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Non-analytic finite-size corrections in the one-dimensional Bose gas and Heisenberg chain

F Woynarovich†, H-P Eckle‡ and T T Truong‡

† Central Research Institute for Physics, POB 49, H-1525 Budapest 114, Hungary

‡ Fachbereich Physik, Freie Universität Berlin, Arnimalle 14, D-1000 Berlin 33, Federal Republic of Germany

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Abstract. The energy spectra of the one-dimensional Bose gas and Heisenberg chain in an external field (chemical potential in the case of the Bose gas and magnetic field in the case of the Heisenberg chain) are calculated. It is found that, at general values of the external field, the spectra are not of the form expected on the basis of conformal invariance. The conformal structure can be recovered only if some extra conditions are imposed on the size of the system and the external field. It is argued that these additional conditions must be satisfied when taking the continuum limit in order to arrive at a conformally invariant theory.

1. Introduction

Progress in understanding the critical state of two-dimensional classical systems is greatly enhanced by the hypothesis of conformal symmetry put forward by Belavin *et al* (1984). This large symmetry was shown to be described by an infinite-dimensional algebra: the Virasoro algebra for which the representation theory yields a complete abstract classification, according to a *conformal anomaly number* c (Friedan *et al* 1984). The scaling dimensions of *primary* conformal order parameters can be then obtained by the so-called Kac formula.

A further step was made when Blöte *et al* (1986) and Affleck (1986) showed that the conformal anomaly and scaling dimensions are directly accessible through the finite-size effects of an affiliated system defined on infinitely long but finitely wide strips at criticality. Finally Cardy (1986) showed that, as another consequence of conformal invariance at criticality for systems with *modular invariance* (with torus boundary conditions), the form of the scaling dimensions in a theory where c is known is completely fixed.

This succession of theoretical results has prompted many groups of workers to seek confirmation either numerically or using exactly solvable models. We shall not dwell on numerical works which are numerous (von Gehlen *et al* 1986, Iglói and Zittartz 1988, etc) but concentrate our discussion on the study of systems solvable by the method of the Bethe ansatz wavefunction. The prototype is the well known XXZ chain of N spins with various boundary conditions (Hamer 1986, de Vega and Karowski 1987, Woynarovich and Eckle 1987, Woynarovich 1987, Alcaraz, Barber and Batchelor 1987, etc). Through this model of a spin chain many of the two-dimensional classical systems can be discussed, such as the Potts, Ashkin–Teller, O(N), etc, models. On the whole one may say that the extraction of the central charge and scaling dimensions is a smooth procedure and leads to expected results.

Recently Bogoliubov *et al* (1986, 1987) extended the study to another class of XXZ chains: chains with periodic boundary conditions but in the presence of a magnetic field. They also consider the case of the one-dimensional Bose gas with delta function pair potential and finite chemical potential. They concentrate on the discussion of the influence of the external field on the scaling dimensions essentially and the behaviour of correlation functions.

The object of the present work is to show that, within the framework of the two models considered by Bogoliubov *et al* (1986, 1987), the obtaining of the conformal quantities through the finite-size method should be done with care. We use a systematic procedure developed earlier (de Vega and Woynarovich 1985, Woynarovich and Eckle 1987) to show that the approach to large size of a system may not necessarily be smooth and, in fact, proceeds by discontinuous steps causing an apparent violation of the expected behaviour. We shall also show that a remedy to this behaviour is to allow some quantities to take only rational values, but not irrational ones, before taking the thermodynamic limit.

This aspect leads us directly to question the procedure of constructing the *continuum* limit of a lattice model. Presumably a naive construction would fail to yield a consistent answer for conformal invariant quantities characterising the system or the quantum field theory which one recovers at the end of the continuum limit. Since this field theory is more or less the universal representation of a whole class of lattice systems having the same conformal characteristics, it is important to know how to construct it properly.

Before discussing the two models in detail let us briefly review the generalities concerning the finite-size effects of critical systems. A one-dimensional quantum system is critical at zero temperature if the long-distance correlations decay algebraically. In particular such behaviour is characteristic of gapless systems with a linear dispersion relation. However, some correlation functions may also show, besides the usual power law decay, spatial oscillations due to intermediate processes involving excitations of particles from one Fermi point to the other. The operators responsible for these processes are not conformal ones but are shown to be (Bogoliubov *et al* 1986, 1987) weighted sums of conformal operators. The relations between the spectrum of the one-dimensional quantum system on a strip of finite width L and the bulk scaling indices are given by (Bogoliubov *et al* 1987)

$$E_n - E_0 = \frac{2\pi v_F}{L}(x_n + N^+ + N^-) \tag{1}$$

$$P_n = \frac{2\pi}{L}(s_n + N^+ - N^-) + 2Dk_F \tag{2}$$

where E_n and P_n are the energy and momentum of the nth excited state, v_F is the Fermi velocity and N^+, N^- are non-negative integers. D is the number of particles excited from the left Fermi point to the right one and finally x_n and s_n are the scaling dimensions of the corresponding bulk operators. The ground-state energy E_0 has the usual form (Blöte *et al* 1986, Affleck 1986)

$$E_0 = L\varepsilon_\infty - \pi v_F c/6L \tag{3}$$

ε_∞ being the ground state energy density of the infinite system and c the conformal anomaly characterising the system.

To illustrate the extended finite-size effects put forward in (1)-(3), Bogoliubov *et al* (1987) have worked on the one-dimensional Bose gas with delta function pair potential and finite chemical potential, as well as on the XXZ Heisenberg chain in a magnetic field, and discussed the dependence of the bulk scaling dimensions of the external field. In the following we shall apply the systematic method of de Vega and Woynarovich (1985) and Woynarovich and Eckle (1987) to derive in detail the finite-size corrections to these two one-dimensional quantum systems. The upshot of this calculation is the occurrence of *non-conformal* terms in equations of the type (1)-(3). However, as will be explicitly shown, appropriate restrictions may be required in order to recover the equations predicted by conformal invariance. These restrictions have physical grounds and pave the way for performing a continuum limit of the theory.

In appendix 1, we show that the main conclusion of this paper can be observed in a simple system: the XX spin chain in a magnetic field. The case of an XY chain in a transverse magnetic field has been treated by Hoeger *et al* (1985), where incommensurable and oscillatory structures appear. This should help the reader not too familiar with Bethe ansatz techniques to understand the scope of the paper which is by no means restricted to non-interacting systems. Appendix 2 describes an attempt to construct a continuum limit in a simple situation to demonstrate to the reader how delicate the procedure really is.

