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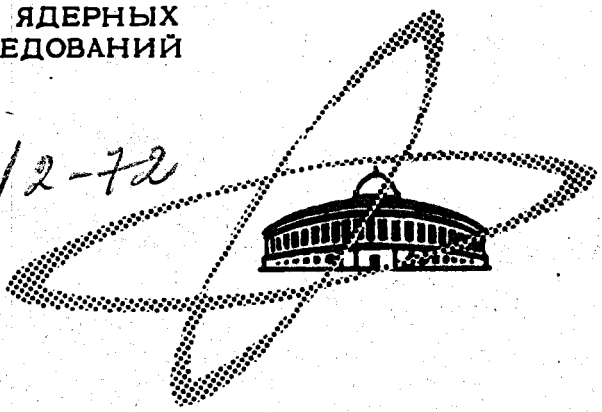

E4 - 6097

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DENSITY OF STATES IN THE ONE-DIMENSIONAL HUBBARD MODEL

ЛАБОРАТОРИЯ ТЕОРЕТИЧЕСКОЙ ФИЗИКИ

1971

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Submitted

to physica status solidi

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1. Introduction

A simple model describing electrons in narrow energy bands is the so-called Hubbard-model /1/

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

where $c^{+}_{i\sigma}$, $c_{i\sigma}$ are, respectively, the creation and annihilation operators for an electron of spin σ in the Wannier state at the i th lattice site, T_{ij} is the hopping integral, and U is the electron-electron repulsion between two electrons of opposite spins occupying the same lattice site.

Although the Hamiltonian (1) has a very simple form (in many respects it is the simplest many-body operator at all), nevertheless, at its application, all known difficulties of the many-body problem appear. Therefore many approximations have been developed (see e.g. ref./2/), to study especially the behaviour of the density of states in dependence on the parameter U/Δ, where Δ is a measure of the band width.

In consequence of the simple form of (1), some exact conclusions can be derived for different extreme cases. They are especially important as a test for different approximations used at present. Such an exact solvable case is e.g. the one-dimensional model with nearest-neighbour interaction[3], i.e.

$$H = \sum_{i\sigma} \left[c^{+}_{i\sigma} \left(c_{i+1,\sigma} + c_{i-1,\sigma} \right) + \frac{U}{2} n_{i,-\sigma} n_{i\sigma} \right] . \qquad (2)$$

(We have chosen $T_{01} = 1$).

Besides the possibility to test approximations, the model (2) is of importance also with respect to really existing systems, which can be well approximated by the one-dimensional narrow band model. Such a system is, for instance, the TCNQ-molecule, forming tetragonal body-centred crystals with $c/a \gg 1$[4].

For the Hamiltonian (2), Lieb and Wu have obtained an exact result for the ground state energy and its dependence on U[3]. Beyond it, in the present paper the density of states depending on U and $n_\sigma = \langle n_{i\sigma} \rangle$ is calculated. Therefore we use the analogy to the one-dimensional δ-gas and the disordered oscillator chain. For these systems, the density of states can be obtained numerically using the so-called phase method[5], which we apply to the system (2).

For the special case $U = \infty$ and $n = 1$, Brinkman and Rice[6] have also calculated the density of states of the system (2). They obtain the strange result, that the density of states in the strong correlated limit $U = \infty$ is the same as in the free electron case

$U = 0$, in contradiction to our result, which gives significant differences between these two cases. Likewise, the ground state energy in the solution of Brinkman and Rice is the same as in the free electron case, which is in contradiction with the exact result of Lieb and Wu[3] and also with general properties of interacting systems. My opinion is, that the transformation $H \to H'$ in the paper of Brinkman and Rice can contain some incorrectnesses even for $U \to \infty$, since the neglected terms are of the form $\infty \cdot 0$. It is possible, that these terms have different effects in the one-dimensional and in the three-dimensional case, analogically to the behaviour of δ-potentials.

2. Functional Equation for the Density of States

We consider an appropriate function

$$G^{\nu}_{i\sigma}(\omega) = \int dt\, e^{i\omega t} \sum_{j\sigma'} \gamma^{\nu}_{j\sigma'} \langle c_{i\sigma}(t) c^{+}_{j\sigma'} \rangle^{\nu}, \quad c_{i\sigma}(t) = e^{iHt} c_{i\sigma} e^{-iHt}, \tag{3}$$

where ν represents a special distribution "ν" of N_e electrons on spins and on N_a lattice sites. The $\gamma^{\nu}_{j\sigma'}$ are free parameters, which can be chosen arbitrarily.

