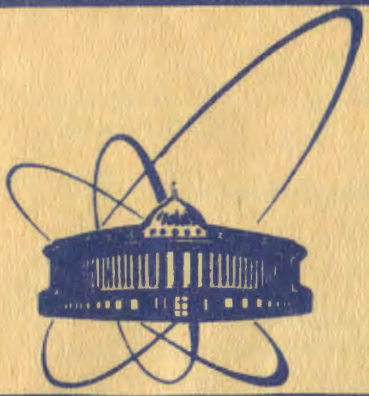

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SINGLE-SITE AND ALL-SITE POISSON APPROXIMATION FOR THE HUBBARD MODEL

1980

1. INTRODUCTION

In a previous paper [1] it was shown that the Green function for the Hubbard model [2] can be represented as the functional average

$$G_{\uparrow}(1,1') = \int D\nu P[\nu] G_{\uparrow}(1,1';\nu), \tag{1}$$

where $G_{\uparrow}(1,1';\nu)$ is the Green function to the one-particle Hamiltonian

$$H_{\uparrow} = \sum_{i,j} t_{ij,\uparrow} a^{+}_{i\uparrow} a_{j\uparrow} + U \sum_{i} \nu_i(t)\, n_{i\uparrow} \tag{2}$$

describing the motion of a spin $\uparrow$-electron in the local time-dependent potential $U\nu(t)$. The $\nu_i(t)$ jump between 0 and 1 and are governed by the functional measure $P[\nu]$ containing the many body aspects and the information about the spin $\downarrow$-electrons.

To obtain explicit results we have to calculate the functional average (1) approximatively. The alloy analogy [3], for instance, is reproduced if we put the bandwidth of the spin $\downarrow$-electrons equal to zero. Then the itinerant spin $\uparrow$-electrons move in an alloy with static energy levels 0 and U. The measure $P[\nu]$ is easily calculated [1]. Because of the serious drowbacks of the alloy analogy [4-7] there is considerable interest to go beyond "static" approximations.

In this paper we propose a "dynamic" approximation based on the following idea. The functional integral in (1) is restricted to the class of ν-functions jumping between 0 and 1. We approximatively look upon this jumps as random events governed by a Poisson distribution. Thus the functional average is calculated with an ad hoc assumed Poisson distribution*. The mean number of jumps in unit time (the parameter of the Poisson distribution) has to be determined self consistently, e.g., by a sum rule.

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* An approximation of this type was already used in quite a different context [8].

ИНСТИТУТ ... ИССЛЕДОВАНИЙ ... БИБЛИОТЕКА

In order to describe a metal-insulator transition we consider a half-filled band in the paramagnetic case and calculate the Poisson averaged Green function in a simple scheme interpolating between band limit and atomic limit. Explicit results for the density of states are obtained in two different approximations. The single site approximation (SSA) neglects the correlation of jumps on different lattice sites. The self-energy is $\vec{k}$-independent. The mean number of jumps a decreases smoothly with increasing Coulomb repulsion U. For strong Coulomb repulsion we obtain two subbands separated by a deep minimum of the density of states. A real gap, however, is found only in the atomic limit.

The all site approximation (ASA) overestimates the correlation of jumps on different lattice sites. The self-energy has a simple $\vec{k}$-dependence. The mean number of jumps decreases to zero if U approaches the critical value U_c equal to the unperturbed bandwidth. For $U \geq U_c$ the spin $\downarrow$-electrons are resting on their lattice sites ($a = 0$) and a gap appears. The mechanism producing a gap is different from that of the alloy analogy.

The paper is organized as follows. In Section 2 we introduce the Poisson approximation. In Section 3 the average procedure for the Green function is described in the following two Sections the results for the SSA and the ASA are presented, respectively.

