Electronic Properties of Armchair Carbon Nanotubes : Bosonization Approach

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The phase Hamiltonian of armchair carbon nanotubes at half-filling and away from it is derived from the microscopic lattice model by taking the long range Coulomb interaction into account. We investigate the low energy properties of the system using the renormalization group method. At half-filling, the ground state is a Mott insulator with spin gap, in which the bound states of electrons at different atomic sublattices are formed. The difference from the recent results [Phys. Rev. Lett. 79, 5082 (1997)] away half-filling is clarified.

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Single wall carbon nanotubes (SWNTs) with diameters of a few atomic distances and lengths of several micrometers can be considered as the ultimate miniaturization of metallic wires \cite{1}. Recent experiments have demonstrated electron transport through individual SWNTs and multiple SWNTs as well as provide evidence of scattering amplitudes in Ref. \cite{9}, which accounts for all types of scattering processes. The most important part of the forward scattering was incorporated into the Tomonaga-Luttinger-like Hamiltonian, whereas the other types of scattering were treated as perturbations. The realistic long-range Coulomb interaction was considered in Refs. \cite{9,10}. Kane, Balents and Fisher \cite{10} discussed the effects of the Coulomb interaction in finite size armchair nanotubes (ANs) in terms of the Tomonaga-Luttinger low energy theory. The most important part of the forward scattering was incorporated into the Tomonaga-Luttinger-like Hamiltonian, whereas the other types of scattering were treated as perturbations. Egger and Gogolin (EG) developed an effective low energy theory of ANs starting from a microscopic model \cite{10}, which accounts for all types of scattering processes. They derived a bosonic phase Hamiltonian and discussed possible ground state away from half-filling.

In this Letter we derive the phase Hamiltonian of ANs and evaluate its parameters from the microscopic lattice model. The difference between our Hamiltonian and that by EG stems from the distinction in the form of kinetic term and the use of oversimplified approximation for $2k_F$-component of scattering amplitudes in Ref. \cite{9}, which overlooks $C_3$ symmetry of the microscopic lattice model. The renormalization group (RG) method is applied to the Hamiltonian, and the low energy states are investigated. At half-filling the ground state is the Mott insulator with spin gap, in agreement with the conclusion of Hubbard-like models \cite{11,12}. In this state, the electronic bound states are formed between the different sublattices. Away from half-filling we predict gaps for both symmetric and antisymmetric spin modes, in contrast to the result of Ref. \cite{11} for the case of equal amplitudes of intrasublattice and intersublattice forward scattering.

We start from the standard tight-binding single particle Hamiltonian \cite{11} for $p_z$ electrons on the honeycomb lattice (inset of Fig. 1),

$$\mathcal{H}_k = \sum_{s,\bar{k}} \left\{ \xi(\bar{k}) a^\dagger_{\bar{k},s} a_{\bar{k},s} + h.c. \right\}. \quad (1)$$

Here $a_{\bar{k},s}(\bar{k})$ are the Fermi operators for electrons at the sublattice $p = \pm$ with the spin $s = \pm$ and the wavevector $\bar{k} = (k_x, k_y)$. The matrix elements are given by $\xi(\bar{k}) = -t(e^{-ik_ya/\sqrt{3}} + 2e^{ik_ya/2\sqrt{3}} \cos k_y a/2)$, $t$ being the hopping amplitude between neighboring atoms. The eigenvalues of the Hamiltonian vanish at two points of the Brillouin zone, $\bar{k} = (\alpha K_0, 0)$ with $\alpha = \pm$ and $K_0 = 4\pi/3a$, which constitute the Fermi surface of a graphene layer \cite{11,12}.

We consider the armchair $(N, N)$ SWNT parallel to the $x$ axis so that the wrapping vector $\bar{w} = N(\bar{a}_+ + \bar{a}_-)$ points in $y$ direction (inset of Fig. 1). In this case the Fermi points lie on the allowed quantized transverse wavevector $k_y = 0$ for any $N$. Expanding Eq. (1) near the Fermi points to the lowest order in $q = k_x - \alpha K_0$ and introducing slowly varying Fermi fields $\psi_{p,s}(x)$, we obtain

$$\mathcal{H}_k = -i\nu_0 \sum_{p,s,\bar{s}} \alpha \int dx \psi^\dagger_{-p,s} \partial_x \psi_{p,s}, \quad (2)$$

$\nu_0 = \sqrt{3}ta/2 \approx 8 \times 10^6$ m/s being the Fermi velocity. It should be noted \cite{12} that Eq. (2) differs from Eq. (2) of...
Ref. [3]. Despite identical energy spectra of both Hamiltonians, the phase relations between the components of an eigenfunction at the two sublattices are different. The consequences of this fact will be discussed later on.

