Method of Image and Transmission through

Semi-infinite Nanowires

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Abstract

The method of functional integral bosonization is extended to examine the transmission properties of semi-infinite nanowires. In particular, it is shown that edge states will arise at the end point of the dimerized semi-infinite spin-chain and by combining the method of image and the bosonization technique, the system can be properly bosonized. Based on the bosonized action and a renormalization group analysis, it is shown that unlike scattering due to single bulk impurity in the nanowire, the scattering potential remains relevant even for slightly attractive potential due to the interaction between the edge state and its image. When the strength of potential goes beyond a critical strength, the tip of the semi-infinite nanowire may become insulating.

\textit{Key words:} nanowire, method of image, bosonization

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1 Introduction

Nanowires have been considered as ideal tools for probing nano-materials[1,2]. In real applications, the scanning probe microscopes (SPM) represent the typical realization[3]. In this approach, the tip of the probe is crucial. It is therefore important to understand the properties of the tip. From theoretical point of view, the tip can be ideally considered as the end of a one dimensional nanowire. The physics is thus embedded in the semi-infinite nanowires. In various situations, it is known that edge states may arise at the end. Nevertheless, conventional studies of the 1D wire have mostly been focused on its bulk properties, whereas assembled nanowires can only have finite lengths and must terminate at some sites (the ends, or the edges). It is therefore important to investigate effects that are due to the ends.

In the absence of interactions, the presence of the edge can be handled by method of image or its generalization[4,5,6]. In this case, effects due to the ends are identified and reflected in the tunneling spectrum. For example, because the end couples $k$ and $-k$, the wavefunction is modulated by $\sin(kx)$ so that the van Hove singularity is suppressed in the local density of states near the end[4,5,6]. The more interesting situation occurs when the reflection symmetry is broken. In that case, it is shown that localized edge states may arise and result in peaks in the tunneling spectrum[7]. These conclusions are based on free electrons in which the problem is linear so that method of image is applicable. In real materials, particularly in nano-materials, interactions can not be neglected. In that case, the applicability of method is called into question. It is therefore of important to examine the applicability of method of image or find a general method to handle the boundary.
In this work, we shall show that indeed the method of image can be generalized even in the presence of interactions. The generalization results from a combination of method of image and the bosonization technique. By adopting the method of the functional bosonization, recently developed by Yurkevich[8], we show that the boundary conditions can be easily implemented. The marriage of the two methods allows one to investigate effects due to the edge states in the most general situations. To illustrate our method, we shall consider the simplest situation that supports the edge states: spinless electrons in dimerized semi-infinite nanowires, which would correspond to fermionized spin-chains. We shall first establish the existence of the edge state in the presence of interactions. This will be investigated by considering a dimerized spin chain. The method of functional bosonization is then combined with the method of image to calculate the two-point correlation function for dimerized nanowires. Finally, the bosonization of the partition function for semi-infinite nanowire will be derived. Based on the derived partition function, we perform a renormalization group (RG) analysis and obtain the RG flow equation. The implication of the effect of the edge state on itinerary electrons will be discussed.

2 Existence of the edge state

We shall first illustrate that under appropriate conditions, the edge states exist and persist even in the presence of strong interaction. For this purpose, we start by considering a dimerized semi-infinite spin-chain in which the transverse spin...
coupling changes alternatively. The Hamiltonian can be written as

\[
H_S = \sum_{i=1}^{i=\infty} 2J_i(S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) + J_z(S_i^z + 1/2)(S_{i+1}^z + 1/2) + hS_i^z,
\]

(1)

where \( h \) is the magnetic field, \( J_i = t_1 \) when \( i \) is odd and \( J_i = t_2 \) when \( i \) is even. By applying the Jordan-Wigner transformation \( \psi_i^\dagger = K(i)S_i^+ \) and \( \psi_i = S_i^- K(i) \) with \( K(i) = \exp[i\pi \sum_{j=1}^{i-1}(S_j^z + 1/2)] \), \( H_S \) is then mapped into the Hamiltonian of spinless electrons with interaction between nearest neighbors

\[
H = \sum_{i=1}^{i=\infty} J_i(\psi_i^\dagger \psi_{i+1} + \psi_{i+1}^\dagger \psi_i) + J_z\psi_i^\dagger \psi_i \psi_{i+1}^\dagger \psi_{i+1} + h(\psi_i^\dagger \psi_i - 1/2).
\]

Here the applied \( h \) field is equivalent to the chemical potential. In the absence of the \( J_z \) term, \( H \) reduces to free electron model with dimerized hopping amplitudes. This is the model that can describe polyacetylene[9]. In this case, the bulk dispersion can be solved exactly and is given by \( \varepsilon_k^z = t_1^2 + t_2^2 + 2t_1 t_2 \cos 2ka \) with \( a \) being the lattice constant. It is clear that the spectrum has a gap \( 2\Delta = 2|t_2 - t_1| \). For semi-infinite chains, previous studies show that when \( t_1 < t_2 \), there is an edge state that decays exponentially from the edge with energy right at zero[7]. It is conceivable by continuity that the edge state survives when \( J_z \) is turned on as long as \( J_z \) is small in comparison to the gap. To check how the edge state evolves in the presence of interaction, we solve \( H_S \) (instead of \( H \)) by resorting to method of exact diagonalization. The energy of the edge state can be found by tuning \( h \) and measuring the local density of electrons at the 1st site. As \( h \) sweeps across the edge state, a large change of the local density occurs due to the fact that the edge state is localized. In Fig. 1, we show the numerical result of 7 sites of spin chain. The jump in the local density is clearly manifested.
The energy of the edge state can be read out by finding the magnitude of \( h \) at the jump. In Fig. 2, we show the energy of the edge state versus \( J_z \). Clearly, one sees that in presence of interactions, the edge state persists except that the energy is no longer right at zero.

