

KFKI-1980-62

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IN A HUBBARD CHAIN  
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*Hungarian Academy of Sciences*

CENTRAL  
RESEARCH  
INSTITUTE FOR  
PHYSICS

BUDAPEST

2017

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HU ISSN 0368 5330  
ISBN 963 371 697 7  
ISBN 963 371 698 5 /összkiadás/

## ABSTRACT

Singlet states of the 1-d Hubbard chain with several pairs of complex wavenumbers are studied. The original set of Lieb-Wu equations is replaced by an equivalent set in which only real wavenumbers appear, the total number of which is equal to the sum of the number of complex wavenumbers and the number of electrons needed to make the band half-filled. In a sense discussed in the text, the new set of equations refers to excitations only. The energy-momentum dispersion is also found. Based on the energy spectrum and the  $U \rightarrow \infty$  limiting form of the wavefunction, the excitations can be identified as interacting quasi-particles.

## АННОТАЦИЯ

Исследуются синглетные состояния одномерных Хаббард-цепей, описываемые многими парами комплексных волновых векторов. Оригинальные уравнения ЛИБ-ВУ замещаются эквивалентной им системой уравнений, в которых появляются уже только действительные волновые векторы, число которых равно сумме чисел комплексных волновых векторов и электронов, нужных для полузаполнения зоны. В данном смысле новая система уравнений относится уже только к возбуждениям. Определяется энергия возбуждений. По форме энергетического спектра, так же как и по форме волновой функции, действительной в пределе  $U \rightarrow \infty$ , возбуждения можно считать взаимодействующими квазичастицами.

## KIVONAT

1-d Hubbard láncok több komplex hullámszám párral leírható singlet állapotait vizsgáljuk. Az eredeti Lieb-Wu egyenleteket helyettesítjük egy ekvivalens egyenletrendszerrel; ebben már csak valós hullámszámok szerepelnek, ezek száma megegyezik a komplex hullámszámok és a sáv félig töltöttségéhez szükséges elektronok számának összegével. A szövegben tárgyalt értelemben az új egyenletrendszer már csak a gerjesztésekre vonatkozik. Meghatározzuk a gerjesztések energiáját. Az energia spektrum formája, valamint a hullámfüggvények az  $U \rightarrow \infty$  határesetben felvett alakja alapján a gerjesztések kölcsönható kvázirészecskéknek tekinthetők.

## 1. INTRODUCTION

In Paper I. (previous paper, F. Woytarovich 1980 ) those eigenstates of the 1-d Hubbard Hamiltonian

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

have been studied which correspond to states in which the amplitude of finding electron pairs occupying the same site does not vanish even if  $U$  is large. It has been established, that these states are to be described by such solutions of the Lieb-Wu (1968) equations

$$Nk_j = 2\pi I_j - \sum_{\beta=1}^{\frac{N_e - S^z}{2}} 2 \operatorname{arctg} \frac{4}{U} (\sin k_j - \lambda_{\beta}) \quad (1.2)$$

$$\sum_{j=1}^{N_e} 2 \operatorname{arctg} \frac{4}{U} (\lambda_{\alpha} - \sin k_j) = 2\pi J_{\alpha} + \sum_{\beta=1}^{\frac{N_e - S^z}{2}} 2 \operatorname{arctg} \frac{2}{U} (\lambda_{\alpha} - \lambda_{\beta})$$

in which some of the wavenumbers  $k$  are complex. Solutions with one pair of complex wavenumbers were discussed in Paper I. for  $S^z = \frac{1}{2}N - 1$ , and for singlet states, with  $N_e/N$  electrons. In the latter case we have found that to the wavenumber pair  $k \pm i\chi$  there is one  $\Lambda$  coupled by the equation

$$\sin(k \pm i\chi) = \Lambda \mp i \frac{U}{4} \quad (1.3)$$

(This equation is correct up to terms exponentially small in  $N$ ).  $\Lambda$  is determined by an equation of the type

$$2 \operatorname{arctg} \frac{4}{u} (\Lambda - \sin k_e) + 2 \operatorname{arctg} \frac{4}{u} (\Lambda - \sin k_m) = 2\pi f' \quad (1.4)$$

where  $k_e$  and  $k_m$  are the wavenumbers defined by Eq. (1.2) to correspond to the  $I$ -s left out of the ground state  $I$  set. They have to satisfy the equations

$$k_{e(m)} + \int_0^\infty \frac{e^{-\omega \frac{u}{4}} J_0(\omega)}{\omega \cdot \operatorname{ch} \omega \frac{u}{4}} \sin(\omega \sin k_{e(m)}) d\omega = \frac{2\pi}{N} I_{e(m)} + \quad (1.5)$$

$$+ \frac{1}{N} \int_0^\infty \frac{e^{-\omega \frac{u}{4}}}{\operatorname{ch} \omega \frac{u}{4}} \cdot \frac{\sin(\omega(\sin k_{e(m)} - \sin k_{m(e)}))}{\omega} d\omega - \frac{2}{N} \operatorname{arctg} \frac{4}{u} (\sin k_{e(m)} - \Lambda)$$

With  $k_e, k_m$  and  $\Lambda$ , all the other unknowns could be expressed; in particular, the densities of the real  $k$ -s, and "normal"  $\lambda$ -s, could be given as

$$\rho(k) = \frac{1}{2\pi} \left\{ 1 + \cos k \int_0^\infty \frac{e^{-\omega \frac{u}{4}} J_0(\omega)}{\operatorname{ch} \omega \frac{u}{4}} \cos(\omega \sin k) d\omega \right\} + \frac{2 \cos k}{2\pi \cdot N} \cdot \frac{u/4}{(u/4)^2 + (\sin k - \Lambda)^2} \quad (1.6)$$

$$- \frac{1}{2\pi N} \cos k \int_0^\infty \frac{e^{-\omega \frac{u}{4}}}{\operatorname{ch} \omega \frac{u}{4}} (\cos(\omega(\sin k - \sin k_e)) + \cos(\omega(\sin k - \sin k_m))) d\omega$$

and

$$\rho(\lambda) = \left\{ \frac{1}{2\pi} \int_0^{\infty} \frac{J_0(\omega)}{\operatorname{ch} \omega \frac{u}{4}} \cos \omega \lambda \, d\omega \right\} - \frac{1}{N \cdot u} \left( \frac{1}{\operatorname{ch}(\lambda - \operatorname{sink}_e) \frac{2\pi}{u}} + \frac{1}{\operatorname{ch}(\lambda - \operatorname{sink}_m) \frac{2\pi}{u}} \right) \quad (1.7)$$

with the first terms in curly brackets being the groundstate densities  $\rho_0(k)$  and  $\rho_0(\lambda)$

