Tomonaga-Luttinger-Liquid Theory of Metallic Carbon Nanotubes with Open Boundaries

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Tomonaga-Luttinger-liquid theory is formulated for metallic carbon nanotubes with open boundaries. Both cases of single- and multi-wall nanotubes are discussed. Based on this theory, spatial variation of the charge density from an edge is investigated with taking account of the shift of the chemical potential which expresses the carrier injection to the nanotube. The charge density has the spatially independent part and the oscillatory component. Roles of Coulomb interaction on the amplitude of the oscillation, the wavenumbers of it and the uniform component of the charge density are clarified.

KEYWORDS: carbon nanotubes, Tomonaga-Luttinger-liquid, bosonization, Friedel oscillation

§1. Introduction

A carbon nanotube is composed of a coaxially rolled graphite sheet and its actual length is of the order of 1µm or less than it. The material is characterized by two integers, \( (N_+, N_-) \), corresponding to a wrapping vector along the waist, \( \mathbf{w} = N_+ \mathbf{a}_+ + N_- \mathbf{a}_- \), where \( \mathbf{a}_\pm = (\pm a/2, \sqrt{3} a/2) \) are primitive lattice vectors of the graphite and \( |\mathbf{a}_\pm| = a \) is the lattice spacing. It has been shown that the carbon nanotubes have peculiar band structures. When \( N_+ - N_- = 0 \mod 3 \), the metallic one-dimensional dispersions appear near the center of the bands. The low energy properties less than \( v_0/R \) (\( v_0 \): Fermi velocity, \( R \): radius of the tube) are well described by taking into account only the metallic one-dimensional dispersions. Thus, the metallic carbon nanotubes are considered as the typical one-dimensional conductors.

It has been well known that physical properties of the one-dimensional interacting electron systems cannot be described by conventional Fermi-liquid-theory. Instead, the systems show the behaviors called as Tomonaga-Luttinger-liquid. The Tomonaga-Luttinger-liquid state is characterized by separation of the charge and spin degrees of freedom, and the anomalous exponents of

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correlation functions, which depend on the interaction. Carbon nanotubes are one of the most promising candidates where such exotic correlation effects can be observed. The electronic states of the metallic carbon nanotube have been theoretically investigated with taking account of the long-range Coulomb interaction and the novel correlation effects have been found. Experimentally, in the transport measurements for single-wall nanotubes (SWNTs), power-law dependences of the conductance as a function of temperature and of the differential conductance as a function of bias voltage have been observed in the metal-SWNT junctions and in the SWNT-SWNT junctions. These results have been interpreted to be due to tunneling between the Fermi-liquid and the Tomonaga-Luttinger-liquid in the former case, and that between the Tomonaga-Luttinger-liquid and the Tomonaga-Luttinger-liquid in the latter case.

The correlation effects of the semi-infinite and finite length carbon nanotube have been studied theoretically. The local density of state of the semi-infinite SWNT calculated by the bosonization theory explains the transport experiments quantitatively. In ref, the local tunneling density of states of the finite length carbon nanotube has been investigated at absolute zero temperature ($T = 0$). It has been found that the new energy scale, which reflects the spin-charge separation in the Tomonaga-Luttinger-liquid, appears in Coulomb blockade behavior in addition to usual charging energy and single-particle level spacing. However, in the above theories, the relationship between the original electron operator and the slowly varying Fermi field describing the low energy physics has not been clarified. The relationship is important for discussing the concrete physical quantities, especially the spatial dependence of those with rapid oscillation determined by Fermi wavelength. Note that the oscillatory component of the local density of states has been neglected in refs. and because the transport measurements are considered to observe the local density of states averaged over several lattice constants. In the present paper, we develop the bosonization theory of the metallic carbon nanotube with open boundaries based on the theory for one-dimensional system with paying attention to the relationship between the two kinds of electron operators. The theory is extended to the case of the multi-wall nanotube (MWNT). By utilizing the theory, the spatial variation of the charge density from an edge is investigated in the presence of the shift of the chemical potential expressing doping of carriers to the nanotube. It is found that the uniform component of the charge density and the wavenumber of the oscillation become smaller compared with the non-interacting case due to the effects of the interaction on the zero modes. The amplitude of the oscillation determined by the bosonic fluctuation is shown to be larger than that in the absence of the interaction. The amplitude for MWNT depends on the number of the metallic shells included in the MWNT, and the effect of the interaction on the amplitude vanishes when the number tends to infinity.

The organization of this paper is as follows. In §2, the bosonization theory with open boundaries is developed for the SWNT. The theory is extended to the case of the MWNT in §3. The charge
distribution of the SWNT and of the MWNT are calculated in §4. Section 5 is devoted to summary and discussion.

§2. Bosonization for SWNTs with open boundaries

We formulate the bosonization theory of the metallic SWNT with open boundaries. As a model of the metallic carbon nanotube, we consider the \((N, N)\) armchair nanotube.

2.1 Non-interacting case

We consider the armchair carbon nanotube with the length, \(L\), and the radius, \(R = \sqrt{3}Na/(2\pi)\), schematically shown in Fig. 1. The Hamiltonian in the tight-binding model is written as \(\mathcal{H} = \mathcal{H}_k + \mathcal{H}_{\text{int}}\), where \(\mathcal{H}_k\) is the kinetic part,

\[
\mathcal{H}_k = -t \sum_{\mathbf{r}, \mathbf{s}, \mathbf{p}} a_{p,s}^\dagger(\mathbf{r}) \left\{ a_{-p,s}(\mathbf{r}) + a_{-p,s}(\mathbf{r} - pa_+ + a_{-p,s}(\mathbf{r} - pa_-) \right\},
\]

and \(\mathcal{H}_{\text{int}}\) describes the mutual interaction,

\[
\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_{\mathbf{r}, \mathbf{r}', \mathbf{s}, \mathbf{s}'} U(\mathbf{r} - \mathbf{r}' - (p - p')d/2) a_{p,s}(\mathbf{r})a_{p,s}(\mathbf{r})a_{p,s}(\mathbf{r'})a_{p,s}(\mathbf{r}).
\]