3 Two-point Green’s functions in dimerized infinite chains

To understand how the localized edge state interacts with extended states, we shall first consider the case without the boundary to illustrate the effect of dimerization on the extended states. In this case, the Hamiltonian of the extended states for spinless electrons is

\[
H = \sum t_i \psi_i^\dagger \psi_{i+1} + h.c. + V n_i n_{i+1}.
\]

(2)

Here when \( i \) is odd, \( t_i = t_1 \), otherwise, \( t_i = t_2 \). In the absence of \( V \), there are two bands separating by a gap. We shall set the Fermi energy \( \varepsilon_f \) in the upper band. After the Fourier transformation, the kinetic term becomes

\[
H_0 = \sum_k (\psi_{\text{odd}}^\dagger(k), \psi_{\text{even}}^\dagger(k)) \begin{pmatrix} 0 & \Delta_k \\ \Delta_k^* & 0 \end{pmatrix} \begin{pmatrix} \psi_{\text{odd}}(k) \\ \psi_{\text{even}}(k) \end{pmatrix},
\]

(3)

where \( \Delta_k = t_1 e^{ika} + t_2 e^{-ika} \). Note that because the lattice consists of two sublattices: even sites and odd sites, the theory is a two-component theory with the obvious notations: \( \psi_{\text{odd}} \) represents \( \psi \) at odd sites and \( \psi_{\text{even}} \) represents \( \psi \) at even sites. To focus on the itinerant electrons, we linearize \( H_0 \) in \( k \) near the Fermi wavevector \( \pm k_f \). By replacing \( i(k \pm k_f) \) by \( \partial_x \), the action for the kinetic terms becomes
\[ S_0 = \int dxd\tau \hat{\psi}^\dagger_L \begin{pmatrix} \partial_\tau - \varepsilon_f & \varepsilon_f + iv_f \partial_x \\ \varepsilon_f + iv_f^* \partial_x & \partial_\tau - \varepsilon_f \end{pmatrix} \hat{\psi}_L \] (4)

\[ + \hat{\psi}^\dagger_R \begin{pmatrix} \partial_\tau - \varepsilon_f & \varepsilon_f - iv_f^* \partial_x \\ \varepsilon_f - iv_f \partial_x & \partial_\tau - \varepsilon_f \end{pmatrix} \hat{\psi}_R. \]

Here \( \tilde{v}_f = a(2t_1t_2\sin 2k_f a - it_2^2 + it_2^2)/\varepsilon_f \) and phase factors, \( e^{i\delta} = (t_1 e^{ik_f a} + t_2 e^{-ik_f a})/\varepsilon_f \), have been absorbed into \( \psi^L_{\text{even}} \) or \( \psi^R_{\text{even}} \). \( R \) and \( L \) represent right and left movers with corresponding energy dispersions: \( i\omega = -v_f k \) and \( i\omega = v_f k \), found by diagonalizing \( S_0 \) \[\text{(10)}\]. Note that \( v_f = \text{Re}[\tilde{v}_f] \) is the Fermi velocity.

In the absence of interaction, the Green’s function can be found by rotating to a new basis so that the action is diagonalized. For example, for the left mover, the relation between the new basis and the old basis is \( (c^L_{\text{upper}}, c^L_{\text{lower}})^T \equiv \hat{M}(\psi^L_0, \psi^L_e)^T \) with \( \hat{M} \) being given by (in the \( k \) space)

\[ \hat{M} = \frac{1}{\sqrt{2}} \begin{pmatrix} \exp[i\text{Im}[\tilde{v}_f]k/2\varepsilon_f] & \exp[-i\text{Im}[\tilde{v}_f]k/2\varepsilon_f] \\ \exp[i\text{Im}[\tilde{v}_f]k/2\varepsilon_f] & -\exp[-i\text{Im}[\tilde{v}_f]k/2\varepsilon_f] \end{pmatrix}. \] (5)

To the 1st order in \( k \), the action for the left mover becomes

\[ S^L_0 \approx \sum \omega \int dk c^L_{\dagger} \begin{pmatrix} i\omega - v_f k & 0 \\ 0 & i\omega - 2\varepsilon_f + v_f k \end{pmatrix} c^L, \] (6)

where \( c^L_{\dagger} = (c^L_{\text{upper}}, c^L_{\text{lower}})^T \). Obviously, \( c^L_{\text{upper}} \) and \( c^L_{\text{lower}} \) correspond to bonding and anti-bonding bands respectively. Since the lower band is filled and so we are left with only \( c^L_{\text{upper}} \) whose two-point correlation function is
\[
< c_{\text{upper}}^\dagger c_{\text{upper}} > = \frac{1}{\beta v_f \sin \left[ \frac{\beta}{v_f} \left( i (x - x')/v_f + (\tau - \tau') \right) \right]}.
\]  
(7)

By using Eq. (5), the relations between \(c\) and \(\psi\) are

\[
\begin{align*}
\psi^R_0(x, \tau) &= \frac{1}{\sqrt{2}} c_{\text{upper}}^L (x - \frac{Lm|v|}{2\xi_f}, \tau) \\
\psi^c_0(x, \tau) &= \frac{1}{\sqrt{2}} c_{\text{upper}}^L (x + \frac{Lm|v|}{2\xi_f}, \tau)
\end{align*}
\]  
(8)

We thus obtain the Green’s functions for electrons

\[
\begin{align*}
G^L_{\text{odd} \rightarrow e} &= G^L_{e \rightarrow e} = \frac{1}{2 \beta v_f \sin \left[ \pi ((\tau - \tau') + i(x - x')/v_f) / \beta \right]} \\
G^L_{\text{odd} \rightarrow \text{odd}} &= \frac{1}{2 \beta v_f \sin \left[ \pi ((\tau - \tau') + i(x - x' + \frac{Lm|v|}{\xi_f})/v_f) / \beta \right]} \\
G^L_{e \rightarrow \text{odd}} &= \frac{1}{2 \beta v_f \sin \left[ \pi ((\tau - \tau') + i(x - x' - \frac{Lm|v|}{\xi_f})/v_f) / \beta \right]}
\end{align*}
\]  
(9)

