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# Acoustic phonon exchange, attractive interactions, and the Wentzel-Bardeen singularity in single-wall nanotubes

A. De Martino and R. Egger Institut für Theoretische Physik, Heinrich-Heine Universität, D-40225 Düsseldorf, Germany (Date: February 1, 2008)

We derive the effective low-energy theory for interacting electrons in metallic single-wall carbon nanotubes taking into account acoustic phonon exchange within a continuum elastic description. In many cases, the nanotube can be described as a standard Luttinger liquid with possibly attractive interactions. We predict surprisingly strong attractive interactions for thin nanotubes. Once the tube radius reaches a critical value  $R_0 \approx 3.6 \pm 1.4$  Å, the Wentzel-Bardeen singularity is approached, accompanied by strong superconducting fluctuations. The surprisingly large  $R_0$  indicates that this singularity could be reached experimentally. We also discuss the conditions for a Peierls transition due to acoustic phonons.

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#### I. INTRODUCTION

Superconductivity in carbon nanotubes has lately generated a lot of excitement. Experimental observations include an unexpectedly strong proximity effect in singlewall nanotubes (SWNTs) [1,2], fluctuation superconductivity in ultrathin SWNTs [3], and intrinsic BCStype behavior in "ropes" containing many SWNTs [4]. These experiments have in turn led to a number of theoretical papers [5–8]. In particular, the authors of Refs. [5,6] argue that phonon exchange holds responsible for some attractive electron-electron interaction. The value or even order of magnitude of the electronphonon coupling was however left open or simply extracted by fitting experimental curves. In this work, we wish to fill this gap and provide a quantitative analysis of phonon-mediated retarded electron-electron interactions in a metallic SWNT. (The theory also holds qualitatively for a heavily doped semiconducting SWNT.) Below we include the usual (repulsive) Coulomb interactions in the effective low-energy theory valid at energies  $|E| < v_F/R$ , with Fermi velocity  $v_F$  and SWNT radius R. We assume that the SWNT is doped away from the charge neutrality point,  $E_F \neq 0$ , i.e., an incommensurate situation, which is normally encountered in practice. Then electron-phonon and electron-electron Umklapp processes can be neglected.

Besides mediating possibly attractive interactions, the effect of phonons on the electronic system could in principle lead to two instabilities, namely the Peierls transition [9] and the Wentzel-Bardeen (WB) singularity [10]. All

these issues can be investigated by integrating out the phonons and studying the electron system alone, since the relevant backscattering electron-phonon interactions are weak [11]. This is the approach taken in our paper. Our treatment of phonons expands on recent work by Suzuura and Ando [12], where the field theory for acoustic phonons and their coupling to electrons in SWNTs was derived. Optical phonons are ignored in this theory as well as in ours. This should create no major problem for the issues at stake here, since optical phonons do not produce sizeable attractive interactions nor a WB singularity. Their relevance for the Peierls transition is discussed briefly below. The theory of Ref. [12] is analytically tractable and, moreover, appears to be in excellent agreement with local-density-functional calculations even for ultrathin  $(R \approx 2 \text{ Å})$  nanotubes [13]. For instance, we find that the frequency of the breathing mode computed in Ref. [13] coincides to within 4% with the value extracted from the continuum theory of Ref. [12]. Furthermore, the predicted value for the twist velocity  $v_T$  below is consistent with Refs. [14,15]. This is fortunate since previous estimates for the electron-phonon coupling [16,17] were only qualitative in nature and did not even agree on orders of magnitude. For related theoretical work on acoustic phonons and electron-phonon interactions in SWNTs, see Ref. [18].

As we show in detail below, the phonon-mediated effective attraction among electrons is very strong for sufficiently thin nanotubes. The dominant phonon exchange processes involve two phonon modes, namely the stretching and the breathing mode. The stretching mode has a linear dispersion characterized by a velocity  $v_S$ , while the breathing mode has a finite frequency  $\omega_B$  at long wavelengths. Following general arguments [11,19], for a large part of the relevant parameter space, the influence of the stretching mode is negligible. Then the system can be described as a Luttinger liquid (LL) with standard interaction parameter  $K_{c+}$  in the charged channel [20], where  $K_{c+} = 1$  for noninteracting electrons. Phonon exchange involving the breathing mode implies

$$K_{c+} = \frac{K_{c+}^0}{\sqrt{1 - (K_{c+}^0)^2 R_B / R}},\tag{1.1}$$

with  $R_B=2.4\pm0.9$  Å. Here  $K_{c+}^0\leq 1$  characterizes the repulsive Coulomb interactions, where  $K_{c+}^0\approx 0.2$  for unscreened interactions [20]. Notice that without external screening, phonon exchange is not relevant, and

 $K_{c+} \approx K_{c+}^0$ . However, once Coulomb interactions are externally screened off, e.g. by nearby gate electrodes, we get  $K_{c+}^0 \approx 1$  and Eq. (1.1) predicts surprisingly strong attractive interactions ( $K_{c+} > 1$ ). For a (10,10) armchair tube with R = 6.79 Å, the LL parameter is then  $K_{c+} \approx 1.3$ , i.e. significantly larger than the noninteracting value. These attractive interactions get stronger for thinner nanotubes.

