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The Ground State Energy of the Hubbard Model in Hubbard's Approximation

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(Z. Naturforsch. **27 a**, 889—893 [1972]; received 24 March 1972)

We have calculated the ground state energy of the Hubbard model in the approximation of Hubbard's first paper [1]. For the neutral model with nearest neighbour interaction the energy resulting from the selfconsistent paramagnetic solution is compared with those ones following from the (ferromagnetic) Hartree-Fock and an (antiferromagnetic) single particle theory. The energy of the latter one turns out to be the best approximation of the true ground state energy of the model for all values of the coupling constant V_0, but the energy derived from Hubbard's approximation, in spite of the absence of magnetic ordering, is a reasonable approximation at least for sufficiently large values of V_0.

1. Introduction

During the last years the Hubbard model [1] of electron interactions in narrow energy bands has been the object of detailed investigations both with respect to its magnetic and its conductivity properties.

This model is stated by the Hamiltonian

$$H = \sum_{j,k,\sigma} T_{jk}\, c^+_{j\sigma}\, c_{k\sigma} + \frac{V_0}{2} \sum_{j,\sigma} n_{j\sigma}\, n_{j,-\sigma} \qquad (1)$$

where $c^+_{j\sigma}$ generates an electron of spin σ in a Wannier state centred at the lattice site $\boldsymbol{j}$, $n_{j\sigma} = c^+_{j\sigma}\, c_{j\sigma}$, T_{jk} is the hopping constant for electron transitions from the site $\boldsymbol{j}$ to $\boldsymbol{k}$ and V_0 is the matrix element of the Coulomb repulsion, which electrons of opposite spin feel, when they are brought together to the same lattice site.

Hubbard himself in a series of papers [1, 2] not only discusses the usual Hartree-Fock (HF) approach to this Hamiltonian (1) but also takes into account correlations between the electrons by introducing different decouplings of quantum statistical Greens functions. In his first paper [1, *] he uses a decoupling which gives interesting results for the band-splitting but does not yield a selfconsistent solution for ferromagnetism for reasonable shapes of the density of states of the free electrons, whereas, on the other hand the HF approach yields ferromagnetism for sufficiently strong coupling V_0. Later on a single particle (SP) approach [3, 4] to the Hamiltonian (1) was set up allowing for antiferromagnetic ordering of the electron-spins, which for the neutral model (i. e. number of electrons N_e = number of lattice sites N) led to the prediction of antiferromagnetism for all values of $V_0 > 0$. This theory may be deduced from a variational principle [3, 5], such giving an upper bound for the true groundstate energy of the problem and may be shown to yield a much better approximation to the groundstate energy than the HF approach does.

Recently this approach was extended to an investigation of the stability of antiferromagnetism versus ferromagnetism [5] with the result that (at least) for the neutral Hubbard model with nearest neighbour interactions the antiferromagnetic phase is stable for all values of the coupling V_0.

Contrary to these theories the decoupling of H I goes beyond a single particle approach and takes into account correlations between the band electrons.

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* This paper will be hereafter referred to as H I.

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Hubbard did not calculate the groundstate energy resulting from this approximation, but clearly it should be revealing to compare the energy for his self-consistent (i. e. paramagnetic) solution with those ones computed from the (ferromagnetic) HF and the (antiferromagnetic) SP approach mentioned above. This comparison shall be performed in the present paper for a neutral Hubbard model in a simple cubic lattice; but the formulae for the groundstate energy will be derived in full generality.

2. Formulation of the Green's Function Approach

Defining the groundstate energy as the zero-temperature limit of the internal energy we find

$$E_0 = \sum_{\boldsymbol{j},\boldsymbol{k},\sigma} T_{\boldsymbol{jk}} \langle c^+_{\boldsymbol{j}\sigma}\, c_{\boldsymbol{k}\sigma}\rangle_0 + \frac{V_0}{2}\sum_{\boldsymbol{j},\sigma}\langle n_{\boldsymbol{j}\,\sigma}\, n_{\boldsymbol{j},\,-\sigma}\rangle_0 . \quad (2)$$

where $\langle \ldots \rangle_0$ means the $T \to 0$ limit of the grand canonical average.

