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I. STATES WITH ONE PAIR OF COMPLEX WAVENUMBERS

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ABSTRACT

Those excited states of a half filled 1-d Hubbard chain are studied which are connected with electron pairs occupying the same sites. It is argued, that these states are to be described by such solutions of the Lieb-Wu equations in which some of the wavenumbers are complex. Solutions of this type, corresponding to $S^z = 1/2N-1$ and singlet states are found. The energy-momentum dispersion is also calculated. The gap in the spectrum of the singlet excitations is found to be equal to the discontinuity of the chemical potential calculated by Lieb and Wu.

АННОТАЦИЯ

Исследуются возбужденные состояния полузаполненных Хуббард-цепей, которые связаны с электронными парами, занимающими одинаковое место. Показано, что эти состояния описываются решениями уравнения ЛИБ-ВУ, содержащими комплексные волновые векторы. Найдены решения уравнения ЛИБ-ВУ, содержащие одну пару комплексных волновых векторов, соответствующие $S^z = 1/2\ N-1$ и синглетному спиновым состояниям. В обоих случаях определяются дисперсионные соотношения энергии-импульса. "Gap" в спектре синглетных возбуждений соответствует скачку химического потенциала, вычисленному Либ и Ву.

KIVONAT

A félig töltött Hubbard láncok azon gerjesztett állapotait vizsgáljuk, amelyek azonos rácshelyet elfoglaló elektron-párokkal kapcsolatosak. Megmutatjuk, hogy ezeket az állapotokat a Lieb-Wu egyenletek komplex hullámszámot is tartalmazó megoldásai irják le. Megkeressük a Lieb-Wu egyenletek $S^z = 1/2N-1$ és singlet spinállapotoknak megfelelő egy komplex hullámszám-párt tartalmazó megoldásait. Mindkét esetre meghatározzuk az energia-momentum diszperziót is. A singlet gerjesztések spektrumában található gap azonos a kémiai potenciál Lieb és Wu által kiszámolt ugrásával.

1. INTRODUCTION

The one-dimensional Hubbard model, being a non-trivial but exactly treatable model for interacting spin 1/2 fermions, is of great theoretical interest. It describes electrons, which can hop between the Wannier states of neighbouring sites in a chain, and have a repulsion if two of them /with opposite spins/ occupy the same site. Its Hamiltonian is

$$\hat{H} = t \sum_{i=1}^{N} \sum_{\sigma} (c_{i\sigma}^{+} c_{i+1\sigma} + c_{i+1\sigma}^{+} c_{i\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow} \qquad (1.1)$$

Here N is the number of sites on the chain, $c_{i\sigma}^{+}$, $c_{i\sigma}$ and $n_{i\sigma}$ are the creation, annihilation and number operators, respectively, for an electron with spin σ in the Wannier state centered around the site i . The problem is uniquely defined by imposing periodic boundary conditions on the system.

In the exact solution of the model the first step, which made all further work possible, was made by Lieb and Wu (1968), who, starting from Youg's (1967) work, showed that the diagonalisation of (1.1) is equivalent to solving a set of coupled nonlinear equations. They calculated the ground state energy of the system for half filled band, and the gap in the spectrum of the one particle type excitations at this bandfilling (half filled band $\pm$ one particle). Based on the equations set up by Lieb and Wu, Ovchinnikov calculated (1970) the lower edge of the continuum of the triplet excitations of a half filled band. In his paper calculations for the singlet excitations can be found, too. Coll (1974) calculated the spin--wave type and one-particle type excitations for general band filling. The $T = 0$ magnetic properties of the model have been worked out by Takahashi (1969) and Shiba (1972); in particular Takahashi found the magnetisation curve for the half filled band, and extending this work Shiba gave the magnetic susceptibility for an orbitrary concentration of electrons.

The aim of the present work is to study those excitations of a Hubbard chain which are connected with charge rearrangement. In a non-half-filled band two kinds of such excitations exist. The first kind, which have been described by Coll (1974), differ from the ground state only in the momentum distribution of the electrons. The number of this type of excitations disappears as the bandfilling aproaches 1/2; a fact which suggests that in all these states the electrons occupy different lattice sites. The other type of "charge excitations" is connected with electron pairs occupying the same lattice sites. Our aim is to find a way to describe such excitations. For the sake of symplicity, for this purpose the half filled band is studied first, since in this case charge excitations of the first kind do not exist.

The paper is organised as follows. In Chapter 2. after introducing the general formalism an analysis of the wave function leads us to argue that complex wavenumbers have to be used to describe the states in question. In Chapter 3. we study the simplest case in which such excitations can exist, namely the one in which all but one of the spins point in the same direction, but the electron with the opposite spin propagates along occupied sites. In these states the spin degrees of freedom are highly excited. Chapter 4. is devoted to the description of such an excitation if the spin degrees of freedom are not excited.

2. THE LIEB-WU EQUATIONS; SOME PROPERTIES OF THE EIGENSTATES

2.1 The symmetries of the Hamiltonian

In deriving the secular equations for the model, the following symmetries of the Hamiltonian (1.1) have been exploited:

i, $\hat{H}$ does not act on the spin coordinates of the electrons (this becomes apparent if we write (1.1) in first quantised form), i.e. it commutes with both the z component and the square of the total spin. This means that the eigenstates can be characterised by these quantisies (of course S^z and S^2 do not define the state uniquely, thus together with these quantities other quantum numbers must be introduced, too).

ii, Introducing holes instead of electrons, the form of $\hat{H}$ does not change (apart from an additive constant) thus it is sufficient to describe those states in which the number of electrons (N_e) is less than or equal to the number of sites (N). It is also apparent that it is enough to deal with states in which the number of down spins (M) is less than or equal to the number of up spins $(M'=N_e-M)$.

iii, Without the loss of generality t can be taken as $t=-1$.

2.2 The Lieb-Wu equations and the eigenfunctions

Using a generalisation of Bethe's hypothesis Lieb and Wu showed that finding an eigenstate of (1.1) which corresponds to (ii) is equivalent to solving the system of equations

$$N k_j = 2\pi I_j - \sum_{\beta=1}^{M} 2\,\mathrm{arctg}\,\frac{4}{U}(\sin k_j - \lambda_\beta) \tag{2.1}$$

$$(j = 1, 2, \ldots N_e)$$

$$\sum_{j=1}^{N_e} 2\,\mathrm{arctg}\,\frac{4}{U}(\lambda_\alpha - \sin k_j) = 2\pi J_\alpha + \sum_{\beta=1}^{M} 2\,\mathrm{arctg}\,\frac{2}{U}(\lambda_\alpha - \lambda_\beta) \tag{2.2}$$

$$(\alpha = 1, 2, \ldots M)$$

where the parameters I are integers (or half odd-integers) if M is even (or odd) and the parameters J are integers (or half odd-integers) if $N_e - M$ is odd (or even). In this system of equations the k -s and λ -s are the unknowns and the parameters I and J are the actual quantum numbers specifying the state. Only those solutions are meaningful, for which all the k -s and λ -s are different. It is a special difficulty that it is not clear to which sets of I and J can a meaningful solution of (2.1 -2) be found. Thus solving (2.1-2) means a twofold task: finding the appropriate I and J sets and finding the k -s and λ -s.