2. Finite-size effects in the energy spectra

As is well known, both the Bose gas, defined in a box of length L with a chemical potential $h>0$ and a repulsive delta function interaction of strength $\kappa \geqslant 0$

$$\mathscr{H}_{\mathrm{BG}} = \int_0^L (\partial_x\psi^\dagger\partial_x\psi + \kappa\psi^\dagger\psi^\dagger\psi\psi - h\psi^\dagger\psi)\,\mathrm{d}x \tag{4}$$

and the anisotropic Heisenberg chain of N sites with anisotropy $\cos\theta$ and external magnetic field h $(0 \leqslant h \leqslant (1+\cos\theta))$

$$\mathscr{H}_{\mathrm{HC}} = \sum_{i=1}^{N} (-S_i^x S_{i+1}^x - S_i^y S_{i+1}^y + \cos\theta\, S_i^z S_{i+1}^z - hS_i^z) - \tfrac{1}{4}N(\cos\theta - 2h) \tag{5}$$

are solvable by the Bethe ansatz (BA) method.

An eigenstate of $\mathscr{H}_{\mathrm{BG}}$ containing M bare particles is completely described by the M parameters $\eta_\alpha (\alpha = 1, 2, \ldots, M)$ satisfying the algebraic equations (the BA equations)

$$L\eta_\alpha = 2\pi J_\alpha - 2\sum_{\beta=1}^{M} \tan^{-1}\frac{\eta_\alpha - \eta_\beta}{\kappa} \tag{6}$$

where $J_\alpha = (M+1)/2 \pmod 1$ are the quantum numbers of this state. The energy and momentum of the state are, respectively,

$$E = \sum_{\alpha=1}^{M} (\eta_\alpha^2 - h) \tag{7}$$

$$P = \frac{2\pi}{L}\sum_{\alpha=1}^{M} J_\alpha . \tag{8}$$

Analogously, an eigenstate of $\mathscr{H}_{HC}$ is also defined by M spin waves of parameters η_α obeying the Bethe ansatz equations

$$2N\tan^{-1}\left(\cot\frac{\theta}{2}\tanh\frac{\eta_\alpha}{2}\right)=2\pi J_\alpha+2\sum_{\beta=1}^{M}\tan^{-1}\left(\cot\theta\tanh\frac{\eta_\alpha-\eta_\beta}{2}\right) \tag{9}$$

where $J_\alpha=(M+1)/2(\text{mod } 1)$ are the quantum numbers of this state. The energy and momentum of the state are, respectively,

$$E=\sum_{\alpha=1}^{M}\left(h-\frac{\sin^2\theta}{\cosh\eta_\alpha-\cos\theta}\right) \tag{10}$$

$$P=-\frac{2\pi}{N}\sum_{\alpha=1}^{M}J_\alpha. \tag{11}$$

Finally, N being the total number of sites on the chain, the total magnetisation of the chain is

$$S^z=\sum_{i=1}^{N}S_i^z=\tfrac{1}{2}N-M.$$

We observe that the two sets of Bethe ansatz equations are very similar in nature. We shall outline our calculations for the Heisenberg chain, but the results can be readily translated to the case of the Bose gas.

We start by specifying the set of numbers J_α. We choose two numbers J^+ and J^-, both equal to $M/2 \bmod 1$, so that $J^+-J^-=M$ and $-\frac{1}{2}(J^++J^-)=D$. For J_α we take all the numbers equal to $(M+1)/2 \bmod 1$ between J^+ and J^-. It is not hard to see that this corresponds to a Fermi sea of M particles with D particles placed from the left Fermi point to the right one. Later on one can introduce holes and particles by removing J_α from the sea and introducing J_α outside the sea. In order not to change M and D, however, the number of holes and particles should be equal both in the vicinity of the right, and in the vicinity of the left, Fermi point.

As in the earlier works (de Vega and Woynarovich 1985, Woynarovich and Eckle 1987) we define the density of roots for the finite system:

$$z_N(\eta)=\frac{1}{2\pi}\left(p_0(\eta)-\frac{1}{N}\sum_\alpha\phi_0(\eta-\eta_\alpha)\right) \tag{12}$$

$$\sigma_N(\eta)=\mathrm{d}z_N(\eta)/\mathrm{d}\eta \tag{13}$$

with

$$p_0(\eta)=2\tan^{-1}\left(\cot\frac{\theta}{2}\tanh\frac{\eta}{2}\right) \tag{14}$$

$$\phi_0(\eta)=2\tan^{-1}\left(\cot\theta\tanh\frac{\eta}{2}\right). \tag{15}$$

With these notations the Bethe ansatz equations are

$$z_N(\eta_\alpha)=J_\alpha/N. \tag{16}$$

We use the Euler-Maclaurin formula to write up an integral equation for $\sigma_N(\eta)$:

$$\frac{1}{N}\sum_\alpha f(\eta_\alpha)=\int_{\Lambda^-}^{\Lambda^+}f(\eta)\sigma_N(\eta)\,\mathrm{d}\eta+\frac{1}{24N^2}\left(\frac{f'(\Lambda^-)}{\sigma_N\Lambda^-)}-\frac{f'(\Lambda^+)}{\sigma_N(\Lambda^+)}\right)+\mathrm{O}\left(\frac{1}{N^3}\right). \tag{17}$$

The integration boundaries $\Lambda^{\pm}$ are defined through

$$z_N(\Lambda^{\pm}) = J^{\pm}/N. \tag{18}$$

Applying (17) to (12) and (13) one obtains

$$\sigma_N(\eta) = \frac{1}{2\pi}\left[\frac{\mathrm{d}p_0(\eta)}{\mathrm{d}\eta} + \frac{1}{24N^2}\left(\frac{1}{\sigma_N(\Lambda^-)}\frac{\mathrm{d}K(\eta-\Lambda^-)}{\mathrm{d}\eta} - \frac{1}{\sigma_N(\Lambda^+)}\frac{\mathrm{d}K(\eta-\Lambda^+)}{\mathrm{d}\eta}\right)\right.$$
$$\left. - \int_{\Lambda^-}^{\Lambda^+} K(\eta-\eta')\sigma_N(\eta')\,\mathrm{d}\eta'\right] \tag{19}$$

where the kernel of the integral is given by

$$K(\eta) = \mathrm{d}\phi_0(\eta)/\mathrm{d}\eta. \tag{20}$$

This linear integral equation is completed by the equations determining Λ^+ and Λ^- (obtained from (12), (13) and (18)):

$$\int_{\Lambda^-}^{\Lambda^+} \sigma_N\,\mathrm{d}\eta = \frac{M}{N} \tag{21}$$

$$\frac{1}{2}\left(\int_{\Lambda^+}^{\infty} \sigma_N(\eta)\,\mathrm{d}\eta - \int_{-\infty}^{\Lambda^-} \sigma_N(\eta)\,\mathrm{d}\eta\right) = \frac{D}{N}. \tag{22}$$