With H from (2), we get the relation

$$\omega\, G^{\nu}_{i\sigma}(\omega) = U\, \Gamma^{\nu}_{i\sigma}(\omega) + G^{\nu}_{i-1,\sigma}(\omega) + G^{\nu}_{i+1,\sigma}(\omega), \tag{4}$$

where

$$\Gamma^{\nu}_{i\sigma}(\omega) = \int dt\, e^{i\omega t} \sum_{j\sigma'} \gamma^{\nu}_{i\sigma'} \langle n_{i,-\sigma}(t)\, c_{i\sigma}(t)\, c^{+}_{i\sigma'} \rangle^{\nu} =$$

$$= \int dt\, e^{-i\omega t} \sum_{j\sigma'} \gamma^{\nu}_{i\sigma'} \langle n_{i,-\sigma}\, c_{i\sigma}\, c^{+}_{j\sigma'}(t) \rangle^{\nu} . \qquad (5)$$

In the last equation we use the fact, that the expectation value depends only on time differences.

With the definitions

$$\tan \frac{\phi_i}{2} = \frac{G^{\nu}_{i-1\sigma}(\omega)}{G^{\nu}_{i\sigma}(\omega)} , \qquad g^{\nu}_{i\sigma} = \frac{\Gamma^{\nu}_{i\sigma}(\omega)}{G^{\nu}_{i\sigma}(\omega)} , \qquad (6)$$

we obtain from (4) the relation

$$\phi_i = 2 \tan^{-1} \left(\omega - U g^{\nu}_{i\sigma} - \cot \frac{\phi_{i+1}}{2} \right) \qquad (7)$$

between neighbour phases. In this relation the only important fact is, whether or not, in the distribution "ν" an electron with spin $-\sigma$ is present at the i th atom. This is completely analogical to the case of the disordered oscillator chain, in which only the masses m_i appear in the phase relation[5]. Assuming an infinite system (N_e , $N_a \to \infty$, $N_e / N_a = n$) and taking into account a set of states "ν" the phase relation (7) is independent of the special lattice site. Then, using the Knotensatz, we obtain the functional equation (see ref.[5] for the detailed derivation of an analogical equation in the case of oscillator chains)

$$W_\sigma [\phi ; \omega] = (1-n_{-\sigma}) W_\sigma [2 \tan^{-1} (\omega - \cot \frac{\phi}{2}); \omega] + \\ + n_{-\sigma} W_\sigma [\tan^{-1} (\omega - U - \cot \frac{\phi}{2}); \omega] - W_\sigma [-\pi ; \omega] \quad (8)$$

in the range $0 \leq \phi < 2\pi$ and

$$W_\sigma [\phi + 2\pi ; \omega] = 1 + W_\sigma [\phi ; \omega] \quad (9)$$

elsewhere. Herein $n_{-\sigma}$ is the probability for an electron with spin $-\sigma$ at any site, resulting in the value 1 for the belonging g from (6), and $(1 - n_{-\sigma})$ is the probability for $g = 0$, respectively.

The density of states $D_\sigma (\omega)$ follows from (8) directly with

$$M_\sigma (\omega) = \int^{\omega} d\omega' \, D_\sigma (\omega') = -W_\sigma [-\pi ; \omega] \quad (10)$$

where $M_\sigma (\omega)$ is the integrated density of states.

For $U \to \infty$ we obtain from (8)

$$W_\sigma^\infty [\phi ; \omega] = (1-n_{-\sigma}) \{ W_\sigma^\infty [2 \tan^{-1} (\omega - \cot \frac{\phi}{2}); \omega] - W_\sigma^\infty [-\pi ; \omega] \} . \quad (11)$$

Consequently, also in the strong correlated limit the density of states can be calculated exactly.

3. Numerical Calculations

The functional equations (8) and (11) can be numerically solved dividing the range $0 \leq \phi < 2\pi$ into finite steps. Then a purely algebraic system of equations follows, which is solvable with usu-

al methods. As widths of steps are chosen $\Delta\phi = 2\pi/60$ and $\Delta\omega = 0.1$, for several special ranges also $\Delta\phi = 2\pi/120$ and $\Delta\omega = 0.01$. The numerical errors of $M_\sigma(\omega)$ are at most smaller than 2%, only for small U they are larger at the band edges. We have calculated $M_\sigma(\omega)$ and $D_\sigma(\omega)$ for $n_{-\sigma} = 0.01$, 0.1, 0.3, 0.5, 0.6, 0.8 and 0.99 and $U = 0.1$, 0.5, 1.41, 4.0, 20.0 and ∞. The numerical calculations are carried out at the BESM-6 in Dubna.