Following the reasoning which led to Eqs. (2.1-2), the wavefunction can be constructed. One finds that the amplitude of finding the electrons at the positions $n_1, n_2, \ldots n_{N_e}$

with spins $\sigma_1, \sigma_2, \ldots \sigma_{N_e}$ is (up to a normalization factor)

$$f(n_1\sigma_1; n_2\sigma_2; \ldots n_{N_e}\sigma_{N_e}) = \sum_P (-1)^Q (-1)^P \exp\{i\sum_j k_{Pj} n_{Qj}\} \, \phi_P(\sigma_{Q1}\sigma_{Q2}\cdots\sigma_{QN_e}) \tag{2.3}$$

where the permutation Q is defined by the condition that

$$1 \le n_{Q1} \le n_{Q2} \le \ldots \le n_{QN_e} \le N \tag{2.4}$$

and the summation is extended over all permutations P of the k -s. The function ϕ_P is given in the form

$$\phi_P(\sigma_{Q1}\sigma_{Q2}\cdots\sigma_{QN_e}) = \sum_\pi A(\lambda_{\pi 1}\lambda_{\pi 2}\cdots\lambda_{\pi M}) \left(\prod_{l=1}^{M} F_P(\lambda_{\pi l}; y_l)\right) \tag{2.5}$$

with

$$F_P(\lambda; y) = \left(\prod_{j=1}^{y-1} \frac{i(\sin k_{Pj} - \lambda) - \frac{U}{4}}{i(\sin k_{Pj} - \lambda) + \frac{U}{4}}\right) \cdot \frac{1}{i(\sin k_{Py} - \lambda) + \frac{U}{4}} \tag{2.6}$$

$$\frac{A(\ldots \lambda_{\pi i}\lambda_{\pi i+1}\ldots)}{A(\ldots \lambda_{\pi i+1}\lambda_{\pi i}\ldots)} = \frac{i(\lambda_{\pi i+1} - \lambda_{\pi i}) - \frac{U}{2}}{i(\lambda_{\pi i+1} - \lambda_{\pi i}) + \frac{U}{2}} \tag{2.7}$$

where the y -s are the positions of the down spins in the series $\sigma_{Q1}, \sigma_{Q2}, \ldots \sigma_{QN_e}$ in increasing order

$$1 \le y_1 < y_2 < \ldots < y_M \le N_e \tag{2.8}$$

and $\sum_{\pi}$ in (2.5) refers to summation over all permutations of the λ -s.

In connection with the wavefunction (2.3-8) the following can be established:

α, f is uniquely defined even if Q is not: if for example n_i and n_j are equal, there are two permutations, Q and $Q' = QP_{ij}$ which arrange the spatial coordinates into non--decreasing order but the value of f does not depend on wether we choose Q or Q' in (2.3)

β, f is antisymmetric (due to the factor $(-1)^Q$)

γ, f satisfies the eigenvalue equation with the energy

$$E = -\sum_{j=1}^{N_e} 2\cos k_j \tag{2.9}$$

δ, f is periodic with a period N . Its momentum is

$$p = \sum_{j=1}^{N_e} k_j \tag{2.10.a}$$

which, by summing up (2.1) and (2.2), yields

$$p = \frac{2\pi}{N}\left\{\sum_{j=1}^{N_e} I_j + \sum_{\alpha=1}^{M} J_\alpha\right\} \tag{2.10.b}$$

2.3 The ground state and simple excitations

According to Lieb and Wu the ground state is characterised by the parameter set in which both the I_j -s and J_α -s are consecutive integers (or half odd-integers) centered around the origin.

Taking the $N \to \infty$ (N_e/N , M/N : fixed) limit, the k and λ variables will be distributed continuously in the regions $-Q < k < Q \leq \pi$, $-B < \lambda < B \leq \infty$ with density functions $\rho(k)$ and $\sigma(\lambda)$, respectively. (2.1) and (2.2) then leads to the integral equations

$$2\pi \rho(k) = 1 + \cos k \int_{-B}^{B} \frac{2 \cdot (U/4)}{(U/4)^2 + (\sin k - \lambda)^2} \cdot \sigma(\lambda) d\lambda \qquad (2.11)$$

$$\int_{-Q}^{Q} \frac{2 \cdot (U/4)}{(U/4)^2 + (\lambda - \sin k)^2} \rho(k) dk = 2\pi \sigma(\lambda) + \int_{-B}^{B} \frac{2(U/2)}{(U/2)^2 + (\lambda - \lambda')^2} \sigma(\lambda') d\lambda' \qquad (2.12)$$

where Q and B are determined by the conditions

$$\int_{-B}^{B} \sigma(\lambda) d\lambda = M/N \quad , \quad \int_{-Q}^{Q} \rho(k) dk = N_e/N \qquad (2.13)$$

The ground state is a singlet (if N is even) with $M = N_e/2$, $S^z = S^2 = 0$, or a doublet, $S^z = \pm 1/2$, $S^2 = 3/4$ (if N is odd). For this state $B = \infty$ is to be chosen, as it can be checked by integrating (2.12) over λ . For a half-filled band $Q = \pi$ is to be taken. For this state (2.11-12) can be solved in closed form by Fourier transformation giving

$$\rho_0(k) = \frac{1}{2\pi}\left\{1 + \cos k \int_0^\infty \frac{e^{-\omega\frac{u}{4}}}{ch(\omega\frac{u}{4})} J_0(\omega)\cos(\omega \sin k)\, d\omega\right\} \tag{2.14}$$

$$\sigma_0(\lambda) = \frac{1}{2\pi}\int_0^\infty \frac{J_0(\omega)}{ch(\omega\frac{u}{4})} \cos\omega\lambda \, d\omega \tag{2.15}$$

The groundstate-energy for a half filled band is

$$E_0 = -N\int_{-\pi}^{\pi} 2\cos k\, \rho(k) dk = -2N\int_0^\infty \frac{e^{-\omega\frac{u}{4}} \cdot J_0(\omega)\cdot J_1(\omega)}{ch(\omega\frac{u}{4})} \cdot \frac{d\omega}{\omega} \tag{2.16}$$

where J_0 and J_1 are the zeroth and first order Bessel functions, respectively.

The simplest excited states can be obtained by making small changes in the I set, or in the J set, or in both. The simplest excitations with one spin turned over are triplet spin waves and are described by a J set in which one J_α is missing ("hole in the λ distribution" in Lieb and Wu's classification). The simplest excitations connected with the k distribution may be "hole", "particle" and "particle-hole" type ones, which are described by certain well defined modifications of the I set belonging to the ground state. In the cases of "hole" or "particle" like excitations the essential changes in the I sets are removing one I from the "bulk" of the set, or adding one I to the set far from its ends, respectively. (Changing the number of I -s, i.e. the number of electrons, by one may be accompanied by a change in the parity of the numbers $2J$, and may necessitate the change of the number of J -s, and of the parity of $2I$ -s as well. A pure "charge" type excitation is defined by choosing the spin part so as to get the lowest excitation energy.) The "particle-hole" type excitations are defined by I sets which are obtained from the ground state set by removing one I from the bulk of the set and adding to it an other I which is larger (or smaller) than the largest (or smallest) I in the ground state set. All these states are discussed in detail in Coll's paper.

Note, that if the band is half filled i.e. $N_e = N$, from the "particle", "hole" and "particle and hole in the k distribution" states only the "hole" type can exist. This can be seen by the following reasoning: All I_j can be taken to satisfy $-\frac{N}{2} < I_j \leq \frac{N}{2}$ as changing k_j by 2π does not effect anything. In the above region there are N different integers or half odd-integers, thus if we originally had N different I_j -s, we can not displace an I outside of the region covered by the ground state I -set.

2.4 Eigenstates with real k -s in the large U limit

Looking at (2.2) one sees that in the large U limit all $\lambda_\alpha - \sin k_j$ must be of the order of U . As for real k-s $|\sin k_j| \leq 1$, the λ_α-s must be proportional to U . This means that for states described by a k -set in which all k -s are real, the limiting values of the λ -s must satisfy the equations which are obtained by neglecting the $\sin k_i$-s in the l.h.s. of (2.2). These equations are essentially the secular equations of an isotropic Heisenberg spin chain with N_e sites (See f. eg. Griffits (1964)) independently of the actual values of the k -s(in fact, the substitution $2\,\mathrm{arc\,tg}\frac{4\lambda_\alpha}{U} = \pi - k_\alpha$ leads to the form of equations used in the literature of the Heisenberg chain.) The limiting values of the wavenumbers can be obtained by neglecting the $\sin k$ -s in the r.h.s. of Eq. (2.1). They are

$$k_i = \frac{2\pi}{N} I_j + \frac{1}{N}\sum_\alpha 2\,\mathrm{arc\,tg}\frac{4\lambda_\alpha}{U} = \frac{2\pi}{N} I_j + \frac{1}{N}\left(\frac{2\pi}{N_e}\sum_\alpha J_\alpha\right) \tag{2.17}$$

This resembles the k -set of a noninteracting spinless fermi system, except that all k -s are displaced by $1/N$ times the total momentum of the given state of the Heisenberg chain.

