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LETTER TO THE EDITOR

Massive particles in the relativistic limit of the non-half-filled 1D attractive Hubbard model

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Abstract. The continuum limit of the Bethe ansatz solution for an attractive Hubbard chain is considered in which the particle number per site n is kept finite ($0 < n < 1$). It is shown that by adjusting the hopping t, the Hubbard U and the lattice constant a in a proper way the excitations connected to unbound electrons will be relativistic with a finite mass. The higher level Bethe ansatz equations for these particles are given. The spectrum and the phase shifts of these particles show close analogy to those of the massive particles of the SU(2) chiral invariant Gross–Neveu model.

The one-dimensional (1D) Hubbard model, being completely integrable (Shastry 1988) and exactly solvable by the Bethe ansatz (BA) (Lieb and Wu 1968), plays a central role in the theory of strongly correlated electron systems (Korepin and Eßler 1994). At the same time, by direct linearization around the Fermi points (Sólyom 1979), the model can be related to relativistic field theory models (Gross and Neveu 1974, Wiegmann and Larkin 1977), particularly to the SU(2) Gross–Neveu model. Since the Gross–Neveu model can also be diagonalized by BA (Andrei and Lowenstein 1979), constructing the relativistic limit of the BA solution of the Hubbard chain can be of two-fold interest. On one hand it provides a possibility to study the details of the relationship of the two models, and on the other hand, if equivalence is established, the Hubbard chain can be considered as a regularization of the Gross–Neveu model. Earlier Filev (1977), and more recently Melzer (1995), studied the relativistic limit of the half-filled Hubbard chain. While Filev (1977) concentrated on the massive particles, Melzer (1995) has shown that in the scaling limit the half-filled Hubbard chain has one massive and two massless excitations, which based on the spectrum and the phase shifts can be identified to those of the SU(2) chiral invariant Gross–Neveu model. In the present letter we give the scaling (relativistic) limit of the non-half-filled attractive Hubbard chain. We construct the spectrum of the massive particles, and we show that they have the same spectrum and phase shifts as the analogous particles of the half-filled chain and SU(2) chiral invariant Gross–Neveu model.

The model is described by the Hamiltonian

$$\hat{H} = -t\sum_{i=1}^{N}\sum_{\sigma=\uparrow,\downarrow}(c^{+}_{i,\sigma}c_{i+1,\sigma} + \mathrm{HC}) + U\sum_{i=1}^{N}(\hat{n}_{i,\uparrow} - \tfrac{1}{2})(\hat{n}_{i,\downarrow} - \tfrac{1}{2}) + \mu\sum_{i=1}^{N}(\hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}) \qquad (1)$$

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in which $c^+_{i,\sigma}$ $(c_{i,\sigma})$ creates (destroys) an electron at the site i with spin σ, $\hat{n}_{i,\sigma} = c^+_{i,\sigma} c_{i,\sigma}$, and according to the periodic boundary condition the site $i = N + 1$ is the same as the site $i = 1$. The hopping t is positive while the interaction U is negative, and the value of the chemical potential μ is choosen to fix the desired particle number per site n. The eigenvalue equation of this Hamiltonian has been reduced to a set of nonlinear equations by Lieb and Wu (1968):

$$Nk_j = 2\pi I_j - \sum_{\alpha=1}^{M} 2\tan^{-1}\frac{\sin k_j - \lambda_\alpha}{U/4} \qquad (2a)$$

$$\sum_{j=1}^{N_e} 2\tan^{-1}\frac{\lambda_\alpha - \sin k_j}{U/4} = 2\pi J_\alpha + \sum_{\beta=1}^{M} 2\tan^{-1}\frac{\lambda_\alpha - \lambda_\beta}{U/2}. \qquad (2b)$$

Here N_e is the number of electrons, M is the number of down spins, i.e. $S^z = (N_e/2 - M)$, and the I_j and J_α quantum numbers are integers or half-odd-integers depending on the parities of N_e and M. Once these equations are solved the wavefunction can be given (Woynarovich 1982), and also the energy and the momentum of the corresponding state can be calculated:

$$E = NU/4 - \sum_{j=1}^{N_e}(2t\cos k_j + U/2 - \mu) \qquad P = \sum_{j=1}^{N_e} k_j. \qquad (3)$$