Following EG, the interaction term of the Hamiltonian reads,

$$
\mathcal{H}_{\text{int}} = \frac{1}{2} \sum_{l,l'} \sum_{p'p} \sum_{s's} \sum_{\alpha_1 \cdots \alpha_4} U_{pp'} (x_l - x_{l'}) \psi_{p\alpha_1 s_1}^\dagger (x_l) \psi_{p'\alpha_2 s_2}^\dagger (x_{l'}) \psi_{p\alpha_3 s_3} (x_{l'}) \psi_{p\alpha_4 s_4} (x_l),
$$

with \( x_l = la/2 \). The effective 1D interaction between the sublattices \( p \) and \( p' \), \( U_{pp'} (x_l) \), is the average of the Coulomb potential \( U(x,y) = e^2 / \sqrt{\alpha_0^2 + x^2 + 4R^2 \sin^2 (y/2R)} \) over the nodes of a sublattice along the \( y \) direction,

$$
U_{pp'} (x_l) = \frac{1}{\Gamma} \sum_n U \left( x_l, a\sqrt{3} (n + \Delta_{pp'}) \right),
$$

with \( \Delta_{pp'} = \text{mod}(l, 2)/2 + \delta_{pp'}/3 \). Here \( \kappa \) is an effective dielectric constant of the system (the estimate [3] for the parameters of the experiment [2] gives \( \kappa = 1.4 \) and \( a_0 \approx a \) characterizes the radius of the orbital wave function in the graphite plane.

The Hamiltonian \( \mathcal{H}_{\text{int}} \) can be separated into the "forward scattering" \( \mathcal{H}_C = \mathcal{H}_f (a_1 = a_4, a_2 = a_3) \) and "backscattering" \( \mathcal{H}_b = \mathcal{H}_{\text{vb}} (a_1 = -a_4, a_2 = a_3) \) [3].

$$
\mathcal{H}_C = \frac{V_{pp}(0)}{2} \int dx \rho^2(x),
$$

$$
\mathcal{H}_b = -\frac{\delta V(0)}{2} \sum_{\alpha\sigma} \int dx \psi_{p\alpha s}^\dagger \psi_{p\alpha s} \psi_{p\alpha s}^\dagger \psi_{p\alpha s},
$$

$$
\mathcal{H}_{\text{vb}} = -\frac{\delta V(2K_0)}{2} \sum_{\alpha\sigma} \int dx \psi_{p\alpha s}^\dagger \psi_{p\alpha s} \psi_{p\alpha s}^\dagger \psi_{p\alpha s},
$$

where \( \rho = \sum_{\alpha\sigma} \psi_{p\alpha s}^\dagger \psi_{p\alpha s} \) is the total electron density, \( \delta V(0) = V_{pp}(0) - V_{pp'}(0) \), and \( \delta V(2K_0) = V_{pp}(2K_0) - V_{pp'}(2K_0) \), with \( V_{pp'}(q) = (a/2) \sum_{l} e^{iql} U_{pp'} (x_l) \) being the Fourier transformed interaction.

