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Finite-size bosonization and self-consistent harmonic approximation

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Abstract

The self-consistent harmonic approximation is extended in order to account for the existence of Klein factors in bosonized Hamiltonians. This is important for the study of finite systems where Klein factors cannot be ignored *a priori*. As a test we apply the method to interacting spinless fermions with modulated hopping. We calculate the finite-size corrections to the energy gap and the Drude weight and compare our results with the exact solution for special values of the model parameters.

1. Introduction

Bosonization techniques have been extensively used in the study of one-dimensional electron and spin systems [1–3]. The success of the method is based on the fact that the low energy properties of fermions are determined by the states close to the Fermi surface which in one dimension consists only of two points. When the spectrum is linearized around the Fermi points the Hamiltonian can be expressed in terms of bosonic operators associated with particle–hole excitations of momentum q . In addition, scattering processes between left and right Fermi points require us to introduce extra operators, the so-called Klein factors.

Perturbations like impurity scattering or a modulation of the hopping lead to nonlinearities in the bosonized Hamiltonian, for which an exact solution is known only in some special cases [4]. In general one has to resort to approximative methods like renormalization group calculations. Another more intuitive method is the self-consistent harmonic approximation (SCHA) where the non-linear terms are replaced by a harmonic potential with parameters to be determined self-consistently according to a variational principle for the energy.

The SCHA has been successfully applied to various non-linear field theories [5–11]. In the context of bosonized Hamiltonians, however, the existence of Klein factors has been ignored in these approaches. This may be justified for infinite systems [3], but in general the Klein factors have to be treated carefully as pointed out for example in the context of impurity models and

two-leg ladders [2, 12–14]. In the following we present an extension of the SCHA which treats the bosonic fields and the Klein factors on equal footing. As a prototype model for this study we consider the lattice model of spinless fermions at half filling including nearest-neighbour interaction and a modulation of the hopping due to a periodic lattice distortion.

In the next section the Hamiltonian of this model is bosonized and a trial Hamiltonian is constructed which serves as the basis for the SCHA. In section 3 we calculate the energy gap and the Drude weight and compare our results with exact results that are available for certain values of the model parameters. Finally, we conclude with a brief summary in section 4.

2. Model and formalism

We consider a one-dimensional model of spinless fermions with static dimerization

$$H = -t \sum_i (1 + (-1)^i u) (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) + V \sum_i n_i n_{i+1} \quad (1)$$

where u is the dimerization parameter that leads to a periodic modulation of the hopping amplitude t , and V is the strength of the nearest-neighbour interaction. At half filling and in the range $-2 < V/t < 2$ the bosonized Hamiltonian of this model reads [2]

$$H = \int_0^L \frac{dx}{2\pi} \left\{ \frac{v}{g} :(\partial_x \phi)^2: + v g :(\partial_x \theta)^2: \right\} + \frac{\pi v}{2Lg} N^2 \\ + \frac{\pi v g}{2L} J^2 - \frac{i t u}{\pi a} \int_0^L dx F_L^\dagger F_R e^{2i\phi(x)} + \text{h.c.} \quad (2)$$

where ϕ and θ are conjugate fields. The renormalized Fermi velocity $v = \pi t \sin(2\eta)/(\pi - 2\eta)$ and the Luttinger parameter $g = \pi/4\eta$ are related to the interaction according to $V = -2t \cos(2\eta)$. The normal ordering operation $(: :)$ is introduced to avoid the divergences associated with unphysical states assumed by the Luttinger model. The parameter a is needed in the bosonization formalism to remove ultra-violet divergences in certain k -summations, and appears in equation (2) since the exponential $\exp(2i\phi(x))$ is not normal ordered. For a lattice model, $1/a$ can be interpreted as a kind of effective band-width [2], whereas in the continuum the limit $a \rightarrow 0$ has to be performed in order to obtain the correct δ -function anticommutators of the fermionic field operators [1]. N and J are the charge and current operators, defined as $N = N_L + N_R$ and $J = N_L - N_R$, respectively, where N_L and N_R count the numbers of left and right moving particles with respect to the filled Fermi sea. The Klein factors $F_{L/R}^\dagger$ and $F_{L/R}$ raise or lower the number of left and right moving fermions by one (which no combination of bosonic operators can ever do), and they assure also that fermions of the two different species anticommute. The dimerization, described by the non-linear term of the Hamiltonian, breaks the conservation of the current J and is responsible for the opening of an energy gap.

