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DIAGRAM ANALYSIS OF THE STATIC AND THE SINGLE-SITE APPROXIMATIONS FOR THE HUBBARD MODEL

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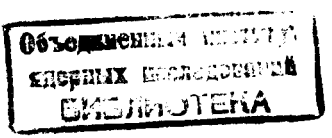

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Веллер В. **E4 - 8448**

Диаграммный анализ статического и одноузельного приближения в модели Хаббарда

Получено диаграммное представление для статического и одноузельного приближений, использованных в недавних работах для модели Хаббарда. Обсуждается нарушение теоремы Латтинжера при статическом приближении.

Сообщение Объединенного института ядерных исследований
Дубна, 1974

Weller W. **E4 - 8448**

Diagram Analysis of the Static and the Single-Site Approximations for the Hubbard Model

The static and the single-site approximations applied to the Hubbard model in recent papers are presented in diagrammatical form. The violation of the Luttinger theorem as a consequence of the static approximation is discussed.

Communications of the Joint Institute for Nuclear Research.
Dubna, 1974

1. Introduction

The Hubbard model [1] given by the Hamiltonian

$$H = \sum_{ij\sigma} T_{ij}\, a^{+}_{i\sigma}\, a_{j\sigma} + U \sum_{i} n_{i\uparrow}\, n_{i\downarrow} \qquad (1)$$

is the simplest model for the description of electron-electron correlation in a single narrow band. This model providing an interpolation between the limit cases of band electrons and localized electrons is widely used in the theory of metal-insulator transitions, the theory of Mott insulators and the theory of itinerant magnetism. $a^{+}_{i\sigma}$ and $a_{i\sigma}$ are the creation and annihilation operators for an electron of spin σ in the Wannier state at lattice site i, $n_{i\sigma} = a^{+}_{i\sigma}\, a_{i\sigma}$; T_{ij} is the hopping amplitude and U denotes the Coulomb repulsion energy between two electrons at the same lattice site.

A number of recent approximations for the Hubbard model are based on the so-called static and single-site approximations. Here we present those approximations as a natural generalization of the Hartree-Fock approximation. It is then shown in section 2 what approximations in the diagram expression for the self-energy correspond to the static and the single-site approximations.

The simplest approximation one can apply to the Hubbard

model is the Hartree-Fock approximation. It is obtained by substituting the Hamiltonian (1) by

$$H = \sum_{ij\sigma} T_{ij}\, a^{+}_{i\sigma}\, a_{j\sigma} + U \sum_{i\sigma} n_{i\sigma}\, \nu_{i,-\sigma} \qquad (2)$$

and determining the c-numbers $\nu_{i,-\sigma}$ by the Hartree-Fock condition

$$\nu_{i,-\sigma} = \langle n_{i,-\sigma} \rangle .$$

$\langle \cdots \rangle$ here denotes the thermodynamical average.

Now a very natural way to improve the Hartree-Fock approximation is given by the following generalized scheme: The $\nu_{i,-\sigma}$ in (2) are not considered as fixed c-numbers (determined by the Hartree-Fock condition) but as a field of random c-numbers characterized by a distribution function

$$P_{i,-\sigma}(\nu_{i,-\sigma}).$$

Obviously, the Hartree-Fock condition now has to be generalized to the form

$$\langle \nu_{i,-\sigma} \rangle_{\nu} = \langle n_{i,-\sigma} \rangle , \qquad (3)$$

$\langle \cdots \rangle_{\nu}$ denotes the average over the ν with respect to the distribution function p, and $\langle \cdots \rangle$ now means the thermodynamical average and the ν-average. The distribution function p (of course not fixed by (3)) has to be determined on the basis of further considerations.

The described approximation can be characterized by saying that the interaction of a σ-electron with the $(-\sigma)$-electrons is replaced by an interaction of a

σ-electron with the time-independent random c-number field $\nu_{i,-\sigma}$. This substitution is called static approximation in the following.