Making use of the famous relation [6]

$$\langle B\, A\rangle = i \lim_{\varepsilon \to +0}\int_{-\infty}^{+\infty} \mathrm{d}E \frac{\{\langle\langle A; B\rangle\rangle_{E+i\varepsilon} - \langle\langle A; B\rangle\rangle_{E-i\varepsilon}\}}{e^{\beta(E-\mu)}+1} \quad (3)$$

such averages may be derived from the knowledge of the respective temperature dependent Green's functions [6]. To become concrete, in order to derive E_0 we must consider the Green's functions

$$G^{\sigma}_{\boldsymbol{kj}}(E) = \langle\langle c_{\boldsymbol{k}\sigma}\,;\, c^+_{\boldsymbol{j}\sigma}\rangle\rangle_E \quad (4\,\mathrm{a})$$

and

$$\Gamma^{\sigma}_{\boldsymbol{kj}} = \langle\langle n_{\boldsymbol{k},-\sigma}\, c_{\boldsymbol{k}\sigma}\,;\, c^+_{\boldsymbol{j}\sigma}\rangle\rangle_E , \quad (4\,\mathrm{b})$$

which in fact are the same ones, which Hubbard considers in H I. After performing a decoupling of the hierarchy of Green's functions, he finds a system of equations, [Eqs. (43) and (50) of H I] by which G and Γ are coupled, and which read

$$E\, G^{\sigma}_{\boldsymbol{l}}(E) = \frac{1}{2\pi}\,\delta_{\boldsymbol{l},0} + \sum_{\boldsymbol{l}'} T_{\boldsymbol{l}'}\, G^{\sigma}_{\boldsymbol{l}-\boldsymbol{l}'} + V_0\, \Gamma^{\sigma}_{\boldsymbol{l}} \quad (5\,\mathrm{a})$$

and

$$\Gamma^{\sigma}_{\boldsymbol{l}}(E) = \frac{n_{-\sigma}}{E - V_0}\left\{\frac{1}{2\pi}\,\delta_{\boldsymbol{l},0} + \sum_{\boldsymbol{l}'} T_{\boldsymbol{l}'}\, G^{\sigma}_{\boldsymbol{l}-\boldsymbol{l}'}\right\}, \quad (5\,\mathrm{b})$$

when we allow for the fact that due to translation symmetry both $T_{\boldsymbol{jk}}$ and the Green's functions will depend only on the difference $\boldsymbol{l}$ of the lattice sites $\boldsymbol{j}$ and $\boldsymbol{k}$, to which they refer; $n_{-\sigma}$ is the expectation value $\langle n_{\boldsymbol{j},\,-\sigma}\rangle$, which Hubbard takes to be independent of the lattice site $\boldsymbol{j}$; this is equivalent to the assumption of ferromagnetic ordering.

These equations may be solved by a Fourier-transformation

$$G^{\sigma}_{\boldsymbol{q}}(E) = N^{-1/2}\sum_{\boldsymbol{l}} G^{\sigma}_{\boldsymbol{l}}(E)\, e^{-i\boldsymbol{q}\boldsymbol{l}} \quad (6)$$

with the results

$$G^{\sigma}_{\boldsymbol{q}}(E) = \frac{N^{-1/2}}{2\pi}\,\frac{E - V_0(1-n_{-\sigma})}{E(E-V_0) - \varepsilon_{\boldsymbol{q}}(E - V_0(1-n_{-\sigma}))}, \quad (7\,\mathrm{a})$$

$$\Gamma^{\sigma}_{\boldsymbol{q}}(E) = \frac{N^{-1/2}}{2\pi}\,\frac{E\, n_{-\sigma}}{E(E-V_0) - \varepsilon_{\boldsymbol{q}}(E - V_0(1-n_{-\sigma}))}. \quad (7\,\mathrm{b})$$

In these formulae $\varepsilon_{\boldsymbol{q}}$ means the Fourier transformed of $T_{\boldsymbol{l}}$

$$\varepsilon_{\boldsymbol{q}} = \sum_{\boldsymbol{l}} T_{\boldsymbol{l}}\, e^{-i\boldsymbol{q}\boldsymbol{l}} \quad (8)$$

and Eq. (7 a) is identical with Hubbards Eq. (54), but we have omitted the self-energy term T_0, which leads to a simple additive constant in the energy, because its contribution to the Hamiltonian (1) is diagonal for fixed number of electrons N_e.