Here \(t\) denotes the hopping integral between the nearest-neighbor atoms, and \(a_{p,s}^\dagger(\mathbf{r})\) is the creation operator of the electron with spin \(s = \pm\) at the location \(\mathbf{r} - pd/2\) where \(\mathbf{r} = (al, \sqrt{3}am)\) or \((a(l + 1/2), \sqrt{3}a(m + 1/2))\) \((l, m: \text{integer})\), \(p = \pm\) and \(d = (0, a/\sqrt{3})\). The interaction, \(U(\mathbf{r})\), is given by \(U(\mathbf{r}) = \epsilon^2/\{\kappa \sqrt{a_0^2 + x^2 + 4R^2 \sin^2(y/2R)}\}\) with \(\mathbf{r} = (x, y)\) where \(e, \kappa\) and \(a_0\) are the electric charge, dielectric constant and short-range cut-off of the interaction, respectively.

At first, we consider the non-interacting case. In order to diagonalize \(\mathcal{H}_k\), we solve Schrödinger equation,

\[
-t \left\{ \phi_{\mathbf{K}}^{p,-}(\mathbf{r}) + \phi_{\mathbf{K}}^{p,-}(\mathbf{r} - pa_+) + \phi_{\mathbf{K}}^{p,-}(\mathbf{r} - pa_-) \right\} = E^r(\mathbf{K})\phi_{\mathbf{K}}^{p}(\mathbf{r}),
\]

with the boundary condition, \(\phi_{\mathbf{K}}^{p}(0, y) = \phi_{\mathbf{K}}^{p}(L, y) = 0\) and \(\phi_{\mathbf{K}}^{p}(\mathbf{r}) = \phi_{\mathbf{K}}^{p}(\mathbf{r} + \mathbf{w})\) where \(\mathbf{w} = N(a_+ + a_-) = (0, \sqrt{3}Na)\). The solution and eigenvalue are obtained as follows,

\[
\phi_{\mathbf{K}}^{p}(\mathbf{r}) = \sqrt{\frac{a}{NL}} A^{r,p}(\mathbf{K}) \sin K_x x e^{iK_y y},
\]

\[
E^r(\mathbf{K}) = -rt|\alpha(\mathbf{K})|,
\]

where \(r = \pm\), \(A^{r,+}(\mathbf{K}) = 1/\sqrt{2}\) and \(A^{r,-}(\mathbf{K}) = r\alpha(\mathbf{K})/(\sqrt{2}|\alpha(\mathbf{K})|)\) with \(\alpha(\mathbf{K}) = 1 + 2\cos(K_x a/2)e^{iK_y \sqrt{3}a}/2\). The wavenumbers, \(K_x\) and \(K_y\), are quantized as \(K_x = n_x \pi/L\) \((n_x = 1, 2, \cdots, L/a)\) and \(K_y = 2\pi n_y/(\sqrt{3}Na)\) \((n_y = 1, 2, \cdots, 2N)\). We note that the energy dispersions with \(K_y = 2\pi/(\sqrt{3}a) \equiv K_0^F\) touch the Fermi energy \((E^F(\mathbf{K}) = 0)\) at \(K_x = 2\pi/(3a) \equiv K_0\), and the others do not cross the Fermi energy. The Hamiltonian is written as \(\mathcal{H}_k = \cdots\).
$\sum K \sum_{r,s} E_r(K)c_{r,s}(K)\phi^p_r(r)c_{r,s}(K)$ where $a_{p,s}(r) = \sum K \sum_{r} \phi^p_r(r)c_{r,s}(K)$. When the chemical potential, $\mu$, stays the energy bands with $K_y = K_y^0$ (see Fig.2), the charge density in the absence of the interaction is given at $T = 0$ for the semi-infinite case, $L \to \infty$, as

$$\langle \sum_s a_{p,s}^\dagger(r)a_{p,s}(r) \rangle = \frac{(K_+ - K_-)a}{2N\pi} - \frac{a(\sin 2K_+x - \sin 2K_-x)}{4N\pi x}, \quad (6)$$

where $K_\pm \simeq K_0 \pm \mu/v_0$ and $v_0 = \sqrt{3}a/2$. The charge distribution has two parts. One is the uniform part due to the shift of the chemical potential and the other expresses the oscillation (Friedel oscillation). We find that there exit the two kinds of oscillation with the wavenumbers, $2K_\pm$, and those are out of phase. The oscillatory behavior is absent for $\mu = 0$.

We apply the bosonization procedure on the system with the open boundaries\(^{14}\) to the present model. Energy dispersion is linearized by substituting $K = (K_0 + k, K_y^0)$ into $E^r(K)$. When we define the right/left moving electron operator, $a_{R/L,s}(K_0 + k)$, as

$$a_{R,s}(K_0 + k) = \begin{cases} c_{-,s}(K), & k \geq 0 \\ c_{+,s}(K), & k < 0 \end{cases}, \quad (7)$$

$$a_{L,s}(K_0 + k) = \begin{cases} c_{+,s}(K), & k \geq 0 \\ c_{-,s}(K), & k < 0 \end{cases}, \quad (8)$$

the Hamiltonian, $H_k$, and the electron operator are respectively written as follows,

$$H_k = \sum_{k,s} v_0 k \left\{ a_{R,s}^\dagger(K_0 + k)a_{R,s}(K_0 + k) - a_{L,s}^\dagger(K_0 + k)a_{L,s}(K_0 + k) \right\}, \quad (9)$$
Fig. 2. Energy dispersion, $E(K)$, of the (5,5) armchair nanotube as a function of $K_x$. Fermi energy in the absence of the chemical potential, $\mu$, is $E(K) = 0$ and $K_\pm \approx K_0 \pm \mu/v_0$ where $K_0 = 2\pi/(3a)$ and $v_0 = \sqrt{3ta}/2$.