Some characteristic graphs of the integrated density of states $M_\uparrow(\omega)$ are plotted in the figures 1 and 2. A representation of $D_\uparrow(\omega)$ does not contain additional information, but by differentiation of $M_\uparrow(\omega)$ the errors are larger. Therefore we have renounced to draw $D_\uparrow(\omega)$.

4. Discussion

As is shown in fig. 1 and 2, the behaviour of the integrated density of states $M_\sigma(\omega)$ depends very sensitively on U as well as on $n_{-\sigma}$. At first, we obtain band splitting into two subbands, if U becomes greater than a critical value $U_c = 4$ $(= 2z\,T_{01}$, where z is the number of nearest neighbours). The centres of gravity of these subbands are separated by U and the maximal possible occupation of the lower and upper subband is given by $(1-n_{-\sigma})$ and $n_{-\sigma}$, respectively.

Furthermore we obtain a strong change of the form (in contradiction to Hubbard's simple approximation[1]), yielding especially at the band edges a significant flattening of the density of states. Thereby the singularities, which are typical for one-dimensional

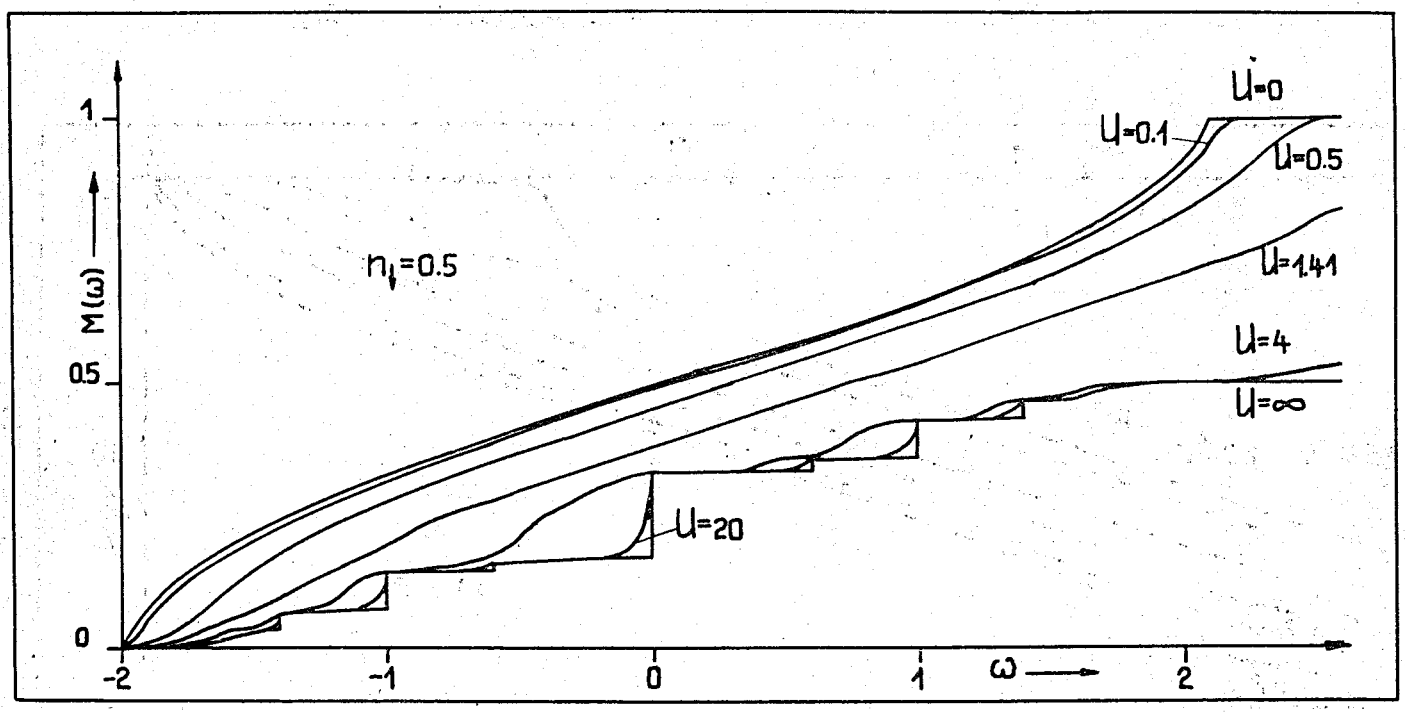

Fig. 1. Integrated density of states $M_{\uparrow}(\omega)$ in dependence on U for $n_{\downarrow} = 0.5$.