Here except for the position shift, \(\Delta \equiv \frac{Lm|v|}{\xi_f}\), between even sites and odd sites, the Green’s functions are the same as those for a single band. From the point of view of the wavefunction, if one denotes \(\psi_{\text{odd}} = e^{ikx}\), one can write \(\psi_{\text{even}} = e^{ikx - i\delta(k)}\) with \(\delta(k)\) being the phase shift. Thus linearizing with respect to \(k_f\) results in a shift of \(x\). We then obtain

\[
\Delta = \partial_k \delta(k_f) = -a \frac{t_2^2 - t_1^2}{t_1^2 + t_2^2 + 2t_1 t_2 \cos 2k_f},
\]  
(10)

Therefore, the position shift can be attributed to the phase shift between even sites and odd sites. Clearly, when \(t_2 \gg t_1\), \(\Delta\) approaches \(-a\). In this case, \(G^L_{\text{odd} \rightarrow \text{even}}(x - x') = G^L_{\text{odd} \rightarrow \text{odd}}(x - (x' + a))\). This is consistent with the fact that when \(t_2 \gg t_1\), electrons on two neighboring sublattice points have the same amplitudes.
We now include the effect of the interaction which takes the following form in the continuum approximation

\[
\frac{1}{4} \hat{V}_0 = \int dx dx' \left( \rho_o(x), \rho_e(x) \right) \begin{pmatrix} 0 & V_0 \\ V_0 & 0 \end{pmatrix} \begin{pmatrix} \rho_o(x') \\ \rho_e(x') \end{pmatrix},
\]

(11)

where \( \rho = \rho^R + \rho^L \) is the density operator at odd sites(\( o \)) or even sites(\( e \)) and \( V_0(x, x') = \frac{1}{2} V_0[\delta(x - x' - a) + \delta(x - x' + a)] \). Following [8], we first apply the Hubbard-Stratonovich (HS) transformation to decouple the density operators

\[
e^{-\frac{1}{4} \hat{V}_0} = \frac{1}{Z} \int D\sigma e^{-\hat{V}_0^{-1} - i(\sigma_o \rho_o + \sigma_e \rho_e)},
\]

(12)

where \( \hat{V}_0^{-1} = (\sigma_o, \sigma_e) \begin{pmatrix} 0 & V_0^{-1} \\ V_0^{-1} & 0 \end{pmatrix} \begin{pmatrix} \sigma_o \\ \sigma_e \end{pmatrix} \) and \( Z = \int D\sigma e^{-\hat{V}_0^{-1}} \). For fixed \( \sigma \), the \(-i\sigma \rho\) term in combination with Eq.(5) constitute the quadratic term. However, due to the matrix nature of the action, the \( \sigma \) fields cannot be expressed as a phase factor, \( e^{i\phi} \), as what happens in the case when \( t_1 = t_2 \) [8]. To avoid this difficulty, we first perform the transformation of Eq.(5). We shall take the left mover as a demonstration. The right mover can be handled by the same method. To 1st order in \( k \), the transformed action \( \hat{M}_L \hat{S}_c^L \hat{M}^{-1} \) becomes

\[
S_c^L = \int d\tau \int dx \hat{c}^L \begin{pmatrix} \partial_\tau + iv_f \partial_x - i\sigma_+ & -i\sigma_- \\ -i\sigma_- & \partial_\tau - 2\varepsilon_f - iv_f \partial_x - i\sigma_+ \end{pmatrix} \hat{c}^L,
\]

(13)

where \( \sigma_+ = (\sigma_o + \sigma_-)/2 \) and \( \sigma_- = (\sigma_o - \sigma_e)/2 \). In the above derivation, we have neglected the commutator of \( \partial_x \) and \( \sigma \) because it is of 2nd order in \( V_0 \) and \( 1/\beta \). Furthermore, its effect is to induce a shift in the position of \( \sigma;\)
equivalently, it induces a shift in the space dependence of $V_0(x, x')$. Since we shall be concerning the long distance behavior, this position shift should not matter. Because the anti-bonding states are $2\varepsilon_f$ below the Fermi energy, we can drop the anti-bonding states and keep the bonding states with the action being given by

$$S_L = \int d\tau \int dx c_{\text{upper}}^L(x', \tau)(\partial_\tau + iv_f \partial_x - i\sigma_+)c_{\text{upper}}^L(x, \tau) . \quad (14)$$

At this stage, the effect of $\sigma$ can be absorbed as a phase factor by defining

$$c_{\text{upper}}^L(x, \tau) \equiv \tilde{c}_{\text{upper}}^L(x, \tau)e^{i\phi_L(x, \tau)} . \quad (15)$$

Here if we require

$$(\partial_\tau + iv_f \partial_x)\phi_L(x, \tau) = \sigma_+ . \quad (16)$$

the $i\sigma \rho$ term is canceled out so that $\tilde{c}_{\text{upper}}^L$ is completely free and its two-point correlation function of $\tilde{c}_{\text{upper}}^L$ is exactly the same as Eq.(7). As a result, the correlation function $\langle c_{\text{upper}}^L c_{\text{upper}}^L \rangle$ is determined by $\langle e^{i\phi_L(x, \tau) - i\phi_L(0, 0)} \rangle$. Furthermore, the relation between $\sigma_+$ and $\phi_L$ in Eq.(16) implies that to evaluate $\langle e^{i\phi_L(x, \tau) - i\phi_L(0, 0)} \rangle$, one needs to find the Lagrangian for $\sigma_+$.