The energy of these states, evaluated by the formula

$$E = \sum_{\text{real } k} (-2 \cos k) - 4 \cos k \operatorname{ch} x \quad (1.8)$$

is

$$E = E_0 + \epsilon(k_e) + \epsilon(k_m) + U \quad (1.9)$$

with  $E_0$  being the groundstate energy and

$$\epsilon(k) = 2 \cos k + 2 \int_0^{\infty} \frac{e^{-\omega \frac{u}{4}}}{\operatorname{ch} \omega \frac{u}{4}} \cdot \frac{J_1(\omega)}{\omega} \cdot \cos(\omega \operatorname{sink}) \, d\omega \quad (1.10)$$

while the momentum evaluated by

$$p = \frac{2\pi}{N} (\sum I + \sum J) \quad (1.11)$$

is

$$\rho = \rho_0 - \rho(k_e) - \rho(k_m) \quad (1.12)$$

with

$$\rho(k) = k + \int_0^{\infty} \frac{e^{-\omega \frac{y}{4}} J_0(\omega) \sin(\omega \sin k)}{\omega \cdot \text{ch} \omega \frac{y}{4}} d\omega \quad (1.13)$$

In this paper we intend to generalise our results in two directions: we look for states with several ( $L$ ) pairs of complex wavenumbers and at the same time we do not fix the bandfilling which can be less than half. We denote the number of electrons needed to make the band half filled by  $H$  :  $H = N - N_e$ . To separate charge and spin redistribution effects, we will look for states in which the spin part is in its ground state. To make sure, that the state can be singlet, we take  $N_e$  even.

The states with several pairs of complex  $k$ -s are expected to have many parameters, thus we will not be able to solve the Lieb-Wu equations completely. What we want to show is that even if the number of complex  $k$ -s is large, they can be separated from the real  $k$ -s and "normal"  $\lambda$ -s and a system of equations analogous to (1.4) (1.5) can be derived, which contains only the parameters of the excitations.

We note that allowing for  $N_e < N$  , the treatment becomes general enough to involve both kinds of charge-excitations (Paper I. Point 2.3).

In Chapter 2. we will derive the system of equations determining the parameters of the excitations. In Chapter 3. the symmetry of the equations found is examined while Chapter 4. is devoted to the discussion of the nature of the states in question.

## 2. EQUATIONS FOR THE STATES WITH SEVERAL COMPLEX WAVENUMBERS

### 2.1 Elimination of the complex wavenumbers from the Lieb-Wu equations

We suppose that, similarly to the case of one complex  $k$ -pair, to each complex  $k$ -pair a  $\Lambda$  is coupled by the equations:

$$\sin(\kappa_n + i\chi_n) = \Lambda_n - i\frac{u}{4} + O(e^{-\eta_n N}) \quad (2.1)$$

$$\sin(\bar{\kappa}_n - i\bar{\chi}_n) = \Lambda_n + i\frac{u}{4} + O(e^{-\bar{\eta}_n N})$$

These equations are the generalisations of (1.3) allowing for the possibility of  $\Lambda$  being complex. The  $\kappa$ -s and  $\chi$ -s satisfying (2.1) (up to exponentially small corrections) are

$$\begin{aligned} \kappa_n &= \arcsin \frac{1}{2} \left\{ \sqrt{\left(\frac{u}{4} - \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n + 1)^2} - \sqrt{\left(\frac{u}{4} - \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n - 1)^2} \right\} \\ \chi_n &= \text{arccosh} \frac{1}{2} \left\{ \sqrt{\left(\frac{u}{4} - \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n + 1)^2} + \sqrt{\left(\frac{u}{4} - \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n - 1)^2} \right\} \end{aligned} \quad (2.2a)$$

$$\chi_n > 0, \quad \text{sign}(\cos \kappa_n) = -\text{sign}\left(\frac{u}{4} - \text{Im}\Lambda_n\right)$$

$$\begin{aligned} \bar{\kappa}_n &= \arcsin \frac{1}{2} \left\{ \sqrt{\left(\frac{u}{4} + \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n + 1)^2} - \sqrt{\left(\frac{u}{4} + \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n - 1)^2} \right\} \\ \bar{\chi}_n &= \text{arccosh} \frac{1}{2} \left\{ \sqrt{\left(\frac{u}{4} + \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n + 1)^2} + \sqrt{\left(\frac{u}{4} + \text{Im}\Lambda_n\right)^2 + (\text{Re}\Lambda_n - 1)^2} \right\} \end{aligned} \quad (2.2b)$$

$$\bar{\chi}_n > 0, \quad \text{sign}(\cos \bar{\kappa}_n) = -\text{sign}\left(\frac{u}{4} + \text{Im}\Lambda_n\right)$$

Note that also in this case the set of complex  $k$ -s consists of complex conjugate pairs provided the  $\Lambda$  set consists of real  $\Lambda$ -s and complex conjugate pairs. In the following we will suppose this, but later we will see that the equations determining the  $\Lambda$ -s indeed define such  $\Lambda$ -sets.

Now the equations for the complex  $k$ -s are

$$N(\kappa_n + i\chi_n) = 2\pi I_n - \sum_{\beta=1}^{\frac{N_0-L}{2}} 2 \operatorname{arctg} \frac{4}{u} (\sin(\kappa_n + i\chi_n) - \lambda_\beta) - \sum_{m=1}^L 2 \operatorname{arctg} \frac{4}{u} (\sin(\kappa_n + i\chi_n) - \Lambda_m) \quad (2.3.a)$$

$$N(\bar{\kappa}_n - i\bar{\chi}_n) = 2\pi \bar{I}_n - \sum_{\beta=1}^{\frac{N_0-L}{2}} 2 \operatorname{arctg} (\sin(\bar{\kappa}_n - i\bar{\chi}_n) - \lambda_\beta) - \sum_{m=1}^L 2 \operatorname{arctg} (\sin(\bar{\kappa}_n - i\bar{\chi}_n) - \Lambda_m) \quad (2.3.b)$$

It is not hard to verify that (2.1) and so (2.2.a-b) are the solutions of the imaginary parts of (2.3.a-b) if the conditions

$$\kappa_n + \frac{1}{N} \operatorname{Im} \left\{ \sum_{\beta} 2 \operatorname{arctg} \frac{4}{u} (\sin(\kappa_n + i\chi_n) - \lambda_\beta) + \sum_{m \neq n} 2 \operatorname{arctg} \frac{4}{u} (\sin(\kappa_n + i\chi_n) - \Lambda_m) \right\} = \eta_n > 0 \quad (2.4)$$

$$-\bar{\kappa}_n + \frac{1}{N} \operatorname{Im} \left\{ \sum_{\beta} 2 \operatorname{arctg} \frac{4}{u} (\sin(\bar{\kappa}_n - i\bar{\chi}_n) - \lambda_\beta) + \sum_{m \neq n} 2 \operatorname{arctg} \frac{4}{u} (\sin(\bar{\kappa}_n - i\bar{\chi}_n) - \Lambda_m) \right\} = -\bar{\eta}_n < 0$$

are fulfilled. These inequalities are to be checked at the end when the  $\lambda$ -s and  $\Lambda$ -s are known.