The forward scattering [5] has the strongest amplitude, \( V_{pp}(0) = 2e^2/\kappa \ln(R_d/R) \), where \( R_d \approx \min(L, D) \) characterizes the screening of the Coulomb interaction due to a finite length \( L \) of the AN and/or the presence of metallic electrodes at a distance \( D \). The amplitude \( V_{pp}(0) \) is relatively insensitive to the choice of \( R \) due to logarithmic dependence. From Eq. [10], one sees that the amplitudes \( \delta V(0) \) and \( V_{pp}(2K_0) \) decay as \( 1/R \) for \( R \gg a \). It should be noted that the matrix element \( NV_{pp'}(2K_0) \) vanishes identically in case of a graphite plane (\( R \to \infty \)) due to the \( C_4 \) symmetry of the lattice. For this reason, \( V_{pp'}(2K_0) \) is much smaller than \( \delta V(0) \) and \( V_{pp}(2K_0) \). All the matrix elements decrease with increasing \( a_0 \). Numerical evaluation for \( a_0 = a/2 \) and \( R \gg a \) gives \( \delta V(0) = 0.21 \), \( V_{pp}(2K_0) = 0.60 \), \( V_{pp'}(2K_0) = 9.4 \times 10^{-4} \) in units of \( a^2/2\pi \) is estimated for \( N = 10 \). This result shows that the approximation \( V_{pp}(2K_0) = V_{pp'}(2K_0) \) used in Ref. [1] is questionable.

In order to bosonize the Hamiltonian \( \mathcal{H} = \mathcal{H}_C + \mathcal{H}_{\text{int}} \), Eqs. (3), (5), (6), we diagonalize the kinetic term Eq. (4) by the unitary transformation

$$
\psi_{\alpha s} = \left( \psi_{\alpha s} + \alpha \psi_{\alpha s} \right) / \sqrt{2},
$$

which maps the basis of atomic sublattices \( \pm \) to the basis of right- and left-movers \( \pm \). This transformation is different from one by EG due to the different form of the kinetic term.

We bosonize the Fermi fields \( \psi_{\alpha s} \),

$$
\psi_{\alpha s} = \eta_{\alpha s} \exp \left[ i r q_F x + i \frac{\pi}{2} \left( \theta_{\alpha s} + r \phi_{\alpha s} \right) \right],
$$

and decompose the phase variables \( \theta_{\alpha s}, \phi_{\alpha s} \) into symmetric \( \delta = + \) and antisymmetric \( \delta = - \) modes of the charge \( \rho \) and spin \( \sigma \) excitations, \( \theta_{\alpha \sigma} = \theta_{\alpha +} + s \theta_{\alpha +} + \alpha \theta_{\alpha -} \), and \( \phi_{\alpha \sigma} = \phi_{\alpha +} + s \phi_{\alpha +} + \alpha \phi_{\alpha -} \) + \( s \phi_{\alpha -} \).

The bosonic fields satisfy the commutation relation, \( \left[ \theta_{\phi} (x), \phi'_{\eta} (x') \right] = (\pi/2) \text{sign}(x - x') \delta_{\phi} \delta_{\eta} \). The Majorana fermions \( \eta_{\alpha s} \) are introduced to ensure correct commutation rules for different species \( \sigma, r, a \) of electrons, and satisfy \( \left[ \eta_{\alpha s}, \eta'_{\alpha s'} \right] = 2 \delta_{\alpha \alpha'} \delta_{\sigma \sigma'} \delta_{s s'} \).

The spin-conserving products \( \eta_{\alpha s} \eta'^{\dagger}_{\alpha s'} \) in the Hamiltonian \( \mathcal{H} \) can be represented as \( \frac{\eta_{\alpha s}}{\sqrt{2}} \exp \left[ -i r q_F x + i \frac{\pi}{2} \left( \theta_{\alpha s} + r \phi_{\alpha s} \right) \right] \).

Hence, the bosonized Hamiltonian has the form,

$$
\mathcal{H} = \sum_{j = r, \sigma} \sum_{\delta = \pm} \frac{v j}{2 \pi} \int dx \left\{ K_j^{-1} \left( \partial_x \eta_j \right)^2 + K_j \left( \partial_x \phi_j \right)^2 \right\} + \frac{1}{2} \frac{\delta (\alpha \sigma)}{a^2} \int dx \{ \left[ \delta V(0) - 2 \left( 2V(2K_0) \right) \right] \cos(4q_F x + 2\theta_{\sigma +}) \cos 2\theta_{\sigma +} \\
- \delta V(0) \cos(4q_F x + 2\theta_{\sigma +}) \cos 2\theta_{\sigma -} \\
+ \delta V(0) \cos(4q_F x + 2\theta_{\sigma +}) \cos 2\sigma_{\sigma -} \\
- \delta V(0) \cos 2\theta_{\sigma +} \cos 2\theta_{\sigma -} \\
- \delta V(2K_0) \cos(4q_F x + 2\theta_{\sigma +}) \cos 2\phi_{\sigma -} \\
+ 2V(2K_0) \cos 2\theta_{\sigma +} \cos 2\phi_{\sigma -} \\
+ \delta V(2K_0) \cos 2\theta_{\sigma +} \cos 2\phi_{\sigma -} \{ \right\}. 
$$
\[ v_{j\delta} = v_0 \sqrt{A_{j\delta} B_{j\delta}} \] and \[ K_{j\delta} = \sqrt{B_{j\delta} / A_{j\delta}} \] being the velocities of excitations and exponents for the modes \( j, \delta \). The parameters \( A_{j\delta}, B_{j\delta} \) are given by