$$a_{p,s}(r) = \sqrt{\frac{a}{2N_L}} \sum_k \sin(K_0 + k)x e^{iky} \left\{ p a_{R,s}(K_0 + k) + a_{L,s}(K_0 + k) \right\}. \quad (10)$$

Here we define the slowly varying Fermi field, $\psi_{R/L,\alpha,s}(x)$, as

$$\psi_{R,+s}(x) = -i \sqrt{\frac{2}{L}} \sum_k e^{ikx} a_{R,s}(K_0 + k), \quad (11)$$

$$\psi_{L,+s}(x) = -i \sqrt{\frac{2}{L}} \sum_k e^{ikx} a_{L,s}(K_0 + k), \quad (12)$$

$$\psi_{L,-s}(x) = i \sqrt{\frac{2}{L}} \sum_k e^{-ikx} a_{R,s}(K_0 + k), \quad (13)$$

$$\psi_{R,-s}(x) = i \sqrt{\frac{2}{L}} \sum_k e^{-ikx} a_{L,s}(K_0 + k), \quad (14)$$

where $\alpha = \pm$ is the index corresponding to valleys for the case for periodic boundary condition. The electron operator is expressed by the slowly varying fields as

$$a_{p,s}(r) = \sqrt{\frac{a}{4N}} e^{iK_0y} \left\{ e^{iK_0x} [p\psi_{R,+s}(x) + \psi_{L,+s}(x)] + e^{-iK_0x} [p\psi_{L,-s}(x) + \psi_{R,-s}(x)] \right\}. \quad (15)$$

The expression is the same as that in case of the periodic boundary condition. The slowly varying field operators are not independent, but satisfy,

$$\psi_{L,+s}(x) = -\psi_{R,-s}(-x), \quad (16)$$

$$\psi_{L,-s}(x) = -\psi_{R,+s}(-x). \quad (17)$$
Therefore we can actually work with the right moving operator only. The boundary condition, 
\[ a_{p,s}(0, y) = 0, \] is automatically satisfied due to eqs. (16) and (17). However, the condition, 
\[ a_{p,s}(L, y) = 0, \] implies,

\[
\psi_{R,\alpha,s}(-L) = e^{i2\alpha K_0 L} \psi_{R,\alpha,s}(L). \tag{18}
\]

So we can regard the field \( \psi_{R,\alpha,s}(x) \) as defined for \( 0 \leq x \leq 2L \) with the boundary condition,

\[
\psi_{R,\alpha,s}(x + 2L) = e^{-i2\alpha K_0 L} \psi_{R,\alpha,s}(x) = e^{i2\alpha \pi \nu/3} \psi_{R,\alpha,s}(x), \tag{19}
\]

where \( \nu = 0, \pm 1 \) is defined as \( L = (3n_L + \nu)a \) \((n_L : \text{integer satisfying } L > 0)\). In terms of the right moving operators, eqs.(9) and (10) are expressed as

\[
\mathcal{H}_k = v_0 \sum_{\alpha,s} \int_{-L}^{L} \frac{dx}{\pi L} \psi_{R,\alpha,s}^\dagger (-i\partial_x) \psi_{R,\alpha,s}, \tag{20}
\]

\[
a_{p,s}(r) = e^{iK_y^0 y} \sqrt{\frac{a}{4N}} \sum_\alpha p^{(1+\alpha)/2} \left\{ e^{i\alpha K_o x} \psi_{R,\alpha,s}(x) - e^{-i\alpha K_o x} \psi_{R,\alpha,s}(-x) \right\}. \tag{21}
\]

The above Hamiltonian and the right moving electron operators are straightforwardly bosonized by utilizing Haldane prescription. The bosonized form for \( \psi_{R,\alpha,s} \) is given by

\[
\psi_{R,\alpha,s}(x) = \frac{\eta_{\alpha,s}}{\sqrt{2\pi a}} e^{-i\theta_{\alpha,s}} e^{i\pi x/4} \left( \Delta N_{\alpha,s} + \alpha \nu/3 \right) e^{i\phi_{\alpha,s}(x)}, \tag{22}
\]

where \( \Delta N_{\alpha,s} \) is the extra electron with the index \((\alpha, s)\) and satisfies, \[ \left[ \theta_{\alpha,s}, \Delta N_{\alpha',s'} \right] = i\delta_{\alpha,\alpha'}\delta_{s,s'}. \]

The operator, \( \eta_{\alpha,s} \), is Majorana Fermion satisfying \( \{ \eta_{\alpha,s}, \eta_{\alpha',s'} \} = 2\delta_{\alpha,\alpha'}\delta_{s,s'} \) and \( \tilde{a} \) is the ultra violet cut-off of the order of \( 1/R \). The function, \( \phi_{\alpha,s}(x) \), is given by

\[
\phi_{\alpha,s}(x) = \sum_{q > 0} \sqrt{\frac{\pi}{\pi L}} \left\{ e^{i q x - \tilde{a} q / 2} b_{\alpha,s}(q) + \text{h.c.} \right\}, \tag{23}
\]

and satisfy \( \phi_{\alpha,s}(x + 2L) = \phi_{\alpha,s}(x) \) because \( q = n\pi/L \) \((n : \text{integer})\). Here \( b_{\alpha,s}(q) \) is the boson operator, so satisfies \( \left[ b_{\alpha,s}(q), b_{\alpha',s'}^\dagger(q') \right] = \delta_{\alpha,\alpha'}\delta_{s,s'}\delta_{q,q'} \). The density operator, \( \rho_{R,\alpha,s}(x) \equiv \psi_{R,\alpha,s}^\dagger(x) \psi_{R,\alpha,s}(x) \), is given by