The equations defining the real  $k$ -s are

$$Nk_j = 2\pi I_j - \left\{ \sum_{\beta=1}^{\frac{N_e}{2}-L} 2 \operatorname{arctg} \frac{4}{u} (\sin k_j - \lambda_\beta) + \sum_{m=1}^L 2 \operatorname{arctg} \frac{4}{u} (\sin k_j - \Lambda_m) \right\}_{\text{discont.}} \quad (2.5)$$

$$- \left\{ \sum_{\beta=1}^{\frac{N_e}{2}-L} 2 \operatorname{arctg} \frac{4}{u} (\sin k_j - \lambda_\beta) + \sum_{m=1}^L 2 \operatorname{arctg} \frac{4}{u} (\sin k_j - \Lambda_m) \right\}_{\text{cont.}}$$

where we understand

$$\operatorname{Re} \left\{ 2 \operatorname{arctg} \frac{4}{u} (\sin k - \Lambda) \right\}_{\text{cont.}} = \operatorname{arctg} \frac{\sin k - \operatorname{Re} \Lambda}{\frac{u}{4} + \operatorname{Im} \Lambda} + \operatorname{arctg} \frac{\sin k - \operatorname{Re} \Lambda}{\frac{u}{4} - \operatorname{Im} \Lambda} \quad (2.6.a)$$

$$i \operatorname{Im} \left\{ 2 \operatorname{arctg} \frac{4}{u} (\sin k - \Lambda) \right\}_{\text{cont.}} = \frac{1}{2i} \ln \frac{\left(\frac{u}{4} + \operatorname{Im} \Lambda\right)^2 + (\sin k - \operatorname{Re} \Lambda)^2}{\left(\frac{u}{4} - \operatorname{Im} \Lambda\right)^2 + (\sin k - \operatorname{Re} \Lambda)^2}$$

$$\operatorname{Re} \left\{ 2 \operatorname{arctg} \frac{4}{u} (\sin k - \Lambda) \right\}_{\text{discont.}} = \begin{cases} \pi \operatorname{sign}(\sin k - \operatorname{Re} \Lambda) & \text{if } |\operatorname{Im} \Lambda| > \frac{u}{4} \\ 0 & \text{if } |\operatorname{Im} \Lambda| < \frac{u}{4} \end{cases} \quad (2.6.b)$$

$$\operatorname{Im} \left\{ 2 \operatorname{arctg} \frac{4}{u} (\sin k - \Lambda) \right\}_{\text{discont.}} = 0$$

The  $I$  set in (2.5) consists of integers if  $N_e/2$  is even and half-odd-integers if  $N_e/2$  is odd. Note that the  $I'$  set defined as

$$I_i' = I_i - \frac{1}{2\pi} \left\{ \sum_{\beta} 2 \operatorname{arctg} \frac{u}{u} (\sin k_i - \lambda_{\beta}) - \sum_m 2 \operatorname{arctg} \frac{u}{u} (\sin k_i - \Lambda_m) \right\}_{\text{discont.}} \quad (2.7)$$

consists of integers (or half odd-integers) if the  $I$ -s are integers (or half odd-integers). Thus, depending on the parity of  $(N-H)/2$  we have to choose  $N-2L-H$  different  $I'$ -s from one of the sets

$$-\frac{1}{2}(N-1), -\frac{1}{2}(N-3), \dots \quad \frac{1}{2}(N-3), \frac{1}{2}(N-1) \quad (2.8.a)$$

$$-\frac{1}{2}(N-2), -\frac{1}{2}(N-4), \dots \quad \frac{1}{2}(N-1), \frac{1}{2}N \quad (2.8.b)$$

Equation (2.5) defines  $k$ -s also to the  $I'$ -s left out from (2.8.a) or (2.8.b). We will denote this  $k$ -s by the index  $h$  (for "hole"). The density of the  $k$ -s, satisfying (2.5) is

$$\rho(k) = \frac{1}{2\pi} + \frac{1}{2\pi N} \cdot 2 \cos k \sum_{\beta} \frac{(u/u)}{(u/u)^2 + (\sin k - \lambda_{\beta})^2} + \frac{1}{2\pi N} 2 \cos k \sum_m \frac{(u/u)}{(u/u)^2 + (\sin k - \Lambda_m)^2} \quad (2.9)$$

As this  $\rho(k)$  contains also the contribution of the variables  $k_h$ , to replace  $k$ -sums, we have to use

$$\rho^*(k) = \rho(k) - \frac{1}{N} \sum_{h=1}^{H+2L} \delta(k - k_h) \quad (2.10)$$

The equations for the "normal"  $\lambda$ -s are

$$\begin{aligned} \sum_{j \neq h} 2 \operatorname{arctg} \frac{4}{u} (\lambda_\alpha - \sin k_j) + \sum_{m=1}^L 2 \operatorname{arctg} \frac{4}{u} (\lambda_\alpha - \sin(\kappa_m + i\bar{\kappa}_m)) + \\ + \sum_{m=1}^L 2 \operatorname{arctg} \frac{4}{u} (\lambda_\alpha - \sin(\bar{\kappa}_m - i\bar{\kappa}_m)) = 2\pi \mathcal{F}'_\alpha + \sum_{\beta=1}^{\frac{N_0-L}{2}} 2 \operatorname{arctg} \frac{2}{u} (\lambda_\alpha - \lambda_\beta) + \\ + \sum_{m=1}^L 2 \operatorname{arctg} \frac{2}{u} (\lambda_\alpha - \Lambda_m) \end{aligned} \quad (2.11)$$

Now using (2.1) and the identity

$$\begin{aligned} 2 \operatorname{arctg} \frac{4}{u} (\lambda_\alpha - \Lambda_m - i\frac{u}{4}) + 2 \operatorname{arctg} \frac{4}{u} (\lambda_\alpha - \Lambda_m + i\frac{u}{4}) = \\ = 2 \operatorname{arctg} \frac{2}{u} (\lambda_\alpha - \Lambda_m) + \pi \operatorname{sign}(\operatorname{Re}(\lambda_\alpha - \Lambda_m)) \end{aligned} \quad (2.12)$$

One has (up to exponentially small terms)

$$\sum_{j \neq h} 2 \operatorname{arctg} \frac{4}{u} (\lambda_\alpha - \sin k_j) = 2\pi \mathcal{F}'_\alpha + \sum_{\beta=1}^{\frac{N_0-L}{2}} 2 \operatorname{arctg} \frac{2}{u} (\lambda_\alpha - \lambda_\beta) \quad (2.13)$$

with

$$\mathcal{F}'_\alpha = \mathcal{F}_\alpha - \sum_m \frac{1}{2} \operatorname{sign}(\operatorname{Re}(\lambda_\alpha - \Lambda_m)) \quad (2.14)$$

$\mathcal{F}'_\alpha$  is integer if  $(N-H-2L)/2$  is odd and half odd-integer if  $(N-H-2L)/2$  is even. Note that (2.13) is formally the same as the corresponding equation for a system with  $N-2L-H$

electrons, all described by real  $k$ -s.