Neglecting the $\sin k$-s also in the wavefunction, one finds that in f ϕ_P becomes independent of the permutation P and f turns into a product of a space coordinate dependent and a spin dependent function. The former is essentially the wave function of a spinless Fermi-system, and the latter is an eigenfunction of a Heisenberg spin chain.

The same separation can be seen in the energy of the system, too. To calculate the energy, one has to find the limiting values of the k -s up to first order in $1/U$. This can be done by expanding Eqs. (2.1) and (2.2) up to first order in $1/U$(in $\sin k/U$ and in $\delta\lambda_\alpha/U$). In this way one gets that the energy of such a state is the sum of the energy of the Fermi-system and the energy of the Heisenberg chain with an effective coupling constant proportional to $1/u$.

Thus we can conclude, that in the large u limit, in all states described by a real wavenumber set, the system behaves like an uncoupled ensemble of a spinless Fermi-system and a Heisenberg chain. The ground state corresponds to the ground state of both the Fermi-system and the Heisenberg chain. The excited states connected with the J -set go over to the excited states of the spin chain, while excitations connected with the I set correspond to the excitations of the spinless Fermi-system. This is why the excitations connected with the J or I set can be regarded as "spin" or "charge" excitations. The maximum number of the spin excitations is N_e^2 as this is the number of different states of the spins while the maximum number of charge excitations described by real k -s is $\binom{N}{N_e}$. This implies that excitations connected with the I -set can be described by real k -sets only if $N_e < N$ i.e. the band is less than half filled. (See: "particle" and "particle--hole in the k distribution".)

As in a spinless Fermi-system all particles occupy different sites, in all states described by real k -sets the amplitude of finding electron pairs occupying the same sites must disapper as $u \to \infty$. All the states in which this amplitude does not vanish, must be described by k -sets containing complex wavenumbers, too. The energy of these states is expected to have a term proportional to u , i.e. these states are important if u is of the order of unity, but they are also important when the bandfilling is near to 1/2 being the only excitations connected with charge distribution. Finding the solutions of (2.1-2) corresponding to these states is the goal of the present study.

Our strategy will be as follows: as we mentioned already, solving the Eqs (2.1) and (2.2) means a twofold task: findig the appropriate quantum numbers and determining the k and λ sets. Now we will not separate these two steps: we will not specify all of the quantum numbers in advance, only the quantum numbers corresponding to the real k-s and the λ-s belonging to them will be chosen at the beginning. These k-s and λ-s will be determined as functions of the parameters belonging to the excitations, and will be eliminated from the equations for the complex k-s. The quantum numbers belonging to the complex wavenumbers will be specified only at this stage, so as to have solution for the equations obtained in this process.

3. $S^z = \frac{1}{2}N-1$ STATES WITH COMPLEX WAVENUMBERS

According to our program in this chapter we investigate, for a half filled band, the simplest possible case in which Eqs (2.1-2) may have complex solutions. As these solutions are expected to correspond to states in which at least one site is doubly occupied even in the large U limit, there should be at least one spin which is turned down. That's why we investigate first the states with $S^z = \frac{1}{2}N-1$.

It is clear that if the k -set contains a complex k, it should contain its complex conjugate, too. We look for solutions in which there is only one pair of complex wave-numbers, and denote them by $\kappa \pm i\chi$.

3.1 Basic equations

The equations for the real k -s are:

$$Nk_j = 2\pi I_j - 2\,\mathrm{arctg}\,\frac{4}{U}(\sin k_j - \Lambda) \tag{3.1}$$

For the complex k pair we have

$$N(\kappa \pm i\chi) = 2\pi I - 2\,\mathrm{arctg}\,\frac{4}{U}(\sin(\kappa \pm i\chi) - \Lambda) \tag{3.2}$$

which by separating the real and imaginary parts is equivalent to

$$N\kappa = 2\pi I - 2\,\mathrm{Re}\,\mathrm{arctg}\,\frac{4}{U}(\sin(\kappa + i\chi) - \Lambda) \tag{3.3}$$

$$N x = \frac{1}{4} \ln \frac{(u/4 - \cos\kappa\, sh\, x)^2 + (\sin\kappa\, ch\, x - \Lambda)^2}{(u/4 + \cos\kappa\, sh\, x)^2 + (\sin\kappa\, ch\, x - \Lambda)^2} \tag{3.4}$$

In (3.1) and (3.2) the I -s are half odd integers as M is one. Thus for the I_j -set we have to choose $N-2$ half odd--integers with $-\frac{N}{2} < I_j \leq \frac{N}{2}$ i.e. the series

$$-\tfrac{1}{2}(N-1)\, , \; -\tfrac{1}{2}(N-3)\, , \; \dots \qquad \tfrac{1}{2}(N-1) \qquad (N \text{ even}) \tag{3.5.a}$$

or

$$-\tfrac{1}{2}(N-2)\, , \; -\tfrac{1}{2}(N-4)\, , \; \dots \qquad \tfrac{1}{2} N \qquad (N \text{ odd}) \tag{3.5.b}$$

with two holes left in it. Eq (3.1) defines k -s also for the I -s left out of the series and we will denote them as k_ℓ and k_m . The parameter I in (3.3) will be fixed later.

The equation for Λ is given by

$$\sum_{j \neq m,\ell} 2\,\mathrm{arctg}\, \frac{4}{u}(\Lambda - \sin k_j) + 4\,\mathrm{Re}\; \mathrm{arctg}\, \frac{4}{u}(\Lambda - \sin(\kappa + i x)) = 2\pi J \tag{3.6}$$

where J is an integer if N is even and a half odd-integer if N is odd.

3.2 Solution of the system (3.1), (3.3), (3.4) and (3.6)

We start with (3.4). If x is finite, the l.h.s. is of the order of N . It means that to satisfy the equation κ , x

and Λ must be near to those values at which the r.h.s. is singular. Choosing the $\varkappa$ to be positive, these values are defined by the equations

$$\begin{aligned} &\sin k_0 \cdot ch\, \varkappa_0 - \Lambda = 0 \\ &\cos k_0 \cdot sh\, \varkappa_0 + \frac{u}{4} = 0 \end{aligned} \tag{3.7}$$

i.e.

$$k_0 = \arcsin \frac{1}{2}\left(\sqrt{\left(\frac{u}{4}\right)^2 + (\Lambda+1)^2} - \sqrt{\left(\frac{u}{4}\right)^2 + (\Lambda-1)^2}\right) \tag{3.8}$$
$$\frac{\pi}{2} \leq |k_0| \leq \pi$$

$$(0 <)\, \varkappa_0 = \operatorname{arech} \frac{1}{2}\left(\sqrt{\left(\frac{u}{4}\right)^2 + (\Lambda+1)^2} + \sqrt{\left(\frac{u}{4}\right)^2 + (\Lambda-1)^2}\right) \tag{3.9}$$

(the allowed regions for k_0 in (3.8) come from the condition that $\cos k_0$ must be negative as both $\varkappa_0$ and u are positive). Looking for the solution in the form $\varkappa = \varkappa_0 + \delta\varkappa$ and $k = k_0 + \delta k$ one finds that

$$\begin{aligned} \delta k &= r \cdot \cos\varphi \\ \delta \varkappa &= r \cdot \sin\varphi \end{aligned} \tag{3.10}$$

$$r = 2\, \frac{\frac{u}{4}}{\left\{\left[\left(\frac{u}{4}\right)^2 + \Lambda^2 - 1\right]^2 + 4\left(\frac{u}{4}\right)^2\right\}^{1/4}} \cdot e^{-\varkappa_0 N}$$

with φ as yet unspecified. This solution is accurate up to terms of the order of $N \cdot exp(-2Nx_0)$.