\[
\rho_{R,\alpha,s}(x) = \frac{\Delta N_{\alpha,s} + \alpha \nu/3}{2L} + \frac{1}{2\pi} \partial_x \phi_{\alpha,s}(x), \tag{24}
\]

and \( \rho_{L,\alpha,s}(x) = \rho_{R,-\alpha,-s}(-x) \). The bosonized form of \( \mathcal{H}_k \) is given as

\[
\mathcal{H}_k = \pi v_0 \sum_{\alpha,s} \int_{-L}^{L} dx : \rho_{R,\alpha,s}(x) \rho_{R,\alpha,s}(x) :
= \frac{\pi v_0}{2L} \sum_{\alpha,s} \left( \Delta N_{\alpha,s} + \frac{\alpha \nu}{3} \right)^2 + \sum_{\alpha,s} \sum_{q > 0} v_0 q b_{\alpha,s}^\dagger(q) b_{\alpha,s}(q). \tag{25}
\]

Before including the mutual interaction, we change the variables of \((\alpha, s)\) to those for charge/spin \((j = \rho/\sigma)\) degree of freedom of symmetric/antisymmetric \((\delta = +/-)\) combination between the
valley index. We define

\[
\begin{align*}
    b_{\rho+}(q) &= \frac{1}{2} \sum_{\alpha,s} b_{\alpha,s}(q), \\
    b_{\rho-}(q) &= \frac{1}{2} \sum_{\alpha,s} \alpha b_{\alpha,s}(q), \\
    b_{\sigma+}(q) &= \frac{1}{2} \sum_{\alpha,s} s b_{\alpha,s}(q), \\
    b_{\sigma-}(q) &= \frac{1}{2} \sum_{\alpha,s} \alpha s b_{\alpha,s}(q), \\
    \Delta N_{\rho+} &= \sum_{\alpha,s} \Delta N_{\alpha,s}, \\
    \Delta N_{\rho-} &= \sum_{\alpha,s} \alpha \Delta N_{\alpha,s}, \\
    \Delta N_{\sigma+} &= \sum_{\alpha,s} s \Delta N_{\alpha,s}, \\
    \Delta N_{\sigma-} &= \sum_{\alpha,s} \alpha s \Delta N_{\alpha,s}.
\end{align*}
\]

Then \([b_{j\delta}(q), b_{j'\delta'}(q')]=\delta_{j,j'}\delta_{\delta,\delta'}\delta_{q,q'}\), \([\theta_{\alpha,s}, \Delta N_{\rho+}]=i\alpha\), \([\theta_{\alpha,s}, \Delta N_{\rho-}]=i\alpha\), \([\theta_{\alpha,s}, \Delta N_{\sigma+}]=i\alpha s\) and \([\theta_{\alpha,s}, \Delta N_{\sigma-}]=i\alpha s\). Since the eigenvalue of \(\Delta N_{\alpha,s}\) is an integer, that of \(\Delta N_{j\delta}, Q_{j\delta}\) has a constraint,

\[
Q_{\rho+} + \alpha Q_{\rho-} + s Q_{\sigma+} + \alpha s Q_{\sigma-} = 4 \times \text{integer}.
\]

In terms of the new variables, \(H_k\) and \(\psi_{R,\alpha,s}(x)\) are respectively expressed as follows,

\[
H_k = \frac{\pi v_0}{8L} \sum_{j,\delta} \left( \Delta N_{j\delta} + \frac{4\nu}{3} \delta_{j,\rho} \delta_{\delta,\rho} \right)^2 + \sum_{j,\delta} \sum_{q>0} v_0 q b_{j\delta}^\dagger(q) b_{j\delta}(q)
\]

\[
\psi_{R,\alpha,s}(x) = \frac{\eta_{\alpha,s}}{\sqrt{2\pi\alpha}} e^{-i\theta_{\alpha,s}} e^{\frac{\pi}{3} i \Delta N_{\rho+} + \alpha \Delta N_{\rho-} + 4\nu/3} \Delta N_{\sigma+} + \alpha s \Delta N_{\sigma-} \times e^{i\theta_{\rho+}(x) + \alpha \theta_{\rho-}(x) + s \theta_{\sigma+}(x) + \alpha s \theta_{\sigma-}(x)},
\]

with

\[
\phi_{j\delta}(x) = \sum_{q>0} \sqrt{\frac{\pi}{qL}} \left\{ e^{i q x - \delta q/2} b_{j\delta}(q) + \text{h.c.} \right\}.
\]

2.2 Effects of interaction

We take into account of the mutual interaction, eq.(2). Among the various interaction processes, the term with the strongest amplitude is written in terms of slowly varying Fermi fields as

\[
H_{\text{int}} = \frac{V(0)}{2} \int_0^L dx \left\{ \sum_{\alpha,s} [\rho_{R,\alpha,s}(x) + \rho_{L,\alpha,s}(x)] \right\}^2,
\]

\[
= \frac{V(0)}{2} \int_{-L}^L dx \left\{ \left[ \sum_{\alpha,s} \rho_{R,\alpha,s}(x) \right]^2 + \sum_{\alpha,s} \sum_{\alpha',s'} \rho_{R,\alpha,s}(x) \rho_{R,\alpha',s'}(-x) \right\},
\]