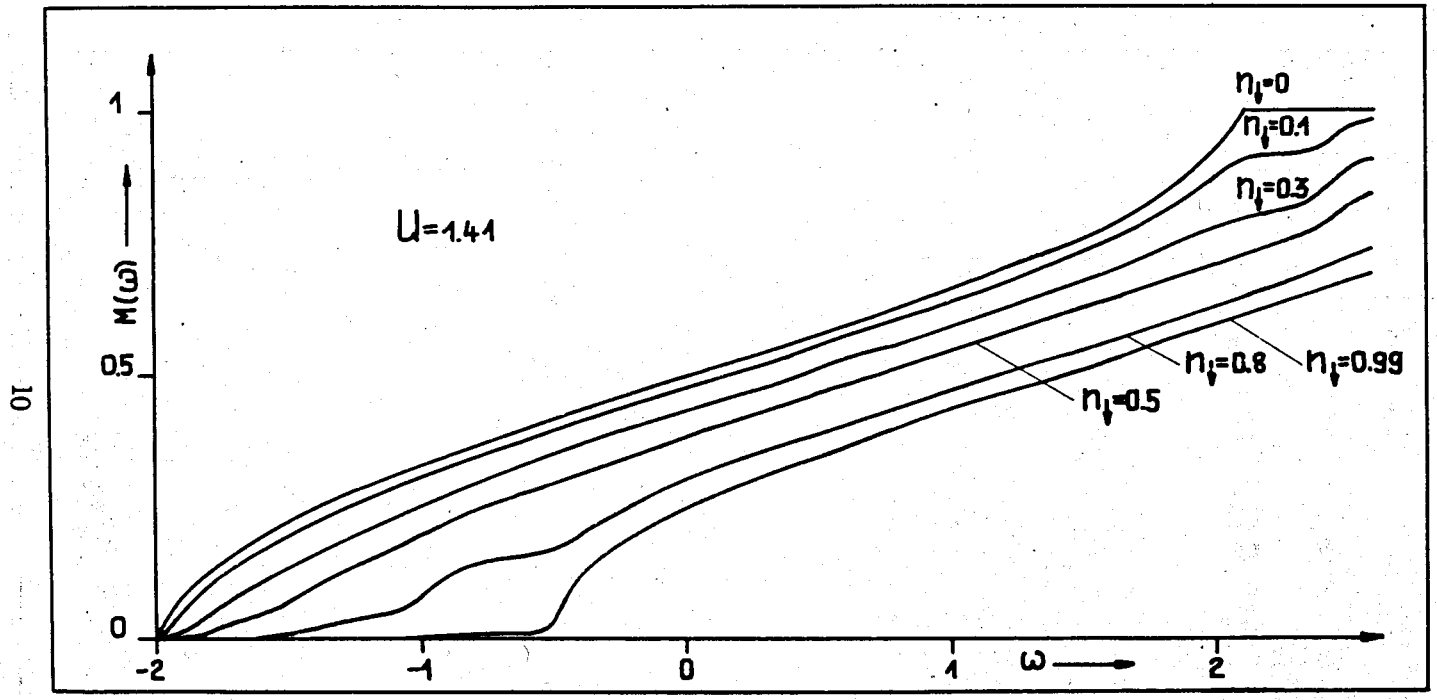

Fig. 2a. Integrated density of states $M_{\uparrow}(\omega)$ in dependence on $n_{\downarrow}$ for $U = 1.41$.