3. Derivation of the Groundstate Energy

Now we are going to derive the groundstate energy E_0 from the Green's functions given by Equations (7).

At first we note that due to the linearity of both the averaging process and Eq. (3) the contribution of the first sum in (2) may be derived by application of (3) to the function

$$N\sum_{\boldsymbol{l},\sigma} T_{\boldsymbol{l}}\, G^{\sigma}_{\boldsymbol{l}}(E) = N^{1/2}\sum_{\boldsymbol{q},\sigma}\varepsilon_{\boldsymbol{q}}\, G^{\sigma}_{\boldsymbol{q}}(E) \quad (9\,\mathrm{a})$$

whereas for the second sum we can start from

$$\frac{V_0}{2}\sum_{\boldsymbol{j},\sigma}\Gamma^{\sigma}_{\boldsymbol{jj}}(E) = \frac{V_0}{2}\,N^{1/2}\sum_{\boldsymbol{q},\sigma}\Gamma^{\sigma}_{\boldsymbol{q}}(E). \quad (9\,\mathrm{b})$$

Moreover, G and Γ are rational functions, which can be denoted by

$$G^{\sigma}_{\boldsymbol{q}}(E) = \frac{N^{-1/2}}{2\pi}\,\frac{P^{\sigma}_1(E)}{Q^{\sigma}_{\boldsymbol{q}}(E)} \quad (10\,\mathrm{a})$$

and

$$\Gamma^{\sigma}_{\boldsymbol{q}}(E) = \frac{N^{-1/2}}{2\pi}\,\frac{P^{\sigma}_2(E)}{Q^{\sigma}_{\boldsymbol{q}}(E)}, \quad (10\,\mathrm{b})$$

where P_1, P_2 and Q_q are polynomials in E and $Q_q(E)$ is in common to G and Γ. Therefore these functions may be resolved into partial fractions by

$$G_q^\sigma(E) = \frac{N^{-1/2}}{2\pi} \sum_{\lambda=1,2} \frac{P_1^\sigma(E_{q\sigma}^\lambda)}{Q_q^{\sigma'}(E_{q\sigma}^\lambda)} \frac{1}{E-E_{q\sigma}^\lambda} \tag{11 a}$$

and

$$\Gamma_q^\sigma(E) = \frac{N^{-1/2}}{2\pi} \sum_{\lambda=1,2} \frac{P_2^\sigma(E_{q\sigma}^\lambda)}{Q_q^{\sigma'}(E_{q\sigma}^\lambda)} \frac{1}{E-E_{q\sigma}^\lambda} \tag{11 b}$$

where $E_{q,\sigma}^\lambda$ are the two roots of $Q_q^\sigma(E)$ for fixed $\boldsymbol{q}$ and σ and $Q_q^{\sigma'}(E_{q\sigma}^\lambda)$ is the derivative $\mathrm{d}Q/\mathrm{d}E$ taken at the point of the zero $E_{q\sigma}^\lambda$.

Having inserted (11) into (9) we may apply the relation (3) and with help of Dirac's identity we get the result

$$E_0^{(1)} = \sum_{j,k,\sigma} T_{jk} \langle c_{j\sigma}^+ c_{k\sigma} \rangle_0 = \sum_\sigma \int_{-\infty}^{\mu} \mathrm{d}E \sum_q \varepsilon_q \varrho_{q\sigma}^{(1)}(E) \tag{12 a}$$

and

$$E_0^{(2)} = \frac{V_0}{2} \sum_{\lambda,\sigma} \langle n_{j\sigma} n_{j,-\sigma} \rangle_0 = \frac{V_0}{2} \sum_\sigma \int_{-\infty}^{\mu} \mathrm{d}E \sum_q \varrho_{q\sigma}^{(2)}(E) \tag{12 b}$$