\[
\begin{align*}
A_{\mu+} &= 1 + \frac{4\tilde{V}(0)}{4\pi v_0} - \frac{\delta V(0)}{4\pi v_0} - \frac{\tilde{V}(2K_0)}{2\pi v_0} - \frac{\delta V(2K_0)}{4\pi v_0}, \\
B_{\mu+} &= B_{\sigma+} = 1 + \frac{\delta V(0)}{4\pi v_0} + \frac{\tilde{V}(2K_0)}{2\pi v_0} - \frac{\delta V(2K_0)}{4\pi v_0}, \\
A_{\mu-} &= A_{\sigma-} = 1 - \frac{\delta V(0)}{4\pi v_0} + \frac{\tilde{V}(2K_0)}{2\pi v_0} + \frac{\delta V(2K_0)}{4\pi v_0}, \\
B_{\mu-} &= B_{\sigma-} = 1 + \frac{\delta V(0)}{4\pi v_0} - \frac{\tilde{V}(2K_0)}{2\pi v_0} + \frac{\delta V(2K_0)}{4\pi v_0},
\end{align*}
\]

with \( \tilde{V}(q) = |V_{pp}(q) + V_{p\rho}(q)|/2 \). The sublattice-independent forward scattering \( V(0) \) strongly renormalizes the exponent for the symmetric charge mode, \( K_{\sigma \pm} \approx 0.2 \) \[9\], whereas for the other modes the interaction is weak, \( K_{j\delta} = 1 + O(a/R) \) \[8\].

We now compare the Hamiltonian \[11\] with that derived by EG \[9\] away from half-filling. In this case, the non-linear terms containing the misfit parameter \( q_F \) can be neglected due to the breakdown of the momentum conservation. Despite the equal forward scattering parts of both Hamiltonians, there is difference in the backscattering parts. Namely, the Hamiltonian by EG can be obtained from ours by substituting \( \tilde{V}(2K_0) \to 0 \) and \( \delta V(2K_0) \to 2V(2K_0) \). The absence of \( \cos 2\theta_{\sigma+} \cos 2\phi_{\sigma-} \) term in the Hamiltonian by EG originates from the use of the approximation \( \delta V(2K_0) = 0 \), whereas the difference in the coefficient in front of the three other non-linear backscattering terms stems from the difference in the unitary transformation \[9\].

The low energy properties of the Hamiltonian Eq. \[11\] can be investigated by the renormalization group (RG) method. The RG equations can be derived by assuming scale invariance of the correlation functions \( \langle \exp \{ i(\eta_{j\delta}(x_1, \tau_1) - \eta_{j\delta}(x_2, \tau_2)) \} \rangle \) \[10\]. At half-filling, \( q_F = 0 \), we obtain