As we discuss below, the neglect of the retarded interaction due to the stretching mode, leading to a (fourchannel) LL with interaction parameter  $K_{c+}$  given by Eq. (1.1) and interaction parameters  $K_{\lambda} = 1$  in the three neutral channels (see below), is valid provided Ris sufficiently large compared to the "critical radius"  $R_c = (K_{c+}^0)^2 R_0$ , where  $R_0$  is slightly larger than  $R_B$ ,  $R_0 = 3.6 \pm 1.4$ Å. Only in the immediate vicinity of this radius, the retarded interaction mediated by the stretching phonon mode has to be kept explicitly. This critical radius defines the location of the so-called Wentzel-Bardeen (WB) singularity [10]. For  $R \leq R_c$ , our model breaks down, and a transition to a phase-separated state is expected. Previous work by Loss and Martin [21] studied the WB singularity in detail for one-dimensional (1D) systems, but a concrete physical realization seemed out of reach due to the small ratio between sound and Fermi velocity in all systems considered so far. We argue below that SWNTs with screened-off interactions may offer the possibility to reach this elusive singularity, which has never been observed experimentally. This is remarkable since the ratio between sound and Fermi velocity is still small. However, in a SWNT the stretching and the breathing phonon modes collaborate in driving the system towards the WB singularity in a very efficient manner.

Moreover, the closeness to the WB singularity holds responsible for rather strong superconducting fluctuations. From our theory, estimates for the attractive interactions generated via phonon exchange are obtained. To describe most of the issues raised by the experiments of Refs. [3,4] in a quantitative way, it will however be important to also analyze the effect of various inter-tube couplings in SWNT ropes or crystals in more detail. Employing a mean-field approximation for Josephson couplings, the standard 1D Ginzburg-Landau description can be obtained [22]. In this paper, we focus on the phonon-mediated electron-electron interaction within a given nanotube, and postpone a full discussion of experimentally relevant quantities to a future publication [23].

The present paper also sheds light on the recent discussion about the possibility of a Peierls transition in SWNTs [15,24–26]. Notably, even in the incommensurate situation studied here, in principle a Peierls transition can occur [27], although the resulting pseudogap is expected to be wiped out by quantum fluctuations [11]. Within a mean-field approximation, the Peierls transi-

tion due to optical phonons has been studied in Refs. [24–26], resulting in a Kekulé-type modulation. Since we only treat acoustic phonons, we have nothing to say about this issue. However, recent theoretical work including acoustic phonons has pointed out the possibility of a sizeable Peierls gap in thin armchair SWNTs [15]. This Peierls modulation was found to correspond to a twist distortion of the SWNT. Below we study arbitrary metallic SWNTs, and indeed confirm that the relevant Peierls distortion for an armchair SWNT would correspond to a tube twisting. In addition, we find the proper mode for any metallic SWNT. Our findings follow from analyzing backscattering phonon exchange, which operates at the doping-dependent wavevector  $2q_F$ , where  $q_F = |E_F|/v_F$ . Based on our essentially exact results, we do not expect that the Peierls transition predicted in Ref. [15] is observable, at least not for an individual SWNT away from the neutrality point. According to our theory, a Peierls gap in the 1D sense [11] could only be possible for very thin SWNTs and under rather stringent conditions.

The outline of the paper is as follows. In Sec. II we briefly summarize the elastic continuum theory for phonons and the electron-phonon interaction. The resulting effective electron-electron interaction generated by phonon exchange is derived in Sec. III. The dominant forward scattering process, the Luttinger liquid with attractive interactions, and the Wentzel-Bardeen singularity are discussed in Sec. IV. The remaining phonon exchange terms and the Peierls transition is studied in Sec. V. Some details concerning Sec. V have been transferred to an appendix. Finally, we discuss the relevance of inter-tube phonon exchange and conclude in Sec. VI.

# II. ACOUSTIC PHONONS AND ELECTRON-PHONON COUPLING

Here we shall always assume a suspended (free-standing) tube. With regard to the important phonon modes coupling to the low-energy electrons, this should be an accurate assumption both for SWNTs embedded in a zeolite matrix [3] or in a rope [4]. However, modifications may arise for individual SWNTs on a substrate, where phonon modes could be pinned. Let us then briefly summarize the main results of Ref. [12], where acoustic phonons in SWNTs are described by an elastic continuum theory. The Euclidean action is (we put  $\hbar = 1$ )

$$S = \int d\tau d^2r \left\{ (M/2)\dot{\mathbf{u}}^2 + U[\mathbf{u}] + U_c[\mathbf{u}] \right\}, \qquad (2.1)$$