As a next step we solve (3.6) for Λ . We turn the summation on the l.h.s. into on integral: to do this we use the fact that the number of k -s satisfying (3.1), and falling into the interval $(k\,;\,k+dk)$, is $N\,\rho(k)\,dk$ with

$$\rho(k) = \frac{1}{2\pi} + \frac{1}{2\pi}\cdot\frac{1}{N}\cdot 2\cos k\,\frac{(u/4)}{(u/4)^2 + (\sin k-\Lambda)^2} \qquad (3.11.a)$$

As the $\rho(k)$ contains also k_ℓ and k_m , we have to use

$$\rho^*(k) = \rho(k) - \frac{1}{N}\,\delta(k-k_\ell) - \frac{1}{N}\,\delta(k-k_m) \qquad (3.11.b)$$

Then

$$\sum_{j\neq \ell,m} 2\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin k_j) \cong 2N\int_{-\pi}^{\pi} \mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin k)\cdot\rho^*(k)\,dk \qquad (3.12)$$

where the equality holds up to terms of the order of $1/N$.
Making this substitution, we have

$$\begin{aligned} &2Nk(\Lambda) - 2\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin k_\ell) - 2\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin k_m) + \\ &\quad + 4\,\mathrm{Re}\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin(\kappa+ix)) = 2\pi J \end{aligned} \qquad (3.13)$$

with

$$k(\Lambda) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \operatorname{arctg} \frac{4}{U}(\Lambda - \sin k)\, dk = \arcsin \frac{1}{2}\left(\sqrt{\left(\frac{U}{4}\right)^2 + (\Lambda+1)^2} - \sqrt{\left(\frac{U}{4}\right)^2 + (\Lambda-1)^2}\right) \tag{3.14}$$

$$-\frac{\pi}{2} \leq k(\Lambda) \leq \frac{\pi}{2}$$

Multyplying (3.3) by 2 and adding it to (3.13) we get

$$2N(K_0 + k(\Lambda)) - 2\pi(\mathcal{J} + 2I) = 2\operatorname{arctg}\frac{4}{U}(\Lambda - \sin k_\ell) + 2\operatorname{arctg}\frac{4}{U}(\Lambda - \sin k_m) \tag{3.15}$$

Note that

$$K_0 + k(\Lambda) = \pi \operatorname{sign} \Lambda \tag{3.16}$$

i.e. the l.h.s. of (3.15) is of the form $2\pi \mathcal{J}'$ where $\mathcal{J}'$ is an integer if $\mathcal{J}$ is integer and half odd-integer if $\mathcal{J}$ is half odd-integer. At the same time the r.h.s. changes between -2π and $+2\pi$ as Λ runs from $-\infty$ to ∞, thus we have a solution only if the l.h.s. is -2π , 0 or 2π ($\mathcal{J}$ integer) or $-\pi$ or π ($\mathcal{J}$ half odd-integer). The possible solutions are

$$N \cdot \operatorname{sign}\Lambda - (\mathcal{J} + 2I) = 0 \qquad \Lambda = \frac{1}{2}(\sin k_\ell + \sin k_m) \tag{3.17.a}$$

$$\pm N - (\mathcal{J} + 2I) = \pm 1 \qquad \Lambda = \pm\infty \tag{3.17.b}$$

or

$$N \operatorname{sign} \Lambda^{\pm} - (J + 2I) = \pm \frac{1}{2} \qquad \Lambda^{\pm} = \frac{\sin k_\ell + \sin k_m}{2} \pm \sqrt{\left(\frac{\sin k_\ell - \sin k_m}{2}\right)^2 + \left(\frac{U}{4}\right)^2} \tag{3.18}$$

Solutions (3.17.a) and (3.18) are proper solutions of the system in the sense that all quantities are finite in the equations and in the corresponding wavefunction. We discuss these solutions now and come back to the interpretation of (3.17.b) later.

Using the form of κ and χ ((3.8-10)) we have with exponential accuracy

$$\kappa_0 = \frac{2\pi}{N} I - \frac{1}{N} \operatorname{arctg}\left(\frac{\cos\kappa_0 \operatorname{ch}\chi_0 \cos\varphi + \sin\kappa_0 \operatorname{sh}\chi_0 \sin\varphi}{-\sin\kappa_0 \operatorname{sh}\chi_0 \cos\varphi + \cos\kappa_0 \operatorname{ch}\chi_0 \sin\varphi}\right) \tag{3.19}$$

which, if Λ is given, can be solved easily for φ and I.

Thus we see, that all unknowns can be expressed by $\sin k_\ell$ and $\sin k_m$, and the quantum numbers J and I can also be determined if k_ℓ and k_m are known. Thus the system (3.1), (3.2), (3.6) is reduced to the determination of k_ℓ and k_m with (3.1) and (3.17) or (3.18), if I_ℓ and I_m are given. The solutions correct up to terms of the order of $1/N^2$ are

$$k_{\ell(m)} = 2\pi I_{\ell(m)} - \frac{2}{N} \operatorname{arctg} \frac{4}{U}\left(\sin \frac{2\pi}{N} I_{\ell(m)} - \Lambda(I_\ell, I_m)\right) \tag{3.20}$$

where by $\Lambda(I_\ell, I_m)$ we understand the Λ determined by (3.17), or (3.18), where $\sin k_{\ell(m)} = \sin \frac{2\pi}{N} I_{\ell(m)}$.

3.3 Energy and momentum

The energy of the state calculated above is, according to (2.9)

$$E = -\sum_{j\neq \ell,m} 2\cos k_j - 4\cos k_0 \, ch\chi_0 \qquad (3.21)$$

Using $\rho^*(k)$ to evaluate the sum, and also using the identity

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{(U/4)}{(U/4)^2 + (\sin k - \Lambda)^2} \cos^2 k \, dk = \cos k(\Lambda) \cdot e^{-\chi_0} \qquad (3.22)$$

with $k(\Lambda)$ given by (3.14), and χ_0 given by (3.1), one has

$$E = 2\cos k_\ell + 2\cos k_m + U \qquad (3.23)$$

The momentum, according to (2.10.b) is

$$p = \frac{2\pi}{N}\Big(\sum_{j\neq m,\ell} I_j + 2I + J\Big) \qquad (3.24)$$

which gives for (3.17.a)

$$p = 2\pi \operatorname{sign}\Lambda - \frac{2\pi}{N} I_\ell - \frac{2\pi}{N} I_m \qquad (3.25)$$

and for (3.18)

$$p^\pm = 2\pi \operatorname{sign}\Lambda^\pm - \frac{2\pi}{N} I_\ell - \frac{2\pi}{N} I_m \pm \frac{\pi}{N} + \pi \qquad (3.26)$$

Expressing (3.25) and (3.26) by k_l and k_m yields

$$p = -k_m - k_l + \psi \tag{3.27}$$

where ψ is zero if N is even and π if N is odd.

3.4 Interpretation of the solution with infinite Λ (3.17.b)

We try to interpret this solution so that all k -s, κ_0, $\varkappa_0$ $\delta\kappa$, $\delta\varkappa$ and φ should be treated as functions of Λ, and the $\Lambda \rightarrow +\infty$ (or $-\infty$) limit must be taken. Whether this interpretation is possible or not depends on whether the wavefunction obtained through this limiting process is meaningful or not. Note that if this interpretation is reasonable, both (3.23) and (3.27) remain valid.