Due to the linearity of (19) σ_N can be written in the following form:

$$\sigma_N(\eta) = \sigma(\eta\,|\,\Lambda^+,\Lambda^-) - \frac{1}{24N^2}\left(\frac{\rho(\eta\,|\,\Lambda^+,\Lambda^-)}{\sigma_N(\Lambda^+)} + \frac{\rho(-\eta\,|\,-\Lambda^-,-\Lambda^+)}{\sigma_N(\Lambda^-)}\right) \tag{23}$$

where $\sigma(\eta\,|\,\Lambda^+,\Lambda^-)$ and $\rho(\eta\,|\,\Lambda^+,\Lambda^-)$ are defined by the equations

$$\sigma(\eta\,|\,\Lambda^+,\Lambda^-) = \frac{1}{2\pi}\left(\frac{\mathrm{d}p_0(\eta)}{\mathrm{d}\eta} - \int_{\Lambda^-}^{\Lambda^+} K(\eta-\eta')\sigma(\eta'\,|\,\Lambda^+,\Lambda^-)\,\mathrm{d}\eta'\right) \tag{24}$$

and

$$\rho(\eta\,|\Lambda^+,\Lambda^-) = \frac{1}{2\pi}\left(\frac{\mathrm{d}K(\eta-\Lambda^+)}{\mathrm{d}\eta} - \int_{\Lambda^-}^{\Lambda^+} K(\eta-\eta')\rho(\eta'|\Lambda^+,\Lambda^-)\,\mathrm{d}\eta'\right). \tag{25}$$

It will become clear later that it is sufficient to define $\Lambda^{\pm}$ with an accuracy of order $1/N$. Therefore we may replace σ_N by $\sigma(\eta\,|\,\Lambda^+,\Lambda^-)$ in (21) and (22):

$$\int_{\Lambda^-}^{\Lambda^+} \sigma(\eta\,|\,\Lambda^+,\Lambda^-)\,\mathrm{d}\eta = \frac{M}{N} \tag{26}$$

$$\frac{1}{2}\left(\int_{\Lambda^+}^{\infty} \sigma(\eta\,|\,\Lambda^+,\Lambda^-)\,\mathrm{d}\eta - \int_{-\infty}^{\Lambda^-} \sigma(\eta\,|\,\Lambda^+,\Lambda^-)\,\mathrm{d}\eta\right) = \frac{D}{N}. \tag{27}$$

The equations (23)-(27) form a closed system and determine *completely* the state under consideration.

By the application of (17) to (10) and using also (23) we have for the energy

$$E = N\varepsilon\left(\frac{M}{N},\frac{D}{N}\right) - \frac{1}{24N}\frac{e(\Lambda^+,\Lambda^-)}{\sigma(\Lambda^+)} - \frac{1}{24N}\frac{e(-\Lambda^-,-\Lambda^+)}{\sigma(\Lambda^-)} \tag{28}$$

with

$$\varepsilon\left(\frac{M}{N}, \frac{D}{N}\right)=\int_{\Lambda^+}^{\Lambda^-} \varepsilon_0(\eta)\sigma(\eta\,|\,\Lambda^+, \Lambda^-)\,\mathrm{d}\eta \tag{29}$$

and

$$e(\Lambda^+, \Lambda^-)=\frac{\mathrm{d}\varepsilon_0(\Lambda^+)}{\mathrm{d}\Lambda^+}+\int_{\Lambda^+}^{\Lambda^-} \varepsilon_0(\eta)\rho(\eta\,|\,\Lambda^+, \Lambda^-)\,\mathrm{d}\eta \tag{30}$$

$\varepsilon_0(\eta)$ being the bare energy

$$\varepsilon_0(\eta)=\left(h-\frac{\sin^2\theta}{\cosh\eta-\cos\theta}\right). \tag{31}$$

If we make the limit $N\to\infty$ keeping $M/N\to\mu$, $D/N\to\delta$ finite, $\varepsilon(\mu, \delta)$ will give the energy density of the infinite system. In the ground state of the infinite system $\varepsilon(\mu, \delta)$ is minimal with respect to μ and δ. This minimisation can be performed, and $\varepsilon(M/N, D/N)$ be expanded around the minimum. This is a somewhat lengthy but straightforward procedure and leads to the following. At the minimum we have $\delta=0$ and $\Lambda^+=-\Lambda^-=\Lambda$. Denoting the minimal value of $\varepsilon(\mu, 0)$ by ε_∞, and the value of μ for which $\varepsilon(\mu, 0)$ reaches its minimum by $\mu(h)$, we finally obtain

$$\varepsilon\left(\frac{M}{N}, \frac{D}{N}\right)=\varepsilon_\infty+\frac{e(\Lambda, -\Lambda)}{\sigma(\Lambda\,|\,\Lambda, -\Lambda)}\left[\frac{1}{(2\xi(\Lambda))^2}\left(\frac{M}{N}-\mu(h)\right)^2+(\xi(\Lambda))^2\left(\frac{D}{N}\right)^2\right] \tag{32}$$

where $\xi(\Lambda)$ is the dressed charge (Korepin 1979) at the Fermi surface, the dressed charge function $\xi(\eta)$ being defined through the integral equation

$$\xi(\eta)=1-\frac{1}{2\pi}\int_{-\Lambda}^{\Lambda} K(\eta-\eta')\xi(\eta')\,\mathrm{d}\eta'. \tag{33}$$

Without spoiling the accuracy we may replace Λ^+ by Λ, Λ^- by $-\Lambda$ and $\sigma_N(\Lambda^+)$ by $\sigma(\Lambda\,|\,\Lambda, -\Lambda)$ in (28). Therefore we obtain

$$\begin{aligned}E(M, D)-N\varepsilon_\infty=&\frac{1}{N}\frac{e(\Lambda, -\Lambda)}{\sigma(\Lambda\,|\,\Lambda, -\Lambda)}\\&\times\left(\frac{1}{(2\xi(\Lambda))^2}(M-N\mu(h))^2+(\xi(\Lambda))^2D^2-\tfrac{1}{12}\right).\end{aligned} \tag{34}$$