After having performed the static approximation, the coherent potential approximation /2,3/ well known from the theory of disordered alloys can be applied to the Hamiltonian (2). We restrict the considerations to the single-site approximation. The one-electron Green function is then given by

$$\left(G_{\sigma}^{-1}(\omega)\right)_{ij} = \left(G^{(0)-1}(\omega)\right)_{ij} - \Sigma_{i\sigma}(\omega)\,\delta_{ij} . \qquad (4)$$

$G^{(0)}$ is the Green function for the noninteracting electrons. The CPA self-energy $\Sigma_{i\sigma}(\omega)$ is the solution of the CPA condition

$$\left\langle T_{i\sigma}(\omega) \right\rangle_{\nu} = 0 ; \qquad (5)$$

$T_{i\sigma}$ denotes the t-matrix for the scattering of an electron of spin σ at a lattice site i by the potential

$$v_{i\sigma} = U \nu_{i,-\sigma} - \Sigma_{i\sigma}(\omega) . \qquad (6)$$

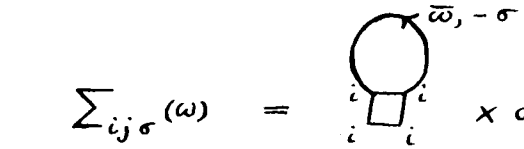
A number of approximations for the Hubbard model fit into the described scheme. The simplest one is the alloy analogy introduced by Hubbard /4/. In the alloy analogy, where for the motion of a σ-electron the $(-\sigma)$-electrons are considered as randomly distributed and not moving, the distribution function $P_{i,-\sigma}$ confines $\nu_{i,-\sigma}$ to the values 0 and 1 corresponding to absence or presence of a $(-\sigma)$-electron at site i. (It was first noted in /3/ that Hubbard's

treatment of the alloy analogy corresponds to the single-site CPA). The motion of the $(-\sigma)$-electrons neglected in the alloy analogy is included to some extend by Hubbard's broadening correction [4]. For a half-filled band ($\langle n_{i\uparrow} + n_{i\downarrow} \rangle = 1$) Hubbard's solution including the broadening correction also fits into the described scheme as was shown by Weller and Gobsch [5]. Recently, Puff and Weller [6] developped an approximation scheme for the Hubbard model based on the functional differential equation for the self-energy with source potentials $\lambda_{i\sigma}(t)$ as the independent variables. There the static approximation is introduced by neglecting the time-dependence of the $\lambda_{i\sigma}$; in this way the Hubbard problem is reduced to an alloy problem which is treated in single-site approximation. The final equations then coincide with those of the above described scheme (**equations** (2 to 6)) closed by an integral equation for the distribution function $P_{i,-\sigma}$. Solutions for this distribution function are considered in [7,8]. Furthermore, also the approximations based on the functional integral method [9,10,11] are very similar to the here described scheme. A detailed comparison, however, cannot be immediately done because in the functional integral method the interaction term is transformed by means of the Mühlschlegel identity

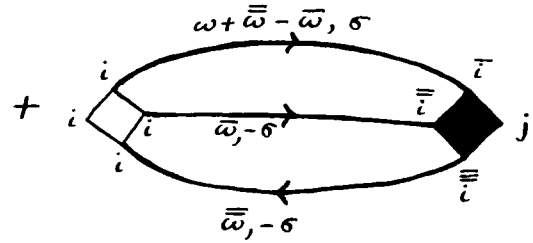
$$n_{i\uparrow} n_{i\downarrow} = \frac{1}{4}(n_{i\uparrow} + n_{i\downarrow})^2 - \frac{1}{4}(n_{i\uparrow} - n_{i\downarrow})^2 .$$

2. Diagram Analysis

In this **section** we derive **equation** (5) determining the self-energy in the static and the single-site approximations starting from the diagram expression for the self-energy. The exact diagram for the self-energy of the model (1) is given by (**compare**, e.g. /12/)

$\Sigma_{ij\sigma}(\omega) =$ 

$\times \delta_{ij} +$



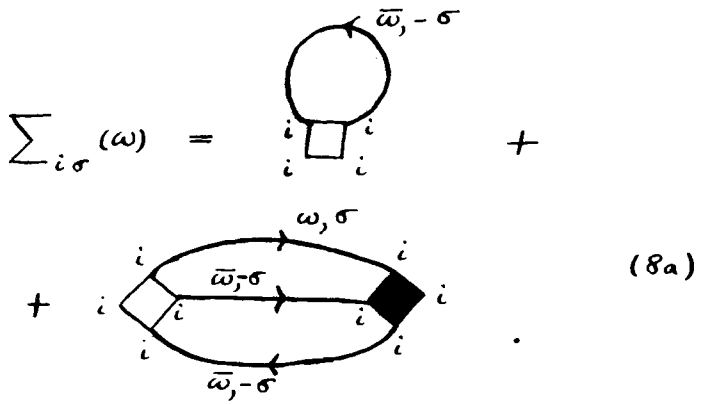
(7)

□ = U is the bare vertex, ■ = Γ is the total vertex for the model (1), ⟶ denotes the Green function; the variables $\bar{\omega}$, $\bar{\bar{\omega}}$ and $\bar{i}$, $\bar{\bar{i}}$, $\bar{\bar{\bar{i}}}$ are summed over. The first term in (7) gives the Hartree-Fock approximation.