The Lagrangian for $\sigma_+$ can be found by first noting that the transformation of Eq. (15) induces a Jacobian
By expanding in powers of \( \sigma \), the above Jacobian becomes

\[
\ln J^L = \text{Tr}[\ln \left( \begin{pmatrix}
\partial_\tau - \varepsilon_f - i\sigma_o & \varepsilon_f + i\tilde{v}_f \partial_x \\
\varepsilon_f + i\tilde{v}_f^* \partial_x & \partial_\tau - \varepsilon_f - i\sigma_e
\end{pmatrix} \right)]
\]

(17)

where \( \hat{G} \) is the 2 \( \times \) 2 matrix of the Green’s function in the absence of interactions and

\[
\hat{\sigma} = \begin{pmatrix}
\sigma_o & 0 \\
0 & \sigma_e
\end{pmatrix}
\]

(19)

Using the loop cancelation theorem[8], we retain only the \( n = 2 \) term

\[
\frac{1}{2}(\sigma_o, \sigma_e) \hat{J}^L/R \begin{pmatrix}
\sigma_o \\
\sigma_e
\end{pmatrix} = -\frac{1}{2} \text{Tr}[\hat{\sigma} \hat{G}^L/R \hat{\sigma} \hat{G}^L/R]
\]

(20)

After adding contributions from left and right movers and retaining only the lowest orders in \( q \) and \( \omega \), we obtain

\[
\hat{J} \equiv \hat{J}^L + \hat{J}^R \approx \frac{v_f q^2}{2\pi^2 \beta (\omega^2 + v_f^2 q^2)} \begin{pmatrix}
1 & 1 \\
1 & 1
\end{pmatrix}
\]

(21)
Combining $\frac{1}{2} \hat{J}$ with $V_0^{-1}$, we obtain the action for the $\sigma$ fields

$$\hat{S}_\sigma = \frac{1}{4\pi\beta} \sum_{\Omega} \int_0^\infty dq \left[ \sigma_+(V_0^{-1} + \frac{v_f q^2}{\pi(\omega^2 + v_f^2 q^2)})\sigma_+(q, \omega) - \sigma_-(q, \omega) V_0^{-1} \sigma_-(q, \omega) \right].$$

(22)

Using Eqs. (16) and (22), we obtain

$$<\phi_L(x, \tau)\phi_L(0, 0)> = \ln \sin \left[ \frac{\pi}{\beta v_f} (ix + v_f \tau) \right] - \frac{g + g^{-1}}{2} \ln |\sin \left[ \frac{\pi}{\beta v} (ix + v \tau) \right]| + i \arg \left[ \sin \left[ \frac{\pi}{\beta v} (ix + v \tau) \right] \right],$$

(23)

where $v^2 \equiv v_f^2(1 + V_0/\pi v_f)$ and $g \equiv v_f/v$. Therefore, the two-point correlation function of $c_{\uparrow \downarrow}^{L}$ is given by

$$<c_{\uparrow \downarrow}^{L}(x, \tau)c_{\uparrow \downarrow}^{L}(x', \tau')> = \frac{1}{\beta v_f} e^{i \arg \left[ \sin \left[ \frac{\pi}{\beta v} (ix + v_f \tau + v_f \tau') \right] \right]}.$$ 

(24)

It is clear that the interaction changes not only the exponent but also the phase in correlation functions. Similar procedure applies to the right mover, the correlation function for the right mover turns out to be the complex conjugate of $<c_{\uparrow \downarrow}^{L}(x, \tau)c_{\uparrow \downarrow}^{L}(x', \tau')>$. Finally, the two-point Green’s functions for electrons are obtained by combining Eqs. (8) and (24). The net effect of the relation Eq. (8) is to shift positions of even sites by $\Delta$, given by Eq. (10). Clearly, the shift is not changed by the interaction and the same conclusion applies to other Green’s functions.

We conclude this section by noting that the bosonization of dimerized chains is almost the same as that for one band model except when calculating Green’s functions, positions have to be shifted appropriately as indicating in Eq. (9). Obviously, this also applies to the general case when the system contains more
than two sublattices. In that case, one first bosonizes the energy band cut by the Fermi energy. The important information one needs for calculating Green’s functions is then contained in the transformation matrix, similar to Eq.(5), which determines the position shift of each site.

4 Generalized method of image for semi-infinite chains

We now apply method of functional bosonization to semi-infinite chains. A generalized method of image will be developed in the presence of interactions. We first set the boundary right at site 0, thus $\psi(0) = 0$. In the continuum approximation, the Hamiltonian for the energy band cut by the Fermi energy can be generally written as $H = \hat{H}_R + \hat{H}_L + \hat{V}_0$ with the interaction term being given by

$$\hat{V}_0 = \frac{1}{2} \int_0^\infty dx \int_0^\infty dx' \rho(x) V_0(x - x') \rho(x'), \quad (25)$$

and the kinetic terms be given by

$$\hat{H}_{R/L} = \mp iv_f \int_0^\infty dx \psi_R^\dagger \partial_x \psi_{R/L}. \quad (26)$$

Here the operator $\psi = e^{ik_f x} \psi_R + e^{-ik_f x} \psi_L$ is the continuum operator for electrons in the energy band cut by the Fermi energy. In an infinite chain, the right-mover and the left-mover are independent. This independence, however, is lifted in the semi-infinite chain due to the boundary condition

$$\psi(0) = \psi_R(0) + \psi_L(0) = 0. \quad (27)$$
To satisfy the boundary condition, it is useful to extend the defining domain of $\psi_R$ and $\psi_L$ to $x < 0$. For this purpose, we define

$$\psi_{R/L}(-x, \tau) = -\psi_{L/R}(x, \tau),$$

so that the boundary condition is automatically satisfied. The kinetic term can be then rewritten in terms of a single chiral field

$$\hat{H}_R + \hat{H}_L = -iv_f \int_{-\infty}^{\infty} dx \psi_R^\dagger \partial_x \psi_R.$$  