For the momentum of the state considered (11) gives

$$P(M, D)=\frac{2\pi}{N}MD. \tag{35}$$

The above calculations can be easily extended to the case where particle-hole-like excitations are also introduced in the vicinity of the Fermi points. We characterise the holes and particles in the vicinity of J^+ by the quantum numbers J_{h}^+ and J_{p}^+:

$$J_{\mathrm{h}}^+=J^+-n_{\mathrm{h}}^+ \tag{36}$$

$$J_{\mathrm{p}}^+=J^++n_{\mathrm{p}}^+ \tag{37}$$

respectively, and the holes and particles near J^- by the quantum numbers

$$J_{\mathrm{h}}^-=J^-+n_{\mathrm{h}}^- \tag{38}$$

$$J_{\mathrm{p}}^-=J^--n_{\mathrm{p}}^-. \tag{39}$$

The numbers $n_h^{\mp}$, $n_p^{\pm} > 0$ are half-odd integers. In addition to (34) and (35) we get the contributions

$$\frac{1}{N} \frac{e(\Lambda, -\Lambda)}{\sigma(\Lambda|\Lambda, -\Lambda)} (N^+ + N^-) \tag{40}$$

and

$$-\frac{2\pi}{N}(N^+ - N^-) \tag{41}$$

to the energy and to the momentum, respectively, whereby

$$N^{\pm} = \sum (n_h^{\pm} + n_p^{\pm}).$$

(Note that N^+ (N^-) are integers since the number of $J_p^+(J_p^-)$ is equal to the number of $J_h^+(J_h^-)$.) The expression (40) justifies the notation

$$v_F = \frac{e(\Lambda, -\Lambda)}{2\pi\sigma(\Lambda|\Lambda, -\Lambda)}. \tag{42}$$

So we have finally the expressions for the energy and momentum

$$E(M, D) = N\varepsilon_\infty + \frac{2\pi v_F}{N}\left(\frac{1}{(2\xi(\Lambda))^2}(M - N\mu(h))^2 + (\xi(\Lambda))^2 D^2 - \tfrac{1}{12} + N^+ + N^-\right) \tag{43}$$

$$P(M, D) = \frac{2\pi}{N}(MD - N^+ + N^-). \tag{44}$$

As we said, the treatment of the Bose gas is practically the same as that of the Heisenberg chain. Actually all the formulae remain valid, if we replace N by L and take

$$p_0(\eta) = \eta \tag{45}$$

$$\phi_0(\eta) = -2\tan^{-1}(\eta/\kappa) \tag{46}$$

$$\varepsilon_0(\eta) = (\eta^2 - h) \tag{47}$$

and substitute P by $-P$ (compare (4), (6), (7) and (8) with (5), (9), (10) and (11)). So for the Bose gas one has

$$E(M, D) = L\varepsilon_\infty + \frac{2\pi v}{L}\left(\frac{1}{(2\xi(\Lambda))^2}(M - L\mu(h))^2 + (\xi(\Lambda))^2 D^2 - \tfrac{1}{12} + N^+ + N^-\right) \tag{48}$$

$$P(M, D) = \frac{2\pi}{L}(-MD + N^+ - N^-) \tag{49}$$

where ε_∞, v, $\xi(\Lambda)$ and $\mu(h)$ are now the corresponding quantities of the Bose gas.

3. Non-analytic finite-size behaviour of the spectra

For both the Bose gas and Heisenberg chain the finite system is in the ground state if N^+, $N^- = 0$ and if $(M - L\mu(h))^2$ and $(M - N\mu(h))^2$, respectively, is minimal. We denote by M_0 the particle number (Bose gas) or spin wave number (Heisenberg chain) in the ground state (the following equations are given for the Heisenberg chain case only: the corresponding equations for Bose gas are readily obtained by replacing the number of sites on the chain N by the length of the system L):

$$M_0 = \begin{cases} [N\mu(h)] & \text{if } \{N\mu(h)\} < \frac{1}{2} \\ 1 + [N\mu(h)] & \text{if } \{N\mu(h)\} > \frac{1}{2}. \end{cases} \qquad (50)$$

The braces [ ] and { } denote integer and fractional parts, respectively. The ground state energy is then given by

$$E_0^{\rm HC} = N\varepsilon_\infty - \frac{\pi v_{\rm F}}{6N}\left(1 - \frac{3}{(\xi(\Lambda))^2}\min((\{N\mu(h)\})^2, (1-\{N\mu(h)\})^2)\right). \qquad (51)$$

This expression is not of the conformal form (3) since the coefficient of the term proportional to $1/N$ is still dependent on N. The first gap in the energy connected with the change in spin wave number (particle number in the case of the Bose gas) is determined by M_0+1 if $\{N\mu(h)\}<\frac{1}{2}$ and by M_0-1 otherwise:

$$E_1^{\rm HC} - E_0^{\rm HC} = \frac{2\pi v_{\rm F}}{N}\frac{1}{(2\xi(\Lambda))^2}|1-2\{N\mu(h)\}| \qquad (52)$$

which is also not immediately of the conformal form (1) for the same reason.

To illustrate the analytical results of the previous section we have solved numerically the BA equations for long ($N = 150, 152, \ldots, 170$) Heisenberg chains. We have chosen $\theta = \pi/3$ as the higher-order corrections are expected to decay fast at this value of θ (Woynarovich and Eckle 1987). Our results for $h = 1.3282$ (which corresponds to $\mu(h) = 0.174\,63$ or $\Lambda = 0.35$) are shown in figure 1. Full circles denote the non-analytical part of the ground-state energy as a function of N, in units of $\pi v_{\rm F}/6N$, i.e. $(E_0^{\rm HC} - N\varepsilon_\infty)6N/(\pi v_{\rm F})+1$. Open circles correspond to the first gap in units of $2\pi v_{\rm F}/N$, i.e. $(E_1^{\rm HC} - E_0^{\rm HC})N/2\pi v_{\rm F}$. The broken curves and lines show the theoretical expectations if N were continuous (as is the case for L in the Bose gas).