Analysing the wavefunction one finds that some of the terms will be divergent in the above outlined limiting process. The most divergent amplitudes are those in which two coordinates are equal, (and the down spin belongs to one of these coordinates.) The terms with the strongest divergence in these amplitudes belong to those permutations for which in the exponent $\kappa + i\varkappa$ and $\kappa - i\varkappa$ are multiplied by the equal coordinates. These terms diverge as $|\Lambda|^{N+1}$. The coefficient of this factor is given by

$$\sum_{P'} (-1)^{Q'} (-1)^{P'} \exp\left\{ i \sum_j{}' k_{P'_j} n_{Q'_j} \right\} \cdot e^{i\pi n} \tag{3.28}$$

where n denotes the coordinate of the electron pair, Q' orders the remaining coordinates into increasing order, $\sum_{j}'$ means summations over the real k-s and $\sum_{P'}$ means summation over all possible permutations of the $N-2$ real k-s. This form is independent of the sign of the Λ, and we have used that $k(\Lambda) \to \pm\frac{\pi}{2}$ if $\Lambda \to \pm\infty$. It is clear that the normalised wavefunction will have a limiting form proportional to (3.28)

At the same time the limiting values of the real k-s can be given as

$$k_j = \frac{2\pi}{N} I_j \,(\pm)\, \frac{\pi}{N} \tag{3.29}$$

The wavefunction (3.28) can be given also in second quantised form:

$$\Big(\sum_{n=1}^{N} C^+_{n\uparrow} C^+_{n\downarrow} e^{i\pi n}\Big)\cdot\Big(\prod_{j\neq l,m} \cdot C^+_{k_j\uparrow}\Big)|\mathrm{vacuum}\rangle \tag{3.30}$$

It is easy to see that the commutator of the operator

$$\hat{C} = \sum_{n=1}^{N} c^+_{n\uparrow} c^+_{n\downarrow} e^{i\pi n} \tag{3.31}$$

with $\hat{H}$ is

$$[\hat{H},\hat{C}] = U\cdot\hat{C} \tag{3.32}$$

thus (3.30) and so (3.17.b) is indeed a good eigenstate with its energy and momentum given by (3.23) and (3.28), respectively. (Note, that (3.32) holds if N is even only, otherwise operators with indeces 1 and N do not cancel. At the same time infinite Λ solution exists also only if N is even.)

3.5 Visualisation of the states described by (3.17) and (3.18)

In the eigenstates studied here the appearence of complex wavenumbers would suggest at the first sight that we have some sort of bound states. In what follows we show that the same states can arrive at via another route which makes them appear as unbound states. Describing the $N-1$ up-spin electrons as a filled band with one hole in it, one gets a Hamiltonian for the system consisting of the hole and the down-spin electron which is similar to (1.1) with the difference that now these two particles have an onsite attraction instead of repulsion. This Hamiltonian can be diagonalised by elementary methods giving N bound states and $N(N-1)$ scattering states. Inspecting their energies and momenta, one finds that the scattering states are those which correspond to our complex k-states: a complex k-state characterised by k_ℓ and k_m corresponds to a state which is a combination of the states with a hole in the filled band of the up-spin electrons with wavenumber k_ℓ and a down--spin electron propagating along occupied sites with a wavenumber $\pi - k_m$, and vice versa. (This can be seen directly on the state corresponding to the solution (3.17.b) i.e. on the eigenstate (3.30), by expressing the operator $\hat{C}$ as $\sum_{\text{all } k} c^+_{\pi-k\downarrow} c^+_{k\uparrow}$ and taking into account that in this sum only those terms can act in which k is either k_ℓ or k_m). This result, namely that our complex k-states are those which correspond to the scattering states of the electron-hole pair, is not surprising, as in a state with all k-s real the electrons most occupy different sites as $U \to \infty$ i.e. the electron with down spin is "bound" into the hole in the band of up spin electrons.

Unfortunately the picture becomes less clear if the bandfilling is less than 1/2, as it can be illustrated on states analogous to (3.30). The operator $\hat{C}$ acting on eigenstates of the Hamiltonian creates an other eigenstate with two more electrons. In this new state certainly there is at least one pair of electrons occupying the same site, but to regard these electrons as bound ones makes sense only if they are surrounded mainly by empty sites i.e. when the bandfilling is much less than 1/2. In the opposite limit, when the doubly occupied sites are surrounded by singly occupied sites, one of the electrons can move any way, and we can not tell which electron is bounded to which other one. In the intermediate case neither the electron-hole nor the bound electron pair picture seems well established.

4. SINGLET STATES WITH ONE PAIR OF COMPLEX WAVENUMBERS

4.1 The Lieb-Wu equations for singlet states with two complex k -s

To describe $S^z = 0$ states we have to introduce $N/2$ λ -s. We take N as an even number, otherwise the state with the smallest spin belongs to $S^z = \pm 1/2$. This restriction makes no difference concerning the nature of the excitations since if N were odd both the ground state and the excited states analogous to those discussed here would belong to $S^z = \pm 1/2$, and so, both for even and odd N the excitations themselves can be regarded as singlet ones. We suppose that among the $N/2$ λ -s there is one (which we denote by Λ) for which, as in the case discussed in the previous chapter,

$$\sin(\kappa \pm i\chi) = \Lambda \mp i\frac{U}{4} + O(e^{-\eta N}) \tag{4.1}$$

where η is a positive number of the order of unity and $O(e^{-\eta N})$ means terms of the order of $e^{-\eta N}$.

The equations for the complex k pair are

$$\begin{aligned} N(\kappa \pm i\chi) = 2\pi I - \sum_{\beta=1}^{\frac{N}{2}-1} 2\,\mathrm{arc\,tg}\,\frac{4}{U}(\sin(\kappa \pm i\chi) - \lambda_\beta) - \\ - 2\,\mathrm{arc\,tg}\,\frac{4}{U}(\sin(\kappa \pm i\chi) - \Lambda) \end{aligned} \tag{4.2}$$

and (4.1) is actualy the solution of their imaginary part, provided that

$$\varkappa + \operatorname{Im} \sum_{\beta=1}^{\frac{N}{2}-1} \frac{1}{N} 2 \operatorname{arctg} \frac{4}{u} \left(\sin(\kappa + i\varkappa) - \lambda_\beta \right) = \eta > 0 \tag{4.3}$$

It is easy to see that if (4.3) holds, then κ and $\varkappa$ are the same functions of Λ as given by (3.8-9-10) with the only difference that in the r of (3.10) in the exponent we have η instead of $\varkappa_o$. The validity of (4.3) (and so of (4.1)) can not be proven in general. What one has to do is to solve the remaining part of the equations using (4.1) and at the end, having the λ -s at hand, to check whether (4.3) holds or not. This is what we will do.

The real part of (4.2), using the identity

$$2 \operatorname{Re} \operatorname{arctg} \frac{4}{u} (\sin(\kappa + i\varkappa) - \lambda) =$$

$$= \operatorname{arctg} \frac{\sin\kappa \operatorname{ch}\varkappa - \lambda}{\frac{u}{4} - \cos\kappa \operatorname{sh}\varkappa} + \operatorname{arctg} \frac{\sin\kappa \operatorname{ch}\varkappa - \lambda}{\frac{u}{4} + \cos\kappa \operatorname{sh}\varkappa} + \psi \tag{4.4}$$

$$\psi = \begin{cases} \pi \operatorname{sign}(\sin\kappa \operatorname{ch}\varkappa - \lambda) & \text{if } \frac{u}{4} < |\cos\kappa \operatorname{sh}\varkappa| \\ 0 & \text{if } \frac{u}{4} > |\cos\kappa \operatorname{sh}\varkappa| \end{cases}$$

combined with (4.1) can be written in the form (up to terms exponentially small in N)

$$\begin{aligned} N\kappa = 2\pi I &- \frac{\pi}{2} \sum_{\beta=1}^{\frac{N}{2}-1} \operatorname{sign}(\Lambda - \lambda_\beta) - \sum_{\beta=1}^{\frac{N}{2}-1} 2 \operatorname{arctg} \frac{2}{u} (\Lambda - \lambda_\beta) \\ &- 2 \operatorname{Re} \operatorname{arctg} \frac{4}{u} (\sin(\kappa + i\varkappa) - \Lambda) \end{aligned} \tag{4.5}$$

The real k -s are defined by the equations

$$Nk_j = 2\pi I_j - \sum_{\beta=1}^{\frac{N}{2}-1} 2\,\mathrm{arctg}\,\frac{4}{U}(\sin k_j - \lambda_\beta) - 2\,\mathrm{arctg}\,\frac{4}{U}(\sin k_j - \Lambda) \tag{4.6}$$

Now the I_j -s are integers if $N/2$ is even and half odd integers if $N/2$ is odd. Thus, depending on the parity of $N/2$ we have to choose one of the sets

$$-\tfrac{1}{2}(N-2)\ ,\ -\tfrac{1}{2}(N-4)\ ,\ \dots\qquad \tfrac{1}{2}(N-2)\ ,\ \tfrac{1}{2}N \tag{4.7.a}$$

$$-\tfrac{1}{2}(N-1)\ ,\ -\tfrac{1}{2}(N-3),\ \dots\qquad \tfrac{1}{2}(N-3),\ \tfrac{1}{2}(N-1) \tag{4.7.b}$$

with two holes left in it.

