One-dimensional Hubbard–Luttinger model for carbon nanotubes

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Abstract
A Hubbard–Luttinger model is developed for qualitative description of one-dimensional motion of interacting Pi-conductivity-electrons in carbon single-wall nanotubes at low temperatures. The low-lying excitations in one-dimensional electron gas are described in terms of interacting bosons. The Bogolyubov transformation allows one to describe the system as an ensemble of non-interacting quasi-bosons. Operators of Fermi excitations and Green functions of fermions are introduced. The electric current is derived as a function of potential difference on the contact between a nanotube and a normal metal. Deviations from Ohm law produced by electron–electron short-range repulsion as well as by the transverse quantization in single-wall nanotubes are discussed. The results are compared with experimental data.

Keywords: Hubbard–Luttinger model, single-wall carbon nanotubes, electron transport.

1. Introduction
We consider a system of interacting electrons in one-dimensional approximation. It is known that the standard Landau–Fermi liquid theory of interacting fermions is inapplicable to the one-dimensional case. In this case the one-dimensional Hubbard model [1, 2] is applied, which relies on the following two basic assumptions: (i) strong repulsion between two electrons in the same narrow potential well and (ii) small probability for the electron jump to the neighboring well. Another known model, the Luttinger liquid model [3, 4], allows one to analytically describe the one-dimensional system of electrons with short-range repulsion between them at low temperature using two other assumptions: (i) all electrons have energies near the Fermi level and the energy spectrum is linear, i.e. $\varepsilon = (p - p_F)p_F$ (here and hereafter the electron mass is assumed $m = 1$), and (ii) after the collisions with each other the electrons may move either in the same direction (transferred momentum then is $\Delta p = 0$) or in the opposite direction (transferred momentum in this case is $\Delta p = 2p_F$).

In the Luttinger model, even weak coulomb interactions cause strong perturbations. For instance, tunneling into a Luttinger liquid at energies near the Fermi level is predicted to be strongly suppressed, unlike what happens in the case of two- and three-dimensional metals. Besides, the differential conductivity scales as power law with respect to bias voltage [5]. Thus, one may expect that the electrically conducting single-wall carbon nanotubes may exhibit Luttinger liquid behavior.

On the other hand, one should account for the bound electrons’ influence on the pure Luttinger behavior. To discuss the role of this subsystem of electrons, one may apply the one-dimensional Hubbard model [2]. Usually, such a treatment uses the Bethe ansatz, which suggests a convenient variational wave function for a many-particle system [6]. Using this approach, a gas of one-dimensional Bose particles interacting via a repulsive delta function potential has been considered in [7]. The energies and wave functions for the ground state and low-lying excited states of a system of one-dimensional fermions also interacting via a repulsive delta function potential have been calculated in [8].

The influence of electron–electron interactions on transport in disordered systems has been extensively investigated for the past two decades. It is well known that the interaction has a very strong effect on one-dimensional systems. Electron tunneling into a one-dimensional conductor is suppressed by interactions even in the absence of disorder. This suppression,
which yields vanishing tunneling density of states at the Fermi level, can be described in the framework of the Luttinger liquid theory. The recently discovered carbon nanotubes provide a unique opportunity for studying interaction effects in quantum wires. The transport in single-wall nanotubes is described by the Luttinger liquid theory, but it is still not very well understood. The number of channels, disorder strength, and carrier concentrations in these systems can vary over a wide range and they are difficult to control experimentally. Tunneling into a Luttinger liquid at energies near the Fermi level is predicted to be strongly suppressed, unlike in two- and three-dimensional metals. Experiments on one-dimensional semiconductor wires have been interpreted using Luttinger liquid theory, but an unequivocal verification of the theoretical predictions has not yet been obtained. Similarly, the edge excitations seen in fractional quantum Hall conductors are consistent with Luttinger liquid behavior, but recent experiments failed to confirm the predicted relationship between the electrical properties of the bulk state and those of the edge states.

In the present paper, a Hubbard–Luttinger model is developed for qualitative description of one-dimensional motion of interacting $\pi$-conductivity electrons in carbon single-wall nanotubes at low temperatures. The low-lying excitations in one-dimensional electron gas are described in terms of interacting bosons. Using the Bogolyubov transformation, the system is further described as an ensemble of non-interacting quasi-bosons. Then operators of Fermi-excitations and Green functions of fermions are introduced. Finally, the electric current is calculated as a function of voltage on contact between a nanotube and a normal metal. Deviations from Ohm law produced by electron–electron short-range repulsion [9] as well as by the transverse quantization in single-wall nanotubes [10] are discussed. Comparison of the obtained results with the experimental data of [11] shows qualitative agreement in quantum interference oscillations of conductivity.