The  $\Lambda$ -s coupled to the complex  $k$ -s are determined by the equations:

$$\begin{aligned} & \sum_{j \neq h} 2 \operatorname{arctg} \frac{y}{u} (\Lambda_n - \sin k_j) + \sum_{m=1}^L 2 \operatorname{arctg} \frac{y}{u} (\Lambda_n - \sin(\kappa_m + i\bar{\chi}_m)) + \\ & + \sum_{m=1}^L 2 \operatorname{arctg} \frac{y}{u} (\Lambda_n - \sin(\bar{\kappa}_m - i\bar{\chi}_m)) = 2\pi f_n + \sum_{\beta=1}^{N_0-L} 2 \operatorname{arctg} \frac{z}{u} (\Lambda_n - \lambda_\beta) + \\ & + \sum_{m=1}^L 2 \operatorname{arctg} \frac{z}{u} (\Lambda_n - \Lambda_m) \end{aligned} \quad (2.15)$$

If in the first term of the l.h.s. we replace the continuous part of the sum over the real  $k$ -s by the corresponding integral, then we have, up to terms proportional to  $1/N^2$  (calculating also the sum of the discontinuous parts by means of  $\hat{p}(k)$  would introduce an error of the order of  $1/N$ )

$$\begin{aligned} & \frac{1}{N} \sum_{j \neq h} \left\{ 2 \operatorname{arctg} \frac{y}{u} (\Lambda_n - \sin k_j) \right\}_{\text{cont}} \cong -\frac{1}{N} \sum_{h=1}^{H+2L} \left\{ 2 \operatorname{arctg} \frac{y}{u} (\Lambda_n - \sin k_h) \right\}_{\text{cont}} \\ & + \operatorname{sign}\left(\frac{y}{u} - \operatorname{Im} \Lambda_n\right) \operatorname{arcsin} \frac{1}{2} \left\{ \sqrt{\left(\frac{y}{u} - \operatorname{Im} \Lambda_n\right)^2 + (\operatorname{Re} \Lambda_n + 1)^2} - \sqrt{\left(\frac{y}{u} - \operatorname{Im} \Lambda_n\right)^2 + (\operatorname{Re} \Lambda_n - 1)^2} \right\} + \\ & + \operatorname{sign}\left(\frac{y}{u} + \operatorname{Im} \Lambda_n\right) \operatorname{arcsin} \frac{1}{2} \left\{ \sqrt{\left(\frac{y}{u} + \operatorname{Im} \Lambda_n\right)^2 + (\operatorname{Re} \Lambda_n + 1)^2} - \sqrt{\left(\frac{y}{u} + \operatorname{Im} \Lambda_n\right)^2 + (\operatorname{Re} \Lambda_n - 1)^2} \right\} - \\ & - i(\chi_n - \bar{\chi}_n) \end{aligned} \quad (2.16)$$

We used here the identities (2.6.a) and

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \operatorname{arctg} \frac{\Lambda - \sin k}{\gamma} dk = \operatorname{arcsin} \frac{1}{2} \left\{ \sqrt{\gamma^2 + (\Lambda + 1)^2} - \sqrt{\gamma^2 + (\Lambda - 1)^2} \right\} \quad (2.17)$$

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{z} \ln \frac{z^2 + (\Lambda - \sin k)^2}{z^2 + (\Lambda - \sin k)^2} dk = \int_0^{\infty} \frac{e^{-z_2 \omega} - e^{-z_1 \omega}}{\omega} J_0(\omega) \cos \omega \Lambda d\omega \quad (2.18.a)$$

$$\int_0^{\infty} \frac{J_0(\omega) (1 - e^{-z \omega})}{\omega} d\omega = \operatorname{arccch} \frac{1}{z} \left\{ \sqrt{z^2 + (\Lambda+1)^2} + \sqrt{z^2 + (\Lambda-1)^2} \right\} \quad (2.18.b)$$

Thus summing up Eqs. (2.3.a), (2.3.b) and (2.15), and using also (2.1) and (2.12), one obtains

$$\sum_{k=1}^{2L+H} 2 \operatorname{arctg} \frac{y}{u} (\Lambda_n - \sin k_k) = 2\pi \mathcal{F}'_n + \sum_{m=1}^L 2 \operatorname{arctg} \frac{z}{u} (\Lambda_n - \Lambda_m) \quad (2.19)$$

with

$$\begin{aligned} \mathcal{F}'_n &= N \cdot \operatorname{sign}(\operatorname{Re} \Lambda_n) - \mathcal{F}_n - I_n - \bar{I}_n + \sum_{m \neq n} \operatorname{sign}(\operatorname{Re}(\Lambda_n - \Lambda_m)) \\ &+ \sum_{\text{all } k} \frac{\operatorname{sign}(\frac{y}{u} - |\operatorname{Im} \Lambda_n|) - 1}{2} \cdot \frac{\operatorname{sign}(\operatorname{Re} \Lambda_n) - \operatorname{sign}(\operatorname{Re} \Lambda_n - \sin k)}{2} \quad (2.20) \\ &+ \frac{1}{2} \sum_{\beta} \operatorname{sign}(\operatorname{Re}(\Lambda_n - \lambda_{\beta})) \end{aligned}$$

$\mathcal{F}'_n$  being integer if  $N-L-H$  is odd and half odd-integer if  $N-L-H$  is even.

The actual system to be solved is the system of (2.5), (2.13) and (2.19). Knowing all the  $k_i$ -s and  $k_h$ -s,  $\lambda_{\beta}$ -s, and

$\Lambda_n$ -s , the complex wavenumbers can be calculated, the original  $I$  , and  $J$  quantum numbers can be determined and through (2.3.a-b) also the exponentially small corrections to the  $k$ -s and  $\chi$ -s of (2.2.a-b) can be obtained.