The equations for the λ -s are

$$\begin{aligned}\sum_{j\neq l,m} 2\,\mathrm{arctg}\,\frac{4}{U}(\Lambda - \sin k_j) - 4\,\mathrm{Re}\,\mathrm{arctg}\,\frac{4}{U}(\sin(\kappa+i\chi) - \Lambda) &= \\ = 2\pi J + \sum_{\beta=1}^{\frac{N}{2}-1} 2\,\mathrm{arctg}\,\frac{2}{U}(\Lambda - \lambda_\beta)&\end{aligned} \tag{4.8}$$

(k_l and k_m being the k -s defined by (4.6) for the holes in the I set) and

$$\begin{aligned}\sum_{j\neq l,m} 2\,\mathrm{arctg}\,\frac{4}{U}(\lambda_\alpha - \sin k_j) - 4\,\mathrm{Re}\,\mathrm{arctg}\,\frac{4}{U}(\sin(\kappa+i\chi) - \lambda_\alpha) &= \\ = 2\pi J_\alpha + \sum_{\beta=1}^{\frac{N}{2}-1} 2\,\mathrm{arctg}\,\frac{2}{U}(\lambda_\alpha - \lambda_\beta) + 2\,\mathrm{arctg}\,\frac{2}{U}(\lambda_\alpha - \Lambda)&\end{aligned} \tag{4.9}$$

This second equation combined with (4.4) and (4.1) is equivalent to the equation

$$\sum_{j\neq l,m} 2\,\mathrm{arctg}\,\frac{4}{u}(\lambda_\alpha - \sin k_j) = 2\pi J'_\alpha + \sum_{\beta=1}^{\frac{N}{2}-1} 2\,\mathrm{arctg}\,\frac{2}{u}(\lambda_\alpha - \lambda_\beta)$$

$$J'_\alpha = J_\alpha - \frac{1}{2}\,\mathrm{sign}(\lambda_\alpha - \Lambda) \tag{4.10}$$

Since J_α is an integer if $N/2$ is odd and half odd-integer if $N/2$ is even, J'_α is integer if $N/2$ is even and half odd-integer if $N/2$ is odd. It is interesting to note that (4.10) is formally the same, as the corresponding equation for a system of $N-2$ electrons. Based on this analogy, we suppose that it is the J' set which defines the state of the spin system. According to our program, now we want to describe states for which the spin degrees of freedom are not excited, thus for the J'-s we choose the same set which would correspond to the ground state of a system of $N-2$ electrons, i.e. the set

$$-\frac{1}{2}\left(\frac{N}{2}-2\right),\ -\frac{1}{2}\left(\frac{N}{2}-4\right),\ \dots \qquad \frac{1}{2}\left(\frac{N}{2}-2\right) \tag{4.11}$$

4.2 Solutions of the system (4.2), (4.6), (4.8), (4.10)

In the following we suppose that in the large N limit all the k_j-s and λ_α-s can be described by their density functions $\rho(k)$ and $\sigma(\lambda)$ *. Equations for these functions can be derived from (4.6) and (4.10):

*See p. 39.

$$\rho(k) = \frac{1}{2\pi} + \frac{2\cos k}{2\pi}\int_{-\infty}^{\infty} \frac{(U/4)}{(U/4)^2 + (\sin k - \lambda)^2}\,\sigma(\lambda)d\lambda + \frac{2\cos k}{2\pi N}\cdot\frac{(U/4)}{(U/4)^2 + (\sin k - \Lambda)^2} \tag{4.12}$$

$$2\int_{-\pi}^{\pi} \frac{(U/4)}{(U/4)^2 + (\lambda - \sin k)^2}\,\rho^*(k)dk = 2\pi\,\sigma(\lambda) + 2\int_{-\infty}^{\infty} \frac{(U/2)}{(U/2)^2 + (\lambda - \lambda')^2}\,\sigma(\lambda')d\lambda' \tag{4.13}$$

with

$$\rho^*(k) = \rho(k) - \frac{1}{N}\delta(k-k_\ell) - \frac{1}{N}\delta(k-k_m) \tag{4.14}$$

($\rho(k)$ being the density of k -s satisfying (4.6), with the whole set (4.7), it contains also k_ℓ and k_m , i.e. the k -s belonging to the two holes.) This system can be solved by Furier transformation giving

$$\sigma(\lambda) = \sigma_0(\lambda) - \frac{1}{N\cdot U}\left(\frac{1}{ch(\lambda - \sin k_\ell)\frac{2\pi}{U}} + \frac{1}{ch(\lambda - \sin k_m)\frac{2\pi}{U}}\right) \tag{4.15}$$

and

$$\begin{aligned}\rho(k) = \rho_0(k) &+ \frac{1}{2\pi\cdot N}\cdot 2\cos k\,\frac{(U/4)}{(U/4)^2 + (\sin k - \Lambda)^2} - \\ &- \frac{1}{2\pi N}\cos k\int_0^{\infty} \frac{e^{-\omega\frac{U}{4}}}{ch\,\omega\frac{U}{4}}\left(\cos(\omega(\sin k - \sin k_\ell)) + \cos(\omega(\sin k - \sin k_m))\right)d\omega\end{aligned} \tag{4.16}$$

with $\rho_0(k)$ and $\sigma_0(\lambda)$ given by (2.14) and (2.15), respectively.

Having $\rho(k)$ at hand, also (4.5) and (4.8) can be reduced: (4.8) after carrying out the summation over the k -s (using $\rho^{*}(k)$) yields

$$2Nk(\Lambda) - 2\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin k_l) - 2\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin k_m) + \tag{4.17}$$
$$+ 4\,\mathrm{Re}\,\mathrm{arctg}\,\frac{4}{u}(\Lambda-\sin(\kappa+ix)) = 2\pi \mathcal{J} + \sum_{\beta=1}^{\frac{N}{2}-1} 2\,\mathrm{arctg}\,\frac{2}{u}(\Lambda-\lambda_\beta)$$

with $k(\Lambda)$ given by (3.14). (4.5) and (4.17) are the analogues of (3.3) and (3.13). Their solution for Λ can be obtained in the same way. Thus we have

$$N\,\mathrm{sign}\,\Lambda - \Big(\mathcal{J} + 2I - \frac{1}{2}\sum_{\beta=1}^{\frac{N}{2}-1}\mathrm{sign}(\Lambda-\lambda_\beta)\Big) = 0 \qquad \Lambda = \frac{1}{2}(\sin k_m + \sin k_l) \tag{4.18.a}$$

$$\Big(N - \frac{1}{2}\big(\frac{N}{2}-1\big)\Big)\,\mathrm{sign}\,\Lambda - (\mathcal{J}+2I) = \pm 1 \qquad \Lambda \to \pm\infty \tag{4.18.b}$$

(Note that now the solutions corresponding to (3.18) do not exist, as $\mathcal{J} - \frac{1}{2}\sum_\beta \mathrm{sign}(\Lambda-\lambda_\beta)$ is always an integer. The solution (4.18.b) is to be understood as (3.17.b)). At the same time, we have from (4.17) (with the sum turned into an integral with $\sigma(\lambda)$ given by (4.15))

$$\frac{2N}{2\pi}\int_0^\infty \frac{J_0(\omega)\sin\omega\Lambda}{\omega\cdot \mathrm{ch}\,\omega\frac{u}{4}}\,d\omega = 2\pi\mathcal{J} + 4\,\mathrm{Re}\,\mathrm{arctg}\,\frac{4}{u}(\sin(\kappa+ix)-\Lambda) \tag{4.19}$$

which is the equivalent of (3.19) to determine $\mathcal{J}$ (and through (4.18), I) and φ of (3.10).