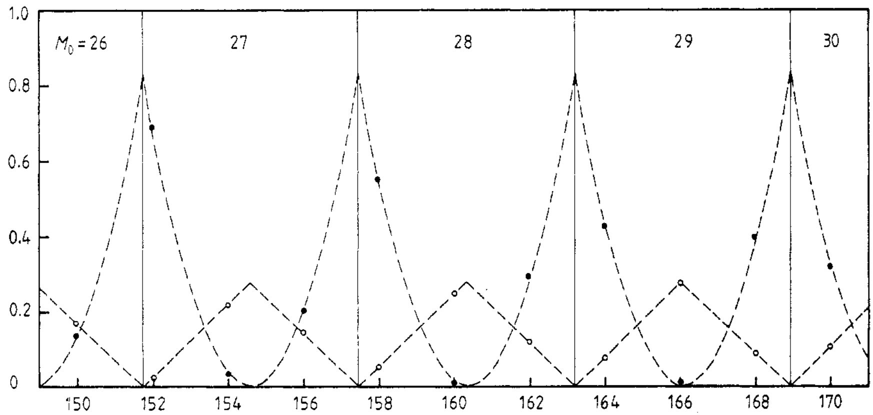

Figure 1. Non-analytic finite-size corrections in the anisotropic Heisenberg chain at $\theta = \pi/3$ and $h = 1.3282$. Full circles denote the non-analytic part of the ground-state energy as a function of N, in units of $\pi v_{\rm F}/6N$, i.e.

$$(E_0^{\rm HC} - \varepsilon_\infty N)6N/(\pi v_{\rm F}) + 1.$$

Open circles correspond to the first gap in units of $2\pi v_{\rm F}/N$, i.e.

$$(E_1^{\rm HC} - E_0^{\rm HC})N/2\pi v_{\rm F}.$$

The broken curves and lines show the theoretical expectations if N were a continuous number. M_0 is the number of spin waves minimising the energy at the given N and h.

4. Discussion of the results

We have to note that the above non-analytic finite-size effects are not consequences of the Bethe ansatz; rather, they should be present in any system, where the particle number of the ground state depends on external parameters such as chemical potential or magnetic field. As examples we refer to the one-dimensional non-interacting spinless Fermi gas with Hamiltonian

$$\mathcal{H} = -\int_0^L \left(\psi^+(x) \frac{d^2}{dx^2} \psi(x) + h\psi^+(x)\psi(x) \right) dx \tag{53}$$

and the XX chain in a magnetic field with Hamiltonian

$$\mathcal{H} = -\sum_{i=1}^{N} (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y + hS_i^z) \tag{54}$$

which can be solved with more elementary techniques. These models show the same or similar non-analytic finite-size effects as the Bose gas or the Heisenberg chain (cf appendix 1). The formal reason for these non-analyticities is that the particle number M_0 in the finite system as a function of the size and external parameter cannot be an analytic function of the external parameter since M_0 must be an integer. However simple this reason is, it seems to spoil the conformal structure of the spectrum and gives rise to the question whether these systems are conformally invariant or not.

In answering this question we recall that in *lattice* systems conformal invariance is an approximate symmetry only, which is valid on a length scale that is large compared to any other scale in the system. In other words, only appropriate scaling limits of these models are conformally invariant. If the energy spectrum is of the form expected on the basis of conformal invariance, this indicates that the model has a conformally invariant scaling limit. If the conformal structure can only be restored by imposing extra conditions on the system, these extra conditions should also be obeyed in constructing the scaling limit.

In the case of the Bose gas the conformal structure is restored if we choose $L = m/\mu(h)$ (m being only an arbitrary integer). Then $M_0 = m$, and denoting $M - M_0 = \Delta M$ we have

$$E(\Delta M, D) = L\varepsilon_\infty + \frac{2\pi v}{L}\left(\frac{1}{(2\xi(\Lambda))^2}(\Delta M)^2 + (\xi(\Lambda))^2 D^2 - \tfrac{1}{12} + N^+ + N^- \right) \tag{55}$$

and

$$P(\Delta M, D) = -\frac{2\pi}{L} M_0 D + \frac{2\pi}{L}(-\Delta MD + N^+ - N^-) \tag{56}$$

from which one can see that $c^{BG} = 1$ and that the scaling dimensions are

$$x(\Delta M, D) = \frac{1}{(2\xi(\Lambda))^2}(\Delta M)^2 + (\xi(\Lambda))^2 D^2 \tag{57}$$

$$s(\Delta M, D) = -\Delta MD \tag{58}$$

which is the result of Bogoliubov *et al* (1987) and Berkovich and Murthy (1988) also. We note that in this case the $2k_F$ for the finite and infinite system are equal, i.e. $2k_F = 2\pi M_0/L$.

For arbitrary L, however, the $2k_F$ of the finite system is $2\pi M_0/L$ while that of the infinite one is $2\pi\mu(h)$, and will in general take different values. This difference has the following reason. While in the infinite system $2k_F$ is determined only by h, in the finite L case $2k_F$ is also subject to the constraint that the number of particles in the system should be an integer. The relation between the critical indices and the spectrum of the Hamiltonian for finite L has been established through the conformal mapping of the plane onto a strip of width L. Our result shows that this relation holds only if the mapping does not change $2k_F$, and this is not true in general for any value of L.

The case of the Heisenberg chain is somewhat more complicated because the chain length can take only integer values, i.e. for arbitrary h, hence $\mu(h)$, the conformal form cannot be recovered. It can be recovered only if $\mu(h)=p/q$ with $2p<q$ and $p, q =$ relative prime integers. Then the allowable values of N are $N=qN'$ with N' integer and $M_0=pN'$ is to be chosen. Denoting $M-M_0=\Delta M$ we have

$$E(\Delta M, D)=N\varepsilon_\infty+\frac{2\pi v_F}{N}\left(\frac{1}{(2\xi(\Lambda))^2}(\Delta M)^2+(\xi(\Lambda))^2D^2-\tfrac{1}{12}+N^++N^-\right) \tag{59}$$

$$P(\Delta M, D)=\frac{2\pi p}{q}D+\frac{2\pi}{N}(\Delta MD-M^++N^-). \tag{60}$$

These equations give $2k_F=2\pi p/q$, $c=1$ and the same scaling indices as in (57) and (58). We observe that the scaling indices are not constants but functions of the coupling and of the magnetic field as expected from general considerations when $c=1$. But in order to satisfy the requirement $\mu(h)=p/q$, $\cos\theta$ and h cannot be changed independently: this means that the marginal operators in the problem (cf Cardy 1987) should also contain the magnetic field and the magnetisation.

In commenting on the requirement $\mu(h)=p/q$ we first recall the case of zero magnetic field. There we have for $h=0$, $S^z=0$ and $\mu(h=0)=\frac{1}{2}$. To recover the structure of (59), N should be even (this condition is well known but has never been emphasised). In particular this restriction shows up in the construction of the continuum limit of the problem. As Luther (1980) has shown, in taking the continuum limit of the fermionised model, the local field operators $\psi_{1,2}(x)$ should be defined in terms of the lattice fermion operators a_j and the lattice spacing s as

$$\psi_1(x)=\frac{1}{\sqrt{2s}}(-1)^j(a_{2j}+\mathrm{i}a_{2j+1}) \tag{61}$$

$$\psi_2(x)=\frac{1}{\sqrt{2s}}(-1)^j(a_{2j}-\mathrm{i}a_{2j+1}). \tag{62}$$

In the limits $s\to 0$, $sN\to L$, $2js\to x$ this construction when applied to the XXZ chain yields the massless Thirring model. The important point is that two sites of the lattice correspond to one point in the continuum limit. Therefore the requirement that N ought to be even appears as a *natural* one. If N is odd, the above procedure leads again to the massless Thirring model but with an extra term corresponding to the a_j which does not belong to any of the operators $\psi_{1,2}(x)$. This extra term is a kind of defect operator which shifts the energy levels by an amount of order $1/L$.