Thus in the absence of interaction, the Green’s function for the right mover is exactly the same as that of the infinite chain. By using Eq.(28), we find that the full Green’s function can be written as

$$g(x, x'; \tau, \tau') = e^{ik_f(x-x')}G^R(x, x'; \tau, \tau') + e^{-ik_f(x-x')}G^R(-x, -x'; \tau, \tau')$$

$$-e^{ik_f(x+x')}G^R(x, -x'; \tau, \tau') + e^{-ik_f(-x')}G^R(-x, x'; \tau, \tau'),$$

where we have denoted the Green’s functions for the right/left mover by $G^R/L$. Note that Eq.(28) also implies $G^R(x, x') = G^L(-x, -x')$. Therefore, Eq.(30) can be cast in the form

$$g(x, x'; \tau, \tau') = G(x, x'; \tau, \tau') - G(x, -x'; \tau, \tau'),$$

where $G(x, x'; \tau, \tau') = e^{ik_f(x-x')}G^R(x, x'; \tau, \tau') + e^{-ik_f(x-x')}G^L(x, x'; \tau, \tau')$ has the form of the Green’s function for the infinite chain. Notice that without interactions, $G^R/L$ are the same as the bulk Green’s functions for infinite chains, thus Eq.(31) demonstrates the validity of method of image. In the presence of the interaction, $G^R/L$ and $G$ appear not to be the bulk Green’s functions and their meaning requires further exploration (see below). Nonetheless, the form
of Eq.(31) is still valid except that one has to resort to Eq.(30) to calculate the Green’s function. Obviously, all the information needed is in $G^R$.

To calculate $G^R$, we first apply the HS transformation[8] on the interaction term for $0 < x < \infty$

$$e^{-\int_0^\beta d\tau \hat V_0(\tau)} = \int D\sigma e^{-\frac{1}{4} \int_0^\beta d\tau [\int_0^\infty dx \int_0^\infty dx' \sigma V_0^{-1}(\tau)\sigma + i \int_0^\infty dx \sigma c^c]/Z},$$

(32)

where $V_0^{-1}(x', x'')$ is the interaction potential that satisfies $\int dx' V_0(x, x') V_0^{-1}(x', x'') = \delta(x - x'')$. Since we shall be interested in the local approximation in which $x \approx x'$ dominates, by extending the HS field, $\sigma(x, \tau)$, into $-\infty < x < 0$

$$\sigma(-x, \tau) \equiv \sigma(x, \tau),$$

(33)

and assuming that $V_0^{-1}$ is symmetric in the real space, the first term on the RHS in Eq.(32) can be rewritten as $\frac{1}{4} \int_0^\beta d\tau \int_\infty^{-\infty} dx \int_\infty^{-\infty} dx' \sigma(x) \hat V_0^{-1} \sigma(x')$. For the second term on the RHS in Eq.(32), we use Eq.(28) and neglect terms that contain the fast-oscillating factor, $e^{\pm 2ik_f x}$. The action for the right mover then becomes

$$\hat S_R = \int_0^\beta d\tau \left[ \int_\infty^{-\infty} dx \psi_R^\dagger (\partial_\tau - i\sigma(x) - iv_f \partial_x) \psi_R ight. + \left. \frac{1}{4} \int_\infty^{-\infty} dx \int_\infty^{-\infty} dx' \sigma(x) \hat V_0^{-1} \sigma(x'). \right]$$

(34)

We have thus transformed the semi-infinite problem into an infinite one except that the $\sigma$ field has to be even: $\sigma(x) = \sigma(-x)$. Clearly, the loop cancelation theorem[8] is still valid so that the action of $\sigma$ is quadratic. By making use of $\sigma(q, \Omega) = \sigma(-q, \Omega)$, we obtain
\[ \hat{S}_\sigma = \frac{1}{4\pi\beta V_0} \sum_\Omega \int_0^\infty dq \sigma(q, \Omega) \frac{\Omega^2 + v^2 q^2}{\Omega^2 + v_f^2 q^2} \sigma(q, -\Omega), \]  

(35)

where \( v^2 = v_f^2 + \frac{v_i V_0}{\pi} \). Note that the correlation function of \( \sigma \) is given by

\[ < \sigma(q, \Omega) \sigma(q', \Omega') >_\sigma = 2\pi\beta V_0 \frac{\Omega^2 + v^2 q^2}{\Omega^2 + v_f^2 q^2} (\delta(q + q') + \delta(q - q')) \delta_{\Omega + \Omega'}. \]  

(36)

Here the term \( \delta(q + q') \) is due to the relation \( \sigma(q, \Omega) = \sigma(-q, \Omega) \); clearly, it is the crucial difference between the infinite chains and semi-infinite chains and reflects the effects of boundary condition.