To solve the system completly we have to solve the equations:

$$k_{\ell(m)} + \int_0^\infty \frac{e^{-\omega\frac{u}{4}}}{\omega\cdot ch\,\omega\frac{u}{4}} J_0(\omega)\sin(\omega\sin k_{\ell(m)})\,d\omega = \frac{2\pi}{N}\cdot I_{\ell(m)} +$$

$$+\frac{1}{N}\int_0^\infty \frac{e^{-\omega\frac{u}{4}}}{\omega\cdot ch\,\omega\frac{u}{4}} \sin\left(\omega\left(\sin k_{\ell(m)} - \sin k_{m(\ell)}\right)\right) - \frac{2}{N}\,arctg\,\frac{4}{u}\left(\sin k_{\ell(m)} - \Lambda\right) \qquad (4.20)$$

which were obtained by evaluating the sum over λ_β-s in (4.6). Λ given by (4.18), (4.20) can be solved numericaly.

Using $\sigma(\lambda)$ the validity of (4.3) can be checked: The l.h.s. can be estimated by replacing the $\sum_\beta$ by $\int d\lambda\,\sigma(\lambda)$ with an error of the order of $\ln N/N$ (This estimated error comes from the supposition that $min(\lambda_\beta - \Lambda) \simeq \frac{1}{N}$. We may suppose this, since if $min(\lambda_\beta - \Lambda)$ is much less then $1/N$ for one Λ (I_ℓ and I_m) then changing I_ℓ (or I_m) by one, Λ will change $\sim \frac{1}{N}\frac{\cos k_\ell}{\rho(k_\ell)}$ while the difference between neighbouring λ_β-s around Λ is $\frac{1}{N}\frac{1}{\sigma(\Lambda)}$, thus $min(\lambda_\beta - \Lambda)$ will be of the order of $1/N$. Thus this estimate may not hold only accidentally for a few points of the dispersion.) Although the integral obtained in this way can not be evaluated in closed form, one can show that the l.h.s.(η) is definitely positive. This means also, that for one pair of complex k-s, there must be a Λ coupled to them by (4.1): if there were no such Λ then instead of (4.1) we would have an equation $\eta = 0$, which has no solution.

4.3 The energy and momentum

The energy of the states is easily calculated by means of $\rho^*(k)$:

$$E = -N\int_{-\pi}^{\pi} 2\cos k\, \rho^*(k)\, dk - 4\cos k\, ch x = \tag{4.21}$$

$$= E_0 + \epsilon(k_e) + \epsilon(k_m) + U$$

with E_0 given by (2.16) and

$$\epsilon(k) = 2\cos k + 2\int_0^\infty \frac{e^{-\omega\frac{U}{4}}}{ch\,\omega\frac{U}{4}} \cdot \frac{J_1(\omega)}{\omega} \cdot \cos(\omega \sin k)\, d\omega \tag{4.22}$$

The momentum, according to (2.10.b), (4.7), (4.10) and (4.11) is

$$p = \frac{2\pi}{N}\left(-I_e - I_m + J + \sum_{\beta=1}^{\frac{N}{2}-1} \frac{1}{2}\, \mathrm{sign}(\lambda_\beta - \Lambda) + 2I\right) + p_0 \tag{4.23}$$

where p_0 , the momentum of the ground state is π if $N/2$ is even and 0 if $N/2$ is odd This combined with (4.18) and (4.20), yields

$$p - p_0 = 2\pi\, \mathrm{sign}\,\Lambda - k_e - \int_0^\infty \frac{e^{-\omega\frac{U}{4}} J_0(\omega) \sin(\omega \sin k_e)\, d\omega}{\omega \cdot ch\,\omega\frac{U}{4}} \tag{4.24}$$

$$- k_m - \int_0^\infty \frac{e^{-\omega\frac{U}{4}} J_0(\omega) \sin(\omega \sin k_m)\, d\omega}{\omega \cdot ch\,\omega\frac{U}{4}}$$

Introducing the notation

$$p(k) = k + \int_0^\infty \frac{e^{-\omega\frac{U}{4}} J_0(\omega)\sin(\omega\sin k)}{\omega\cdot ch\,\omega\frac{U}{4}}\,d\omega \qquad (4.25)$$

we have (up to 2π)

$$p - p_0 = -p(k_\ell) - p(k_m) \qquad (4.26)$$

The energy momentum curve defined by (4.25) and (4.22) is shown in Fig. 1. . Fig. 2. displays the continuum of the excitations in the (ϵ, p) plane.

4.4 Comments

The number of states described above is $N(N-1)$ as there are $N(N-1)/2$ choices of the I_ℓ and I_m parameters and to each choice we have two solutions ((4.18.a) and (4.18.b)). On the other hand, as one can verify, these states in the large U limit correspond to states in which one site is doubly occupied and one site is empty, and the Heisenberg chain of the spins belonging to the singly occupied states is in its ground state. As the number of these states is also $N(N-1)$ we have found all of them.

It is interesting to note that the state with lowest energy is the one in which $k_\ell \simeq k_m \simeq \pi$. Here the energy is

$$(E - E_0)_{min} = U - 4 + 4\int_0^\infty \frac{e^{-\omega\frac{U}{4}}}{ch\,\omega\frac{U}{4}}\cdot\frac{J_1(\omega)}{\omega}\,d\omega \qquad (4.27)$$

which is exactly the same as

$$\mu_+ - \mu_- = [E_0(N+1) - E_0(N)] - [E_0(N) - E_0(N-1)] \tag{4.28}$$

($E_0(N\pm1)$ being the ground state energy of a system with $N\pm1$ electrons) calculated by Lieb and Wu. In other words the gap calculated through the one particle excitations coincides with the gap in the spectrum of particle number conserving charge excitations. A detailed discussion of the results of this chapter is given in the second part of the present work (Woynarovich 1980), where solutions corresponding to an arbitrary number of complex pairs are found for the case of an arbitrary band-filling.

5. SUMMARY

The main points of the present study can be summarised as follows:

1. Based on the analysis of the $U \to \infty$ limiting form of the eigenfunctions of the 1-d Hubbard chain it is shown, that all those states in which the amplitude of finding electron pairs occupying the same sites is finite, even if U is large, are to be described by such solutions of the Lieb-Wu equations in which some of the wavenumbers are complex.

2. Solutions of the Lieb-Wu equations containing one pair of complex wavenumbers, corresponding to $S^z = 1/2 N - 1$ states are found. In these states all but one spins point in the same direction, and the electron with the opposite spin propagates along occupied sites. The states are characterised by three parameters (k_ℓ , k_m and Λ) which are coupled to the corresponding quantum numbers, and to each other, by a set of nonlinear equations (3.1),(3.15). The solution of this system is given by (3.17) or (3.18) and (3.20).

3. Solutions with one pair of complex wavenumbers, corresponding to states in which the spin part is in its ground state (singlet) are also found. Also these states are characterised by three parameters (k_ℓ , k_m and Λ) and these parameters are coupled to each other by Eqs (4.18),(4.20). In the energy and momentum only the parameters k_ℓ and k_m appear explicitely

((4.21), (4.22), (4.25), (4.26)). In the spectrum a gap is found which is of the same magnitude as that calculated by Lieb and Wu for the one-particle type excitations.

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FOOTNOTE (p. 28.)

*Describing the k and λ sets by their density functions is very plausible, but it is not established in a strict mathematical sense. The problem is that one must be sure, that the error introduced by turning the sums into integrals is much less then the $1/N$ terms which are present due to the excitations. Replacing $(1/N)\sum_k$ by $\int dk\,\rho(k)$ introduces an error of the order of $1/N^2$ but the replacement of $(1/N)\sum_\lambda$ by $\int d\lambda\,\sigma(\lambda)$ may introduce a larger error as the integration interval is infinite.

Figure captions

Fig. 1. $\epsilon(p)$ dispersions for different values of U . The individual curves are labelled by the value of U.

