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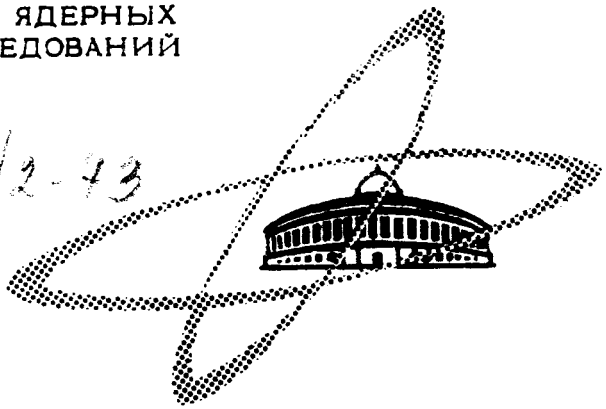

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ANALYTICAL AND NUMERICAL RESULTS OF THE HUBBARD MODEL IN SIMPLE APPROXIMATIONS

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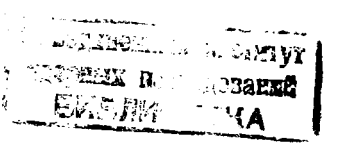

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To study the electron correlation in narrow bands the Hubbard model /1/

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

is frequently used. In (1) $c^{+}_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator of an electron with spin $\sigma\ (=\pm 1)$ in a Wannier state at the site i, T_{ij} is the hopping integral, and U describes the interaction between electrons at the same lattice site. Since (1) describes a many-body system, the corresponding equations of motion for the n-particle Green's functions $G^{(n)}(\omega)$ can be solved only approximately /2-6/. Then, for instance, from the solution for $G^{(1)}(\omega)$ one obtains the one-particle density of states

$$D(\epsilon) = -\frac{1}{\pi N}\, Im\, Tr G^{(1)}(\epsilon + i\delta), \qquad \delta \gtrsim 0. \qquad (2)$$

Unfortunately analytical expressions for $D(\epsilon)$ are only available within the framework of the Hartree-Fock approximation or using Hubbard's decoupling procedure /1/. Then the resulting expressions depend on the density of states $D^{0}(\epsilon)$ of the unperturbed system ($U = 0$, band width $= 2w$), the electron density $n = N_e / N$, and the magnetic structure of the considered states. In most cases only the "neutral" model $(n = 1)$ is considered /7/. Since the operator (1) is proposed to be a model Hamiltonian for narrow d-bands, also the case $n < 1$ is of interest (the case $n > 1$ follows by permutation of electrons and holes).

In the following at first some analytical results of the two mentioned approximations are considered. Further numerical results for the energy of some particular states (paramagnetic [PM], antiferromagnetic [AF] and ferromagnetic [FM] state) are discussed.

In the framework of Hubbard's decoupling procedure one obtains the system of equations[1]

$$\omega G^{(1)}_{ij\sigma}(\omega) = \delta_{ij} + \sum_{\ell} T_{i\ell} G^{(1)}_{\ell j\sigma}(\omega) + U \tilde{G}^{(2)}_{ij\sigma}(\omega), \tag{3}$$

$$(\omega - U)\tilde{G}^{(2)}_{ij\sigma}(\omega) \approx \langle n_{i,-\sigma} \rangle \delta_{ij} + \langle n_{i,-\sigma} \rangle \sum_{\ell} T_{i\ell} G^{(1)}_{\ell j\sigma}(\omega) \tag{4}$$

(with a special two-particle Green's function $\tilde{G}^{(2)}(\omega)$). Using the ansatz

$$\langle n_{i,\sigma} \rangle = \begin{cases} \frac{n}{2} \\ \frac{n}{2}(1 \pm \sigma) \\ n\,\delta_{\sigma,+1} \end{cases} \quad \text{in a sublattice } \begin{matrix} A \\ B \end{matrix} \text{ for } \begin{cases} PM \\ AF \\ FM \end{cases} \tag{5}$$