It is interesting to note, that the system (2.5), (2.13), (2.19) is entirely symmetric (as far as the structure is concerned) in the variables  $k_j$ ,  $\lambda_\alpha$  and  $k_h$ ,  $\Lambda_m$ . The only asymmetry is that the number of  $\lambda_\alpha$  -s is the half of the number of  $k_j$  -s while the number of  $\Lambda_m$  -s can be less than half the number of  $k_h$  -s (if  $H$  is not zero). But this is only due to the fact that we are investigating  $S^z=0$  states. It is not hard to see, that if we were calculating states with  $S^z \neq 0$  , then even this asymmetry would disappear. (In the general case, with  $N_e$  electrons,  $M_1$   $\lambda_\alpha$ -s and  $M_2=L$   $\Lambda_m$ -s (  $S^z = \frac{1}{2} N_e - (M_1 + M_2)$  ) the prescription for the  $I'$ ,  $J'_\alpha$  and  $J'_h$  parameters would be that  $I'$  -s are integer numbers if  $M_1 + M_2$  is even,  $J'_\alpha$  -s are integers if  $N_e - M_1$  is odd, and  $J'_h$  -s are integers if  $N_e - M_2$  is odd).

## 2.2 Elimination of the normal $\lambda$ -s.

Equation (2.13) may have many solutions depending on the choice of the parameters  $J'_\alpha$ . As we stated in our program, we would like to describe such states in which the spin degrees of freedom are not excited. To do this, based on the analogy of (2.13) and the corresponding equation of a system with  $N-H-2L$  electrons, we have to choose that  $J'_\alpha$  -set which is characteristic of the ground state of a system of  $N-H-2L$  electrons, i.e.

the set

$$-\frac{1}{2} \left( \frac{N-H-2L}{2} - 1 \right), -\frac{1}{2} \left( \frac{N-H-2L}{2} - 3 \right), \dots, \frac{1}{2} \left( \frac{N-H-2L}{2} - 1 \right) \quad (2.21)$$

With this choice of the  $\lambda'_\alpha$ -s, the density of the  $\lambda$ -s must satisfy the equation

$$2 \int_{-\pi}^{\pi} \frac{(u/4)}{(u/4)^2 + (\lambda - \sin k)^2} \rho^*(k) dk = 2\pi \sigma(\lambda) + 2 \int_{-\infty}^{\infty} \frac{(u/2)}{(u/2)^2 + (\lambda - \lambda')^2} \sigma(\lambda') d\lambda' \quad (2.22)$$

The solution of (2.22) is easily obtained by Fourier transformation:

$$\sigma(\lambda) = \frac{1}{2\pi} \int_0^{\infty} \frac{J_0(\omega) \cos(\omega \lambda)}{\operatorname{ch} \omega \frac{u}{4}} d\omega - \frac{1}{Nu} \sum_{k=1}^{H+2L} \frac{1}{\operatorname{ch} (\lambda - \sin k) \frac{2\pi}{u}} \quad (2.23)$$

This  $\sigma(\lambda)$  allows us to eliminate the  $\lambda'_\alpha$ -s from  $\rho(k)$  of (2.9), with the result

$$\begin{aligned} \rho(k) &= \frac{1}{2\pi} \left( 1 + \cos k \int_0^{\infty} \frac{e^{-\omega \frac{u}{4}}}{\operatorname{ch} \omega \frac{u}{4}} J_0(\omega) \cos(\omega \sin k) d\omega \right) \\ &\quad - \frac{1}{2\pi \cdot N} \cos k \int_0^{\infty} \frac{e^{-\omega \frac{u}{4}}}{\operatorname{ch} \omega \frac{u}{4}} \sum_{k=1}^{H+2L} \cos(\omega (\sin k - \sin k_k)) d\omega \\ &\quad + \frac{1}{2\pi \cdot N} \cdot 2 \cos k \sum_{m=1}^L \frac{(u/4)}{(u/4)^2 + (\sin k - \Lambda_m)^2} \end{aligned} \quad (2.24)$$

By means of  $\sigma(\lambda)$  from (2.5) equations for the variables  $k_h$  can be obtained

$$N(k_h + \int_0^\infty \frac{e^{-\omega \frac{y}{4}}}{\operatorname{ch} \omega \frac{y}{4}} \mathcal{I}_0(\omega) \frac{\sin(\omega \sin k_h)}{\omega} d\omega) = 2\pi I'_h +$$

$$+ \sum_{h'=1}^{H+2L} \int_0^\infty \frac{e^{-\omega \frac{y}{4}}}{\operatorname{ch} \omega \frac{y}{4}} \cdot \frac{\sin(\omega(\sin k_h - \sin k_{h'}))}{\omega} d\omega - \sum_{m=1}^L \left\{ 2 \operatorname{arctg} \frac{y}{4} (\sin k_h - \Lambda_m) \right\}_{\text{cont.}} \quad (2.25)$$

As by the  $k_h$ -s and  $\Lambda_n$ -s all the other unknowns are determined the problem is reduced to the solving of Eqs. (2.19) and (2.25)

### 2.3 Energy and momentum

The energy is calculated by the formula

$$E = -N \int_{-\pi}^{\pi} 2 \cos k \rho^*(k) dk - \sum_{m=1}^L 2 (\cos(k_m + i\chi_m) + \cos(\bar{k}_m - i\bar{\chi}_m)) \quad (2.26)$$

which gives

$$E = E_0 + \sum_{h=1}^{H+2L} \mathcal{E}(k_h) + LU \quad (2.27)$$

where  $\mathcal{E}(k)$  is given by (1.10). The momentum evaluated by means of the formulas (1.11), (2.7), (2.8), (2.14), (2.20), (2.21) and (2.25), turns out to be (up to  $n \cdot 2\pi$ )

$$p = \sum_{h=1}^{H+2L} -p(k_h) + \psi \quad (2.28)$$

where  $p(k)$  is given by (1.13), and  $\psi$  is zero if  $(N-H)/2$  is odd and  $\pi$  if  $(N-H)/2$  is even (in the general case

when  $N-H$  can be odd,  $\psi = \pi \cdot (1 + (N-H)/2) \text{ mod } 2\pi$ . The appearance of this  $\psi$  is not connected with the presence of complex wave-numbers. It rather resembles the fact, that even the ground state momentum of a Heisenberg chain can be  $0$ ,  $\pi/2$  or  $\pi$  depending on the parity of the number of sites, and that even the ground state momentum of a half filled Hubbard chain can be  $0$  or  $\pi$  depending on the parity of  $N/2$ .