2. Simplification of the Hubbard model

In order to simplify the Hubbard model, we first consider the two-electron Schrödinger equation with the Hamiltonian (here and hereafter we set $\hbar = m = k = 1$)

$$
\hat{H}(x_1, x_2) = -\frac{1}{2} \left( \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} \right) + U\delta(x_1 - x_2) - k [\delta(x_1) + \delta(x_2)].
$$

This Hamiltonian well corresponds to two electrons in delta function potential with (dimensionless) repulsion potential (Hubbard energy) $U$. The problem is not solved analytically; therefore, we use the variational approach. The symmetrical variational wave function of two electrons with a total spin $S = 0$ can be chosen in the form

$$
\Psi(x_1, x_2) = A \left( e^{-\alpha|x_1|} \delta(x_2) + e^{-\beta|x_2|} \delta(x_1) \right).
$$

If $V = 0$, one obtains $\alpha = \beta = 1$ and the total energy is $E = -1$. The system under consideration is analogous to the negative hydrogen ion. The simplification here is due to the delta function repulsion between two electrons instead of the Coulomb repulsion.

The result of numerical simulations is that when $U = 3$, one of the electrons goes to continuum, while the second...
of the outer electron is \( \beta \) of the inner electron is shown in Figure 3. It is seen that the energy increases monotonically with \( U \). In figure 2 the inverse radius \( \alpha \) of the outer electron is shown. It is seen that \( \alpha = 0 \) when \( U = 3 \). The inverse radius \( \beta \) of the inner electron is shown in figure 3. It is seen that \( \beta = 1 \) when \( U = 3 \). Thus, in this model the (dimensionless) critical repulsion potential is \( U = 3 \). The existence of a critical potential is a known peculiarity of the Hubbard model.

Suppose further that we have four electrons in two delta function one-dimensional potential wells with repulsion potential \( U > 3 \). Based on the above consideration, we may conclude that two electrons should go to the continuum. According to the Pauli principle they should have opposite spins, since their spatial wave functions overlap strongly. Respectively, the other two electrons remain in the neighboring potential wells. They also have opposite spins, but, because of the Hubbard assumption, the probability for the electron to jump to the neighboring well is negligible, so that one may disregard the bound electrons. Obviously, this is valid also for the case of a chain of potential wells. As a result, the Hubbard problem reduces to the Luttinger one-dimensional problem of interacting electrons.

3. The Luttinger approach

The Luttinger Hamiltonian of interacting electrons is of the form [9]

\[
\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2,
\]

\[
\hat{H}_0 = p_F \sum_k \left( |p_0 + k| - p_0 \right) \left( \hat{a}^+_k \hat{a}_{p_0 + k} + \hat{a}^+_p \hat{a}_{p_0 - k} \right),
\]

\[
\hat{H}_1 = \frac{g_1}{2} \sum_{k_i, k_\beta} \left( \hat{a}^+_k \hat{a}_{p_0 + k_1} \hat{a}^+_k \hat{a}_{p_0 + k_2} \hat{a}^+_k \hat{a}_{p_0 + k_3} \hat{a}^+_k \hat{a}_{p_0 + k_4} \right),
\]

\[
\hat{H}_2 = g_2 \sum_{k_i, k_\beta} \left( \hat{a}^+_k \hat{a}_{p_0 + k_1} \hat{a}^+_k \hat{a}_{p_0 + k_2} \hat{a}^+_k \hat{a}_{p_0 + k_3} \hat{a}^+_k \hat{a}_{p_0 + k_4} \right),
\]

where \( \hat{H}_0 \) describes the kinetic energy of electrons. The term \( \hat{H}_1 \) describes the scattering of electrons at the collisions with small transferred momentum \( q \ll p_F \), and the term \( \hat{H}_2 \) stands for the scattering of electrons at the collisions with large transferred momentum \( q \approx 2p_F \). In the general case of arbitrary potential, there are two interaction constants in equation (3), but in the case of a delta function potential these constants are equal:

\[
g_1 = V_{q=0} = V_{q=2p_F} = g_2 = g,
\]

\[
V_q = \int \vartheta(x) \exp(-ixq)x dx.
\] (4)