For the considered $U < 0$ attractive chain near the ground state most of the electrons form bound pairs with wavenumbers given (up to correction exponentially small in N) as

$$\sin k^{\pm} = \Lambda \pm \mathrm{i}u \qquad (4)$$

with $u = |U|/4t$ and Λ being a subset of the set λ. By this relation $k^{\pm}$ can be eliminated from equation (2) and one finds that the wavenumbers of the unbound electrons, the λs connected with their spin distribution and the Λs of the bound pairs satisfy the equations (Woynarovich 1983, Woynarovich and Penc 1991)

$$2\pi I_j = Nk_j - \sum_{\alpha=1}^{n(\lambda)} 2\tan^{-1}\frac{\sin k_j - \lambda_\alpha}{u} - \sum_{\eta=1}^{n(\Lambda)} 2\tan^{-1}\frac{\sin k_j - \Lambda_\eta}{u} \qquad (5a)$$

$$\sum_{j=1}^{n(k)} 2\tan^{-1}\frac{\lambda_\alpha - \sin k_j}{u} = 2\pi J_\alpha + \sum_{\beta=1}^{n(\lambda)} 2\tan^{-1}\frac{\lambda_\alpha - \lambda_\beta}{2u} \qquad (5b)$$

$$2\pi J_\eta = N(\sin^{-1}(\Lambda_\eta - \mathrm{i}u) + \sin^{-1}(\Lambda_\eta + \mathrm{i}u)) - \sum_{j=1}^{n(k)} 2\tan^{-1}\frac{\Lambda_\eta - \sin k_j}{u} - \sum_{\nu=1}^{n(\Lambda)} 2\tan^{-1}\frac{\Lambda_\eta - \Lambda_\nu}{2u}. \qquad (6)$$

Here $n(k), n(\lambda)$ and $n(\Lambda)$ are the number of unbound electrons, the number of unbound electrons with down spins, and the number of bound pairs, respectively ($N_e = n(k) + 2n(\Lambda)$, $M = n(\lambda) + n(\Lambda)$), and the quantum numbers are $I_j = (n(\lambda) + n(\Lambda))/2 \pmod 1$,

$J_\alpha = (n(k) - n(\lambda) + 1)/2 \pmod 1$ and $J_\eta = (n(k) + n(\Lambda) + 1)/2 \pmod 1$. The energy and momentum expressed by these variables is

$$E = -Nu - \sum_j (2t(\cos k_j - u) - \mu) - \sum_\eta \left(2t \left(\sqrt{1-(\Lambda_\eta - \mathrm{i}u)^2} + \sqrt{1-(\Lambda_\eta + \mathrm{i}u)^2} - 2u \right) - 2\mu \right) \tag{7}$$

$$P = \frac{2\pi}{N} \left(\sum_j I_j - \sum_\alpha J_\alpha + \sum_\eta J_\eta \right).$$

We now consider the relativistic limit. In the ground state of N_e = even electrons the J_η are consecutive integers or half-odd-integers between $J_{\mathrm{max/min}} = \pm(N_\mathrm{e}/2 - 1)/2$ and there are no real ks. This state can be excited by combinations of the following three 'elementary' excitations:

(i) introducing holes and particles in the Λ distribution by removing some J_η from the ground-state set and introducing some outside $(J_{\mathrm{max}}, J_{\mathrm{min}})$;

(ii) introducing complex Λs;

(iii) introducing unbound electrons (real ks).