To discuss the gap formation quantitatively, we use the self-consistent harmonic approximation (SCHA) which was originally introduced for the sine-Gordon model [5]. The idea is to construct an exactly solvable trial Hamiltonian H_{tr} where the bosonic fields in (2) are decoupled from the Klein factors and where the non-linear terms $\sim e^{\pm 2i\phi}$ are replaced with a quadratic form $\sim \phi^2$. Accordingly we chose $H_{\text{tr}} = H_{\text{tr}}^\Delta + H_{\text{tr}}^B$ as the sum of two commuting parts

$$H_{\text{tr}}^\Delta = \int_0^L \frac{dx}{2\pi} \left\{ \frac{v}{g} (\partial_x \phi)^2 + v g (\partial_x \theta)^2 + \frac{\Delta^2}{v g} \phi^2(x) \right\} \quad (3)$$

and

$$H_{\text{tr}}^B = -iB(F_L^\dagger F_R - F_R^\dagger F_L) + \frac{\pi v g}{2L} J^2 \quad (4)$$

each of them depending on a single variational parameter, Δ and B , respectively. Notice that from the standard trial Hamiltonian alone (equation (3)), only the trivial solution $\Delta = 0$ can be obtained. Therefore the non-standard term equation (4) is necessarily required to describe the phase transition in the system. Since we are only interested in properties at zero temperature we use the normalized ground state $|\psi_0\rangle$ of H_{tr} as a variational wavefunction for the Hamiltonian (2). This provides us with an upper bound \tilde{E} for the ground state energy E of (2) due to the inequality

$$E \leq \tilde{E} = \langle \psi_0 | H | \psi_0 \rangle. \quad (5)$$

Minimizing \tilde{E} with respect to the variational parameters Δ and B yields the following set of equations:

$$\begin{aligned} \Delta^2 &= -(4vgtu/a)E'_0(B)e^{-2\langle \phi^2 \rangle_{\text{tr}}} \\ B &= (tu/\pi a)L e^{-2\langle \phi^2 \rangle_{\text{tr}}} \end{aligned} \quad (6)$$

where $E_0(B)$ is the ground state energy of H_{tr}^B and $E'_0(B) = dE_0(B)/dB$. Since H_{tr}^B is bilinear in the field operators it is straightforward to calculate the equal time correlation function of the phase field $\phi(x)$ entering equation (6):

$$\langle \phi^2 \rangle_{\text{tr}} = \frac{\pi vg}{L} \sum_{k>0} \frac{e^{-ka}}{\sqrt{v^2 k^2 + \Delta^2}} \quad (7)$$

where the k -values in the sum are multiples of $2\pi/L$.

3. Energy gap and Drude weight

In order to solve the set of equations (6) we have to calculate the ground state energy $E_0(B)$ of the trial Hamiltonian H_{tr}^B . The products of Klein factors $F_L^+ F_R$ and $F_R^+ F_L$ appearing in H_{tr}^B change the quantum number of the current operator from J to $J \pm 2$. H_{tr}^B can therefore be regarded as a particle moving in a harmonic potential along the J -axis. For $L \rightarrow \infty$ the potential energy term in H_{tr}^B vanishes and the kinetic energy term with imaginary hopping iB yields the ground state energy $E_0(B) = -2B$. In this limit we reproduce the results of [11], where the Klein factors have been ignored. Replacing the sum in equation (7) by an integral we obtain

$$\langle \phi^2 \rangle_{\text{tr}} = \frac{g}{2} \ln \frac{\Delta_0}{\Delta} \quad (8)$$

where $\Delta_0 = 2ve^{-\gamma}/a$, $\gamma = 0.5772$ is Euler's constant, and $\Delta \ll \Delta_0$ has been assumed. Inserting equation (8) into (6) and using $E'_0(B) = -2$ yields

$$\frac{\Delta}{\Delta_0} = \left(\frac{u}{u_0} \right)^{1/(2-g)} \quad (9)$$

with $u_0 = e^{-\gamma} \Delta_0 / 4gt$. For $g > 2$ equation (9) diverges as $u \rightarrow 0$ and there is only the trivial solution $\Delta = 0$, i.e. the line $g = 2$ marks the transition from a gapless to a gapped phase in the g - u plane. In the spinless fermion model this corresponds to the line $V/t = -\sqrt{2}$ in the V - u phase diagram. The value $g_c = 2$ obtained within the variational approach is in accordance with the exact result based on a mapping of the bosonized Hamiltonian on the Ashkin-Teller model [15] for $u \rightarrow 0$. However, according to renormalization group calculations [16] and confirmed numerically using the density matrix renormalization group [11], the phase boundary in the g - u plane shifts to larger values of g with increasing u while the SCHA gives a vertical line. On the other hand, the exponent $1/(2-g)$ characterizing the opening of the gap is