2. THE POISSON APPROXIMATION

Since we are not able to evalute the functional integral (1) exactly we calculate the functional average with an ad hoc assumed distribution. The functional integral (1) is restricted to ν-functions jumping between 0 and 1. We assume that the jumps are governed by the Poisson distribution

$$P(k, t) = e^{-at} \frac{(at)^k}{k!} . \tag{3}$$

P is the probability that in the time t occure k jumps. a is the mean number of jumps in unit time. The Poisson distribution is markovian and not compatible with the periodicity condition for ν (see (19) in [1]). Therefore we restrict ourselves to zero temperature where such a condition

does not appear. We consider the electron-hole symmetric case where the chemical potential μ is fixed to U/2 . For convenience we replace $U\nu_i(t) - \mu$ by $U\tilde{\nu}_i(t)$ and let $\tilde{\nu}_i(t)$ jump between 1/2 and -1/2. The autocorrelation function for a Poisson process between 1/2 and -1/2 is

$$W(t) = \langle \tilde{\nu}_i(t)\, \tilde{\nu}_i(0) \rangle_{\text{Poisson}} = \frac{1}{4} e^{-2a|t|} , \tag{4}$$

its Fourier transform is of Lorentzian shape,

$$W(\Omega) = \frac{a}{\Omega^2 + (2a)^2} . \tag{5}$$

The mean number of jumps a enters as a parameter the Poisson distribution. To determine a self consistently we use the sum rule [9]

$$i\frac{\partial}{\partial t} \langle T n_{i\downarrow}(t)\, n_{i\downarrow}(0) \rangle \Big|_{t=0^+} = -\sum_j t_{ij,\downarrow} \langle a^+_{i\downarrow} a_{j\downarrow} \rangle . \tag{6}$$

Taking into account $\langle T n_{i\downarrow}(t)\, n_{i\downarrow}(0) \rangle = \langle \nu_i(t)\, \nu_i(0) \rangle_{\text{Poisson}}$ and replacing after Fourier transformation for the paramagnetic case $\langle n_{\vec{k}\downarrow} \rangle$ by $\langle n_{\vec{k}\uparrow} \rangle$ we obtain the self consistency condition:

$$\frac{a}{2} = -\frac{1}{N} \sum_{\vec{k}} \epsilon_{\vec{k}} \langle n_{\vec{k}\uparrow} \rangle , \tag{7}$$

relating the mean number of jumps with the average kinetic energy. In terms of the retarded Green function (7) reads

$$\frac{a}{2} = \frac{1}{\pi} \operatorname{Im} \frac{1}{N} \sum_{\vec{k}} \epsilon_{\vec{k}} \int_{-\infty}^{0} d\omega\, G_{\vec{k}\uparrow}(\omega) . \tag{8}$$

3. AVERAGE OF THE GREEN FUNCTION

In this Section we calculate the Poisson averaged Green function in a simple approximation interpolating between band

limit and atomic limit. For this reason we consider the Poisson average of the iterated Dyson equation*

$$G[\tilde{\nu}] = G^\circ + U G^\circ \tilde{\nu} G^\circ + U^2 G^\circ \tilde{\nu} G^\circ \tilde{\nu} G[\tilde{\nu}] . \qquad (9)$$

To obtain a Dyson equation for the averaged Green function we brake off the average of the last term,

$$U^2 G^\circ \langle \tilde{\nu} G^\circ \tilde{\nu} G[\tilde{\nu}] \rangle_{\text{Poisson}} \approx U^2 G^\circ \langle \tilde{\nu} G^\circ \tilde{\nu} \rangle_{\text{Poisson}} \langle G[\tilde{\nu}] \rangle_{\text{Poisson}} . \qquad (10)$$

This approximation is correct in the atomic limit (see below). We obtain**

$$G = \langle G[\tilde{\nu}] \rangle_{\text{Poisson}} = G^\circ + G^\circ \Sigma G, \qquad (11)$$

where Σ denotes the second order self-energy,

$$\Sigma = U^2 \langle \tilde{\nu} G^\circ \tilde{\nu} \rangle_{\text{Poisson}} . \qquad (12)$$

In Bloch- and energy-representation we write finally:

$$G_{\vec{k}\uparrow}(\omega) = G^\circ_{\vec{k}\uparrow}(\omega - \Sigma_{\vec{k}\uparrow}(\omega)) , \qquad (13)$$

and

$$\Sigma_{\vec{k}\uparrow}(\omega) = U^2 \frac{1}{N} \sum_{\vec{q}} \int_{-\infty}^{\infty} \frac{d\Omega}{2\pi} G^\circ_{\vec{k}-\vec{q},\uparrow}(\omega - \Omega) W_{\vec{q}}(\Omega) . \qquad (14)$$