Similar to Eq. (16), \( \sigma \) can be absorbed by a phase \( \phi_R \) with the relation \( \phi_R(q, \Omega) = \sigma(q, \Omega) / (i\Omega + v_f q) \). Therefore, the correlation for the phase can be computed by using Eq. (35). After performing appropriate contour integrations, we find that the analytic form for the correlation function of the phase is given by

\[ \langle \phi_R(x, \tau) \phi_R(x', \tau') \rangle = \ln \left[ \sin \left\{ \frac{\pi}{\beta v_f} \left[ i(x - x') - v(\tau - \tau') \right] \right\} \right] - \frac{g + g^{-1}}{2} \ln \left[ \sin \left\{ \frac{\pi}{\beta v_f} \left[ i(x - x') - v(\tau - \tau') \right] \right\} \right] - \frac{g - g^{-1}}{2} \ln \left[ \sin \left\{ \frac{\pi}{\beta v_f} \left[ i(x + x') - v(\tau + \tau') \right] \right\} \right]. \]  

(37)

The Green’s function of the right mover is obtained by computing \( e^{-\frac{1}{2} \langle \phi_R(x, \tau) - \phi_R(x', \tau') \rangle^2} \), we find

\[ G^R(x, x'; \tau, \tau') = \frac{\pi}{v_f} e^{-i \arg[F(x, x'; \tau, \tau')] \left[ F(x, x'; \tau, \tau') \right]^{-\frac{g + g^{-1}}{2} \left[ F(x, x'; \tau, \tau') \right]^{-\frac{g - g^{-1}}{2}}} \times \left[ F(x, -x'; \tau, \tau') \right]^{\frac{g + g^{-1}}{2} \left[ F(x', -x'; \tau', \tau') \right]^{\frac{g - g^{-1}}{2}}}, \]  

(38)

where \( F(x, x'; \tau, \tau') = \sin \left[ \frac{\pi}{\beta v_f} \left[ i(x - x') - v(\tau - \tau') \right] \right] \). From \( G^R \), one obtains the full Green’s function by using Eq. (30) or Eq. (31). Finally, the Green’s functions
of real electrons are obtained by shifting positions according to Eqs. (8) and (10).

In conclusion, the method of image, Eq. (31), is valid even in the presence of interaction except that now the bulk Green’s functions have to be re-interpretated as the Green’s function of the infinite chains with the even $\sigma$ field.

5 The effect of the edge state on itinerary electrons

As demonstrated in Sec. (2), when $t_1 < t_2$, a localized edge state arises. In the absence of interactions, its energy is right at zero with the wavefunction being given by $\psi_0(x) \approx (1, 0, -\epsilon, 0, \epsilon^2, 0, -\epsilon^3, 0, \cdots)$ with $\epsilon \equiv t_1/t_2$ [4,5,6,7]; while in the presence of interactions, the edge state persists with the energy being shifted away from zero.

Since the edge state is localized, it causes higher electron densities near the edge when the Fermi energy exceeds the energy of the edge state. The density-density interaction then induces the potential scattering on electrons near the Fermi energy. This is entirely similar to single bulk impurity in the nanowire, where if there is no interaction between the impurity and the nanowire, the level for the electron residing on the impurity also lies outside the energy bands of the nanowire. The potential scattering due to single bulk impurity was investigated by Kane and Fisher [11]. In the following, instead of performing more detailed analysis such as calculating changes of density of states [12], we shall follow Kane and Fisher and perform the stability analysis on the itinerary electrons qualitatively based the renormalization group analysis. The result
will be conceptually useful in considering the transport properties of semi-
infinite nanowires.

We first note that the electron operator can be represented by \( \hat{\psi}(x) + \hat{\psi}_0(x) \) with \( \hat{\psi}(x) \) denote the operator for itinerary electrons near the Fermi surface. Substituting this representation into the interaction potential, Eq. (25), a potential scattering term is induced:

\[
\hat{V}_p = \int_0^\infty dx \int_0^\infty dx' V_0(x, x') \langle \psi_0(x') \psi_0(x) \rangle \hat{\psi}^\dagger(x) \hat{\psi}(x).
\]

In the continuum approximation, we have \( \hat{\psi}(x) \equiv e^{ik_f x} \psi_R(x) + e^{-ik_f x} \psi_L(x) \) so that

\[
\hat{V}_p = v_f \int_0^\infty dx v(x) [\psi_R^\dagger(x) \psi_R(x) + \psi_L^\dagger(x) \psi_L(x)]
\]

\[
+ \int_0^\infty dx [\lambda(x) \psi_R^\dagger(x) \psi_L(x) + \lambda(x)^* \psi_L^\dagger(x) \psi_R(x)],
\]

where the second equality is obtained by writing \( \hat{\psi} \) in terms of \( \psi_R \) and \( \psi_L \) with \( v_f v(x) \equiv \int_0^\infty dx' V_0(x, x') |\psi_0(x')|^2 \) and \( \lambda(x) \equiv \int_0^\infty dx' V_0(x, x') |\psi_0(x')|^2 e^{2ik_f x} \). By using Eq. (28) and defining \( v(-x) \equiv v(x) \) and \( \lambda(-x) \equiv \lambda^*(x) \), the integration domain can be extended to \(-\infty\). After being combined with the kinetic term, Eq. (29), the first term on the RHS of Eq. (40) becomes

\[
-iv_f \int_{-\infty}^{\infty} dx \psi_R^\dagger(x) [\partial_x - iv(x)] \psi_R(x).
\]

The action induced by the edge state, \( S_{\text{edge}} \), is thus determined by the second term. By writing \( \psi = \psi e^{i\phi}, \lambda = |\lambda| e^{i\eta}, \) and using Eq. (28), we find

\[
S_{\text{edge}} = - \int_0^\beta d\tau \int_{-\infty}^{\infty} dx |\lambda(x)| \langle e^{i\eta} \psi_R^\dagger(x, \tau) \psi_R(-x, \tau) e^{i\phi_R(-x, \tau)} - e^{i\phi_R(x, \tau)} \rangle.
\]
\[ +e^{-i\eta\psi_R^\dagger(-x,\tau)}\psi_R(x,\tau)e^{i\phi_R(x,\tau)-i\phi_R(-x,\tau)}. \]  