(in the AF-state we consider only the case $T_{\vec{k}+\vec{Q}} = -T_{\vec{k}}$, where $(\vec{R}_i^A - \vec{R}_i^B)\cdot\vec{Q} = \pi$ and $T_{\vec{k}}$ = the Fourier transformation of T_{ij}) from (2) one obtains

$$D^{PM}_{H,\sigma}(\epsilon) = D^0\left(\frac{\epsilon(\epsilon - U)}{\epsilon - U(1 - \frac{n}{2})}\right), \tag{6}$$

$$D^{AF}_{H,\sigma}(\epsilon) = \frac{|\epsilon - U(1 - \frac{n}{2})|}{\sqrt{(\epsilon - U)(\epsilon - U(1-n))}} D^0\left(\epsilon\sqrt{\frac{\epsilon - U}{\epsilon - U(1-n)}}\right) \times \tag{7}$$

$$\times [\Theta(\epsilon - U) + \Theta(U(1-n) - \epsilon)],$$

$$D^{FM}_{H,\sigma}(\epsilon) = D^0(\epsilon)\delta_{\sigma,+1} + D^0\left(\frac{\epsilon(\epsilon - U)}{\epsilon - U(1-n)}\right)\delta_{\sigma,-1}. \tag{8}$$

(In (7) $\Theta(x)$ is the step function).

From (6), (7) and (8), expressions follow for band widths and eventually existing gaps. In the PM state a band splitting exists at all U and n with a gap of the width

$$\Delta = \frac{1}{2}\left[\sqrt{(U+w)^2 - 2wUn} + \sqrt{(U-w)^2 + 2wUn} - 2w\right]. \tag{9}$$

The presence of the gap even for $U \to \sigma$ ($\Delta \sim U^2$)[1] shows once more the inadequacy of this decoupling at small U.

The AF state also always splits in two subbands [8]. The upper bound of the gap is situated at $\epsilon = U$, the gap width is approximately $\Delta \simeq U n$. At $\epsilon = U$ a singularity in the density of states exists. In the case $n = 1$ a second singularity exists at $\epsilon = 0$. The vanishing of this second singularity in the case $n < 1$ seems to be an essential cause for the fact, that the ground state is antiferromagnetic if $n = 1$, but not in the case $n \neq 1$.

In the FM state a gap with the width

$$\Delta = \frac{1}{2}\left[U - 3w + \sqrt{(U+w)^2 - 4Uwn} \right] \tag{10}$$

exists, if $U > 2w/(2-n)$.

In the framework of the Hartree-Fock approximation $\tilde{G}^{(2)}(\omega)$ is approximated by

$$\tilde{G}^{(2)}_{ij\sigma}(\omega) \approx \langle n_{i,-\sigma} \rangle G^{(1)}_{ij\sigma}(\omega). \tag{11}$$

This yields (with (5))

$$D^{PM}_{H.-F.,\sigma}(\epsilon) = D^0\left(\epsilon - U\frac{n}{2}\right), \tag{12}$$

$$D^{AF}_{H.-F.,\sigma}(\epsilon) = \frac{\left|\epsilon - U\frac{n}{2}\right|}{\sqrt{\epsilon(\epsilon - Un)}} D^0\left(\sqrt{\epsilon(\epsilon - Un)}\right) \times \left[\Theta(\epsilon - Un) + \Theta(-\epsilon)\right], \tag{13}$$

$$D^{FM}_{H.-F.,\sigma}(\epsilon) = D^0(\epsilon)\delta_{\sigma,+1} + D^0(\epsilon - Un)\delta_{\sigma,-1}. \tag{14}$$

From (12) it follows, that in the PM state a gap does not exist for no values of U and n. Therefore this approximation (replacement of $\langle n_{i\sigma} \rangle$ by the average on all lattice sites) is very bad at larger U, and a CPA calculation [9] (that means a random distribution of $\langle n_{i,\sigma} \rangle$) should give better results. For instance in the CPA a gap appears above a critical U_c. But since the CPA can be done only for a given $D^0(\epsilon)$, the results will be discussed further below.

In the AF state of the Hartree-Fock approximation a gap exists with the width $\Delta = Un$; simultaneously two singularities at the gap bounds $\epsilon = 0$ and $\epsilon = Un$. In the case $n = 1$ the Fermi energy lies in the gap so that the occurrence of the gap is connected with energy

gain, which makes the AF state stable. For $n < 1$, however, the Fermi energy lies in the lower subband below both singularities and this argument does not hold.