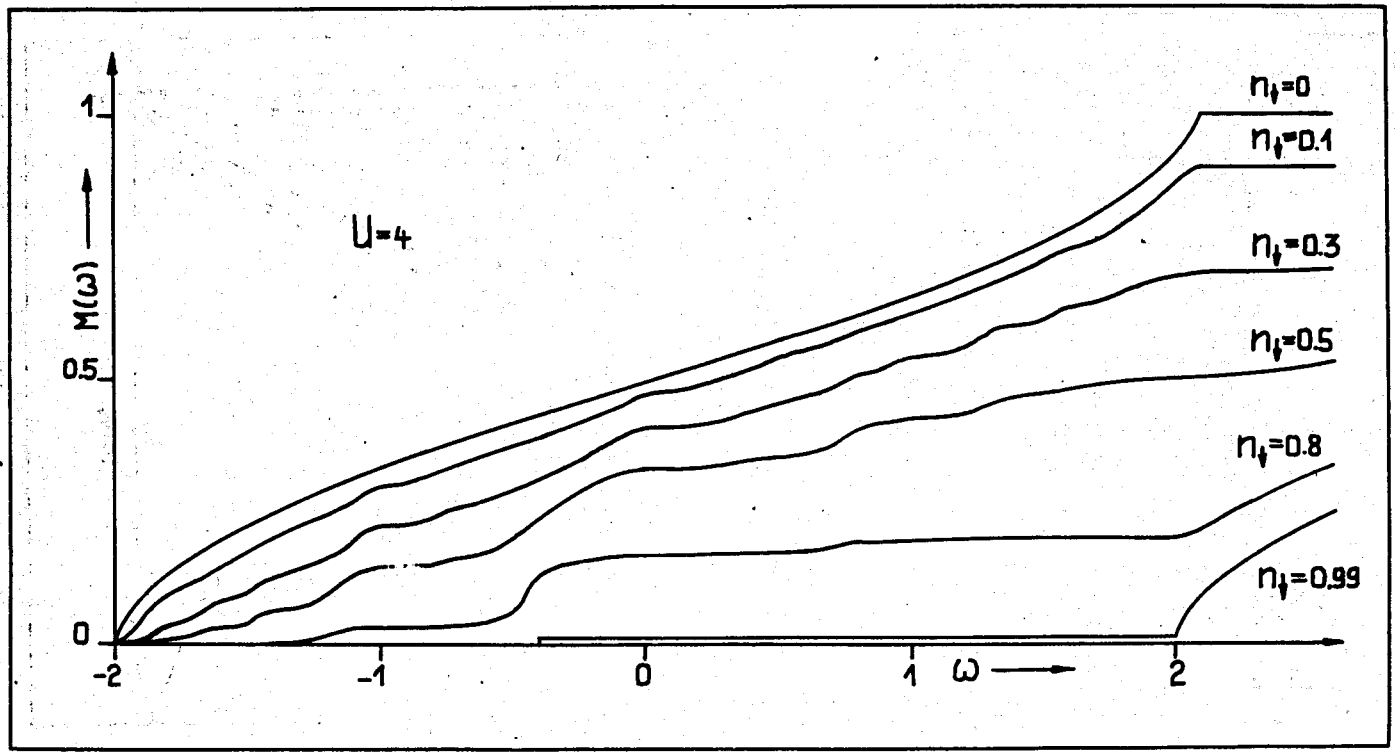

Fig. 2b. Integrated density of states $M_{\uparrow}(\omega)$ in dependence on $n_{\downarrow}$ for $U=4$.