(41)

where we have made use of the relation \( \phi_R(x) = \phi_L(-x) \), which results from the mirror extension of the \( \sigma \) field [see Eq.\( \text{[33]} \)] and the relation between \( \sigma \) and the phases \( \phi_R/L \) [see Eq.\( \text{[16]} \)]. Obviously, the relevant phase is \( \phi_2(x) \equiv \frac{1}{2\tau}(\phi_R(x) - \phi_R(-x)) \), whose correlation function can be found by using Eqs.\( \text{[36]} \) and \( \text{[16]} \). We obtain

\[
<\phi_2(\xi)\phi_2(\xi')> = \frac{1}{2}\ln\left[ \frac{|\sin(\zeta_f - \zeta_f')|}{|\sin(z - z')|^g} \right],
\]

(42)

where \( \xi = (x, \tau) \), \( z_f = \frac{\pi}{\beta}(\tau + ix/v_f) \), \( z = \frac{\pi}{\beta}(\tau + ix/v) \), and \( \overline{\tau} \) is the complex conjugate of \( \tau \). Note that terms that contain the factor \( z_f - \overline{\zeta}_f \) or \( z - \overline{\zeta} \) are contributions from the image, representing the boundary effects. Following Ref.\[12\], the partition function with the edge state \( Z_{\text{edge}} = <e^{-S_{\text{edge}}} \rangle \) can be expanded as

\[
Z_{\text{edge}} = \sum_{n_1,n_2} \frac{1}{n_1!n_2!} \int dx_i d\tau_i |\lambda(x_i)| \langle \prod_{i=1}^{n_1} \psi_R^\dagger(\xi_i)\psi_R(\bar{\xi}_i) e^{2\phi_2(\xi_i) + i\eta} \prod_{j=n_1+1}^{n_1+n_2} \psi_R^\dagger(\xi_j)\psi_R(\xi_j) e^{-2\phi_2(\xi_j) - i\eta} \rangle,
\]

(43)

where \( \bar{\xi}_i = (-x_i, \tau_i) \). By defining \( \zeta_{f,i} = z_{f,i} \) for \( i \leq n_1 \) and \( \zeta_{f,i} = \overline{z_{f,i}} \) for \( i > n_1 \) and applying the Wick’s theorem for averaging over \( \psi_R \), we find

\[
\langle \prod_{i=1}^{n_1} \psi_R^\dagger(\xi_i)\psi_R(\bar{\xi}_i) \prod_{j=n_1+1}^{n_1+n_2} \psi_R^\dagger(\xi_j)\psi_R(\xi_j) \rangle = \left( \frac{1}{2\beta} \right)^n \det\left[ \frac{1}{\sin(\zeta_{f,i} - \zeta_{f,j})} \right].
\]

(44)

On the other hand, the average of the phase field \( \phi_2 \) can be written as

\[
<e^\sum_{i=1}^{n_1} \phi_2(\xi_i) - 2\sum_{j=n_1+1}^{n_1+n_2} \phi_2(\xi_j) \rangle = [P(z)]^g / P(z_f),
\]

(45)
where
\[
P(z) = \prod_i \frac{1}{|\sin(\zeta_i - \zeta_j)|} \prod_{i \neq j} \frac{|\sin(\zeta_i - \zeta_j)|^2}{|\sin(\zeta_i - \zeta_j)|^2}. \quad (46)
\]

By using the Cauchy formula, one obtains \(\text{det} [1/\sin(\zeta_{f,i} - \zeta_{f,j})] = i^{n_2 - n_1} P(z_f)\).

Therefore, \(P(z_f)\) in Eq.(45) gets cancels exactly. As a result, only the velocity \(v\) is retained in the partition function, while terms that depend on \(ix \pm v_f \tau\) are absent. We obtain
\[
Z_{\text{edge}} = \sum_{n, n_1 + n_2 = n} \frac{1}{(2\beta)^n n_1! n_2!} \int \prod_i dx_i d\tau_i |\lambda(x_i)| \left\{ e^{i(\eta - \pi/2)(n_1 - n_2)} [P(z)]^g \right\}. \quad (47)
\]

We now bosonize this system by showing that \(Z_{\text{edge}}\) can be reproduced by a bosonic field \(\vartheta\). For this purpose, we first consider a free boson field, \(\varphi(x)\), described by the action
\[
S_0 = \frac{1}{8\pi g} \int dx d\tau \frac{1}{v} (\partial_\tau \varphi)^2 + v (\partial_x \varphi)^2. \quad (48)
\]

The correlation function for \(\varphi\) is \(-2g \ln |\sin(z - z')|\). To include the effect of boundary, we include the image field \(\varphi(-x)\). The \(\vartheta\) is then constructed as
\[
\vartheta(x, \tau) = \frac{1}{\sqrt{2}} (\varphi(x, \tau) - \varphi(-x, \tau)). \quad (49)
\]

Hence the correlation function for \(\vartheta\) is
\[
\langle \vartheta(x, \tau) \vartheta(x', \tau') \rangle = -2g \left[ \ln |\sin(z - z')| - \ln |\sin(z - z')| \right]. \quad (50)
\]

It is then straightforward to verify that \(Z_{\text{edge}}\) can be written as
\[
Z_{\text{edge}} = \langle \text{exp} \left[ \frac{1}{2\beta} \int_0^\beta d\tau \int_{-\infty}^{\infty} dx |\lambda(x)| (e^{i\vartheta + i\eta - i\pi/2} + e^{-i\vartheta - i\eta + i\pi/2}) \right] \rangle. \quad (51)
\]
In other words, after the bosonization, the action induced by the edge state is

\[ S_{\text{edge}} = -\frac{1}{\beta} \int_0^\beta d\tau \int_{-\infty}^{\infty} dx |\lambda(x)| \cos[\vartheta(x, \tau) + \eta - \pi/2]. \]  

(52)