The excitations type (i) at the proper choice of μ have a dispersion with no gap, whereas those of type (ii) and (iii) possess gaps. The relativistic limit is a continuum limit $N \to \infty$, $a \to 0$ so that $Na = L =$ constant (a and L being the lattice constant and the chainlength, respectively), in which the particle number per site $N_\mathrm{e}/N \to n$ finite, i.e. $N_\mathrm{e} \to \infty$ too. For this the interaction u has also to be adjusted (actually $u \to 0$) to avoid divergences. Finally, although a does not appear explicitly in $\hat{H}$, since $t \propto 1/\text{distance}$, $t \to \infty$ as $a \to 0$. All this is to be performed so that the gap in the spectrum of type (iii) excitations is kept finite. In this limit the excitations of type (i) have a linear dispersion, while the gap of the excitations of type (ii) diverges. In the following, concentrating on the excitations of type (iii), i.e. on the unbound electrons only, we construct the above described limit. We show that if

$$\begin{aligned} &u \to 0, \;\; t \to \infty \\ &N, N_\mathrm{e} \to \infty \text{ at } N_\mathrm{e}/N \to n = \text{constant} < 1 \\ &a \to 0 \text{ at } Na = L = \text{constant} \end{aligned} \tag{8a}$$

so that

$$m_0 = \frac{8t}{\pi} \sqrt{u \sin^3(\pi n/2)} \exp\left\{ -\frac{\pi \sin(\pi n/2)}{2u} \right\} = \text{constant} \tag{8b}$$

$$2at \sin(\pi n/2) = 1 \tag{8c}$$

then the spectrum of type (iii) massive particles is

$$E - E_0 = \sum_\kappa \epsilon(\kappa) \qquad P - p = \sum_\kappa p(\kappa) \tag{9a}$$

where E_0 is the ground-state energy, $p = \pm\pi n/2a$ ($p = 0$) if the number of κs is odd (even),

$$\epsilon(\kappa) = m_0 \cosh(\kappa) \qquad p(\kappa) = m_0 \sinh(\kappa) \tag{9b}$$

and the rapidities κ and the set of variables χ replacing the λs satisfy the higher level BA equations

$$L p(\kappa) = 2\pi I_\kappa - \sum_{\kappa'} \phi\left(\frac{\kappa - \kappa'}{\pi}\right) + \sum_{\chi} 2\tan^{-1}\left(\frac{\kappa - \chi}{\pi/2}\right) \qquad (10a)$$

$$\sum_{\kappa} 2\tan^{-1}\left(\frac{\chi - \kappa}{\pi/2}\right) = 2\pi J_\chi + \sum_{\chi'} 2\tan^{-1}\left(\frac{\chi - \chi'}{\pi}\right) \qquad (10b)$$

$$\phi(x) = \frac{1}{\mathrm{i}} \ln \frac{\Gamma(\frac{1}{2} - \mathrm{i}\frac{x}{2})\Gamma(1 + \mathrm{i}\frac{x}{2})}{\Gamma(\frac{1}{2} + \mathrm{i}\frac{x}{2})\Gamma(1 - \mathrm{i}\frac{x}{2})}.$$

We note, that (10a) and (10b) yield the same phase shifts as those obtained for the half-filled band (Melzer 1995):

$$\psi^{tr} = -\phi\left(\frac{\Delta\kappa}{\pi}\right) \qquad \psi^{s} = -\phi\left(\frac{\Delta\kappa}{\pi}\right) + 2\tan^{-1}\left(\frac{\Delta\kappa}{\pi}\right) \qquad (\Delta\kappa = \kappa - \kappa'). \qquad (11)$$

We now look at the structure of the spectrum. To derive equations (9a) and (9b), and (10a) and (10b) we consider states where the J_η distribution corresponds to that of the ground state ($n(\Lambda)$ consecutive integers or half-odd-integers centred around the origin obeying the parity prescription given above) and there is a number $n(k) \ll N$ of real ks. In this case all the Λ are real, and if $N \to \infty$—as can be derived by standard methods—they will be distributed according to the density

$$\varsigma(\Lambda) = \sigma(\Lambda) + \frac{1}{N}\sum_{k} \varrho(\Lambda, k) \qquad (12)$$