#### 2.4 A special solution for the $\Lambda_n$ -s

The equations (2.19) and (2.25) are highly nonlinear but there is one case when they can be replaced by a linear integral equation. This is the case, when  $H=0$ ,  $L$  is macroscopic (comparable to  $N$ ) and we choose for the  $\zeta_n'$  set the numbers

$$-\frac{1}{2}(L-1), -\frac{1}{2}(L-3), \dots, \frac{1}{2}(L-1) \quad (2.29)$$

With this choice of  $\zeta_n'$ -s all  $\Lambda_n$  will be real, and the number of  $\Lambda$ -s between  $\Lambda$  and  $\Lambda+d\Lambda$  can be given as  $(2L) \cdot f(\Lambda) d\Lambda$ , where

$$f(\Lambda) = \frac{1}{(2L)} \cdot \sum_{k=1}^{2L} \frac{1}{u} \cdot \frac{1}{\text{ch}(\Lambda - \sin k_n) \frac{2\pi}{u}} \quad (2.30)$$

Combining this with (2.23) one finds that the density of all  $\lambda$ -s and  $\Lambda$ -s is the same as the density of  $\lambda$ -s in the ground state

$$\sigma(\lambda) + \frac{2L}{N} f(\lambda) = \frac{1}{2\pi} \int_0^{\infty} \frac{J_0(\omega)}{\text{ch} \omega \frac{u}{4}} \cos \omega \lambda d\omega = \sigma_0(\lambda) \quad (2.31)$$

using the  $f(\lambda)$  to evaluate the sum over the  $\lambda_n$  -s in (2.25), we find that

$$\rho(k_k) = \frac{2\pi}{N} I'_k \quad (2.32)$$

i.e. in this special case the quasiparticles are not interacting. We should emphasize, that this holds only if  $L$  is large and the error introduced by using  $f(\lambda)$  in the summations (for which  $1/L$  is an upper limit) is small enough, and if we choose (2.29) to characterize the system.

#### 2.5 On the conditions (2.4)

Any solution of the system (2.5), (2.13) and (2.19) is meaningful only if substituting the  $\lambda$  -s into (2.4), the inequalities are satisfied. We were not able to show in general that they hold, only in two cases: one in which the number of excitations is small compared to  $N$  (i.e. the number of  $\lambda$  -s is not macroscopic) and at the same time the spin part is near to its ground state. The other case is when although the number of  $\lambda$  -s is macroscopic, the system is near to the state described in Point 2.4. In both cases the sums in (2.4) can be estimated by integrating over the  $\lambda$  -s using their ground state density. This estimation shows that both  $\eta_n$  and  $\bar{\eta}_n$  are definitely positive. It is also true, that for a small number of complex  $k$  -pairs, to each pair there must exist a  $\lambda$  satisfying (2.2.a-b). (If there were complex  $k$  pair without  $\lambda$ , then to that pair  $\eta_n$  and  $\bar{\eta}_n$  should be zero.)

### 2.6 The number of solutions

Eq. (2.19) in the large  $u$  limit goes over into the secular equation of a Heisenberg chain with length  $2L+H$  and with  $L+H$  spins pointing in one direction and  $L$  spins pointing in the other. If Bethe's hypothesis holds, (i.e. all eigenstates of a Heisenberg chain can be described by the Bethe equations) then these equations must have  $\binom{2L+H}{L}$  solutions. At the same time one has  $\binom{N}{2L+H}$  possibilities to choose the  $I_k'$  set. Supposing continuous behaviour in the large  $u$  limit, one can conclude that the equation (2.25) together with (2.19) must have  $N! / \{(N-H-2L)!(L+H)!L!\}$  solutions for all  $u > 0$  and this is exactly the number of states in which there are  $H+L$  empty and  $L$  doubly occupied sites, with the spins belonging to the  $N-H-2L$  singly occupied sites being in ground state. Thus (2.25) and (2.19) describes all of these states (for small enough  $L$  to be sure that (2.4) is valid). It is interesting to note, that with the same reasoning, counting into account the number of different solutions of Eq. (2.13) we have that Eqs. (2.5), (2.13) and (2.19) should have

$$\sum_{L=0}^{\frac{N-H}{2}} \binom{2L+H}{L} \binom{N-2L-H}{(N-2L-H)/2} \binom{N}{2L+H} = \left\{ \binom{N}{\frac{N-H}{2}} \right\}^2 \quad (2.33)$$

different solutions, which is exactly the number of  $S^z=0$  states of  $N-H$  electrons in a chain of length  $N$ . Unfortunately to conclude that the system (2.5), (2.13) and (2.19) describes all solutions of the problem one should have to show that (2.4) holds for all solutions.

3. SYMMETRY OF THE SYSTEM (2.5) (2.13) (2.19)

As we already mentioned, the system (2.5), (2.13) and (2.19) is entirely symmetric in the variables  $k_j, \lambda_\alpha$  and  $k_h, \Lambda_n$ . Now we show that this symmetry is present in some form also in the momentum and the energy of the system.

Let us define the complex wavenumbers  $\kappa_\alpha + i\chi_\alpha$  and  $\bar{\kappa}_\alpha - i\bar{\chi}_\alpha$  for the  $\lambda_\alpha$  variables analogously to (2.1) and calculate

$$\sum_{\text{all } k} k + \sum_{\alpha} \{(\kappa_\alpha + i\chi_\alpha) + (\bar{\kappa}_\alpha - i\bar{\chi}_\alpha)\} + \sum_m \{(\kappa_m + i\chi_m) + (\bar{\kappa}_m - i\bar{\chi}_m)\} \quad (3.1)$$

using (2.5), (2.9) and that

$$\int_{-\pi}^{\pi} \left\{ 2 \operatorname{arctg} \frac{u}{u} (\lambda_{\alpha(m)} - \sin k) \right\}_{\text{cont}} \rho(k) dk = \quad (3.2)$$

$$-(\kappa_{\alpha(m)} + i\chi_{\alpha(m)}) - (\bar{\kappa}_{\alpha(m)} - i\bar{\chi}_{\alpha(m)}) + \pi \operatorname{sign}(\operatorname{Re} \lambda_{\alpha(m)}) \left( 1 + \operatorname{St} \left( \frac{u}{u} - |\operatorname{Im} \lambda_{\alpha(m)}| \right) \right)$$

$\operatorname{St}(x)$  being the step function, we find that the value of (3.1) is simply (up to  $n \cdot 2\pi$ )

$$\frac{2\pi}{N} \sum_{\text{all } I'} I' = \begin{cases} 0 \\ \pi \end{cases} \quad (3.3)$$

depending on whether  $N-M$  ( $M$  being the number of down spins) is even ( $\pi$ ) or odd ( $0$ ). Thus interchanging the roles of the

variables  $k_j, \lambda_\alpha$  and  $k_h, \Lambda_m$  changes the sign of the momentum of the system (up to a term  $\pi$ )

If we calculate the sum

$$\begin{aligned} \sum_{\text{all } k} (-2 \cos k) &= \sum_m 2(\cos(\kappa_m + i\lambda_m) + \cos(\bar{\kappa}_m - i\bar{\lambda}_m)) \\ &= \sum_\alpha 2(\cos(\kappa_\alpha + i\lambda_\alpha) + \cos(\bar{\kappa}_\alpha - i\bar{\lambda}_\alpha)) \end{aligned} \quad (3.4)$$

we find that this is equal to  $M \cdot U$ . Thus in this sense the states in which the roles of the variables  $k_j, \lambda_\alpha$  and  $k_h, \Lambda_n$  are interchanged are "complementers". This complementarity can be used to calculate the energy and wavefunction of highly excited states or low energy states of a Hubbard chain with negative  $U$ . (From this, for example, one knows that the highest energy state of  $N$  electrons is the one in which all  $k$ -s are complex and the distribution of  $\Lambda_n$ -s is the same as the distribution of  $\lambda_\alpha$ -s in the ground state, but this is also the ground state of the chain with  $-U$ .)