The static approximation introduced above is obtained by restricting the summation over the energies in the last term in (7) to $\bar{\omega} = \bar{\bar{\omega}}$; in other words, the σ-electron with external energy ω conserves its energy in the internal line in correspondence to the substitution of its interaction with the $(-\sigma)$-electrons by the interaction with the static random field $\nu_{i,-\sigma}$.

The single-site approximation introduced above is obtained by restricting in (7) to diagonal elements of the Green function and to a local total vertex, that means restriction to $\bar{i} = \bar{\bar{i}} = \bar{\bar{\bar{i}}} = j = i$.

In these approximations equation (7) takes the form



(8a)

The self-energy Σ is now site-diagonal. ■ = $\Gamma^{eff}(\omega,\bar{\omega})$ now means an effective vertex (local in space and depending only on the two energies ω, $\bar{\omega}$), which substitutes the total vertex Γ in (7). In analytical form (8a) writes

$$\Sigma_{i\sigma}(\omega) = U\langle n_{i,-\sigma}\rangle + U\, G_{ii}(\omega)\, G^{2}_{ii}(\bar{\omega})\, \Gamma^{eff}(\omega,\bar{\omega}); \qquad (8b)$$

$\bar{\omega}$ is summed over.

It is easy to see that the static and the single-site approximations performed in the diagram (7) coincide with

those introduced in section 1. We have only to show that the two equations (5) and (8) determining the self-energy Σ coincide. By inserting the equation for the $\mathcal{T}_{i\sigma}$ - matrix into (5) we obtain

$$0 = \langle \mathcal{T}_{i\sigma}(\omega)\rangle_{\nu} =$$

$$= \langle U n_{i,-\sigma} - \Sigma_{i\sigma}(\omega)\rangle_{\nu} + \langle (U n_{i,-\sigma} - \Sigma_{i\sigma}(\omega))\, G_{ii}(\omega)\, \mathcal{T}_{i\sigma}(\omega)\rangle_{\nu} =$$

$$= U\langle n_{i,-\sigma}\rangle - \Sigma_{i\sigma}(\omega) + U\, G_{ii}(\omega)\langle n_{i,-\sigma}\, \mathcal{T}_{i\sigma}(\omega)\rangle_{\nu}; \qquad (9)$$

we have used the condition (3) in getting the last equation. In fact, equations (8) and (9) now become identical if the effective vertex Γ^{eff} is determined by the integral equation

$$G^{2}_{ii}(\bar{\omega})\, \Gamma^{eff}(\omega,\bar{\omega}) = \langle n_{i,-\sigma}\, \mathcal{T}_{i\sigma}(\omega)\rangle_{\nu}. \qquad (10)$$

We close with a remark on the Luttinger theorem /13/. It follows from this theorem for a metallic system states that for $T \to 0$ the imaginary part of the retarded self-energy vanishes at the Fermi energy (chosen equal to 0):

$$Im\, \Sigma^{ret}_{\sigma}(\omega) \propto \omega^{2} \quad \text{for} \quad \begin{matrix}\omega \to 0,\\ T = 0.\end{matrix} \qquad (11)$$

(We consider paramagnetic or ferromagnetic phases where Σ

does not depend on i.) As is well known the proof of the theorem is based on the diagram expression (7) (proceeding step by step beginning with noninteracting Green functions and two bare vertices). It can be shown /14/ that the restriction of the energy summation corresponding to the static approximation leads to the violation of the Luttinger theorem, whereas the single-site approximation has not such a consequence. The violation of the Luttinger theorem by Hubbard's solution /4/ was already remarked by Edwards and Hewson /15/; however we cannot agree with their statement attributing this violation to momentum nonconservation what would mean to the single-site approximation.

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