$W_{\vec{q}}(\Omega)$ is the Fourier transform of $W_{ij}(t) = \langle \tilde{\nu}_i(t) \tilde{\nu}_j(0) \rangle_{\text{Poisson}}$ and $G^\circ_{\vec{k}\uparrow}(\omega) = 1/(\omega - \epsilon_{\vec{k}} + i\delta \operatorname{sgn} \epsilon_{\vec{k}})$. This simple scheme is correct in order U^2 and reproduces the atomic limit: For zero bandwidth the self consistency condition (8) is solved by $\alpha = 0$ so that from (5) results $W(\omega) = \pi\delta(\Omega)/2$. From (14) we obtain after analytical continuation the retarded self-energy $\Sigma^{AL}(\omega) = U^2/4(\omega + i\delta)$ reproducing the atomic limit

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* For the sake of brevity we use a short hand notation dropping all indices and integrations.

** Note, that $\langle \tilde{\nu} \rangle_{\text{Poisson}} = 0$.

Green function $G^{AL}(\omega) = (1/(\omega + U/2 + i\delta) + 1/(\omega - U/2 + i\delta))/2$. To evalute the self-energy (14) we have to know the correlation function $W_{\vec{q}}(\Omega)$. of the Poisson process. In the following Sections the correlation between jumps of ν at different lattice sites is either neglected or drastically over-estimated. In both cases the $\vec{q}$-dependence of $W_{\vec{q}}(\Omega)$ is extremely simple and we need only the autocorrelation function given by (5).

4. SINGLE SITE APPROXIMATION

In the single site approximation (SSA) we neglect the correlation between jumps of $\tilde{\nu}$ at different lattice sites:

$$W_{ij}(\Omega) = W(\Omega)\delta_{ij} \quad \text{or} \quad W_{\vec{q}}(\Omega) = W(\Omega) . \qquad (15)$$

The corresponding self-energy is $\vec{k}$-independent. Performing the Ω-integration one obtains from (14) after analytical continuation the retarded self-energy* **

$$\Sigma(\omega) = \frac{U^2}{4} G^\circ(\omega + 2i\alpha) . \qquad (16)$$

$G^\circ(z)$ is the Hilbert transform of the unperturbed density of states per lattice site

$$G^\circ(z) = \frac{1}{N} \sum_{\vec{k}} G^\circ_{\vec{k}}(z) = \int_{-\infty}^{\infty} dE \frac{\rho^\circ(E)}{z - E} . \qquad (17)$$

The density of states is given by the usual single site result

$$\rho(\omega) = -\frac{1}{\pi} \frac{1}{N} \sum_{\vec{k}} \operatorname{Im} G_{\vec{k}}(\omega) = -\frac{1}{\pi} \operatorname{Im} G^\circ(\omega - \Sigma(\omega)) . \qquad (18)$$

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* In the following we drop the spin index.

** In the SSA the Poisson average procedure can be done exactly with the same result /11/.

The self consistency condition (8) reads in the SSA

$$\frac{a}{2} = \frac{1}{\pi} \mathrm{Im} \int_{-\infty}^{0} d\omega \, F(\omega - \Sigma(\omega)) , \tag{19}$$

with $F(z)$ defined as

$$F(z) = \int_{-\infty}^{\infty} dE \, \frac{\rho^{\circ}(E)E}{z - E} = z\,G^{\circ}(z) - 1 . \tag{20}$$

To simplify the calculations we use in the following the semi-elliptic model density*

$$\rho^{\circ}(E) = \begin{cases} \frac{2}{\pi}\sqrt{1 - E^2} & |E| \leq 1 , \\ 0 & \text{otherwise} . \end{cases} \tag{21}$$