Generalising the above picture for the case $h\neq 0$, $\mu(h)=p/q$ we think that the continuum limit should be constructed as follows. The chain should be cut into blocks of q sites. The local field operators should be associated with these blocks and should be the combinations of operators belonging to the q sites in a block. This is strongly supported by the fact that certain correlation functions show oscillations with period $2k_F = 2\pi p/q$, indicating that *smooth* fields can be obtained by *averaging* over one period of q sites. If h is such that $\mu(h)$ is irrational the period of the oscillations and the period of the lattice are incommensurate and this averaging procedure cannot be properly defined. Hence, if we want to construct the continuum limit for a system of finite size we would have difficulties to define consistently the field operators because the period of the oscillations is determined by $2\pi M_0/N$ and changes with N.

In the case of the XX chain (i.e. $\cos\theta = 0$) the continuum limit can be explicitly constructed (cf appendix 2). The local fields should then be defined as

$$\psi_\mu(x) = \frac{1}{\sqrt{qs}} \sum_{j=1}^{q} \exp[\mathrm{i}(2\mu - 1)k_F(qn+j)s]a_{qn+j} \qquad \mu = 1, \ldots, q \qquad (63)$$

with $x = nqs$. Two of these fields, the ones with $\mu = 1$ and $\mu = q$ corresponding to smooth variations in the amplitudes of fields oscillating with k_F and $-k_F$, respectively, are massless. The others acquire masses in the limit $s \to 0$, which diverge as $1/s$. These infinitely massive fields do not affect the dynamics of the massless ones, and they can be ignored since they correspond to modes deep in the Fermi sea or high above the Fermi level. The resulting Hamiltonian is the one of two fermion fields with linear dispersion corresponding to left and right moving particles.

5. Summary

In the present work we have demonstrated that the spectrum of the one-dimensional Bose gas in the presence of a chemical potential and the spectrum of the Heisenberg chain in an external magnetic field is not immediately of the conformal form: the terms proportional to the inverse of the size of the system depend also in a non-analytic way on the size. This effect is not a consequence of the Bethe ansatz; rather it follows from the dependence of the number of particles or spin waves in the ground state on the external field. Thus the effect is expected to show up in any such system in which the number of particles is determined by an external parameter.

With these non-analytic finite-size effects present it is not possible to extract the conformal invariants from the spectrum of the finite-size system. Thus one must be careful with finite-size scaling.

We show that the conformal structure of the spectrum can be restored, provided some additional conditions imposed on the external field and the size of the system are also satisfied. In the case of the Bose gas one must require that the Fermi momentum of the finite and infinite system are equal. At a given chemical potential this can be ensured if we restrict the length to take only discrete values depending on the chemical potential.

For the Heisenberg chain in an arbitrary magnetic field the conformal form of the spectrum cannot be recovered at any chain length unless the magnetisation density of the infinite system (determined by the magnetic field) is a rational number. Also in this case the chain length can only take some definite discrete values. The Heisenberg model, as a *lattice* system, cannot be conformally invariant by itself. Only certain *continuum* limits of it can be conformally invariant. We argue that this conformally invariant continuum limit can only be constructed at definitive combinations of the coupling constant and magnetic field (at which the magnetisation density is rational).

In other words, the Heisenberg chain is a proper discretisation of a continuum field theory only at these combinations.

At those values of the magnetic field where the spectrum is of the conformal form, the $2k_F$ oscillations and the lattice are commensurate. Moreover the allowable chain lengths are always integer multiples of the period determined by $2k_F$. We therefore propose that the conformally invariant continuum limit should be constructed based on the Fourier transform of certain blocks of operators, which are defined on the lattice sites.

Finally we note that recently Henkel *et al* (1989) have observed similar phenomena in the Ising model with defects, where they have found cases for which a conformally invariant structure is only recovered if certain ratios are rational numbers.

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Appendix 1. Non-analytic finite-size effect in the *XX* spin chain

We study the effect of a magnetic field h on a XX spin chain of N sites and illustrate the findings of the main text through a simple and exact calculation for a non-interacting system.

The Hamiltonian is given by

$$\mathscr{H} = -\sum_{j=1}^{N} (S_j^+ S_{j+1}^- + S_j^- S_{j+1}^+ + 2hS_j^z) \tag{A1.1}$$

where periodic boundary conditions are assumed for the operators S_j^+, S_j^- and S_j^z. As is easily seen, the number of down spins on the chain is a constant of the motion.

Consider first the problem of one spin down defined by

$$|\downarrow\rangle = \sum_{j=1}^{N} \psi(j)|\uparrow\ldots\downarrow\ldots\uparrow\rangle \tag{A1.2}$$

where the down spin is at the jth site. It is an eigenstate of $\mathscr{H}$ with eigenvalue E if

$$\psi(j) = \exp(\mathrm{i}kj) \tag{A1.3}$$

$$E(k) = -2(\cos k - h). \tag{A1.4}$$

Since there cannot be two down spins at the same site, the wavefunction for M down spins $\psi(j_1, j_2, \ldots, j_M)$, where $j_1 < j_2 < \ldots < j_M$, must have a node whenever two arguments are equal. Otherwise it always describes an assembly of independent down spins. Thus it is simply of determinantal form (Slater determinant).

