statistical weights"

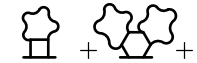
$$w_p = \frac{e^{-\beta\Omega_{(p)}}}{\sum\limits_q e^{-\beta\Omega_{(q)}}} \tag{42}$$

and our single-site atomic problem exactly (naturally) splits into four subspaces $p = 0, 2, \downarrow, \uparrow$.

We can introduce irreducible parts of Green's functions in subspaces $\Xi_{\sigma(p)}(\omega_n)$ by

$$G_{\sigma(p)}(\omega_n) = \frac{1}{\Xi^{-1}_{\sigma(p)}(\omega_n) - J_\sigma(\omega_n)}, \tag{43}$$

where

$\Xi_{\sigma(p)}(\omega_n) =$ 

According to the rules of the introduced diagrammatic technique n-vertices are terminated by the fermionic Green's functions (see (27), (30)

and (31)) and this allows to write a Dayson equation for irreducible parts and to introduce a self-energy

$$\Xi^{-1}_{\sigma(p)}(\omega_n) = g^{-1}_{\sigma(p)}(\omega_n) - \Sigma_{\sigma(p)}(\omega_n), \tag{44}$$

where self-energy $\Sigma_{\sigma(p)}(\omega_n)$ depends on hopping integral $J_{\sigma'}(\omega_{n'})$ only through quantities

$$\begin{aligned} &G_{\sigma'(p)}(\omega_{n'}) - \Xi_{\sigma'(p)}(\omega_{n'}) \\ &\equiv \Xi^2_{\sigma'(p)}(\omega_{n'})\left\{J_{\sigma'}(\omega_{n'}) + J_{\sigma'}(\omega_{n'})\Xi_{\sigma'(p)}(\omega_{n'})J_{\sigma'}(\omega_{n'}) + \cdots\right\}. \end{aligned} \tag{45}$$

Now, one can reconstruct expressions for grand canonical potentials $\Omega_{(p)}$ in subspaces from the known structure of Green's functions. To do this, we scale hopping integral

$$J_\sigma(\omega_n) \to \alpha J_\sigma(\omega_n), \qquad \alpha \in [0,1]$$

which allows to define grand canonical potential as

$$\Omega_{(p)} = \lambda_p + \int_0^1 d\alpha \frac{1}{\beta}\sum_{n\sigma} J_\sigma(\omega_n) G_{\sigma(p)}(\omega_n,\alpha) \tag{46}$$

and after some transformations one can get

$$\begin{aligned} \Omega_{(p)} &= \lambda_p - \frac{1}{\beta}\sum_{n\sigma}\ln\frac{\Xi^{-1}_{\sigma(p)}(\omega_n) - J_\sigma(\omega_n)}{\Xi^{-1}_{\sigma(p)}(\omega_n)} \\ &\quad -\frac{1}{\beta}\sum_{n\sigma}\int_0^1 d\alpha \frac{d\Sigma_{\sigma(p)}(\omega_n,\alpha)}{d\alpha}\left(G_{\sigma(p)}(\omega_n,\alpha) - \Xi_{\sigma(p)}(\omega_n,\alpha)\right), \end{aligned} \tag{47}$$

where $\Sigma_{\sigma(p)}(\omega_n,\alpha)$ depends on α only through quantities $\{G_{\sigma'(p)}(\omega_{n'},\alpha) - \Xi_{\sigma(p)}(\omega_{n'},\alpha)\}$. So, if one find or construct self-energy $\Sigma_{\sigma(p)}(\omega_n)$ he can find Green's functions and grand canonical potentials for subspaces and, according to (38) and (40), solve atomic problem.

For Falicov-Kimball model $J_\downarrow(\omega_n) = 0$ and according to (22) and (28)

$$\Sigma_{\uparrow(p)}(\omega_n) \equiv 0; \quad \Xi_{\uparrow(p)}(\omega_n) = g_{\uparrow(p)}(\omega_n) \tag{48}$$

and

$$\Omega_{(p)} = \lambda_p - \frac{1}{\beta}\sum_n \ln\left(1 - J_\uparrow(\omega_n) g_{\uparrow(p)}(\omega_n)\right), \tag{49}$$

$$G^{(a)}_{\uparrow}(\omega_n) = \frac{1-n_\downarrow}{i\omega_n - \lambda_{\uparrow 0} - J_\uparrow(\omega_n)} + \frac{n_\downarrow}{i\omega_n - \lambda_{2\downarrow} - J_\uparrow(\omega_n)}, \tag{50}$$

$$n_\uparrow = \frac{1}{\beta}\sum_n G^{(a)}_{\uparrow}(\omega_n), \qquad n_\downarrow = w_2 + w_\downarrow \tag{51}$$

which immediately gives results of Ref. [9] (see also Ref. [30]).