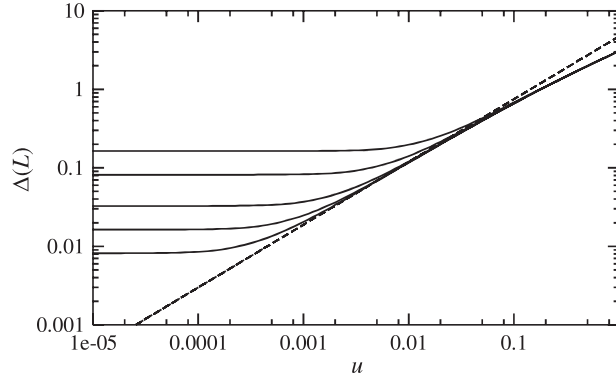


Figure 1. Energy gap $\Delta(L)$ (in units of t) as function of the dimerization parameter u for $L = 100, 200, 500, 1000, 2000$ (from top to bottom). The dashed line is the analytic result of equation (9) valid for $L \rightarrow \infty$ and $\Delta \ll \Delta_0$.

exact [6]. In particular, for non-interacting fermions ($V = 0$) the Luttinger liquid parameter is $g = 1$ and therefore $\Delta \propto u$ in agreement with the exact energy gap $\Delta_{\text{ex}} = 4tu$. At $V = 2t$, where Umklapp scattering becomes relevant and leads to the opening of a correlation gap, equation (9) yields $\Delta \propto u^{2/3}$ which agrees with the exact result $\Delta_{\text{ex}} \propto u^{2/3}/\sqrt{|\ln u|}$ up to the logarithmic correction [17].

In the following we consider a system of finite length L . In order to calculate the ground state energy of H_{tr}^B it is convenient to switch to the momentum representation, $J \rightarrow -i d/dp_J$, where the trial Hamiltonian reads

$$H_{\text{tr}}^B = -\frac{\pi v g}{2L} \frac{d^2}{dp_J^2} + 2B \cos(2p_J) \quad (10)$$

with periodic boundary conditions for the wavefunction, $\Psi(p_J + \pi) = \Psi(p_J)$. The corresponding Schrödinger equation is known as Mathieu's equation. Accordingly, the ground state energy of H_{tr}^B has the following asymptotical behaviour [21]:

$$E_0(B) \approx \begin{cases} -B^2 L / (\pi v g) & \text{for } LB \ll v \\ -2B & \text{for } LB \gg v. \end{cases} \quad (11)$$

Combining the two equations (6) one obtains

$$\Delta^2 L^2 = -4\pi v g E'_0(B) B L \quad (12)$$

which can be used to relate the two limiting cases of equation (11) with two different physical situations: the condition $LB \gg v$ is equivalent with $L\Delta \gg v$ and therefore the results for $\langle \phi^2 \rangle_{\text{tr}}$ and $\Delta(u)$ are the same as for the infinite system i.e. the energy gap depends algebraically on the dimerization. On the other hand, the condition $LB \ll v$ implies that $L\Delta \ll v$. In this case the energy gap is purely due to the finite system size and of order $2\pi v/L$. Thus the crossover from a finite-size gap to a true dimerization gap coincides with the crossover between the regions where Klein factors are relevant or can be ignored.

In general, the set of equations (6) can only be solved numerically. Figure 1 shows the size-dependent energy gap $\Delta(L) = \sqrt{(2\pi v/L)^2 + \Delta^2}$, i.e. the lowest excitation energy of the bosonic modes, as a function of u for several values of the system size L ; notice that we consider a system with periodic boundary conditions, where the smallest wavenumber is $2\pi/L$. The Luttinger parameter is $g = 3/4$ which corresponds to $V/t = 1$.

We now turn to the calculation of the Drude weight D within the SCHA formalism. The Drude weight or charge stiffness is the central quantity to characterize charge transport at zero frequency. At $T = 0$ the real part of the electrical conductivity at frequency ω is of the form $\sigma(\omega) = 2\pi D\delta(\omega) + \sigma_{\text{reg}}(\omega)$ with $\sigma_{\text{reg}}(\omega) \rightarrow 0$ for $\omega \rightarrow 0$ in a system without impurities. Therefore $D = 0$ characterizes an insulator while $D > 0$ describes an (ideal) conductor [20]. The simplest way to calculate D is due to Kohn [19] who has shown that the Drude weight can be expressed as

$$D = \frac{L}{2} \left. \frac{d^2 E}{d\varphi^2} \right|_{\varphi=0} \quad (13)$$