with functions $\varrho^{(1)}$ and $\varrho^{(2)}$ given by

$$\varrho_{q\sigma}^{(1)}(E) = \sum_{\lambda=1,2} \frac{P_1^\sigma(E_{q\sigma}^\lambda)}{Q_q^{\sigma'}(E_{q\sigma}^\lambda)} \delta(E-E_{q\sigma}^\lambda), \tag{13 a}$$

$$\varrho_{q\sigma}^{(2)}(E) = \sum_{\lambda=1,2} \frac{P_2^\sigma(E_{q\sigma}^\lambda)}{Q_q^{\sigma'}(E_{q\sigma}^\lambda)} \delta(E-E_{q\sigma}^\lambda), \tag{13 b}$$

respectively.

Next we shall connect these expressions with the density of states functions of the free electrons. By means of a straightforward discussion of the zeros of the polynomials P and Q we find that $\varrho_{q\sigma}^{(1)}(E)$ may be written as

$$\begin{aligned}\varrho_{q\sigma}^{(1)}(E) &= |P_1^\sigma(E)| \sum_\lambda \frac{\delta(E-E_{q\sigma}^\lambda)}{|Q_q^{\sigma'}(E_{q\sigma}^\lambda)|} \\ &= |E-V_0(1-n_{-\sigma})|\, \delta(Q_q^\sigma(E))\end{aligned} \tag{14 a}$$

whereas

$$\varrho_{q\sigma}^{(2)}(E) = n_{-\sigma} \Lambda(E)\, E\, \delta(Q_q^\sigma(E)) \tag{14 b}$$

holds, with

$$\Lambda(E) = \begin{cases} -1: & E < V_0(1-n_{-\sigma}), \\ +1: & E > V_0(1-n_{-\sigma}). \end{cases} \tag{15}$$

Inserting the explicit expressions for $Q_q^\sigma(E)$ into the δ-functions we find in the next step

$$\begin{aligned}\varepsilon_q \varrho_{q\sigma}^{(1)}(E) &= \varepsilon_q \delta\left\{\frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})} - \varepsilon_q\right\} \qquad (16\text{ a}) \\ &= \frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})} \delta\left\{\frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})} - \varepsilon_q\right\}\end{aligned}$$

and

$$\varrho_{q\sigma}^{(2)}(E) = \frac{n_{-\sigma}E}{E-V_0(1-n_{-\sigma})} \delta\left\{\frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})} - \varepsilon_q\right\}. \tag{16 b}$$

Hence, inserting these formulae into Eqs. (12) and using the relation

$$\delta(a-x) = \int_{-\infty}^{+\infty} \mathrm{d}t\, \delta(a-t)\, \delta(t-x) \tag{17}$$

we get the relatively simple expressions

$$E_0^{(1)} = N \sum_\sigma \int_{-\infty}^{\mu} \mathrm{d}E \frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})} g\left(\frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})}\right) \tag{18 a}$$

and

$$E_0^{(2)} = N \frac{V_0}{2} \sum_\sigma n_{-\sigma} \int_{-\infty}^{\mu} \mathrm{d}E \frac{E}{E-V_0(1-n_{-\sigma})} g\left(\frac{E(E-V_0)}{E-V_0(1-n_{-\sigma})}\right), \tag{18 b}$$

where $g(E)$ is the density of states of the electrons in the absence of interaction, which is defined by

$$g(E) = \frac{1}{N} \sum_q \delta(E-\varepsilon_q) \tag{19}$$

and $g(E(E-V_0)/[E-V_0(1-n_{-\sigma})])$ is the density of states of the pseudo-particles, which Hubbard denotes by $\varrho_\sigma(E)$ in his paper.

4. Application to the Neutral Hubbard Model

Now we are specializing the formulae (18) to the case of the neutral Hubbard model, which is characterized by the equation

$$n_\sigma + n_{-\sigma} = 1; \tag{20}$$

for this case, as has been rigorously proven [7], the chemical potential has the value of $\mu = V_0/2$.