Now requiring periodic boundary conditions for all the arguments of $\psi(j_1, \ldots, j_M)$ means that under the shift $j_s \to j_s + N$ the wavefunction acquires a phase factor $\exp(\mathrm{i}k_s N)$. However, to execute this shift we must move the down spin at j_s through the remaining $(M-1)$ down spins. Each time we go through one down spin we have a phase (-1). The wavefunction would remain invariant if

$$\exp(\mathrm{i}k_s N) = (-1)^{M-1} \qquad s = 1, 2, \ldots, M. \tag{A1.5}$$

Consequently the allowable k_s are

$$k_s = \begin{cases} 2\pi/N \times \text{integer} & \text{if } M \text{ odd} \\ \pi/N \times \text{odd-integer} & \text{if } M \text{ even.} \end{cases} \tag{A1.6}$$

We can now calculate the ground-state energy of M down spins by minimising the total energy of the filled negative-energy states. Suppose M even to fix the ideas, the case of M odd presents no difficulty. This ground-state energy $E_0(N, h)$ is

$$E_0(N, h) = -2 \sum_{s=1}^{M} (\cos k_s - h). \tag{A1.7}$$

Summing on the values of k_s given by (A1.6) we find an energy density

$$\varepsilon_0(\rho, h, N) = -\frac{2\sin(\pi\rho)}{N\sin(\pi/N)} + 2h\rho \tag{A1.8}$$

where $\rho = M/N$ is the density of down spins. It is clear that in the thermodynamic limit we have

$$\varepsilon_0(\rho, h, \infty) = -2\sin \pi\rho/\pi + 2h\rho \tag{A1.9}$$

which has a minimum at $\rho = \rho_0$ defined by

$$\cos \pi\rho_0 = h. \tag{A1.10}$$

Thus $\rho_0 = M_0/N$ is real for $|h| \leq 1$. For N very large, we expect ρ to be very close to ρ_0, i.e. up to the order $1/N$. Then we expand $\varepsilon_0(\rho, h, N)$ with respect to the two independent variables $(\rho - \rho_0)$ and $1/N$:

$$\varepsilon_0(\rho, h, N) = \left(-\frac{2\sin \pi\rho_0}{\pi} + 2h\rho_0 \right) - \frac{2\sin \pi\rho_0}{\pi} \frac{\pi^2}{6N^2}[1 - 3(M - M_0)^2] + \text{higher-order terms.} \tag{A1.11}$$

There are no terms in $(\rho - \rho_0)$ or $1/N$ because of the condition (A1.10). Equation (A1.11) is a special case of (51). It shows clearly that the prediction of conformal invariance is only realised if one chooses h in (A1.10) so that ρ_0 is a rational number p/q. Then one may choose the number of sites N as a multiple of q. Then $M_0 = pN'$ and the quantity $(M - M_0)^2$ does have a minimum at zero.

Appendix 2. Constructing the continuum limit of the *XX* chain in a magnetic field

We shall begin with the fermionised version of the XX chain in a magnetic field:

$$\mathscr{H} = \sum_{j=1}^{N} \left(-\frac{I}{2}(c_j^+ c_{j+1} + c_{j+1}^+ c_j) + hc_j^+ c_j \right) \tag{A2.1}$$

where c_j^+ and c_j are the usual fermion operators.

We shall assume that the number of fermions M_0 and the number of sites N satisfy the conditions

$$N = qN' \qquad M_0 = pN' \tag{A2.2}$$

where p and q are integers and relative primes of each other, satisfying $p < q/2$. The Fermi momentum is defined by

$$2k_F = 2\pi M_0/N = 2\pi p/q. \tag{A2.3}$$

Note that k_F is not a real momentum in the sense that, if M_0 is even then antiperiodic boundary conditions are required (cf (A1.6)) but k_F corresponds to periodic boundary conditions:

$$k_F = \frac{2\pi}{N}\left(\frac{M_0}{2}\right). \tag{A2.4}$$

Similarly, if M_0 is odd then periodic boundary conditions are required but

$$k_F = \frac{2\pi}{N}\left(\frac{M_0}{2}\right) = \frac{2\pi}{N}\left(\left[\frac{M_0}{2}\right] + \frac{1}{2}\right) \tag{A2.5}$$

where [ ] again denotes the integer part of the expression in brackets.

Introducing a q-component fermion representation

$$\psi_\nu(n) = \exp\{ik_F[(n-1)q+\nu]\}c_{[(n-1)q+\nu]} \qquad \nu = 1, \ldots, q \tag{A2.6}$$

we can express $\mathscr{H}$ as

$$\mathscr{H} = \sum_{n=1}^{N'} \sum_{\nu,\mu=1}^{q} \{\phi_\nu^+(n)M_{\nu\mu}\phi_\mu(n) + \phi_\mu^+(n)D_{\mu\nu}^{(1)}(\phi_\nu(n+1) - \phi_\nu(n))$$

$$+ \phi_\mu^+(n)D_{\mu\nu}^{(2)}(\phi_\nu(n) - \phi_\nu(n-1))\} \tag{A2.7}$$

where the matrices **M**, $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ are given by their matrix elements

$$M_{\mu\nu} = h\delta_{\mu\nu} - \tfrac{1}{2}I\delta_{\mu+1,\nu}\,e^{ik_F} - \tfrac{1}{2}I\delta_{\mu-1,\nu}\,e^{-ik_F} \tag{A2.8}$$

$$D_{\mu\nu}^{(1)} = -\tfrac{1}{2}I\delta_{\mu q}\delta_{\nu,1}\,e^{ik_F} \tag{A2.9}$$

$$D_{\mu\nu}^{(2)} = \tfrac{1}{2}I\delta_{\mu,1}\delta_{\nu,q}\,e^{-ik_F}. \tag{A2.10}$$

Performing a canonical transformation Λ, which diagonalises the matrix **M** we can express the Hamiltonian $\mathscr{H}$ in terms of new fermion operators:

$$\psi_\mu(n) = \sum_\nu (\Lambda^{-1})_{\mu\nu}\phi_\nu(n) \tag{A2.11}$$

where the matrix Λ^{-1} is given by

$$(\Lambda^{-1})_{\mu\nu} = \frac{1}{\sqrt{q}}\exp(2ik_F\mu\nu). \tag{A2.12}$$

Then we have

$$\mathscr{H}' = \sum_{n=1}^{N'} \sum_{\mu\nu} \psi_\mu^+(n)M_{\mu\nu}^d\psi_\nu(n) + \psi_\mu^+(n)D_{\mu\nu}'^1[\psi_\nu(n+1) - \psi_\nu(n)]$$

$$+ \psi_\mu^+(n)D_{\mu\nu}'^2[\psi_\nu(n) - \psi_\nu(n+1)] \tag{A2.13}$$

where

$$M_{\mu\nu}^d = \delta_{\mu\nu}\{h - I\cos[2k_F(\nu - \tfrac{1}{2})]\} \tag{A2.14}$$

$$D_{\mu\nu}'^1 = \frac{-I}{2q}\exp[-2ik_F(\nu - \tfrac{1}{2})] \tag{A2.15}$$

$$D_{\mu\nu}'^2 = \frac{I}{2q}\exp[2ik_F(\mu - \tfrac{1}{2})]. \tag{A2.16}$$

We are now in a position to construct the continuum limit of the theory. To this end let s be the lattice constant and set

$$sqN' = L \tag{A2.17}$$

$$sqn = x \tag{A2.18}$$

$$sq = \mathrm{d}x \qquad \text{(the length of one block).} \tag{A2.19}$$

In the limit $s \to 0$ and $N \to \infty$ we obtain the following:

$$\sum_n^{N'} \to \int_0^L \frac{\mathrm{d}x}{sq} \tag{A2.20}$$

$$\delta_{n,n'} \to \delta(x) sq \tag{A2.21}$$

$$\psi_\mu(n) \to (sq)^{1/2} \psi_\mu(x) \tag{A2.22}$$

$$\psi_\mu(n+1) - \psi_\mu(n) \to (sq)^{3/2} \frac{\partial}{\partial x} \psi_\mu(x). \tag{A2.23}$$