Fig. 2. Schematic representation of the continuum of the states with two complex wavenumbers in the energy--momentum plane. Doubly shaded areas represent degenerate states: to one $(\epsilon\ ,p\ )$ point there is two nonequivalent p_1, p_2 pair for which $p_1+p_2 = p$ and $\epsilon(p_1)+\epsilon(p_2)+U = \epsilon$

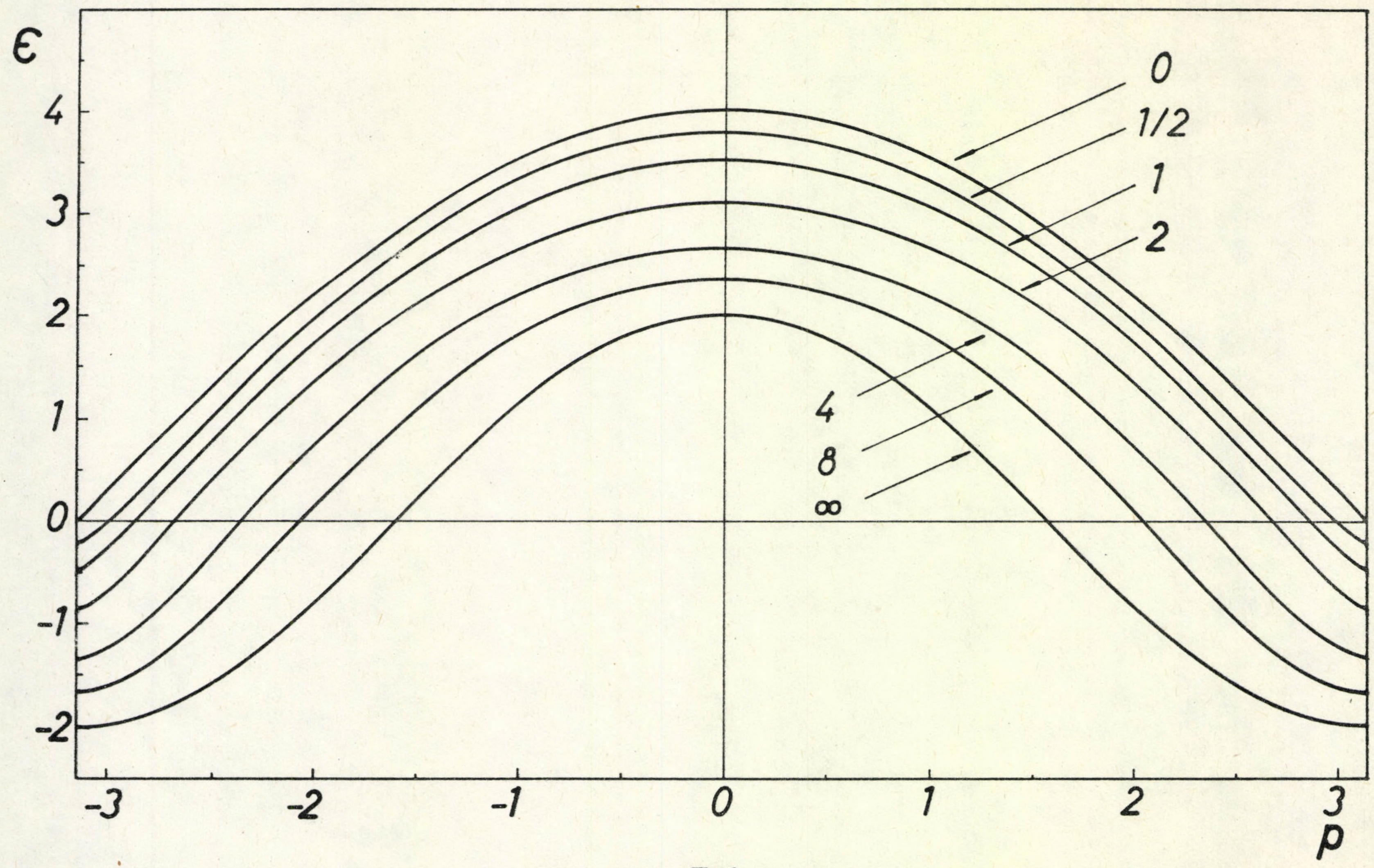
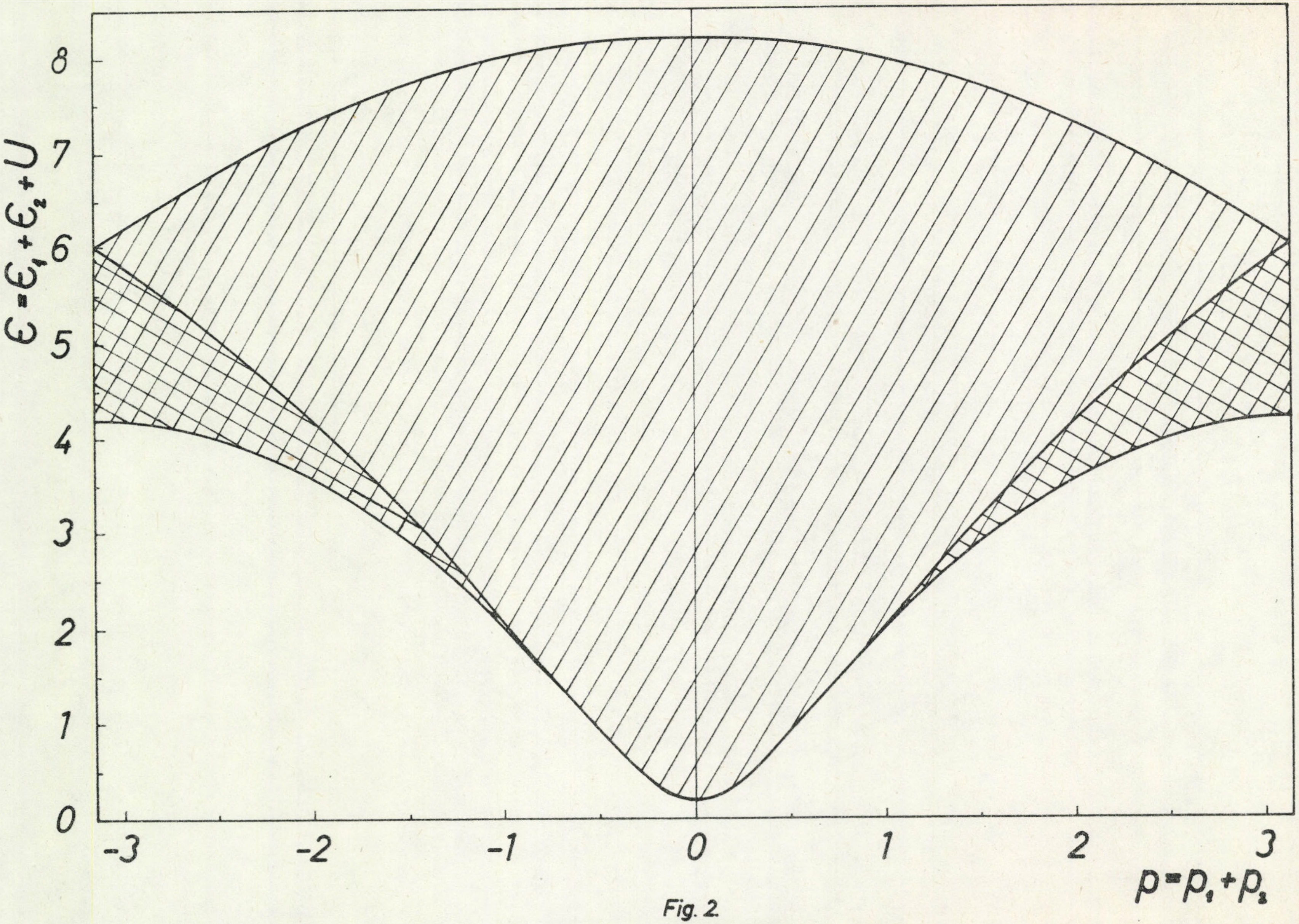


Fig. 1



8
7
6
5
4
3
2
1
0
-3
-2
-1
0
1
2
3
$\varepsilon = \varepsilon_1 + \varepsilon_2 + U$
$p = p_1 + p_2$

Fig. 2.

63.037

Kiadja a Központi Fizikai Kutató Intézet
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