On the other hand we take into account Hubbards important result, that the only self-consistent solution, which exists for a wide class of density functions $g(E)$ is the paramagnetic one with $n_\sigma = n_{-\sigma} = \frac{1}{2}$.

For this case Eqs. (18) simplify to

$$E_0^{(1)} = 2N \int_{-\infty}^{V_0/2} dE \, \frac{E(E-V_0)}{E-V_0/2} \, g\left(\frac{E(E-V_0)}{E-V_0/2}\right) \quad (21\,a)$$

and

$$E_0^{(2)} = N \frac{V_0}{2} \int_{-\infty}^{V_0/2} dE \, \frac{E}{E-V_0/2} \left(\frac{E(E-V_0)}{E-V_0/2}\right) \quad (21\,b)$$

and just the lower one of the two splitted bands is filled up by pseudo-particles.

In these formulae it is possible to eliminate the rational function from the density of states by performing the substitution

$$\varepsilon = E(E-V_0)/(E-V_0/2) \quad (22)$$

which finally leads to the result

$$E_0^{(1)} = -N \int_{-\infty}^{+\infty} d\varepsilon \, g(\varepsilon) \, \frac{\varepsilon^2}{\sqrt{\varepsilon^2 + V_0^2}} \quad (23\,a)$$

and

$$E_0^{(2)} = N \left\{ \frac{V_0}{4} - \frac{V_0^2}{4} \int_{-\infty}^{+\infty} d\varepsilon \, g(\varepsilon) \, \frac{1}{\sqrt{\varepsilon^2 + V_0^2}} \right., \quad (23\,b)$$

thus that the groundstate energy E_0 resulting from the paramagnetic solution of the decoupling of H I is given by

$$E_0 = N \left\{ \frac{V_0}{4} - \int_{-\infty}^{+\infty} d\varepsilon \, g(\varepsilon) \left(\frac{\varepsilon^2 + V_0^2/4}{\sqrt{\varepsilon^2 + V_0^2}} \right) \right\}. \quad (24)$$

5. Comparison of E_0 with the Energies derived from the HF and SP Approaches

We have numerically evaluated Eq. (24) for the case of the s.c. lattice and nearest-neighbour interaction, where the free particle density of states $g(\varepsilon)$ is wellknown [8].

The curve E_0/N versus V_0 is plotted in Fig. 1 in solid lines and is compared with the approximations of the groundstate energy resulting from the antiferromagnetic SP theory (curve SP) and from the HF approach [9] (curve HF). From this comparison we may draw several remarkable conclusions. At first, we see that under all compared methods the antiferromagnetic single particle theory yields the lowest energy for all values of V_0 and – because it has been calculated by a variational procedure – it yields the best approximation of the true groundstate energy of the neutral Hubbard model. The HF-energy lies higher everywhere and is a poor approximation especially for large values of V_0.

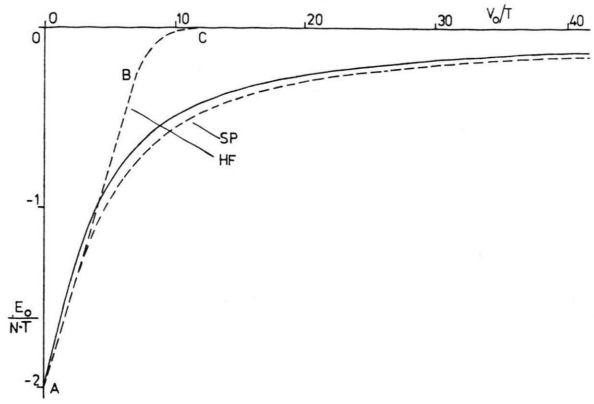

Fig. 1. Approximations of the groundstate energy versus V_0 in the s.c. lattice. – T is the nearest neighbour coupling constant. The solid curve is the energy calculated on the basis of H I, the curve SP is the result of a variational single particle approach [5] and HF is the energy of the Hartree-Fock approach to the same problem. For the s.c. lattice it consists of the straight line ($A\,B$) for values of V_0, where this approach leads to paramagnetism, the curve ($B\,C$) for the range of couplings, where it is partially magnetized, and the abscissa for $V_0 > 2\,\Delta$ (point C, with $2\,\Delta$ is the width of the band of the free electrons). For these couplings the HF approach yields a complete saturated groundstate.