Also we wish to have a fixed Fermi velocity in x space, i.e. $v_{\mathrm{F}}^{\mathrm{discrete}}\, s \to v_{\mathrm{F}}$. Now since on the lattice $v_{\mathrm{F}}^{\mathrm{discrete}} \simeq I$ this would mean that the product Is tends to a finite limit I'.

Taking into account all of these considerations, we see that the continuum limit Hamiltonian on a finite interval of length L is

$$\mathscr{H}^{\mathrm{cont}} = qI' \int_0^L \sum_\mu \left(\psi_\mu^+(x) \psi_\mu(x) \frac{m'_\mu}{qs} + \sum_{\mu\nu} \psi_\mu^+(x) D'_{\mu\nu} \frac{\partial}{\partial x} \psi_\nu(x) \right) \mathrm{d}x. \tag{A2.24}$$

where

$$m'_\mu = \{h' - \cos[2k_{\mathrm{F}}(\mu - \tfrac{1}{2})]\} \tag{A2.25}$$

$$D'_{\mu\nu} = \frac{1}{2q} \{\exp[2\mathrm{i}k_{\mathrm{F}}(\mu - \tfrac{1}{2})] - \exp[-2\mathrm{i}k_{\mathrm{F}}(\nu - \tfrac{1}{2})]\}. \tag{A2.26}$$

This entire procedure makes sense only if we have $h' = \cos(k_{\mathrm{F}})$. Otherwise all masses are of order $\sim 1/s$. Then the modes $\nu = 1$ and $\nu = q$ are massless while the other modes become very massive (of order $\sim 1/s$).

In the $s \to 0$ limit these very massive modes do not intervene in the dynamics of the massless ones. This can be seen as follows. Rewriting the integrand of $\mathscr{H}^{\mathrm{cont}}$ in terms of Fourier components, one can look for the normal modes in momentum space. This amounts to diagonalising the matrix:

$$\begin{pmatrix} -kv_{\mathrm{F}} & k\mathbf{u}^+ & 0 \\ k\mathbf{u} & \mathbf{m} & k\mathbf{v} \\ 0 & k\mathbf{v}^+ & kv_{\mathrm{F}} \end{pmatrix} \tag{A2.27}$$

where we have defined

$$\mathbf{u} = \begin{pmatrix} u_2 \\ u_3 \\ \vdots \\ u_{q-1} \end{pmatrix} \tag{A2.28}$$

$$\mathbf{u}^+ = (u_2^* \quad u_3^* \quad \dots \quad u_{q-1}^*) \tag{A2.29}$$

$$\mathbf{v} = \begin{pmatrix} v_2 \\ v_3 \\ \vdots \\ v_{q-1} \end{pmatrix} \tag{A2.30}$$

$$\mathbf{v}^+ = (v_2^* \quad v_3^* \quad \dots \quad v_{q-1}^*). \tag{A2.31}$$

Here $\mathbf{m}$ is a $(q-2)\times(q-2)$ matrix with non-zero diagonal elements which are proportional to $1/s$.

We look for the first eigenvector in the form

$$\begin{pmatrix} 1 \\ \vdots \\ \mathbf{x} \\ \vdots \\ y \end{pmatrix} \tag{A2.32}$$

$\mathbf{x}$ being a $(q-2)$ column vector. Then the eigenvalue equations with eigenvalue $-kv'_{\mathrm{F}}$ are

$$-v_{\mathrm{F}}+\mathbf{u}\cdot\mathbf{x}=-v'_{\mathrm{F}} \tag{A2.33}$$

$$\mathbf{u}+k^{-1}\mathbf{m}\cdot\mathbf{x}+y\mathbf{v}=-v'_{\mathrm{F}}\mathbf{x} \tag{A2.34}$$

$$\mathbf{v}\cdot\mathbf{x}+v_{\mathrm{F}}y=-v'_{\mathrm{F}}y. \tag{A2.35}$$

Solving these equations we get readily

$$y=-\frac{\mathbf{v}\cdot\mathbf{x}}{(v_{\mathrm{F}}+v'_{\mathrm{F}})} \tag{A2.36}$$

$$\mathbf{x}=-\left(\frac{1}{k}\mathbf{m}+v'_{\mathrm{F}}-\frac{\mathbf{v}\otimes\mathbf{v}}{v_{\mathrm{F}}+v'_{\mathrm{F}}}\right)^{-1}\mathbf{u}. \tag{A2.37}$$

The inverse matrix in the last equation exists. We thus obtain to the order s the following:

$$\left(\frac{1}{k}\mathbf{m}+v'_{\mathrm{F}}-\frac{\mathbf{v}\otimes\mathbf{v}}{v_{\mathrm{F}}+v'_{\mathrm{F}}}\right)^{-1}\sim s$$

$$\mathbf{x}\sim s \qquad y\sim s \tag{A2.38}$$

$$v'_{\mathrm{F}}=v_{\mathrm{F}}+\mathrm{O}(s).$$

So we see that, in the $s\to 0$ limit, the mode $\nu=1$ becomes totally independent from the others as $\mathbf{x}\to\mathbf{0}$ and $y\to 0$. Similarly one can show that the mode with $\nu=q$ will also be independent of the others when $s\to 0$. Thus the modes $\nu=2,\ldots,q-1$ can be omitted in the continuum limit. Finally we can write

$$\mathscr{H}^{\mathrm{cont}}=\mathrm{i}v_{\mathrm{F}}\int_0^L\left(\psi_1^+(x)\frac{\partial}{\partial x}\psi_1(x)-\psi_q^+(x)\frac{\partial}{\partial x}\psi_q(x)\right)\mathrm{d}x \tag{A2.39}$$

with $v_{\mathrm{F}}=I'\sin(k_{\mathrm{F}})$.

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