For Hubbard model there are no exact expression for self-energy but the set of Eqs. 43, 44 and 47 allows to construct different self-consistent approximations.

The first approximation, which can be done, is to put

$$\Sigma_{\sigma(p)}(\omega_n) = 0 \tag{52}$$

which gives

$$\Xi_{\sigma(p)}(\omega_n) = g_{\sigma(p)}(\omega_n) \tag{53}$$

and

$$\Omega_{(p)} = \lambda_p - \frac{1}{\beta}\sum_{n\sigma} \ln\left(1 - J_\sigma(\omega_n) g_{\sigma(p)}(\omega_n)\right) \tag{54}$$

and for the Green's function for atomic problem one can obtain 2-pole expression

$$G^{(a)}_{\sigma}(\omega_n) = \frac{w_0 + w_\sigma}{i\omega_n - \lambda_{\sigma 0} - J_\sigma(\omega_n)} + \frac{w_2 + w_{\bar\sigma}}{i\omega_n - \lambda_{2\bar\sigma} - J_\sigma(\omega_n)} \tag{55}$$

of the alloy-analogy solution for the Hubbard model which is exact for Falicov-Kimball model. In this approximation mean values (10) are equal

$$\begin{aligned} n_\sigma &= \frac{1}{\beta}\sum_n G^{(a)}_{\sigma}(\omega_n) + w_2 + w_\sigma - \frac{w_0 + w_\sigma}{e^{\beta\lambda_{\sigma 0}} + 1} - \frac{w_2 + w_{\bar\sigma}}{e^{\beta\lambda_{2\bar\sigma}} + 1} \\ &\neq \frac{1}{\beta}\sum_n G^{(a)}_{\sigma}(\omega_n) \end{aligned} \tag{56}$$

The next one is to consider only contribution from n-vertices of the (27) and (30) type which allow to construct self-energy in the following form

$$\Sigma_{\sigma(p)}(\omega_n) = \frac{1}{\beta}\sum_{n'} \widetilde{U}_{\sigma\bar\sigma(p)}(\omega_n, \omega_{n'}|0)\left(G_{\bar\sigma(p)}(\omega_{n'}) - \Xi_{\bar\sigma(p)}(\omega_{n'})\right), \tag{57}$$

which besides Hartree-Fock type term

$$\Sigma^{HF}_{\sigma(p)} = U \cdot \frac{1}{\beta}\sum_{n'}\left(G_{\bar\sigma(p)}(\omega_{n'}) - \Xi_{\bar\sigma(p)}(\omega_{n'})\right) \tag{58}$$

contains contributions from the scattering processes involving exchange by bosons: doublons and magnons. These immediately gives for the grand canonical potential (47) the following analytical expression

$$\begin{aligned} \Omega_{(p)} \;=\; & \lambda_p - \frac{1}{\beta}\sum_{n\sigma}\ln\left(1 - J_\sigma(\omega_n)\Xi_{\sigma(p)}(\omega_n)\right) \\ & -\frac{1}{\beta^2}\sum_{nn'}\left(G_{\uparrow(p)}(\omega_n) - \Xi_{\uparrow(p)}(\omega_n)\right)\widetilde{U}_{\uparrow\downarrow(p)}(\omega_n, \omega_{n'}|0) \\ & \times\left(G_{\downarrow(p)}(\omega_{n'}) - \Xi_{\downarrow(p)}(\omega_{n'})\right), \end{aligned} \tag{59}$$

and for Green's function for atomic problem we get 4-pole expression:

$$G^{(a)}_{\sigma}(\omega_n) = \sum_{p=0,2,\uparrow,\downarrow}\frac{w_p}{\Xi^{-1}_{\sigma(p)}(\omega_n) - J_\sigma(\omega_n)}, \tag{60}$$

where irreducible parts $\Xi_{\sigma(p)}(\omega_n)$ are solutions of the set of integral equations ($\sigma = \uparrow, \downarrow$)

$$\Xi^{-1}_{\sigma(p)}(\omega_n) = g^{-1}_{\sigma(p)}(\omega_n) - \frac{1}{\beta}\sum_{n'}\widetilde{U}_{\sigma\bar\sigma(p)}(\omega_n, \omega_{n'}|0)\left(G_{\bar\sigma(p)}(\omega_{n'}) - \Xi_{\bar\sigma(p)}(\omega_{n'})\right) \tag{61}$$

with

$$G_{\bar\sigma(p)}(\omega_{n'}) = \frac{1}{\Xi^{-1}_{\bar\sigma(p)}(\omega_{n'}) - J_{\bar\sigma}(\omega_{n'})}.$$