On the other hand the curve derived on the basis of Hubbard's decoupling procedure yields a much more reasonable approximation for sufficiently large V_0, though this approach does not allow for any kind of magnetic ordering. The somewhat astonishing fact is, that it is for small V_0 a poorer approximation than the simple HF approach (which for the s.c. lattice [5] also leads to paramagnetism in this range of the coupling constant).

To attempt an interpretation of these results we may conclude that the electron correlations incorporated in H I bring about a simulation of part of the effects of antiferromagnetic ordering, which is present in the SP approach but absent in H I.

There is no *ferromagnetic* ordering in Hubbard's approach. Would there be *antiferromagnetism* in the same decoupling of the Green's functions, when we allow the expectation values $\langle n_{j\sigma} \rangle$ to vary periodically in the lattice? This question will be investigated in a subsequent paper.

Acknowledgement

The possibility of carrying out the computations at the Rechenzentrum der Universität Kiel is gratefully acknowledged.

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On the Foundation of Quantal Proposition Systems

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(Z. Naturforsch. **27 a**, 893—900 [1972]; received 18 January 1972)

We investigate the arguments recently given by Jauch and Piron that quantal proposition systems form a complete atomic lattice. Our analysis shows that the reasoning of these authors can not establish the intended result.

1. Introduction

In recent years great efforts have been undertaken to axiomatize quantum mechanics (QM) in the frame of the *proposition calculus*[1,2]. This research aims to deduce QM from a series of simpler and physically well established principles and to clear up to what extend the Hilbert space formalism of QM is uniquely determined by experience — or what other mathematical structures could be used to formulate QM. The justification of the Hilbert space formalism of QM on the basis of the proposition calculus is composed of two parts. The first part consists in elucidating the abstract lattice structure of quantum-mechanical (qm) proposition systems and in tracing back its characteristics to physical principles well confirmed by experience[1,4]; the second part deals with the mathematical representation of qm propositions by closed linear subspaces of an appropriate vector space and aims to justify the distinction of the Hilbert space as the only admissible representation space[4,5,6]. In both parts one still faces open questions and essential characteristics of the Hilbert space formalism of QM are still lacking a convincing experimental confirmation.

Now, in a recent paper[7], JAUCH and PIRON have tried to substantiate the vital lattice-theoretic properties of quantal proposition systems by means of new proof-ideas and relying on the (partly) new hypothesis that every qm object is always in a homogeneous state whereas nonhomogeneous states represent only ensembles of qm objects as a whole (in the sense of *macro-states*)[8]. In detail, Jauch and Piron made the following considerations.

(a) By an explicit instruction for combining special experiments, they try to prove that the propositions of a qm system form a complete lattice.

(b) They define a state concept for QM without recourse to probabilistic concepts.

(c) From the considerations (a) and (b) and the new state hypothesis they derive the atomicity of the proposition lattice.

(d) Finally, Jauch and Piron try to derive the covering law for quantal proposition systems from additional assumptions about the existence of ideal measurements of the first kind.

The present paper examines, by analysing the points (a) to (c), to what extent the reasonings of Ref. [7] really substantiate the asserted lattice structure of quantal proposition systems[9]. For this purpose we accept, disputandi causa, the new state hypothesis though this author does not believe in an experimental decision in favour of this hypothesis as far as it contradicts QM. Our analysis leads to the result that the argumentation of Ref.[7] fails to show that the propositions (0-1-observables) of a qm system form a complete, atomic lattice. Moreover it turns out that a "probability-free" introduction of homogeneous quantum states must be founded on different basic concepts than those used in Ref. [7].

2. The Assumptions of Jauch and Piron

To keep the present paper self-contained, we will first repeat the concepts, considerations and as-

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