In the FM state a gap exists if $U > 2w/n$ (width $\Delta = Un - 2w$).

The comparison of (13) and (14) with (7) and (8) shows, that in the AF and the FM state the Hartree-Fock approximation and Hubbard's decoupling procedure yield equivalent results in the case $n = 1$.

Let us now consider the energy of the states discussed above. Corresponding to (1)

$$E = -\frac{1}{\pi}\int_{-\infty}^{\zeta} d\omega\, \Sigma\, [T_{ij}\, Im\, G^{(1)}_{ij\sigma}(\omega + i\delta) + \frac{U}{2}\delta_{ij}\, Im\, \tilde{G}^{(2)}_{ii\sigma}(\omega + i\delta)], \qquad (15)$$

where ζ is the chemical potential. Using the approximate expressions (4) or (11) for $\tilde{G}^{(2)}(\omega)$ in terms of $G^{(1)}(\omega)$, E can be rewritten in terms of an integral on $D(\epsilon)$:

$$E^{PM}_{H} = 2N \int_{-\infty}^{\zeta} d\omega\, \frac{\omega\,(\omega - U(1 - \frac{n}{4}))}{\omega - U(1 - \frac{n}{2})}\, D^{PM}_{H,+1}(\omega), \qquad (16)$$

$$E^{AF}_{H} = 2N \int_{-\infty}^{\zeta} d\omega\, \frac{\omega\,(\omega - U(1 - \frac{n}{4}))}{\epsilon - U(1 - \frac{n}{2})}\, D^{AF}_{H,+1}(\omega), \qquad (17)$$

$$E^{FM}_{H} = N \int_{-\infty}^{\zeta} d\omega\, [\omega\, D^{FM}_{H,+1}(\omega) + \frac{\omega\,(\omega - U(1 - \frac{n}{2}))}{\omega - U(1 - n)}\, D^{FM}_{H,-1}(\omega)]. \qquad (18)$$

Analogous expressions follow in the Hartree-Fock approximation.

Since $D(\epsilon)$ is given in terms of $D^0(\epsilon)$, we need only to know the unperturbed density of states $D^0(\epsilon)$ in order to be able to compute the energy E. A good approximation for narrow isolated bands is

$$D^0(\epsilon) = \frac{2}{\pi}\sqrt{1 - \epsilon^2}\;\Theta(1 - |\epsilon|), \qquad (19)$$

where the band width $w = 1$. (The case $w \neq 1$ follows by the transformation $U \to U/w$.

In fig. 1 the numerical results versus U are plotted for the cases $n = 1$ and $n = 0.5$. At $n = 1$ the ground state is antiferromagnetic in both considered approximations, if $U < U_{crit}$. At larger U, the ground state is paramagnetic. The phase transition AF - PM occurs at $U = U_{crit} \approx 3$ (Hubbard) or 4 (Hartree-Fock). At $n = 0.5$ the

situation is more complicated. Figure 2 shows the energy versus n at $U=1$. The dependence on n agrees well with general properties of the Hubbard model (AF at $n \simeq 1$, PM at $n \simeq 0$, FM only in a small region of n [10,11]. In fig. 1 and 2 the numbers denote: 1-PM, 2-AF, 3-FM in Hubbard's approximation, 4-PM, 5-AF, 6-PM in the Hartree-Fock approximation, and 7-PM in the CPA.

Since the PM state is very badly approximated by the usual Hartree-Fock method ($\langle n_{i,\sigma} \rangle = \frac{n}{2}$), the results of a CPA calculation[9] are considered also. In the CPA

$$E^{PM}_{CPA} = -\frac{2N}{\pi} Im \int_{-\infty}^{\zeta} d\omega \, (\omega - \frac{1}{2} W(\omega)) \int d\epsilon \frac{D^0(\epsilon)}{\omega - W(\omega) - \epsilon}, \qquad (20)$$

where the complex coherent potential $W(\epsilon)$ follows from

$$W(\omega) = \frac{Un}{2} + W(\omega)(U - W(\omega)) \int d\epsilon \frac{D^0(\epsilon)}{\omega - W(\omega) - \epsilon}. \qquad (21)$$

In the CPA a gap appears, if $U > w$; the gap width $\Delta \approx Un - \sqrt{2}w$ (for $U \gg w$).