where $E(\varphi)$ is the ground state energy of a ring of circumference L which is threaded by the flux φ . Alternatively, the parameter φ can also be associated with a change of boundary conditions; i.e. $\varphi = 0$ corresponds to periodic and $\varphi = \pi$ to antiperiodic boundary conditions. In the fermionic model (1) the hopping parameter t picks up a phase factor $\exp(\pm i\varphi)$ when a flux φ is applied. In the bosonized form (2) the only modification is that the current operator J has to be replaced by [20] $J + \frac{\varphi}{\pi}$. Correspondingly, we modify the B -dependent part of the trial Hamiltonian and write

$$H_{\text{tr}}^B(\varphi) = -iB(F_L^+ F_R - F_R^+ F_L) + \frac{\pi v g}{2L} \left(J + \frac{\varphi}{\pi} \right)^2. \quad (14)$$

Applying the same procedure as in the case $\varphi = 0$ yields a variational estimate \tilde{E} for the ground state energy which now depends on the flux φ , i.e. $\tilde{E} = \tilde{E}(\Delta, B, \varphi)$ where Δ and B , obtained from the gap equations (6), are also functions of φ . On first sight it might seem impossible to calculate the Drude weight using equation (13) since there is no analytical solution of the gap equations (6) even for $\varphi = 0$. However, a closer look reveals a great deal of simplification. From the second derivative

$$\frac{d^2 \tilde{E}}{d\varphi^2} = \frac{\partial^2 \tilde{E}}{\partial \Delta^2} \left(\frac{\partial \Delta}{\partial \varphi} \right)^2 + \frac{\partial^2 \tilde{E}}{\partial B^2} \left(\frac{\partial B}{\partial \varphi} \right)^2 + \frac{\partial \tilde{E}}{\partial \Delta} \frac{\partial^2 \Delta}{\partial \varphi^2} + \frac{\partial \tilde{E}}{\partial B} \frac{\partial^2 B}{\partial \varphi^2} + \frac{\partial^2 \tilde{E}}{\partial \varphi^2} + \text{mixed terms} \quad (15)$$

one retains only

$$\left. \frac{d^2 \tilde{E}}{d\varphi^2} \right|_{\varphi=0} = \left. \frac{\partial^2 \tilde{E}(\Delta, B, \varphi)}{\partial \varphi^2} \right|_{\varphi=0} \quad (16)$$

since

- (i) $\frac{\partial \tilde{E}}{\partial \Delta} = \frac{\partial \tilde{E}}{\partial B} = 0$ due to the minimum condition of the energy and
- (ii) $\frac{\partial \Delta}{\partial \varphi} = \frac{\partial B}{\partial \varphi} = 0$ at $\varphi = 0$ due to symmetry (Δ and B are even functions of φ).

Since the trial Hamiltonian $H_{\text{tr}} = H_{\text{tr}}^{\Delta} + H_{\text{tr}}^B(\varphi)$ consists of two commuting parts we may write $\tilde{E}(\Delta, B, \varphi) = \tilde{E}(\Delta) + E_0(B, \varphi)$ where $\tilde{E}(\Delta)$ depends only on Δ and $E_0(B, \varphi)$ is the ground state energy of $H_{\text{tr}}^B(\varphi)$, i.e. we obtain the simple result

$$D = \frac{L}{2} \left. \frac{\partial^2 E_0(B, \varphi)}{\partial \varphi^2} \right|_{\varphi=0} \quad (17)$$

where B is given by equation (6). To proceed we again represent $H_{\text{tr}}^B(\varphi)$ in terms of the Mathieu equation (10) where now the boundary conditions are $\Psi(p_J + \pi) = e^{i\varphi} \Psi(p_J)$. It is now straightforward to calculate the Drude weight for a finite system of size L in the gapped phase $g < 2$. In the ‘finite size gap’ region ($L\Delta \ll v$) we obtain

$$D = D_0 \left(1 - \frac{q^2}{2} + \dots \right) \quad (18)$$

where $q = 2LB/\pi vg \propto uL^{2-g}$ and $D_0 = vg/2\pi$ is the Drude weight of an unperturbed Luttinger liquid. In the opposite limit ($L\Delta \gg v$) which corresponds to a Mathieu equation with a large cosine potential the variation of the ground state energy with change of boundary conditions is exponentially small (as expected from the WKB approximation). A more careful treatment [21] yields

$$D \simeq D_0 \frac{4}{\pi} \left(\frac{L\Delta}{vg} \right)^{3/2} e^{-2L\Delta/\pi vg} \quad (19)$$

where Δ and u are related via equation (9). In the special case of free fermions i.e. for $g = 1$ and $v = 2t$ we may compare the results obtained within the SCHA with the exact Drude weight (see the appendix)

$$D_{\text{ex}} \simeq D_0 \left(\frac{\pi L \Delta_{\text{ex}}}{v} \right)^{1/2} e^{-L \Delta_{\text{ex}}/2v}. \quad (20)$$

Although the expected exponential behaviour is recovered in the SCHA result, the different numerical factor in the exponent shows the limitations of the method.