where σ and ϱ satisfy equations of the type

$$x(\Lambda) = I_x(\Lambda) - \frac{1}{2\pi}\int_{B^-}^{B^+} K_2(\Lambda - \Lambda')x(\Lambda') \qquad (13)$$

$$K_m(\xi) = \frac{2mu}{(mu)^2 + \xi^2}$$

with inhomogeneous parts

$$\sigma(\Lambda): \qquad I_\sigma = \sigma_0(\Lambda) = \frac{1}{2\pi} 2\,\mathrm{Re}\left(\left(\sqrt{1 - (\Lambda - \mathrm{i}u)^2}\right)^{-1}\right)$$
$$\varrho(\Lambda, k): \qquad I_\varrho = -\frac{1}{2\pi} K_1(\Lambda - \sin k) \qquad (14)$$

respectively, where B^+ and B^- are determined by the equations

$$\int_{B^+}^{\infty} \varsigma(\Lambda) = \frac{1}{2}\left(1 - \frac{2n(\Lambda) + n(k)}{N}\right) \mp \left\{\frac{1}{2N}\right\}$$
$$\int_{-\infty}^{B^-} \varsigma(\Lambda) = \frac{1}{2}\left(1 - \frac{2n(\Lambda) + n(k)}{N}\right) \pm \left\{\frac{1}{2N}\right\} \qquad (15)$$

where the terms in curly brackets are present only if the number of κs is odd. (These terms together with the p term in equation (9a) originate from the parity prescription for the J_η

and fit coherently into the treatment of the massless excitations.) The energy of the system is given by

$$E = -Nu - \sum_j (2t(\cos k_j - u) - \mu) \\ -N \int_{B^-}^{B^+} \left(4t\left(\mathrm{Re}\sqrt{1-(\Lambda_\eta - \mathrm{i}u)^2} - u\right) - 2\mu\right)\varsigma(\Lambda) \quad (16)$$

which through straightforward manipulations (Woynarovich and Penc 1991) can be transformed into the form

$$E = -Nu + N\int_{B^-}^{B^+} \varepsilon(\Lambda)\sigma_0(\Lambda) \\ + \sum_j \left\{ -(2t(\cos k_j - u) - \mu) - \frac{1}{2\pi}\int_{B^-}^{B^+} \varepsilon(\Lambda) K_1(\Lambda - \sin k_j)\right\} \quad (17)$$

where $\varepsilon(\Lambda)$ satisfies equation (13) with an inhomogeneous part:

$$\varepsilon(\Lambda): \qquad I_\varepsilon = \varepsilon_0(\Lambda) = -\left(4t\left(\mathrm{Re}\sqrt{1-(\Lambda - \mathrm{i}u)^2} - u\right) - 2\mu\right). \quad (18)$$

If a function $x(\Lambda)$ satisfies equation (13), it also satisfies the relation (that is an appropriate integral of (13))

$$\int_{B^-}^{B^+} K_m(\xi - \Lambda)x(\Lambda) = -\left(\int_{-\infty}^{B^-} + \int_{B^+}^{\infty}\right) K_m(\xi - \Lambda)x(\Lambda) \\ + \int_{-\infty}^{\infty} K_m(\xi - \Lambda) I_x(\Lambda) - \int_{B^-}^{B^+} K_{m+2}(\xi - \Lambda)x(\Lambda). \quad (19)$$

Through the successive application of this relation the energy takes the form

$$E = N\left(\int_{B^-}^{B^+} \varepsilon(\Lambda)\sigma_0(\Lambda) - u\right) \\ + \sum_j \left\{ -(2t(\cos k_j - u) - \mu) - \frac{1}{4u}\int_{-\infty}^{\infty} \frac{1}{\cosh(\Lambda - \sin k_j)\pi/2u}\varepsilon_0(\Lambda)\right\} \\ + \sum_j \frac{1}{4u}\left(\int_{-\infty}^{B^-} + \int_{B^+}^{\infty}\right)\frac{1}{\cosh(\Lambda - \sin k_j)\pi/2u}\varepsilon(\Lambda). \quad (20)$$