(38)
where \( V(0) = (2e^2/\kappa) \ln(R_s/R) \) where \( R_s \sim L \) characterizes the large distance cut-off of the Coulomb interaction. The other interaction processes, whose couplings scale as \( a/(2\pi R) \) and are extremely small, have been known to play crucial roles in the absence of the carrier doping, \( i.e.\), at half-filling. Since we discuss the case for away from half-filling by introducing the shift of the chemical potential, those are safely neglected. The above interaction has a following bosonized form,

\[
\mathcal{H}_{int} = \frac{V(0)}{2} \left\{ \frac{1}{L} (\Delta N_{p^+})^2 + \sum_{q>0} \frac{4q}{\pi} b^\dagger_{p^+}(q)b_{p^+}(q) - \sum_{q>0} \frac{2q}{\pi} \left( b_{p^+}(q)b_{p^+}(q) + b^\dagger_{p^+}(q)b^\dagger_{p^+}(q) \right) \right\}.
\]

(39)

Since the interaction term, eq.(39), is expressed by \( (p^+) \) mode only, the Hamiltonian except \( (p^+) \) have diagonalized form, \( \mathcal{H}^0_{p^+} \). The Hamiltonian of \( (p^+) \) mode, \( \mathcal{H}_{p^+} \), is diagonalized by Bogoliubov transformation, \( b_{p^+}(q) \to \cosh \varphi b_{p^+}(q) - \sinh \varphi b^\dagger_{p^+}(q) \) with \( e^{2\varphi} = 1/\sqrt{1 + 4V(0)/(\pi v_0)} \equiv K_{p^+} \). As a result, \( \mathcal{H}_{p^+} \) are given as

\[
\mathcal{H}_{p^+} = \frac{\pi v_{p^+} N}{8L} (\Delta N_{p^+})^2 + \sum_{q>0} v_{p^+} q b^\dagger_{p^+}(q)b_{p^+}(q),
\]

(40)

where \( v_{p^+} = v_0/K_{p^+} \) and \( v_{p^+ N} = v_0/K_{p^+}^2 \). The quantity, \( \phi_{p^+}(x) \), is transformed as

\[
\phi_{p^+}(x) \to \cosh \varphi \phi_{p^+}(x) - \sinh \varphi \phi_{p^+}(-x),
\]

(41)

in eqs.(36). From eq.(40), the charge susceptibility per unit length is easily derived as \( 4/(\pi v_{p^+N}) \).

The quantity is suppressed by the long-range Coulomb interaction because \( K_{p^+} < 1 \). For typical metallic nanotubes, the value of \( K_{p^+} \) is estimated as about 0.2 which leads to strong suppression of the charge susceptibility as \( 4/(\pi v_0) \times 0.04 \).

\section*{3. Extension to multi-wall nanotubes}

In this section, we extend the bosonization theory with open boundaries on the SWNT developed in \( \S.2 \) to the case of MWNT. We consider the MWNT where \( N_M \) metallic graphite shells with radii \( R_1 < R_2 < \cdots < R_{N_M} \) are included. For simplicity, we consider the case where all the metallic shells consist of armchair nanotubes. The insulating shells in the MWNT can be incorporated in space-dependent dielectric constant. The electron operator for the \( n \)-th shell, \( a_{p,s,n}(r) \), is given as follows,

\[
a_{p,s,n}(r) = e^{iK_y^g} \sqrt{\frac{\alpha}{4N_a}} \sum_{\alpha} p^{(1+\alpha)/2} \left\{ e^{i\alpha K_{0x}} \psi_{R,\alpha,s,n}(x) - e^{-i\alpha K_{0x}} \psi_{R,\alpha,s,n}(-x) \right\},
\]

(42)

where \( 2\pi R_n = \sqrt{3}N_n a \) and

\[
\psi_{R,\alpha,s,n}(x) = \frac{\eta_{\alpha,s,n}}{\sqrt{2\pi a}} e^{-i\phi_{p,n}(x) + \alpha \phi_{p,n}(x) + s \phi_{p,n}(x) + \alpha \phi_{p,n}(x)} \psi_{p,s,n}(x),
\]

(43)
where \( \{ \eta_{\alpha,s,n}, \eta_{\alpha',s',n'} \} = 2\delta_{\alpha,\alpha'}\delta_{s,s'}\delta_{n,n'} \), \( \alpha \sim 1/R_{N\alpha} \), [\( \theta_{\alpha,s,n}, \Delta N_{\rho+n} \)] = i\delta_{n,n'}, \( [\theta_{\alpha,s,n}, \Delta N_{\rho-n}] = i\alpha\delta_{n,n'}, \) \( \phi_{j\delta n}(x) = \sum_{q>0} \sqrt{\frac{\pi}{qL}} \left( e^{iqx-\delta q/2}b_{j\delta n}(q) + h.c. \right) \), \( \delta_{j,j'}\delta_{s,s'}\delta_{n,n'}\delta_{q,q'} \). The Hamiltonian is written in terms of the bosonic variables as

\[
\mathcal{H}_k = \frac{\pi v_0}{8L} \sum_{n=1}^{N}\sum_{j,d} (\Delta N_{j\delta n} + \frac{4\rho}{3}\delta_{j,\rho}\delta_{\delta,-})^2 + \sum_{n=1}^{N}\sum_{j,d} v_0q\beta_{j\delta n}(q)\beta_{j\delta n}(q),
\]

\[
\mathcal{H}_{\text{int}} = \sum_{n,m=1}^{N} \frac{V_{nm}}{2} \int_{-L}^{L} dx \sum_{\alpha,s} \alpha' \alpha' \{ \rho_{R,\alpha,s,n}(x)\rho_{R,\alpha'\alpha',s',m}(x) + \rho_{R,\alpha,s,n}(x)\rho_{R,\alpha'\alpha',s',m}(-x) \}
\]

\[
= \frac{\pi v_0}{8L} \sum_{n,m=1}^{N} U_{nm} \Delta N_{\rho+n}N_{\rho+m} + \sum_{q>0} \frac{v_0q}{2} \sum_{n,m=1}^{N} U_{nm} \left\{ \beta_{p+n}(q)\beta_{p+m}(q) - \frac{1}{2} \left( \beta_{p+n}(q)\beta_{p+m}(q) + \beta_{p+m}(q)\beta_{p+n}(q) \right) \right\}.
\]