Clearly, \( S_{\text{edge}} \) has the same form as the action induced by impurities in a bulk Luttinger liquid. However, the phase field \( \vartheta \) involved is different. As shown in Eq.(49), the main difference lies in the contribution from the image field \( \phi(-x, \tau) \). Following [11], we perform a gradient expansion. First, since in the local approximation, \( V(x, x') \approx V_0 \delta(x - x') \), we have \( \lambda(x) \approx V_0 |\psi_0(x)|^2 e^{i2k_fx} \). For \( x > 0 \), \( |\psi_0(x)|^2 \approx e^{-2(x-a)/\xi} \) with \( \xi = (\ln t_2/t_1)a \) and \( a \) being the lattice constant, \( \lambda(x) \) peaks at \( x \approx a \). Therefore, after taking \( \lambda(-x) = \lambda(x)^* \) into consideration, in the gradient expansion, \( |\lambda(x)| \) can be approximated by \( \lambda_0[\delta(x-a) + \delta(x+a)] \) with \( \lambda_0 \approx |V_0 \int dx |\psi_0|^2 e^{i2k_fx}| \). As a result, the action induced by the edge reduces to

\[ S_{\text{edge}} = -\frac{\lambda_0 \sin \eta}{\beta} \int_0^\beta d\tau \cos[\vartheta(a, \tau)]. \]  

(53)

Note that \( \eta \) is the phase of \( V_0 \int dx |\psi_0|^2 e^{i2k_fx} \). By setting \( k_f \approx 1/a, \eta \approx \tan^{-1} \xi/a = \tan^{-1}(\ln t_2/t_1) + \pi \text{sign}(V_0) \). Hence when \( t_2 = t_1 \), we obtain \( \eta = 0 \) (repulsive) or \( \psi \) (attractive) and thus \( S_{\text{edge}} = 0 \), which is in consistent with the fact that the edge state disappears in this case.

To completely describe the edge, one needs to specify the action of \( \vartheta(x, \tau) \) at \( x \approx a \). For this purpose, we integrate out \( \phi(x) \) in Eq.(48) for all \( x \) except for \( x = \pm a \) and obtain
\[ S_0 = \frac{1}{4\pi g} \sum_n \frac{|\omega_n|}{1 - e^{-4|\omega_n/v|a}} \Phi^T(-i\omega_n) \begin{pmatrix} 1 & -e^{-2|\omega_n/v|a} \\ -e^{-2|\omega_n/v|a} & 1 \end{pmatrix} \Phi(i\omega_n). \] (54)

Here \( \omega_n \) is the Matsubara frequency and \( \Phi^T(i\omega_n) \equiv [\phi(a, i\omega_n), \phi(-a, i\omega_n)] \).

By diagonalizing \( S_0 \), we find that the eigenmodes consist of symmetric and anti-symmetric combination of \( \phi(a, i\omega_n) \) and \( \phi(-a, i\omega_n) \). Since only the anti-symmetric mode is involved in \( S_{edg} \), the action for \( \vartheta \) is

\[ S^s_0 = \sum_n \frac{1}{4\pi g} \frac{|\omega_n|}{1 - e^{-2|\omega_n/v|a}} |\vartheta(a, i\omega_n)|^2. \] (55)

Following [11], we perform the renormalization-group (RG) transformation. To leading order, the RG flow equation is

\[ \frac{d\lambda_\eta}{dl} = [1 - g(1 - e^{-2\Lambda a/v})]\lambda_\eta, \] (56)

where \( \lambda_\eta \equiv \lambda_0 \sin \eta \) and \( \Lambda \) is a high-frequency cutoff. Eq.(56) is almost the same as the RG flow equation for a single impurity in the bulk Luttinger liquid except for the correction term, \( e^{-2\Lambda a/v} \), due to the interaction of the edge state with its image. Since \( v = v_f/g \) and \( \Lambda \approx O(k_f v_f) \), \( e^{-2\Lambda a/v} = e^{-\alpha g} \) with \( \alpha \) being a numerical factor of order \( O(1) \). The critical value of \( g \) below which \( \lambda_\eta \) grows and is relevant is determined by \( 1 = g_c(1 - e^{-\alpha g_c}) \). Clearly, the exact magnitude of \( g_c \) depends on the microscopic details through \( \alpha \) and is not universal. Nonetheless, qualitatively for \( V_0 > \pi v_f(1/g_c^2 - 1) \), \( V_0 \) is relevant and grows indefinitely under RG transformation. The tip of the nanowire thus may become insulating. This effect is entirely due to the interaction between the edge state and its image. As a result, the critical strength for the tip of the nanowire being insulating is slightly negative.
6 Conclusion and acknowledgments

In conclusion, we have generalized the method of image to be valid in the presence of interactions. The generalization results from a combination of method of image and the bosonization technique. The marriage of the two methods allows one to investigate effects due to the edge states in the most general situations. Based on the derived partition function, it is demonstrated that unlike scattering due to single bulk impurity in the nanowire, the critical strength of interaction when the tip of the semi-infinite nanowire becomes insulating is shifted to be slightly attractive due to the interaction between the edge state and its image. We gratefully acknowledge discussions with Prof. Hsiu-Hau Lin and the support from the National Science Council of the Republic of China.

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In the case when $t_1 = t_2$, our convention of the Fourier transformation is
\[ \psi(x) = e^{ikf x} \psi_R(x) + e^{-ikf x} \psi_L(x), \]
and the kinetic term is
\[ S_0 = \sum_{k, \omega} \psi_R^\dagger (i\omega + vf k) \psi_R + \psi_L^\dagger (i\omega - vf k) \psi_L. \]
Figure Captions

Fig. 1 The local density at the 1st site versus \( h \) for zero temperature and \( 1/k_B T = 100 \). Here \( t_1 = 1, t_2 = 4 \), and \( J_z = 0.1 \).

Fig. 2 The shift of the edge state energy, i.e., with increasing \( J_z \) in zero temperature.
Fig. 2.