\[
\begin{align*}
(K_{\sigma+})' &= -(K_{\sigma+}^2/8)(y_2^2 + y_3^2 + y_7^2), \\
(K_{\sigma-})' &= -(K_{\sigma-}^2/8)(y_7^2 + y_2^2 + y_3^2 + y_7^2), \\
(K_{\rho+})' &= -(K_{\rho+}^2/8)(y_7^2 + y_2^2 + y_3^2 + y_7^2), \\
(K_{\rho-})' &= -(K_{\rho-}^2/8)(y_2^2 + y_3^2 + y_7^2), \\
(y_1)' &= \{ 2 - (K_{\sigma+} + K_{\sigma-}) \} y_1, \\
(y_2)' &= \{ 2 - (K_{\rho+} + K_{\sigma+}) \} y_2, \\
(y_3)' &= \{ 2 - (K_{\rho+} + K_{\sigma+}) \} y_3, \\
(y_4)' &= \{ 2 - (K_{\rho-} + K_{\sigma-}) \} y_4, \\
(y_5)' &= \{ 2 - (K_{\sigma+} + K_{\sigma-}) \} y_5, \\
(y_6)' &= \{ 2 - (K_{\rho+} + K_{\sigma-}) \} y_6, \\
(y_7)' &= \{ 2 - (K_{\rho+} + K_{\sigma-}) \} y_7, \\
(y_8)' &= \{ 2 - (K_{\rho+} + K_{\sigma-}) \} y_8, \\
(y_9)' &= \{ 2 - (K_{\rho-} + K_{\sigma-}) \} y_9.
\end{align*}
\]

where \( (\cdot)' \) denotes \( d/d\tau \) with \( d\tau = d\ln(\tilde{a}/a) \) (\( \tilde{a} \) is the new lattice constant). The initial conditions for the Eqs. \[12\]-\[24\] are \( K_{j\delta}(0) = K_{j\delta}, y_1 = (\delta V(0) - 2V(2K_0))/\langle \pi v_0 \rangle, y_2 = -y_3 = -y_5 = y_6 = -\delta V(0)/\langle \pi v_0 \rangle, y_4 = -\delta V(0) - \delta V(2K_0)/\langle \pi v_0 \rangle, y_7 = -y_8 = -2V(2K_0)/\langle \pi v_0 \rangle, \) and \( y_9 = \delta V(2K_0)/\langle \pi v_0 \rangle \). In deriving the RG equations, the non-linear term \( \cos 2\phi_{\sigma} \cos 2\phi_{\rho-} \) is omitted because this operator stays exactly marginal in all orders and is thus decoupled from the problem \[13\]. The RG equations away from half-filling can be obtained from Eqs. \[13\]-\[24\] by putting \( y_1, y_2, y_3, \) and \( y_7, y_8, y_9 \) to zero. Hereafter we concentrate on the case \( N = 10, \kappa = 1.4, R_s = 100 \) \text{nn} and \( a_0 = a/2 \) where the initial values of the RG parameters correspond to the estimates given below Eq. \[8\].

Away from half-filling, the quantities \( K_{\sigma+}, K_{\rho-} \) and \( K_{\sigma-}^{-1} \) renormalize to zero and the coefficient of \( \cos 2\theta_{\sigma+} \cos 2\phi_{\sigma-} \cos 2\phi_{\sigma-} \) tends to \(-\infty \) \( (\infty) \). As a result, the phases \( \theta_{\sigma+}, \theta_{\rho-}, \) and \( \phi_{\sigma-} \) are locked at \( (\theta_{\sigma+}, \theta_{\rho-}, \phi_{\sigma-}) = (0, 0, \pi/2) \) or \( (\pi/2, \pi/2, 0) \) so that the modes \( \sigma \pm, \rho \) are gapped. In this case, the asymptotic behavior of the correlation functions at \( x \to \infty \) is determined by the correlations of the gapless \( \rho \) mode, \( \langle e^{i\phi_{\sigma+}(x)} e^{-i\phi_{\rho-}(0)} \rangle \sim x^{-n^2 K_{\rho-}^2/2} \) and \( \langle e^{i\phi_{\rho-}(x)} e^{-i\phi_{\sigma-}(0)} \rangle \sim x^{-m^2/2K_{\rho-}} (n = 1 \) and \( 2 \) correspond to \( 2q_F \) and \( 4q_F \) density waves and \( m = 1 \) for a superconducting state). Since \( K_{\rho-} \approx 0.2 \), the \( 2q_F \) density wave correlations seem to be dominant. However, we found that the correlation functions of any \( 2q_F \) density wave decay exponentially at large distances due to the gapped modes. We therefore are looking for the four-particle correlations. The \( 4q_F \) density waves dominate over the superconductivity for \( K_{\rho+} < 1/2 \) \[16\]. Such density wave states are given by the product of the charge \( n_\pm(x) \) or spin \( S_\pm(x) \) densities at different sublattices,