Thus, at least at $n \simeq 1$, the results of both considered approximation, Hartree-Fock (with a CPA treatment of the PM case) and Hubbard's approach, are in a qualitative agreement, although the basic assumptions of these approximations are very different. Thus it can be presumed, that these qualitative results show a general behaviour of the model (1), and are not caused by the approximations used.

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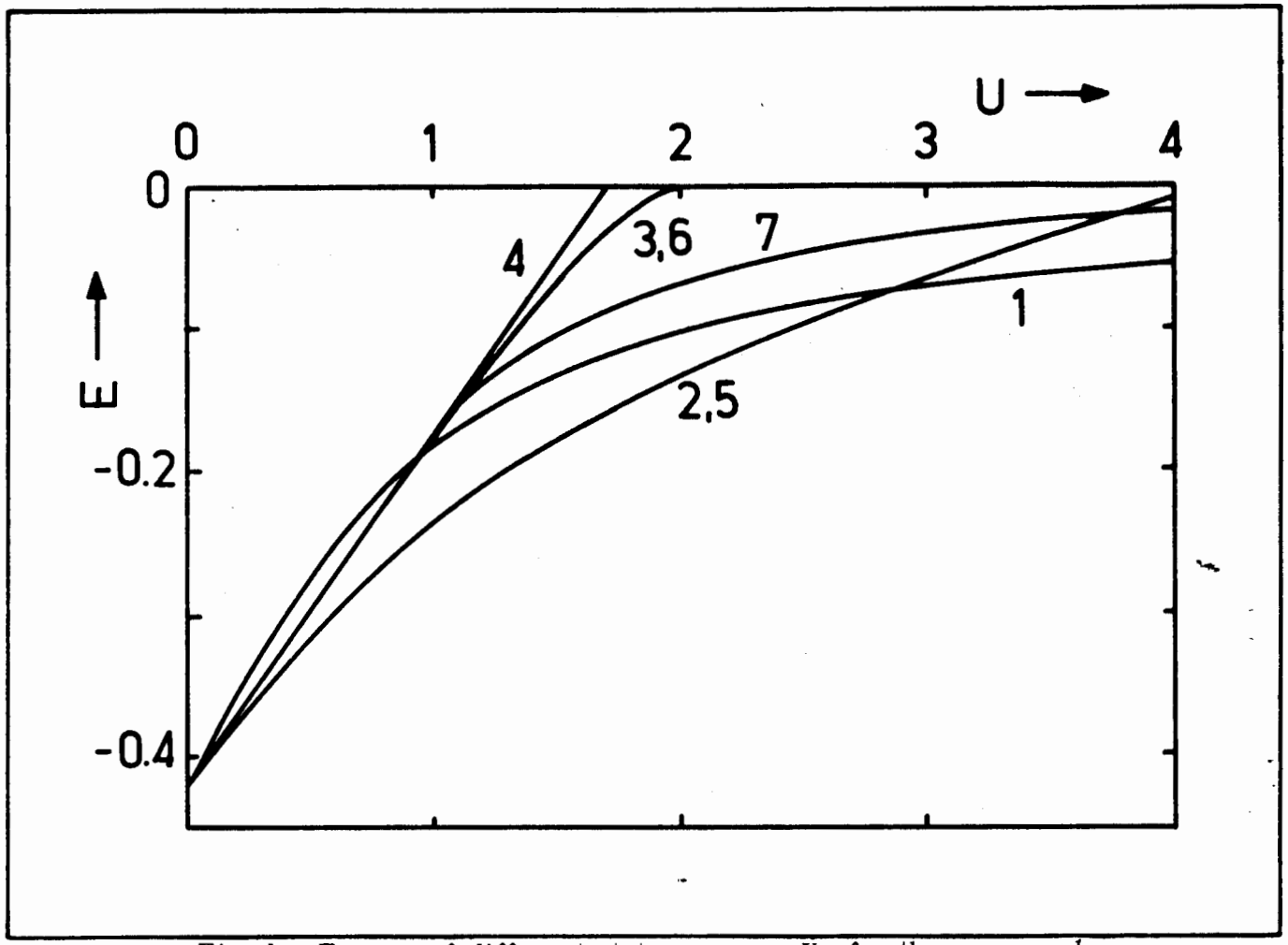

Fig. 1a. Energy of different states versus U for the case $n = 1$.