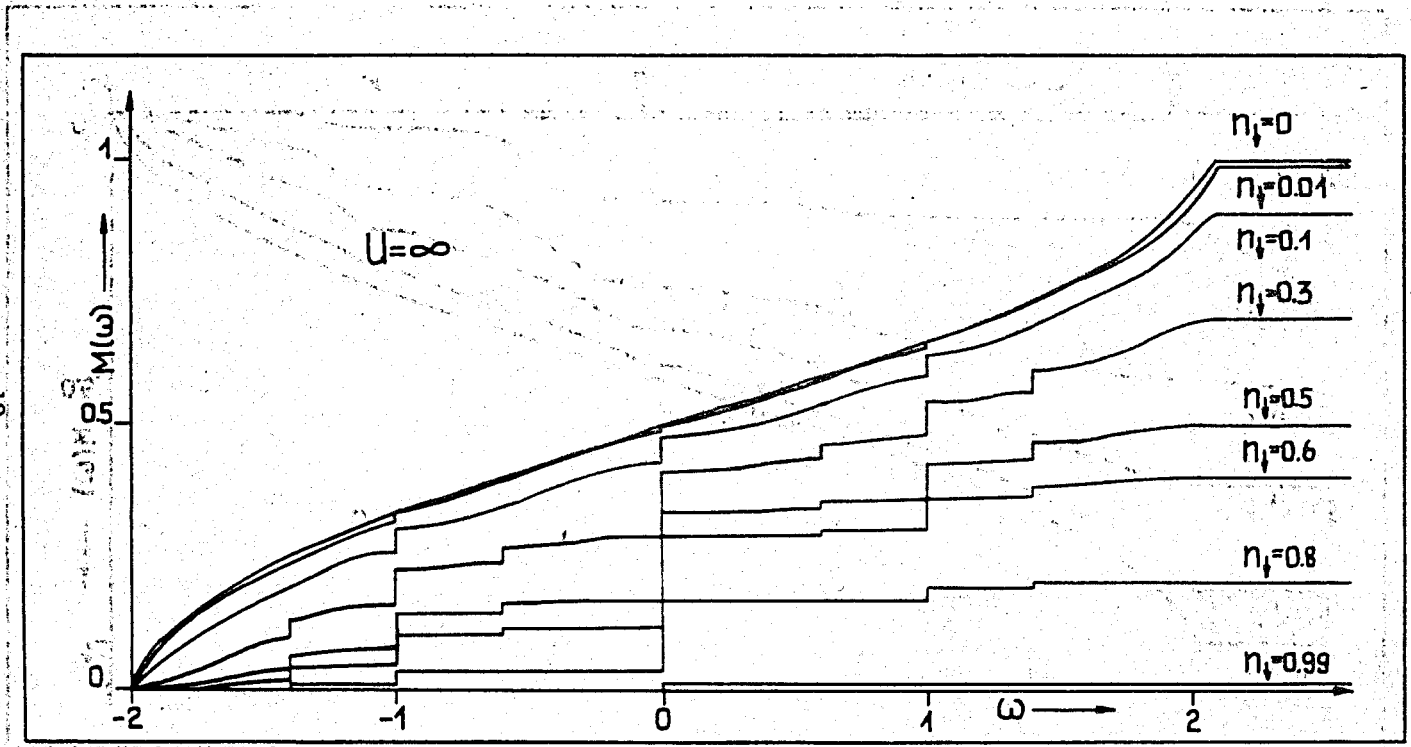

Fig. 2c. Integrated density of states $M_{\uparrow}(\omega)$ in dependence on $n_{\downarrow}$ for $U = \infty$.

systems, vanish. With increasing U and $n_{-\sigma}$ this flattening results in effective narrowing of the band, remaining flat tails extending out to the full free-particle width. For $U \to \infty$ and half-filled bands the bands are narrowed by a factor 0.707, which agrees well witn the approximate result 0.745 of Brinkman and Rice for the three-dimensional sc-lattice[6]. (However, as mentioned above, their prediction for the one-dimensional case is in contradiction with our result). By this effective narrowing the band splitting appears effectively at smaller values of U depending on $n_{-\sigma}$.

Especially it is worth noting the appearance of peaks in the density of states. These peaks become more significant with increasing U, their position depends also on U. At $U = \infty$ the peaks have the form of δ -functions; whereas their strength depends on $n_{-\sigma}$ their position is independent of $n_{-\sigma}$. The largest peak exists in the middle of the band $(\omega = 0)$ and reaches its maximal value at $n_{-\sigma} \sim 0.6$. The physical meaning of these peaks can be related to the existence of localized modes. It is even possible that they exist in such an extreme form only in the one-dimensional system. However, the absence of such peaks in all known approximations applied to the one-dimensional system seems to indicate, that these approximations do not contain the case $U \to \infty$.

Finally it is possible to study the magnetic nature of the ground state by means of different occupation of the up and down spin band. The result is, that for all values $n = n_\uparrow + n_\downarrow$ only the state $n_\uparrow = n_\downarrow$ is stable, in agreement with general properties of one-dimensional systems[7].

5. Concluding Remarks

From the exact solvable one-dimensional Hubbard-model we have obtained some interesting results. Of course, for generalization onto the three-dimensional case some restrictions are necessary. In any case the obtained complete band splitting, changing of form and effective band narrowing of the subbands have real meaning. Moreover, the sharp peaks in the density of states at large values of U indicate directions of further examinations, especially with respect to the basis of approximations.

The author wishes to thank W. John, P. Ziesche, W. Weller and J. Monecke for valuable discussions.

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Received by Publishing Department
on October 22, 1971.