\[
\begin{align*}
n_+(x)n_-(x) &\sim -\frac{1}{2\langle \pi a \rangle^2} \cos(4q_F x + 2\theta_{\rho+}) \\
&\times (2 \cos 2\theta_{\sigma+} + \cos 2\phi_{\sigma-} - \cos 2\theta_{\rho-}), \\
S_+(x)S_-(x) &\sim -\frac{1}{8\langle \pi a \rangle^2} \cos(4q_F x + 2\theta_{\rho+}) \\
&\times (2 \cos 2\theta_{\sigma+} - \cos 2\phi_{\sigma-} + \cos 2\theta_{\rho-}).
\end{align*}
\]
where we neglected the unlocked phases $\phi_{\sigma^+}, \phi_{\sigma^-}, \theta_{\sigma^-}$ whose contribution decays exponentially at large distances. Substituting the values of the locked phases we observe that $n_+(x)n_-(x)$ vanishes, and the dominant state is the $4q_F \rho$ spin density wave with correlation function $(S_+(x)S_-(x)S_+(0)S_-(0)) \sim \cos 4q_F x / a^{2K_{\rho^+}}$.

The modes $\sigma^\pm$ and $\rho^-$ remain gapped also in the limit $\delta V(0) = 0$. In this case EG have obtained that the symmetric modes, $\rho^+$ and $\sigma^+$, are gapless, whereas the $\rho^-$ mode is gapped and $\sigma^- \rho^-$ mode separates into the gapless and gapped parts. The result by EG follows from the special dual symmetry $\theta_{\sigma^-} \leftrightarrow \phi_{\sigma^-}$ of the Hamiltonian and the absence of non-linear terms in the $\rho^+$ and $\sigma^+$ sectors. Both these factors are lacking in Eq. (11). On the other hand, the result by EG for a finite value of $\delta V(0)$ is qualitatively the same as ours.

At half-filling the solution (Fig.1) of the RG equations [17-20] indicates that the phase variables $\theta_{\rho^+}, \theta_{\sigma^+}, \theta_{\sigma^-}$, and $\phi_{\sigma^-}$ are locked and all the kinds of excitation are gapped. In other words, the ground state of the half-filled AN is a Mott insulator with spin gap. The same conclusion has been drawn from the model with short range interactions [22]. The locked phases are given by $(\theta_{\rho^+}, \theta_{\sigma^+}, \theta_{\sigma^-}, \phi_{\sigma^-}) = (0, 0, 0, 0)$ or $(\pi/2, \pi/2, \pi/2, \pi/2)$ since the coefficients tend to $-\infty$ for the first, second and 6-9-th non-linear terms in Eq. (11). The averages $\langle n_+(x)n_-(x) \rangle$ and $\langle S_+(x)S_-(x) \rangle$ are both finite, which indicates the formation of bound states of electrons at different sublattices. The observability of the Mott insulating behavior of ANs depends critically on the magnitude of the gap $\Delta_{\rho^+}$ in the $\rho^+$ mode, which is estimated by the self-consistent harmonic approximation as [18].

$$\Delta_{\rho^+}/(2\nu_{\rho^+}a^{-1}) = \frac{K_{\rho^+}}{\pi\nu_0} \left[ \frac{\delta V(0)^2}{2} + \frac{\bar{V}(2K_0)^2}{2} - \delta V(0)\bar{V}(2K_0) \right]^{-1/2}. \quad (32)$$

Using the value of the matrix elements calculated numerically, the charge gap for $N = 10$ is estimated as $\sim 100K$ for $a_0 = a/2$ and $\sim 10K$ for $a_0 = a$ (in case of $a_0 = a, \delta V(0) = 5.6 \times 10^{-3}$ and $\bar{V}(2K_0) = 6.9 \times 10^{-2}$ in units of $ae^2/2\pi \kappa R$). The resistivity of ANs shows power law temperature dependence, $\rho \sim T^{2K_{\rho^+}-1}/N^2$ at high temperatures $T \gg \Delta_{\rho^+}$ and increases exponentially, $\rho \propto \exp(\Delta_{\rho^+}/T)$, at $T \ll \Delta_{\rho^+}$ [19]. The temperature dependence of the resistivity at half-filling is a characteristic signature of the Mott transition. We conjecture that this signature can be best detected in multiprobe transport measurements [14].

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