The corresponding unperturbed Green function is**

$$G^{\circ}(z) = 2(z - \sqrt{z^2 - 1}) . \tag{22}$$

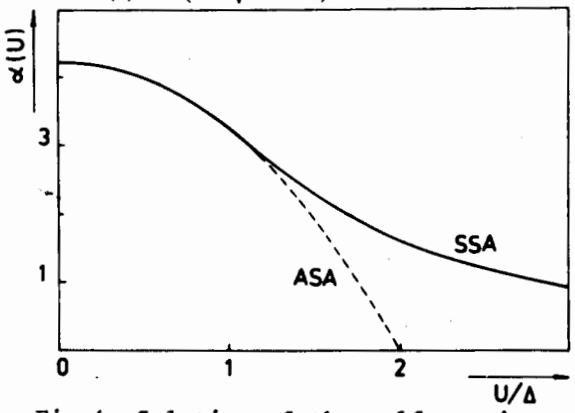

Fig.1. Solution of the self consistency equation: a) SSA (solid line), b) ASA (dashed line).

The set of equations (16,19,20,22) was solved numerically with the result shown in Fig.1. The mean number of jumps a decreases smoothly with increasing Coulomb repulsion U and goes to zero if U goes to infinity. The corresponding density of states is shown in Fig.2. For strong Coulomb repulsion $U \approx 2$ two subbands separated by a deep minimum of the density of states are found. A real gap occures only if U goes to infinity (atomic limit and split band limit). This can be seen analytically: The density of states at zero energy is

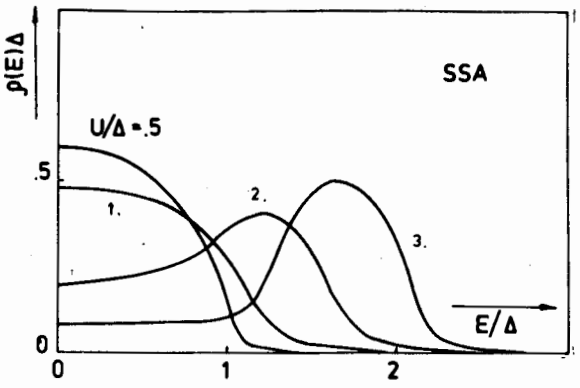

Fig.2. Density of states in SSA.

$$\rho(0) = \frac{2}{\pi}(\sqrt{1 + \mathrm{Im}^2\Sigma(0)} + \mathrm{Im}\,\Sigma(0)) , \tag{23}$$

with

$$\Sigma(0) = i\frac{U^2}{2}(2a - \sqrt{1 + (2a)^2}) . \tag{24}$$

$\rho(0)$ goes to zero only if $\mathrm{Im}\Sigma(0) \to -\infty$, i.e., for $U \to \infty$. It is a common feature of all single site approximations for electron-hole symmetric systems that a gap appears only if $\mathrm{Im}\Sigma(0) \to -\infty$. In the alloy analogy, for instance, $\mathrm{Im}\Sigma(0)$ diverges for $U \to 1$. In approximations with $\vec{k}$-dependent self-energy, however, a gap is possible even if $\mathrm{Im}\Sigma_{\vec{k}}(0) = 0$[10].

5. ALL SITE APPROXIMATION

In the all site approximation (ASA) we assume

$$W_{ij}(\Omega) = W(\Omega) \quad \text{or} \quad W_{\vec{q}}(\Omega) = W(\Omega)\,\delta_{\vec{q},0} . \tag{25}$$

Here, in contrast to the SSA we overestimate the correlation between jumps of $\vec{\nu}$ at different lattice sites. The ASA neglects the momentum transfer between $\uparrow$ - and $\downarrow$-electrons (cf.(13)). The retarded self-energy is $\vec{k}$-dependent

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* The energy is measured in units of the half bandwidth $\Delta = 1$.

** The complex square root has to be taken as $\sqrt{Z^2 - 1} = \sqrt{|Z^2 - 1|}\,\exp\{\frac{i}{2}(\arg(z+1) + \arg(z-1))\}$.

$$\Sigma_{\vec{k}}(\omega) = \frac{U^2}{4} G^{\circ}_{\vec{k}}(\omega + 2ia). \tag{26}$$

Partial fraction evaluation yields for the retarded Green function

$$G_{\vec{k}}(\omega) = \frac{1}{2A}(B_1 G^{\circ}_{\vec{k}}(\omega - B_2) + B_2 G^{\circ}_{\vec{k}}(\omega + B_1)), \tag{27}$$

with

$$A = \sqrt{U^2/4 - a^2},$$
$$B_{1/2} = A \pm ia, \tag{28}$$
$$G^{\circ}_{\vec{k}}(z) = (z - \epsilon_{\vec{k}} + i\delta)^{-1}, \qquad \delta \to +0.$$