Now, electrons with opposite spins do not move independently as it is for the alloy-analogy approximations. Within this approximation, for mean values (10) we obtain

$$n = -\frac{1}{N}\frac{d\Omega}{d\mu} = -\left.\frac{d\Omega_a}{d\mu}\right|_{J=\text{const}} = \sum_p w_p n_{(p)},$$

$$m = -\frac{1}{N}\frac{d\Omega}{dh} = -\left.\frac{d\Omega_a}{dh}\right|_{J=\text{const}} = \sum_p w_p m_{(p)},$$

where

$$\begin{aligned} n_{(p)} \;=\; & -\left.\frac{d\Omega_{(p)}}{d\mu}\right|_{J=\text{const}} \\ =\; & -\frac{d\lambda_p}{d\mu} + \frac{1}{\beta}\sum_{n\sigma}(G_{\sigma(p)}(\omega_n) - \Xi_{\sigma(p)}(\omega_n)) \\ & -\frac{1}{\beta^2}\sum_{nn'}\left(G_{\uparrow(p)}(\omega_n) - \Xi_{\uparrow(p)}(\omega_n)\right)\frac{d\widetilde{U}_{\uparrow\downarrow(p)}(\omega_n\omega_{n'}|0)}{d\mu} \\ & \times\left(G_{\downarrow(p)}(\omega_{n'}) - \Xi_{\downarrow(p)}(\omega_{n'})\right) \end{aligned} \tag{62}$$

and

$$m_{(p)} = -\left.\frac{d\Omega_{(p)}}{dh}\right|_{J=\text{const}}$$
$$= -\frac{d\lambda_p}{dh} + \frac{1}{\beta}\sum_{n\sigma}\sigma\cdot\left(G_{\sigma(p)}(\omega_n) - \Xi_{\sigma(p)}(\omega_n)\right) \qquad (63)$$
$$-\frac{1}{\beta^2}\sum_{nn'}\left(G_{\uparrow(p)}(\omega_n) - \Xi_{\uparrow(p)}(\omega_n)\right)\frac{d\widetilde{U}_{\uparrow\downarrow(p)}(\omega_n\omega_{n'}|0)}{dh}$$
$$\times\left(G_{\downarrow(p)}(\omega_{n'}) - \Xi_{\downarrow(p)}(\omega_{n'})\right).$$

Here

$$\frac{d\widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n\omega_{n'}|0)}{d\mu} = \begin{cases} \mp 2U^2 g_{20}^2(\omega_{n+n'}) & \text{for } p = 0,2 \\ 0 & \text{for } p = \sigma,\bar{\sigma} \end{cases}$$

and

$$\frac{d\widetilde{U}_{\sigma\bar{\sigma}(p)}(\omega_n\omega_{n'}|0)}{dh} = \begin{cases} 0 & \text{for } p = 0,2 \\ \mp 2\sigma U^2 g_{\sigma\bar{\sigma}}^2(\omega_{n-n'}) & \text{for } p = \sigma,\bar{\sigma} \end{cases}.$$

5. Conclusions

A finite-temperature perturbation theory scheme in terms of electron hopping which is based on the Wick's theorem for Hubbard operators and is valid for arbitrary value of U ($U < \infty$) has been developed for Hubbard type models. Diagrammatic series contain single-site vertices, which are irreducible many-particle Green's functions for unperturbated single-site Hamiltonian, connected by hopping lines. The applying of the Wick's theorem for Hubbard operators have allowed to calculate these vertices and it is shown that for each vertice the problem splits into subspaces with "vacuum states" determined by the diagonal (projection) operators and only excitations around these "vacuum states" are allowed. Vertices possesses finite $U \to \infty$ limit when diagrammatic series of the strong coupling approach [5,6] are reproduced. The rules to construct diagrams by the primitive vertices are proposed.

In the limit of infinite spatial dimensions the total auxiliary single-site problem exactly (naturally) splits into subspaces (four for Hubbard model) and a considered analytical scheme allows to build a self-consistent Kadanoff-Baym type theory for Hubbard model. Some analytical results are given for simple approximations. The first one is an alloy-analogy approximation, when 2-pole structure for Green's function

is obtained, which is exact for Falicov-Kimball model. The next approximation besides Hartree-Fock type contributions involves scattering processes from the exchange by bosons and results into the 4-pole structure for Green's function. The applicability and limitations of the proposed approach and considered approximations can be cleared out only by the numerical calculations and it will be the subject of the special investigation.

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Андрій Михайлович Швайка

Підхід сильного зв'язку до розгляду електронних систем з сильними кореляціями

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