This complementarity may be connected with the property of the Hubbard Hamiltonian, that if we introduce holes instead of the up-spin electrons, then

$$\hat{H} \longrightarrow U \cdot \sum_{i=1}^N n_{i\uparrow} - \hat{H}' \quad (3.5)$$

where  $\hat{H}'$  has the same structure as  $\hat{H}$ . Taking into account

the parallelism that in the complementary states the parameters  $\lambda_k$  describing the spin part change role with the  $\Lambda_n$  parameters connected with the charge distribution, and that the transformation which transforms  $\hat{H}$  into  $\hat{H}'$  introduces doubly occupied or empty sites instead of the singly occupied ones (uncompensated spins), and vice versa, the above-suspected connection seems very possible.

#### 4. ON THE NATURE OF STATES WITH COMPLEX WAVENUMBERS

The goal of this chapter is to connect our results obtained through the lengthy algebraic work of the previous chapters with some less rigorous but more or less transparent pictures. A full analysis of the structure of the eigenstates would require the knowledge of the different correlation functions, but this is beyond our grasp. Instead, we have to be satisfied with some indirect reasoning or with the examination of limiting cases. We will base our arguments on the energy-momentum relationship, and on the analysis of the  $U \rightarrow \infty$  behaviour of the wavefunction.

##### 4.1 Quasi-particle picture for the energy-momentum relationship

To have a closer look at the energy and the momentum, let us consider first a system in which there are  $N_e = N - H$  electrons in a state described by real wavenumbers. According to (2.27) and (2.28), the energy measured from the ground state energy of a half filled band, and the momentum are

$$\begin{aligned} E &= \sum_{k=1}^H \epsilon(k_k) \\ P &= \sum_{k=1}^H -p(k_k) + \pi(1 + N_e/2) \end{aligned} \tag{4.1}$$

If we take a system with more electrons than  $N$ , with  $N_e' - N = H'$  we have

$$\epsilon = \sum_{h=1}^{H'} \epsilon(k_h) + H'U \quad (4.2)$$

$$p = \sum_{h=1}^{H'} -p(k_h) + \bar{\pi}(1 + N_e/2)$$

(such a state can be obtained by taking a state with  $N-H'$  electrons and acting on it by the operator  $\exp\left\{-i\sum_{n=1}^N \pi(n+\frac{1}{2})(C_{n+}^+ C_{n+}^+ + C_{n+} C_{n+})\right\}^*$ . This introduces holes instead of particles, and changes the energy by  $H'U$  and the momentum by  $\bar{\pi}H'$ . Now looking at the energy of a state with  $N_e = N-H$  electrons and with  $L$  pairs of complex wavenumbers

$$\epsilon = \sum_{h=1}^{H+2L} \epsilon(k_h) + LU \quad (4.3)$$

$$p = \sum_{h=1}^{H+2L} -p(k_h) + \bar{\pi}(1 + N_e/2)$$

we see that it is like the energy of a state with  $L+H$  holes in a subband with dispersion  $-\epsilon(k(p))$  ((4.1)) and  $L$  particles in an other band with dispersion  $\epsilon(k(p))+U$  ((4.2)). Thus the form of the energy suggests that introducing pairs of complex wavenumbers instead of real  $k$ -s acts like exciting a number of carriers from one band to the other. This picture, however, reflects only the apparent additivity of the energy and momentum, and gives the right coefficient of  $U$ . One should not, however, forget that the states under consideration are excited states of a many-body system, and even if these quasi particles and holes can be identified in some limiting cases as some sort of spatial configurations, their energy and momentum is carried by the system

\* See p. 33.

as a whole. This is expressed in the fact that introducing a pair of complex wavenumbers changes the value of all the other wavenumbers, and consequently the contribution of the other electrons to the total energy and momentum. Another point is that these excitations, if we treat them as quasi particles, should be regarded as interacting ones. This is reflected in the fact that the momenta of the quasi particles are not free parameters, they are connected with the actual quantumnumbers through a system of equations ((2.19), (2.25)). In this respect the picture is very similar to the one we can connect with the motion of the electrons themselves: we have a system of particles which can propagate along a chain, and can scatter on each other. In this scattering processes they can change momentum and depending on their momenta, their phase is shifted as well. To have a stationary state, we have to fit the momenta and the phaseshifts properly. These conditions are expressed in the Lieb-Wu equations and we can put this picture behind the equations (2.19), (2.25), too. This also explains why we can not tell, which momenta are to be associated with the holes and which ones with particles.

The analogy of Eqs. (2.19), (2.25) with the original Lieb-Wu equations makes possible an alternative interpretation. We may regard the quasi particles as identical ones with energy momentum dispersion  $\epsilon(k(p))$ , but carrying an "isospin"  $\pm 1/2$ . Then we do not have to think in terms of two bands but we have to interpret the  $u$  as the creation energy of a pair of these quasi particles with isospins  $+1/2$  and  $-1/2$ .

4.2 The  $u \rightarrow \infty$  limit of the wavefunction

The above detailed interpretation of the states with complex wavenumbers is based merely on the form of the energy and the structure of the equations determining the parameters connected with these excitations. Now we try to find out about the nature of these states in the large  $u$  limit, where also the form of the wavefunction becomes more transparent.