Before evaluating equation (20) in the above-described limit, consider equation (5*a*). Replacing the sum over Λ_η by an integral one has

$$2\pi I_j = Nk_j - \sum_{\alpha=1}^{n(\lambda)} 2\tan^{-1}\frac{\sin k_j - \lambda_\alpha}{u} - N\int_{B^-}^{B^+} 2\tan^{-1}\frac{\sin k_j - \Lambda}{u}\varsigma(\Lambda). \quad (21)$$

This, through the relation (which is actually an integral of equation (19))

$$\int_{B^-}^{B^+} \tan^{-1}\frac{\xi - \Lambda}{mu}x(\Lambda) = -\left(\int_{-\infty}^{B^-} + \int_{B^+}^{\infty}\right)\tan^{-1}\frac{\xi - \Lambda}{mu}x(\Lambda) \\ + \int_{-\infty}^{\infty} \tan^{-1}\frac{\xi - \Lambda}{mu} I_x(\Lambda) - \int_{B^-}^{B^+} \tan^{-1}\frac{\xi - \Lambda}{(m+2)u}x(\Lambda) \quad (22)$$

can be transformed into the form

$$2\pi I_j = N\left\{k_j - \int_{-\infty}^{\infty} 2\tan^{-1}\tanh\frac{\pi(\sin k_j - \Lambda)}{4u}\sigma_0(\Lambda)\right\}$$
$$+N\left(\int_{-\infty}^{B^-} + \int_{B^+}^{\infty}\right)2\tan^{-1}\tanh\frac{\pi(\sin k_j - \Lambda)}{4u}\left(\sigma(\Lambda) + \frac{1}{N}\varrho(\Lambda)\right)$$
$$+\sum_{j'}^{n(k)}\frac{1}{2\pi}\int_{-\infty}^{\infty} 2\tan^{-1}\tanh\frac{\pi(\sin k_j - \Lambda)}{4u}K_1(\Lambda - \sin k_{j'})$$
$$-\sum_{\alpha}^{n(\lambda)} 2\tan^{-1}\frac{\sin k_j - \lambda_\alpha}{u}. \qquad (23)$$

Up to now no approximation has been made, and relations (20) and (23) are exact at any values of U, t, N, and a. Now we make those approximations, which in the scaling limit will become exact. For easy reference let us introduce the system 'r' with no real ks, but with the same number of Λs! This is determined by the equations

$$\sigma_r(\Lambda) = \sigma_0(\Lambda) - \frac{1}{2\pi}\int_{-B}^{B} K_2(\Lambda - \Lambda')\sigma_r(\Lambda') \qquad (24a)$$

with

$$\int_B^{\infty}\sigma_r(\Lambda) = \int_{-\infty}^{-B}\sigma_r(\Lambda) = \frac{1}{2}\left(1 - \frac{2n(\Lambda)}{N}\right) = \frac{1}{2} - n \qquad (24b)$$

and

$$\varepsilon_r(\Lambda) = \varepsilon_0(\Lambda) - \frac{1}{2\pi}\int_{-B}^{B} K_2(\Lambda - \Lambda')\varepsilon_r(\Lambda'). \qquad (25a)$$

We choose μ so that

$$\varepsilon_r(B) = 0. \qquad (25b)$$

Considering (12) and (15) and (24b) it is clear that if $N \to \infty$, so that $n(\Lambda)/N = n$ and $n(k)$ are kept constant, then $B^+ = B + O(1/N)$ and $B^- = -B + O(1/N)$. As a consequence of this and (25b) $\varepsilon(\Lambda) = \varepsilon_r(\Lambda) + O(t/N^2)$ and, in (20), $\varepsilon(\Lambda)$ can be replaced by $\varepsilon_r(\Lambda)$ and $B^+ = -B^- = B$ can be used (therefore introducing an error $O(1/L)$ only). So the first term in (20), being the ground-state energy, although divergent in the $N \to \infty$ limit, need not be considered. The second term is formally the same as the excitation energy in a *half-filled* chain (Filev 1977, Melzer 1995) and it behaves as though proportional to $t\sqrt{u}\exp\{-\pi/2u\}$, i.e. it decays when compared to the third term, which if $u \to 0$ is in leading order:

$$E - E_0 = \sum_{j}^{n(k)}\left(\frac{1}{u}\mathrm{e}^{-B\pi/2u}\int_0^{\infty}\mathrm{e}^{-\Lambda\pi/2u}\varepsilon_r(B + \Lambda)\right)\cosh\frac{\pi\sin k_j}{2u}. \qquad (26)$$