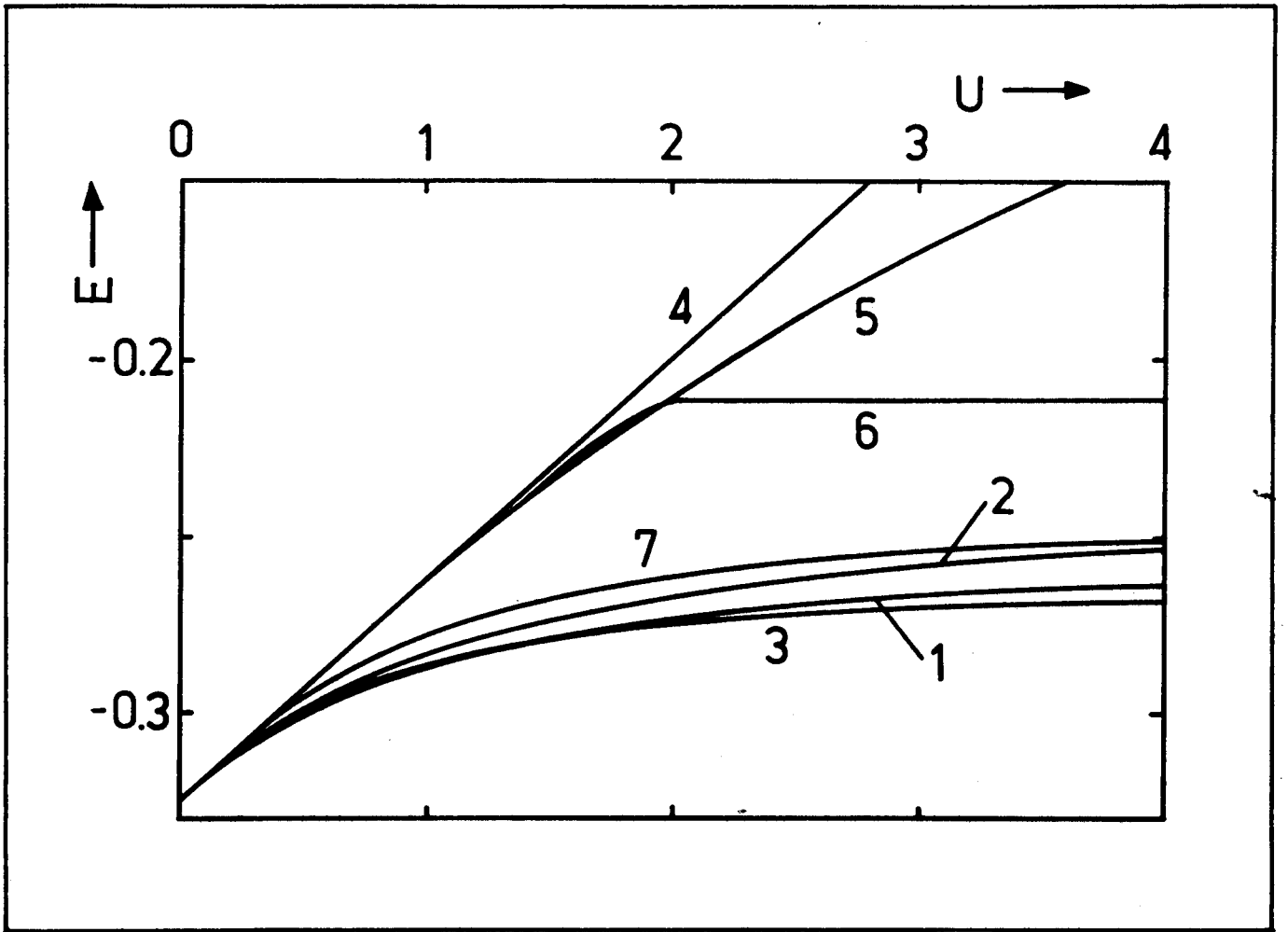

Fig. 1b. Energy of different states versus U for the case $n=0.5$.