Making the  $u \rightarrow \infty$  limit in the wavefunction (see expressions (2.3-8) of Paper I.) one finds, that some of the amplitudes diverge. As in the normalised wavefunction only the terms with the strongest divergence will give finite contributions, picking out the most divergent terms we can separate those configurations which can be realised even if  $u$  is very large. This way we get the result that for large  $u$  only those configurations remain in which the number of doubly occupied sites is equal to the number of complex  $k$ -pairs. In the amplitude of these configurations only those permutations  $P$  and  $\bar{\pi}$  give contributions in which the  $k_m + i\kappa_m$  and  $\bar{k}_m - i\bar{\kappa}_m$  wavenumber pair belongs to one doubly occupied site, and the  $\lambda_m$  belongs to the down spin at this site. Using the fact, that for large  $u$  all the  $\sin k_j$ -s can be neglected compared to the  $\lambda_{\alpha}$ -s and  $\lambda_n$ -s, and also using (2.1) the amplitude of the configurations in question can be given as

$$\begin{aligned}
 & (-1)^Q \left\{ e^{i \sum_{i=1}^L n_i^d} \phi_1(y_1^d, y_2^d, \dots, y_L^d) \right\}_x \\
 & = \left\{ \sum_P (-1)^P e^{i \sum_{j=1}^{N-H-2L} k_{P_j} n_{Q_j}^s} \cdot \phi_2(y_1^s, y_2^s, \dots, y_{N-L}^s) \right\}
 \end{aligned}
 \tag{4.4}$$

Here the permutation  $Q$  arranges the coordinates  $n_1, n_2, \dots, n_{N-H}$  into nondecreasing order with the restriction that from two equal coordinates that of the electron with down spin must come first. The  $n_{Q_i}^s$ -s refer to singly occupied sites, the  $n_i^d$  to doubly occupied ones and  $P$  goes over all permutations of the real wavenumbers. The functions  $\phi_1$  and  $\phi_2$  are essentially the Heisenberg eigenfunctions:

$$\phi_2 = \sum_{\pi} A(\lambda_{\pi_1} \lambda_{\pi_2} \dots \lambda_{\pi_{M-L}}) \left( \frac{i\lambda_{\pi_1} + u/4}{i\lambda_{\pi_1} - u/4} \right)^{y_1^s} \dots \left( \frac{i\lambda_{\pi_{M-L}} + u/4}{i\lambda_{\pi_{M-L}} - u/4} \right)^{y_{M-L}^s} \quad (4.5)$$

$$\frac{A(\dots \lambda_{\pi_i} \lambda_{\pi_{i+1}} \dots)}{A(\dots \lambda_{\pi_{i+1}} \lambda_{\pi_i} \dots)} = \frac{i(\lambda_{\pi_{i+1}} - \lambda_{\pi_i}) - u/2}{i(\lambda_{\pi_i} - \lambda_{\pi_{i+1}}) + u/2}$$

The numbers  $y^s$  are the coordinates of the down spins in the chain of singly occupied sites in increasing order.  $\phi_1$  is formally the same as  $\phi_2$  with the difference that  $u$  must be replaced by  $-u$ , the  $\lambda_x$ -s by the  $\lambda_m$ -s, and the numbers  $y^d$  are the coordinates of the doubly occupied sites in the chain containing only the doubly and unoccupied sites. The amplitude of the configurations in which the number of doubly occupied sites is more or less than  $L$  vanishes at least like  $1/u$  as  $u \rightarrow \infty$ .

To understand (4.4) let us consider a configuration in which the first  $N-H-2L$  sites in the chain are singly occupied, and the remaining  $H+2L$  sites are the empty or doubly occupied ones. In this configuration the electrons can not move (except

the last one) as either the Pauli principle or the large on-site repulsion prevents it. Although in this configuration there is no direct interaction between the electrons, through an intermediate state with energy  $u$  neighbouring electrons can see each other's spins, and electrons with different spins can change position, i.e. the spins can move in the same way as spins move in a Heisenberg chain, the distribution of the spins will correspond to the eigenstates of the Heisenberg Hamiltonian. The situation with the empty and doubly occupied sites is similar: Neighbouring sites can observe each others occupancy through an intermediate state of relative energy  $-u$  ; and also the same intermediate state makes possible for an empty and doubly occupied site to change position. Thus the distribution of the empty and doubly occupied sites will be the same as the distribution of up and down spins in a Heisenberg chain. (See also Chapter 3.) It is clear that neither the spin distribution nor the relative distribution of the empty and doubly occupied sites does change if the chain of singly occupied sites is "diluted" by empty and doubly occupied sites making possible also direct propagation for the electrons.

Now, having the  $u \rightarrow \infty$  form of the eigenfunction at hand, we can see, that complex  $k$  pairs in a solution of the Liebs-Wu equations correspond to doubly occupied and empty sites if  $u$  is large. Thus in this limit the quasi particles corresponding to these excited states should be identified with these objects. We can see also, that if we treat them as particle and hole like

ones, then the filled band corresponds to all sites being occupied by one electron, the holes correspond to the empty sites and the particles to the "second" electrons at the doubly occupied sites. This is in accordance with the intuitive notion of exciting a number of carriers across a Mott-Hubbard gap.

It can be seen also that the alternative interpretation is equivalently good: in this case the carriers are the not singly occupied sites, and the isospin tells us whether a carrier is an empty or a doubly occupied site.

We should emphasize, that what has been said applies only if  $U$  is large, and no discussion of comparable simplicity can be given as one moves away from the  $U \rightarrow \infty$  limit, since it is obvious that for  $U \sim 1$  there are many doubly occupied sites even in the ground state where there is no complex wavenumber in the  $k$ -set. For finite  $U$  we have to be satisfied with the expressions for the energy and momentum of these states without putting behind them a transparent picture.

## 5. SUMMARY

In the present work we have investigated those eigenstates of the 1-d Hubbard model, for which in the wavenumber set there are several pairs of complex  $k$ -s. Our results are the following:

1. For such states solving the Lieb-Wu equations is equivalent to solving the system of Eqs. (2.5), (2.13) and (2.19) provided (2.4) is satisfied by the found solution. This system is similar in structure to the Lieb-Wu equations, the difference is that there are no complex wavenumbers in it.

2. This system can be reduced to a simpler one (Eqs. (2.19), (2.25)) for those states in which the spin degrees of freedom are not excited. For these states the energy and momentum can be given as the energy and momentum of quasi particles. These quasi particles can be regarded as particle-hole like ones but they can be treated as pairs of identical particles with "isospin"  $\pm 1/2$  equivalently well. The form of the energy and momentum of the quasy particles is given by (1.10) and (1.13).

3. A "complementarity" between solutions of the system (2.5), (2.13) and (2.19) corresponding to low and highly excited states can be established, which can be used to describe different states with one solution of the system. In the complementary states the parameters connected with the charge and spin degrees of freedom change role.

In the present study we concentrated on the "charge excitations". To isolate charge rearrangement effects,

we examined such states in which the spin part was in its ground state. We plan to extend our study to those states in which also the spin degrees of freedom are excited. Preliminary results show, that, as it is expected, the presence of spin excitations does not affect drastically the results concerning the states studied so far, just in addition a new type of "elementary excitations" must be introduced.

ACKNOWLEDGEMENT

I am very grateful to Drs. A. Sütő and P. Fazekas for the many valuable discussions.

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Footnote (p. 23.)

\* The state with  $H'$  extra electrons can be constructed this way only if  $N$  is even. If  $N$  is odd, the transformation between particles and holes changes the periodic boundary condition into antiperiodic or changes the sign of the kinetic energy.





63.038

Kiadja a Központi Fizikai Kutató Intézet  
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