4. Summary

We have constructed an extension of the SCHA in order to account for the existence of Klein factors in bosonized Hamiltonians with non-linear perturbations. As an application we have investigated a model of spinless fermions with modulated hopping. For the infinite system, both the value of the Luttinger parameter $g_c = 2$ where the transition from a gapless to a gapped phase takes place and the exponent $1/(2 - g)$ that characterizes the opening of the gap for $u \rightarrow 0$ are correctly obtained within the SCHA. However, the bending of the phase boundary for finite values of u is not reproduced. When considering a finite system Klein factors cannot be ignored *a priori*. Within our approach it turns out that the crossover region from a finite size gap to a true dimerization gap coincides with the crossover to the region where the Klein factors become relevant.

The Drude weight reflects the sensitivity of the system with respect to a change of boundary conditions and is related to the properties of the current operator J in the bosonized version of the Hamiltonian. In a finite system with an energy gap Δ the Drude weight is expected to be nonzero but exponentially small, $D \sim \exp(-\text{const } L\Delta)$. Our extended version of the SCHA allows us to calculate the Drude weight in the insulating phase and we confirm the exponential behaviour.

Using the same concepts the method can also be applied to study finite size effects in more complex models with nontrivial phase diagrams.

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Appendix

For $V = 0$ the ground state energy of Hamiltonian (1) for a system of $N = 4M + 2$ lattice sites is given by

$$E_0(\varphi) = -2t \sum_{n=-M}^M \sqrt{\cos^2 k_n + u^2 \sin^2 k_n} \quad (\text{A.1})$$

where $k_n = (2\pi n + \varphi)/L$ and the lattice constant is set to one. We introduce $z_n = e^{ik_n}$ and the function $f(z) = 1/(z^L - e^{i\varphi})$ which has single poles at z_n with residues $\text{Res} f(z)|_{z=z_n} = z_n e^{-i\varphi}/L$. Expressing equation (A.1) in terms of z_n we may replace the sum by a contour integral and obtain

$$E_0(\varphi) = -\frac{tL e^{i\varphi} \sqrt{1-u^2}}{2} \oint_C \frac{dz}{2\pi i} \frac{\sqrt{z^2 + z^{-2} + 2\gamma}}{z(z^L - e^{-i\varphi})} \quad (\text{A.2})$$

where $\gamma = (1+u^2)/(1-u^2)$ and \mathcal{C} is a contour that encloses the singularities of $f(z)$. We chose \mathcal{C} to be composed of two circles with radii slightly larger or smaller than one, respectively. Substituting $z \rightarrow 1/z$ the integral along the inner circle can be mapped on the integral along the outer circle. The square root in the numerator has branch cuts along the imaginary axis in the interval $[-y_1, y_1]$ and for $|y| > y_0$ where $\pm iy_0$ and $\pm iy_1$ are the zeros of the function under the square root. Now we deform the integration contour along the branch cut from iy_0 to $i\infty$ and obtain for the energy difference $\Delta E = E_0(\pi) - E_0(0)$

$$\Delta E = \frac{4tL\sqrt{1-u^2}}{\pi} \int_{y_0}^{\infty} \frac{dy}{y} \frac{\sqrt{y^2 + y^{-2} - 2\gamma}}{y^L - y^{-L}}. \quad (\text{A.3})$$

Substituting $y = e^x$ yields

$$\Delta E = \frac{4tL\sqrt{1-u^2}}{\pi} \int_{x_0}^{\infty} dx \frac{\sqrt{2 \cosh(2x) - 2\gamma}}{e^{Lx} - e^{-Lx}} \quad (\text{A.4})$$

with $x_0 = \text{arcosh} \gamma = \ln((1+u)/(1-u))$. For $Lx_0 \gg 1$ the integral is rapidly cut off by the exponential and we may expand the square root around $x = x_0$. The Drude weight is then

$$D = \frac{L\Delta E}{4} \simeq t \sqrt{\frac{2uL}{\pi}} \exp\left(-\frac{L}{2} \ln \frac{1+u}{1-u}\right). \quad (\text{A.5})$$

Expanding the logarithm for $u \ll 1$ and inserting $\Delta_{\text{ex}} = 4tu$ yields equation (20).

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