The Hamiltonian of interacting electrons is then expressed via these operators as

\[
\hat{H} = \left( \pi p_F + \frac{g}{2} \right) \sum_q \left( \hat{\rho}_1(q)\hat{\rho}_1(-q) + \hat{\rho}_2(q)\hat{\rho}_2(-q) \right) + g \sum_q \hat{\rho}_1(q)\hat{\rho}_2(-q).
\] (5)

If the density operators are expanded into Fourier series:

\[
\hat{\rho}_1(q) = \frac{1}{\sqrt{2\pi}} \left\{ \begin{array}{ll}
\hat{b}_q; & q > 0 \\
\hat{b}_q^*; & q < 0
\end{array} \right.
\]

\[
\hat{\rho}_2(q) = \frac{1}{\sqrt{2\pi}} \left\{ \begin{array}{ll}
\hat{b}_q^*; & q < 0 \\
\hat{b}_q; & q > 0
\end{array} \right.
\] (6)

where \( \hat{b}_q, \hat{b}_q^* \) are Bose operators, and the Luttinger Hamiltonian takes the form

\[
\hat{H} = \left( \pi p_F + \frac{g}{2} \right) \sum_{q > 0} \left( \hat{b}_q \hat{b}_q^* + \hat{b}_q^* \hat{b}_q \right) + \frac{g}{2\pi} \sum_{q > 0} \left( \hat{b}_q \hat{b}_q^* + \hat{b}_q^* \hat{b}_q \right).
\] (7)

The Bogolyubov transformation allows one to reduce the problem to an effective one for a system of non-interacting
sound bosons:

\[ \hat{H} = \sum_{q} \omega_q \hat{c}^+_q \hat{c}_q, \quad \omega_q = u |q|, \quad u = \sqrt{\nu^2 + \frac{1}{\pi} p_{\text{F}} g}. \]  

where the quantity \( u \) is the speed of sound for this Hamiltonian.

The right density operators in spatial time representation are expressed via the Bose operators as

\[
\hat{\rho}_{1,2}(x, t) = \frac{1}{2} \sum_{q > 0} \sqrt{|q|} \left( \hat{c}_q \cos \theta \exp(\text{i}(q x - ut)) - \hat{c}^+_q \sin \theta \exp(\text{i}(q x - ut)) \right) + \sum_{q > 0} \sqrt{|q|} 2 \pi \times \left\{ \hat{c}_q \cos \theta \exp(-\text{i}(q x - ut)) - \hat{c}^+_q \sin \theta \exp(-\text{i}(q x - ut)) \right\},
\]

where we have introduced the notation

\[
\tan h(2\theta) = g / \left( g + 2\pi p_{\text{F}} \right).
\]

Similarly, we can express the left density operators in spatial time representation via the Bose operators.

The next step is the determination of the Fermi operators via right and left density operators:

\[
\hat{\psi}_{1,2}(x, t) = (2\pi a)^{-1/2} e^{i \hat{\phi}_{1,2}(x, t)},
\]

\[
\hat{\phi}_{1,2}(x, t) = 2\pi \int_{-\infty}^{x} \rho_{1,2}(x', t) dx',
\]

where \( a \) is a small parameter determining the relaxation of the system. It is introduced in order to avoid the divergence of the involved integrals [9].

The explicit form of these functions is derived by the substitution of equation (12) into equation (13) [9]:

\[
G_1(x, t) = \frac{1}{2\pi a} \left( \frac{a}{a - \text{i}(x - ut)} \right)^{\text{cos h}^\theta} \left( \frac{a}{a + \text{i}(x + ut)} \right)^{\text{sin h}^\theta},
\]

\[
G_2(x, t) = \frac{1}{2\pi a} \left( \frac{a}{a + \text{i}(x + ut)} \right)^{\text{cos h}^\theta} \left( \frac{a}{a - \text{i}(x - ut)} \right)^{\text{sin h}^\theta}.
\]

4. The differential tunnel conductivity

Let us derive the general expression for the tunneling current. We consider two parallel one-dimensional systems \( A \) and \( B \) with point-like tunneling contact between them. Both systems are Luttinger fluids; they are described by the Hamiltonian equation (equation (9)), with interaction constants \( g_A \) and \( g_B \), respectively. The total Hamiltonian is of the form

\[ \hat{H} = \hat{H}_A + \hat{H}_B + \hat{H}_{\text{tun}} \]

where the tunneling Hamiltonian is

\[ \hat{H}_{\text{tun}} = w \hat{\psi}_B^+ \hat{\psi}_A |x = x_0 + c.c. \]

and \( w \) is the tunneling amplitude. Fermi operators \( \hat{\psi}_{A,B} \) are determined by equation (12). We assume that the electron tunneling occurs in the small vicinity of the point \( x_0 \); everywhere we have in mind, for certain, that \( \hat{\psi}_{A,B} \) are the right Fermi operators.