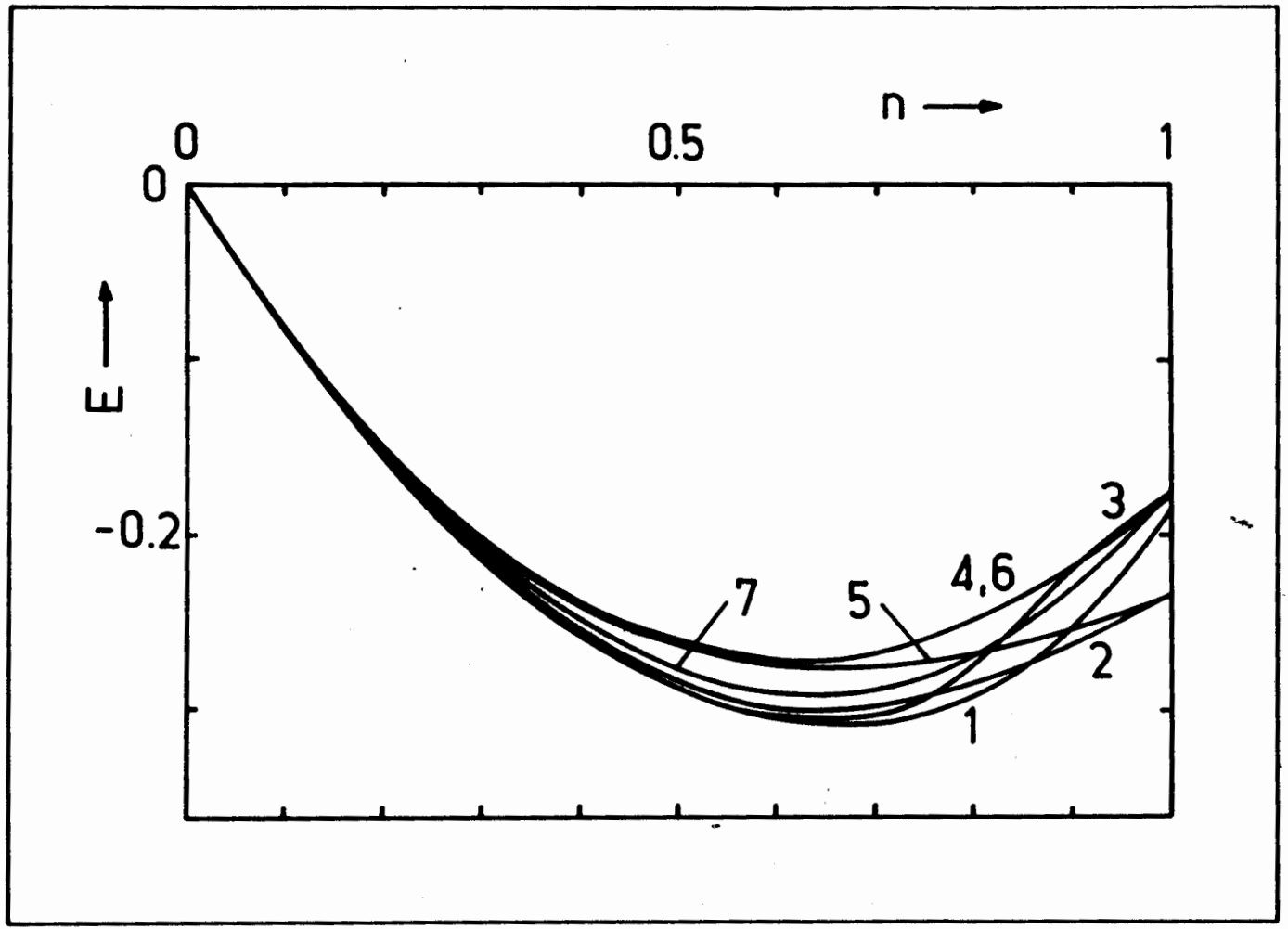

Fig. 2. Energy of different states versus n at $U = 1$.