The density of states is given by

$$\rho(\omega) = -\frac{1}{\pi} \mathrm{Im}\{\frac{1}{2A}(B_1 G^{\circ}(\omega - B_2) + B_2 G^{\circ}(\omega + B_1)\}. \tag{29}$$

It is easily prooved that $\int_{-\infty}^{\infty} d\omega \rho(\omega) = 1$. The self consistency condition reads in ASA

$$\frac{a}{2} = \frac{1}{\pi} \mathrm{Im}\{\frac{1}{2A} \int_{-\infty}^{0} d\omega [B_1 F(\omega - B_2) + B_2 F(\omega + B_1)]\}. \tag{30}$$

Now we examine under which conditions (30) has a solution $a = 0$. For symmetric densities ($\rho^{\circ}(\omega) = \rho^{\circ}(-\omega)$) we obtain from (30) that we have to fulfill

$$0 = \int_{-\infty}^{U/2} d\omega \rho^{\circ}(\omega)\omega. \tag{31}$$

Obviously $a = 0$ is a self consistent solution if $U \geq 2$. In this case the $\downarrow$-electrons are resting on their lattice sites and we get the physical picture of an alloy with static energy levels 0 and U. From (29) we obtain two rigid unperturbed bands shifted by $\pm$ U/2

$$\rho(\omega) = \frac{1}{2}(\rho^{\circ}(\omega - \frac{U}{2}) + \rho^{\circ}(\omega + \frac{U}{2})), \tag{32}$$

Since we have not performed any sophisticated average over the initial configuration $\{\vec{\nu}_i(t=0)\}$ this simple rigid band result has to be expected.

For U < 2 the situation is more difficult. With the semielliptic model density (21) we obtain from (30)

$$\frac{a}{2} = \frac{1}{3\pi}\{U^2 - \mathrm{Im}[\frac{1}{A}(B_1\sqrt{(B_2^2-1)^3} + B_2\sqrt{(B_1^2-1)^3})]\}, \tag{33}$$

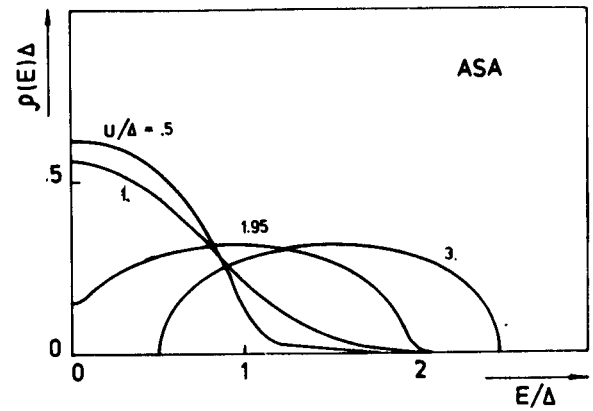

Fig.3. Density of states in ASA. A gap occures if U $\geq$ 2.

which has to be solved numerically. The result is shown in Fig.1. The mean number of jumps a decreases to zero if U $\to$ 2. The density of states is shown in Fig.3. A gap occures if U is larger than the unperturbed bandwidth (U $\geq$ 2).

In the ASA the gap is produced intrinsically by the $\vec{k}$-dependence of the self-energy. As discussed already above the splitting mechanism is different from that in the SS-CPA alloy analogy [3], where a gap occures for U $\geq$ 1, a result suspicious to overestimate the electron correlation.

At last we mention that the ASA does not fulfill the $\downarrow$-electron number conservation as can be seen deriving the result from the equivalent mean field Hamiltonian

$H^{ASA}_{\uparrow} = H^{\circ} + U\nu(t) \sum_i n_{i\uparrow}$. Nevertheless this approximation shows drastically the importance of the $\vec{k}$-dependence of the self-energy. An approximation which takes into account more realistically the correlation of jumps at different lattice sites gives an increased tendency of forming the Hubbard subbands in comparision with the SSA [12].

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