The $N \to \infty$ limit in (23) is made as follows. The first term on the right-hand side is exactly the same as the analogous term in the *half-filled* case; it decays as though proportional to $(1/a)\sqrt{u}\exp\{-\pi/2u\}$ and can be neglected. In the second term we may write

$$2\tan^{-1}\tanh\frac{\pi(\sin k - \Lambda)}{4u} \approx -\mathrm{sgn}(\Lambda)\left(\frac{\pi}{2} - 2\mathrm{e}^{-|\Lambda - \sin k|\pi/2u}\right). \qquad (27)$$

Also in this term $B^{\pm}$ can be replaced by $\pm B$ and $\sigma(\Lambda)$ by $\sigma_r(\Lambda)$, while the $\varrho(\Lambda, k)$ terms can be neglected. Finally, replacing N by L/a leads to

$$\sum_j^{n(k)} L\left(\frac{4}{a}\mathrm{e}^{-B\pi/2u}\int_0^\infty \mathrm{e}^{-\Lambda\pi/2u}\sigma_r(B+\Lambda)\right)\sinh\frac{\pi\sin k_j}{2u}. \tag{28}$$

Evaluating the third term explicitly, and introducing the notations

$$\begin{aligned}
&\left(\frac{1}{u}\mathrm{e}^{-B\pi/2u}\int_0^\infty \mathrm{e}^{-\Lambda\pi/2u}\varepsilon_r(B+\Lambda)\right)=m_0\\
&\left(\frac{4}{a}\mathrm{e}^{-B\pi/2u}\int_0^\infty \mathrm{e}^{-\Lambda\pi/2u}\sigma_r(B+\Lambda)\right)=m_0\\
&\kappa=\frac{\pi\sin k}{2u}\qquad \chi=\frac{\pi\lambda}{2u}
\end{aligned} \tag{29}$$

and also using the momentum in (7) one arrives at (9a) and (9b) and (10a) and (10b).

Finally, one should evaluate m_0, i.e. the integrals in (26), (28), and (29). This is possible in the $u \to 0$ limit in leading order: equations (24a)–(25b) can be solved by Wiener–Hopf techniques. The solution is described by Woynarovich and Penc (1991); here we cite the results only:

$$\int_0^\infty \mathrm{e}^{-\Lambda\pi/2u}x_r(B+\Lambda)=\frac{2u}{\pi}\sqrt{\frac{\pi}{e}}x_r(B)+\frac{4u^2}{\pi^2}\sqrt{\frac{\pi}{e}}\frac{x_0'(B)}{\sqrt{2}} \tag{30}$$

with $x(\Lambda) : \varepsilon(\Lambda)$ or $\sigma(\Lambda)$ and prime means derivative according to Λ,

$$\lim_{u\to 0} x_r(B)=\frac{1}{\sqrt{2}}\lim_{u\to 0} x_0(B) \tag{31}$$

and

$$B=\sin\frac{\pi n}{2}-\frac{u}{\pi}\left(1+\ln\frac{\pi\cos^2\pi n/2\sin\pi n/2}{2u}\right). \tag{32}$$

Using these results and also (25b) one arrives at (8b) and (8c).

We note here that the spectrum of the excitations that we have considered was studied earlier by Krivnov and Ovchinnikov (1975). Our result does not agree completely with theirs.

In the present work we have concentrated on the massive excitations in the relativistic limit of the non-half-filled Hubbard chain. A more detailed study also including the massless excitations and comparison of the half- and non-half-filled cases is planned to be published in another paper.

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