Here \( U_{nm} = 4V_{nm}/(\pi v_0) = \{8e^2/(\pi v_0\kappa_{nm})\} \ln (R_{n}/R_{nm}) \) expresses the interaction between the n-th and m-th shell with \( \kappa_{nm} \) and \( R_{nm} \) being the dielectric constant between the n-th and m-th shell and the “mean radius” of \( R_n \) and \( R_m \) introduced in ref. [13], respectively. The modes except \( (\rho+) \) are already diagonalized. By using the orthogonal matrix satisfying \( \sum_{m=1}^{N} U_{nm}\Gamma_{m,j} = \Gamma_{nj}g_j \), the Hamiltonian for \( (\rho+) \) mode, \( \mathcal{H}_{\rho+} \) is written as

\[
\mathcal{H}_{\rho+} = \frac{\pi v_0}{8L} \sum_{j=1}^{N} (1+g_j)(\Delta \tilde{N}_{\rho+j})^2
\]

\[
+ \sum_{q>0} v_0q \sum_{j=1}^{N} \left\{ (1+g_j/2)\beta_{p+j}(q)\beta_{p+j}(q) - g_j/4 \left( \beta_{p+j}(q)\beta_{p+j}(q) + \beta_{p+j}(q)\beta_{p+j}(q) \right) \right\},
\]

where \( \Delta \tilde{N}_{\rho+n} = \sum_{j=1}^{N} \Gamma_{nj}\Delta \tilde{N}_{\rho+j}, b_{p+n}(q) = \sum_{j=1}^{N} \Gamma_{nj}b_{p+j}(q) \) and \( g_j \) is the eigenvalue of \( U_{nm} \).

Equation (47) is diagonalized by Bogoliubov transformation, \( b_{p+j}(q) \rightarrow \cosh \varphi_j b_j(q) - \sinh \varphi_j \beta_j(q) \) \((e^{2\varphi_j} = 1/\sqrt{1+g_j} \equiv K_j)\) as

\[
\mathcal{H}_{\rho+} = \sum_{j=1}^{N} \left\{ \frac{\pi v_j}{8L}(\Delta \tilde{N}_{\rho+j})^2 + \sum_{q>0} v_jq\beta_j(q)\beta_j(q) \right\},
\]

where \( v_j = v_0/K_j \) and \( v_jN = v_0/K_j^2 \) with \( K_j = 1/\sqrt{1+g_j} \). In terms of \( b_j(q) \) and \( \beta_j(q), \phi_{\rho+n} \) is expressed as

\[
\phi_{\rho+n}(x) = \sum_{j=1}^{N} \Gamma_{nj} \{ \cosh \varphi_j \phi_j(x) - \sinh \varphi_j \phi_j(-x) \},
\]

\[
\phi_j(x) = \sum_{q>0} \sqrt{\frac{\pi}{qL}} \left\{ e^{iqx-aq/2}b_j(q) + h.c. \right\}.
\]
§4. Charge distribution

Based on the bosonization theory formulated above, the distribution of the charge density from the one boundary is discussed with taking account of the shift of the chemical potential, $\mu$. The roles of the zero modes and of the bosonic long wavelength fluctuations are clarified.

At first, we consider the SWNT. The term expressing the shift of the chemical potential, $-\mu \Delta N_{\rho^+}$, is added to the Hamiltonian, eq.(40). Using eq.(21), the charge density is given as follows,

$$\langle \sum_s a_{p,s}^\dagger(r)a_{p,s}(r) \rangle = \frac{a}{4N} \sum_{s,\alpha} \left\{ \langle \psi_{R,\alpha,s}(x) \psi_{R,\alpha,s}(x) \rangle + \langle \psi_{R,\alpha,s}^\dagger(-x) \psi_{R,\alpha,s}(-x) \rangle \right. 
- e^{-i2\alpha K_0 x} \langle \psi_{R,\alpha,s}^\dagger(x) \psi_{R,\alpha,s}(-x) \rangle 
- e^{i2\alpha K_0 x} \langle \psi_{R,\alpha,s}^\dagger(-x) \psi_{R,\alpha,s}(x) \rangle \right\}.$$  (51)

The first and the second terms are spatially independent and given by

$$\sum_{s,\alpha} \left\{ \langle \psi_{R,\alpha,s}^\dagger(x) \psi_{R,\alpha,s}(x) \rangle + \langle \psi_{R,\alpha,s}^\dagger(-x) \psi_{R,\alpha,s}(-x) \rangle \right\} = \frac{\langle \Delta N_{\rho^+} \rangle}{L}.$$  (52)

On the other hand, the third and fourth terms are given by

$$\sum_{s,\alpha} \left\{ e^{-i2\alpha K_0 x} \langle \psi_{R,\alpha,s}^\dagger(x) \psi_{R,\alpha,s}(-x) \rangle + e^{i2\alpha K_0 x} \langle \psi_{R,\alpha,s}^\dagger(-x) \psi_{R,\alpha,s}(x) \rangle \right\}$$

$$= \sum_{\alpha, s} \left\{ e^{-i\pi x/L}\langle \Delta N_{\rho^+} + \alpha(\Delta N_{\rho^-} + 4\mu/v + s \Delta N_{\sigma^+} + s \Delta N_{\sigma^-}) \rangle e^{-i2\alpha K_0 x} e^{f(2x)} + (x \rightarrow -x) \right\}$$

$$\times \frac{1}{2\pi \tilde{a}} \left[ \frac{\sin^2(\pi \tilde{a}/2L)}{\sinh^2(\pi \tilde{a}/2L) + \sin^2(\pi x/L)} \right]^{(K_{\rho^+} + 3)/8}$$