Between systems \( A \) and \( B \) the voltage \( eV = \mu_B - \mu_A \) is applied where \( \mu_B - \mu_A \) is the difference of chemical potentials. After gauge transformation the tunneling Hamiltonian, equation (17), becomes dependent on time \( (\hbar = 1) \):

\[ \hat{H}_{\text{tun}}(t) = w \exp(-\text{i}eVt)\hat{\psi}_B^+\hat{\psi}_A |x = x_0 + h.c. \]

The operator of electron charge for the system \( A \) is determined as

\[ \hat{Q}_A = -e \int_{-\infty}^{\infty} \hat{\psi}_A^+(x)\hat{\psi}_A(x) dx. \]

Then the operator of the tunneling current \( A \rightarrow B \) is

\[ \hat{I}(t) = \left[ \hat{H}_{\text{tun}}(t), \hat{Q}_A \right]. \]

Here \([\ldots]\) is notation for the commutator. Substituting equations (18) and (19) into equation (20), we derive this commutator:

\[ \hat{I}(t) = -\text{i} e \left[ w \exp(-\text{i}eVt)\hat{\psi}_B^+\hat{\psi}_A^+ - \text{w}\exp(-\text{i}eVt)\hat{\psi}_B^+\hat{\psi}_A \right] \]

The next step is averaging the current operator:

\[ I(V) = \left\{ \hat{I}(t) \right\} = \left\{ \hat{U}^{-\dagger} (t) \hat{I}(t) \hat{U}(t) \right\}; \]

\[ \hat{U}(t) = \exp \left(-\int_{-\infty}^{t} \hat{H}_{\text{tun}}(t') dt' \right). \]

The tunneling amplitude is exponentially small. Therefore we can expand \( \hat{U}(t) \) in a Taylor series:

\[ \hat{U}(t) \approx 1 - \text{i} \int_{-\infty}^{t} \hat{H}_{\text{tun}}(t') dt'. \]
Substituting equation (23) into equation (22), one obtains:

\[ I(V) = e^2 |w|^2 \int_{-\infty}^{t'} \text{d}t' \left\{ \left[ \hat{\psi}_R^* (t') \hat{\psi}_A (t'), \hat{\psi}_A^* (t) \hat{\psi}_B (t) \right] \right\} \times \exp(-ieV(t' - t)) \]
\[ - e^2 |w|^2 \int_{-\infty}^{t'} \text{d}t' \left\{ \left[ \hat{\psi}_A^* (t') \hat{\psi}_B (t'), \hat{\psi}_B^* (t) \hat{\psi}_A (t) \right] \right\} \times \exp(iV(t' - t)) \]

Equation (24) contains four terms. After the substitution of \(t' \rightarrow t - t\) in two terms, equation (24) is simplified:

\[ I(V) = e^2 |w|^2 \int_{-\infty}^{t} \{ K_{BA}(t - t') \exp(-ieV(t' - t)) - K_{AB} \times \exp(iV(t' - t)) \} \text{d}t' \]

Here the following notations are introduced:

\[ K_{BA}(t - t') = \langle \hat{\psi}_R^* (t') \hat{\psi}_B (t) \rangle \langle \hat{\psi}_A (t') \hat{\psi}_A^* (t) \rangle; \]
\[ K_{AB}(t - t') = \langle \hat{\psi}_A^* (t') \hat{\psi}_A (t) \rangle \langle \hat{\psi}_B (t') \hat{\psi}_B^* (t) \rangle \]

The brackets (…) are the averaging on the ground states of the systems A and B. It should be noted that equation (25) does not depend on the physics of tunneling.