$$\times \prod_{l=1}^{\infty} \left[ 1 + \frac{\sin^2(\pi x/L)}{\sinh^2(\pi^2 \xi_{\rho^+/L})} \right]^{-K_{\rho^+}/4} \left[ 1 + \frac{\sin^2(\pi x/L)}{\sinh^2(\pi^2 \xi_0/L)} \right]^{-3/4},$$  (53)

where $f(2x) = \tan^{-1}\left\{ \sin(2\pi x/L)/(e^{\pi \tilde{a}/L} - \cos 2\pi x/L) \right\}$, $\xi_{\rho^+} = \nu_{\rho^+}/(2\pi T)$ and $\xi_0 = v_0/(2\pi T)$. Here $\langle \cdots \rangle$ in the r.h.s. in eq. (53) expresses the average in terms of the zero modes. Since the first line in the r.h.s in eq.(53) expresses the oscillation of the charge density, the zero modes determine the uniform shift of the charge density by the chemical potential, eq.(52), and the wavenumbers of the charge density oscillation. On the other hand, the second and third lines are due to the bosonic fluctuation and express the amplitude of the oscillation.

We consider the semi-infinite case, $L \rightarrow \infty$. In this case, the average in terms of zero-modes is easily calculated,

$$\langle \Delta N_{\rho^+} \rangle = \frac{4L \mu}{\pi \nu_{\rho^+}}.$$  (54)

$$\langle e^{i\pi x/L} \Delta N_{\rho^+} + \alpha(\Delta N_{\rho^-} + 4\mu/v + s \Delta N_{\sigma^+} + s \Delta N_{\sigma^-}) \rangle = e^{i2\mu x/\nu_{\rho^+}},$$  (55)

and $f(2x) = (\pi/2)\text{sgn}(x)$. As a result, eq.(51) is calculated as follows

$$\langle \sum_s a_{p,s}^\dagger(r)a_{p,s}(r) \rangle = \frac{\mu a}{\pi N \nu_{\rho^+}} - \frac{a}{N} \left\{ \frac{1}{2\pi \tilde{a}} \left[ \sin(2K_0 + \frac{2\mu}{\nu_{\rho^+}})x - \sin(2K_0 - \frac{2\mu}{\nu_{\rho^+}})x \right] A_S(x) \right\}. $$
\[ A_S(x) = \left( \frac{\tilde{a}}{2x} \right)^{(K_{\rho+}+3)/4} \left\{ \sinh \left( \frac{x}{\xi_{\rho+}} \right) \right\}^{-K_{\rho+}/4} \left\{ \frac{\sinh(x/\xi_0)}{x/\xi_0} \right\}^{-3/4}. \] (56)

Note that eq.(56) together with eq.(57) in case of \( T = 0 \) and \( K_{\rho+} = 1 \) reduces to the non-interacting case, eq.(6). The deviation of the uniform charge density, \( \mu a/(\pi N v_{\rho+N}) = \mu a K_{\rho+}^2/(\pi v_0) \), and the shift of the wavenumber of the oscillation, \( 2\mu/v_{\rho+N} = 2\mu K_{\rho+}^2/v_0 \), are smaller than those in the absence of the interaction. Both quantities are about 0.04 as large as those in the absence of the interaction for the typical SWNT. The fact means that Coulomb interaction prevents the carriers being injected into the nanotube, and has the same origin as suppression of the uniform charge susceptibility. The amplitude of the oscillation, \( A_S(x) \), is large and decays slowly compared to the non-interacting case as is shown in Fig.3. Here, the amplitude of the oscillation is shown as a function of \( x/\tilde{a} \) for \( T/E_c = 0 \) (solid curves) and \( T/E_c = 0.04 \) (dotted curves) with \( E_c = v_0/\tilde{a} \). For each temperature, the upper and lower curves express the amplitude in case of \( K_{\rho+} = 0.2 \) and that in the absence of the interaction, i.e., \( K_{\rho+} = 1 \), respectively. The temperature, \( T/E_c = 0.04 \), corresponds to room temperature for \( N = 10 \). Note that the amplitude delays as \( \exp \left\{ -(K_{\rho+}^2 + 3)x/(4\xi_0) \right\} \) for \( x \gg \xi_{\rho+} \).

Fig. 3. The amplitude of Friedel oscillation of SWNT, \( A_S(x) \), defined in eq.(57) as a function of \( x/\tilde{a} \) for \( T/E_c = 0 \) (solid curves) and \( T/E_c = 0.04 \) (dotted curves) where \( E_c = v_0/\tilde{a} \). For each temperature, the upper (lower) curve expresses the amplitude in case of \( K_{\rho+} = 0.2 \) (\( K_{\rho+} = 1 \)).

Next we consider the case of the MWNT. The charge density of the \( n \)-th shell is obtained for
\( L \to \infty \) as,

\[
\langle : \sum_s a_{p,s,n}^\dagger(\mathbf{r})a_{p,s,n}(\mathbf{r}) : \rangle = \frac{\mu a}{\pi N_n} \sum_{m,j=1}^{N_M} \frac{\Gamma_{n_j} \Gamma_{m_j}}{v_{jN}}
- \frac{a}{N_n} \frac{1}{2\pi a} \left\{ \sin(2K_0 + 2\mu \sum_{m,j=1}^{N_M} \frac{\Gamma_{n_j} \Gamma_{m_j}}{v_{jN}})x - \sin(2K_0 - 2\mu \sum_{m,j=1}^{N_M} \frac{\Gamma_{n_j} \Gamma_{m_j}}{v_{jN}})x \right\}
\times \left( \frac{\tilde{a}}{2x} \right)^{\left( \sum_{j=1}^{N_M} K_j^2 + 3 \right)/4} \prod_{j=1}^{N_M} \left\{ \frac{\sinh(x/\xi_j)}{x/\xi_j} \right\}^{-\Gamma_{m_j}^2 K_j^4/4} \left\{ \frac{\sinh(x/\xi_0)}{x/\xi_0} \right\}^{-3/4},
\]