Substituting equation (14) into equation (26) and using for the sake of simplicity the position of contact \(x_0 = 0\), one finds

\[ K_{BA}(t - t') = \frac{1}{4 \pi^2 R^2} \left( \frac{\tilde{a}}{a - i(t' - t)} \right)^2; \]
\[ \alpha = 2 \left( 1 + \sin h^2 \theta_A + \sin h^2 \theta_B \right); \]
\[ \tilde{a} = \frac{a}{p_F}; \quad K_{AB}(t - t') = K_{BA}(t' - t). \]

The current, equation (25), is derived substituting equation (27). We use at this derivation the well-known expression for the gamma function:

\[ \int_{-\infty}^{\infty} (a + \text{it})^{-z} \exp[(a + \text{it})b] \text{d}t = 2\pi b^{z-1} \Gamma(z); \]
\( b, z > 0. \)

Then at \(V > 0\) only the first term in equation (25) is nonzero, while at \(V < 0\) only the second term in equation (25) is nonzero. Hence, the tunneling current, equation (25), is

\[ I(V) = e^2 |w|^2 \frac{\tilde{a}^2}{2 \pi a^2 \Gamma(a)} \left\{ \frac{(eV)^{a-1}}{eV} + \text{eV}^{a-1}; \quad V > 0; \right\} \]
\[ - \frac{\text{eV}^{a-1}}{(eV)^{a-1}}; \quad V < 0. \]

The differential tunnel conductivity \(\rho(V) = \frac{dI(V)}{dV}\) is

\[ \rho(V) \sim V^{a-2}, \quad \tan h(2\theta_{A,B}) = \frac{g_{A,B}}{g_{A,B} + 2\pi p_F}. \]

Now we generalize this result by taking into account the transverse quantization in single-wall nanotubes. The Fermi energy is shifted by the quantity \([10]\)

\[ E_F \rightarrow E_F - \frac{U^2 m R^2}{2 \hbar^2} + \frac{\hbar^2 (n^2 - 1/4)}{2m R^2}; \]

\(n = 0, 1, 2, \ldots\),

where \(R\) is the radius of the nanotube, \(UR\delta(r - R)\) is the potential of the well, and the transverse quantization is determined by the integer \(n\). Accordingly, the differential tunnel conductivity is modified as

\[ \rho(V) = V^a \sum_{n=0}^{\infty} \frac{1}{\left( E_F - \frac{U^2 m R^2}{2 \hbar^2} + \frac{\hbar^2 (n^2 - 1/4)}{2m R^2} - V \right)^\alpha}. \]

For the typical example of \(\pi\)-electrons in a single-wall carbon nanotube the involved parameters are as follows:

\[ E_F = \frac{U^2 m R^2}{2 \hbar^2} = 1 \text{eV}, \quad \alpha = 2.5, \quad R = 0.3 \text{nm}. \]

With these values, the differential conductivity as a function of the voltage \(V\) is shown in figure 4. It is seen that the conductivity undergoes pronounced oscillations.

5. Conclusion

Thus we conclude that transverse quantization produces non-monotonic dependence of nanotube conductivity on the voltage in comparison with the standard Luttinger one-dimensional model. The next improvement of the model can be done based on the one-dimensional extended Hubbard model.
with a weak repulsive short-range interaction in the non-half–filled band case [12]. This approach will use non-perturbative renormalization group methods and Ward identities coming from the asymptotic gauge invariance of the model. At zero temperature the response functions have anomalous power-law decay with logarithmic corrections. A model shows the phenomenon of spin–charge separation, a manifestation of which is that the 2-point function is factorized into the product of two functions. Note that spin–charge separation occurs in the Hubbard model, but is valid only at large distances and up to logarithmic corrections.

The electrical transport properties of well-contacted ballistic single-wall carbon nanotubes at low temperatures have been experimentally studied in [11]. Signatures of strong electron–electron interactions have been observed (the conductivity exhibits bias voltage–dependent amplitudes of quantum interference oscillations), and the current noise manifests bias voltage–dependent power-law scalings as was predicted in [9] (see equation (17)). We note that figure 3 in [11] demonstrates oscillations in agreement with our predictions given by equation (19) and shown in figure 4.

It should be noted that carbon nanotubes display more complex quasi-1D characteristics, which are required to reconsider and extend the basics of the Luttinger liquid theory [13]. According to results of [13] the density of states varies strongly for small Fermi level shifts, which complicates the extension of analytical results obtained for a 1D channel with constant density of states. Also, we did not take into account the fact that the interaction parameter $g$ depends on the length of the nanotube [14]. We did not discuss coupling parameters between different subbands, assuming, probably, that they are the same. Finally, we derived the Hamiltonian with only one parameter $g$, ignoring Hubbard repulsion energy $U$ between electrons at the same site. The Coulomb repulsion between electrons with Hubbard energy $U=17$ eV was changed by model delta function repulsion. Thus, our approach is a purely qualitative one.

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