where \( \xi_j = v_j/(2\pi T) \). Because of the weak logarithmic dependence of \( U_{nm} \) on \( \bar{R}_{nm} \), we can obtain sensible results by the approximation \( U_{nm} = U \). The approximation leads to \( g_1 = N_M U, g_j = 0 \) for \( j = 2 \cdots N_M \) and \( \Gamma_{n1} = 1/\sqrt{N_M} \). As a result, the charge density is obtained as

\[
\langle : \sum_s a_{p,s,n}^\dagger(\mathbf{r})a_{p,s,n}(\mathbf{r}) : \rangle = \frac{\mu a}{\pi N_n v_{1N}} - \frac{a}{N_n} \frac{1}{2\pi a} \left\{ \sin(2K_0 + 2\mu/v_{1N})x - \sin(2K_0 - 2\mu/v_{1N})x \right\} A_M(x),
\]

\[
A_M(x) = \left( \frac{\tilde{a}}{2x} \right)^{(K_1 - 1)/(4N_M) + 1} \left\{ \frac{\sinh(x/\xi_1)}{x/\xi_1} \right\}^{-K_1/(4N_M)} \left\{ \frac{\sinh(x/\xi_0)}{x/\xi_0} \right\}^{-1 + 1/(4N_M)},
\]

where \( K_1 = 1/\sqrt{1 + N_M U}, \xi_1 = v_1/(2\pi T) \) with \( v_1 = v_0/K_1 \) and \( v_{1N} = v_0/K_1^2 \). The amplitude of the oscillation, \( A_M(x) \), becomes small with increasing \( N_M \) as is shown in Fig.3, where the quantity, \( A_M(x) \), is shown as a function of \( x/\tilde{a} \) for \( T/E_c = 0 \) (solid curves) and \( T/E_c = 0.04 \) (dotted curves) with \( \bar{R}_{nm} = 6nm \) and \( \kappa_{nm} = 1.4 \) for several choices of \( N_M \). For each temperature, the curve from top to bottom corresponds to the case of \( N_M = 1, 2, 5, \infty \). We note that the effects of the interaction on \( A_M(x) \) disappear in the limit, \( N_M \to \infty \).

\section{Summary and discussion}

In the present paper, the bosonization theory with open boundaries was developed for both SWNT and MWNT. We payed attention to the relationship between the electron operator of the tight-binding model and the slowly varying field. Based on this bosonization theory, we investigated the distribution of the charge density from an edge with taking account of the shift of the chemical potential expressing carrier doping to the nanotube.

The bosonized Hamiltonian is written by the sum of symmetric/antisymmetric combination of the charge/spin excitation. Each mode has two contribution, zero modes and bosonic fluctuation. Effects of the Coulomb interaction with the strongest amplitude appear in only the symmetric charge excitation. These facts are the same as the case of the periodic boundary condition. However, the Hamiltonian of zero modes are expressed in terms of only the extra number. This fact is due to the open boundary condition, and different from the periodic boundary condition, where the zero
Fig. 4. The amplitude of Friedel oscillation of MWNT as a function of \( x/\tilde{a} \) for \( T/E_c = 0 \) (solid curves) and \( T/E_c = 0.04 \) (dotted curves) with \( \tilde{R}_{nm} = 6\text{nm} \) and \( \kappa_{nm} = 1.4 \) for several choices of \( N_M \). For each temperature, the curve from top to bottom corresponds to the case of \( N_M = 1, 2, 5, \infty \).

The mode Hamiltonian is written by the extra number and the current. The charge distribution in the presence of the shift of the chemical potential has two component. One is spatially independent and the other shows oscillatory behavior which vanishes in the absence of the chemical potential. The zero modes determine the magnitude of the spatially independent component and the wavenumbers of the oscillation. The long-range Coulomb interaction strongly suppress the both quantities. This means the fact that the interaction prevents carriers from being injected into the nanotubes. For the typical SWNT with \( K_{\rho +} = 0.2 \), the both quantities are about 0.04 as large as those in the absence of the interaction. The quantity, the shift of the chemical potential, corresponds to the applied gate voltage or difference between the work function of the nanotube and that of the substrate material. The carrier doping from the gold substrate has been observed by scanning tunneling spectroscopy (STS)\(^{17,18}\) and scanning tunneling microscopy (STM)\(^{19}\). In the STS experiments, the asymmetry of the density of states has been observed, and it is maintained to be due to the difference between the work function of the nanotube and that of the gold(111) substrate. In the present formalism, the shift of the density of states is just given by the chemical potential even in the presence of the Coulomb interaction,\(^2\) which is the same as the conclusion in refs.\(^{17,18}\). However, the deviation of the Fermi wavenumber, \( \delta k \), in the presence of the chemical potential is given by not the simple form of \( \mu/v_0 \) but \( \mu/v_{\rho +N} = \mu K_{\rho +}^2/v_0 \) as is seen in eq.(56). On the other hand, the STM experiment observes \( \delta k \sim \mu/v_0 \). The discrepancy seems to need the further theoretical study on the
Coulomb interaction of the nanotube. The amplitude of the oscillation determined by the bosonic long wavelength fluctuation shows the non-integer power law behavior as a function of the spatial coordinate at $T = 0$. We found that the amplitude is enhanced by the interaction and it becomes smaller with increasing the number of the metallic shells, $N_M$, in the MWNT and identical with that in the absence of the interaction in the case, $N_M \to \infty$. Finally, we note that the present result of the charge distribution are also valid for the strong impurity potential.

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