where  $\mathbf{u}^T(\vec{r}) = (u_x, u_y, u_z)$  is the displacement field and  $\vec{r} = (x, y)$ . The displacement field in this approximation does not discriminate among the graphite sublattices, and hence will not describe optical phonons. The coordinate system is chosen as follows. The y-axis points

along the tube,  $0 \le x \le 2\pi R$  around the circumference, and z denotes the direction perpendicular to the tube surface. The elastic potential energy density in Eq. (2.1) is given by

$$U[\mathbf{u}] = \frac{1}{2} \left( B(u_{xx} + u_{yy})^2 + \mu [(u_{xx} - u_{yy})^2 + 4u_{xy}^2] \right),$$

where the strain tensor is defined by the relations  $u_{yy} = \partial_y u_y$ ,  $2u_{xy} = \partial_y u_x + \partial_x u_y$ , and, due to the cylindrical geometry,  $u_{xx} = \partial_x u_x + u_z/R$ . Furthermore, the curvature-induced potential energy density is

$$U_c[\mathbf{u}] = (a^2 \Xi/2)[(\partial_x^2 + \partial_y^2 + R^{-2})u_z]^2.$$

In the above expressions, a=2.46 Å is the lattice constant, and the carbon mass per unit area is  $M=3.80\times10^{-7}$  kg/m<sup>2</sup>. The bulk modulus B and the shear modulus  $\mu$  are accurately known for bulk graphite,

$$B/M = 2.90 \times 10^8 \,\mathrm{m^2/sec^2},$$
 (2.2)  
 $\mu/M = v_T^2 = 1.51 \times 10^8 \,\mathrm{m^2/sec^2}.$ 

Finally, the normal-force constant is  $\Xi/M=6.19\times 10^6\,\mathrm{m^2/sec^2}$ . Since  $\Xi\ll B,\mu$  and the curvature-induced terms are additionally suppressed in the long-wavelength limit, terms related to  $\Xi$  are neglected in what follows. It is then convenient to switch to Fourier space,

$$\mathbf{u}(\tau,\vec{r}) = \frac{1}{\beta L} \sum_{\omega_n,q_x} \int \frac{dq_y}{2\pi} e^{-i(\omega_n \tau - \vec{q} \cdot \vec{r})} \mathbf{u}(\omega_n,\vec{q}),$$

where  $\vec{q} = (q_x, q_y)$ ,  $\omega_n = 2\pi n/\beta$  with  $\beta = 1/k_BT$  are Matsubara frequencies,  $L = 2\pi R$  is the circumference of the tube, and  $q_x = n/R$  with integer n denotes the discrete transverse momenta. The action (2.1) then reads

$$S = \frac{1}{2\beta L} \sum_{\omega_n, q_x} \int \frac{dq_y}{2\pi} \mathbf{u}^T(-\omega_n, -\vec{q}) \underline{A}(\omega_n, \vec{q}) \mathbf{u}(\omega_n, \vec{q}),$$
(2.3)

where  $\underline{A}$  is given by the matrix

$$\begin{pmatrix} M\omega_n^2 + \Delta q_x^2 + \mu q_y^2 & Bq_xq_y & -i\Delta\frac{q_x}{R} \\ Bq_xq_y & M\omega_n^2 + \Delta q_y^2 + \mu q_x^2 & -i(B-\mu)\frac{q_y}{R} \\ i\Delta\frac{q_x}{R} & i(B-\mu)\frac{q_y}{R} & M\omega_n^2 + \frac{\Delta}{R^2} \end{pmatrix}$$

with  $\Delta = B + \mu$ .

Our strategy is to integrate out phonons, which is valid unless the electron-phonon coupling is very strong and/or soft phonon modes are present, see Ref. [11]. These requirements are met in our case. In order to proceed, we then need the inverse of  $\underline{A}$ , whose general form is straightforward to obtain but not required here. The only transverse momentum relevant for the effective interaction is  $q_x=0$ , since only the corresponding electronic states have to be kept at low energy scales. Therefore we focus on this special limit henceforth. Putting  $q_y=q$  and  $q_x=0$ , the matrix  $\underline{A}$  reads

$$\underline{A} = \begin{pmatrix} M\omega_n^2 + \mu q^2 & 0 & 0\\ 0 & M\omega_n^2 + \Delta q^2 & -i(B-\mu)q/R\\ 0 & i(B-\mu)q/R & M\omega_n^2 + \Delta/R^2 \end{pmatrix},$$

with eigenvalues (i = 1, 2, 3)

$$\lambda_i = M \left[ \omega_n^2 + \epsilon_i^2(q) \right]. \tag{2.4}$$

The inverse matrix is

$$\underline{A}^{-1} = \begin{pmatrix} \frac{1}{\lambda_1} & 0 & 0\\ 0 & \frac{M\omega_n^2 R^2 + \Delta}{\lambda_2 \lambda_3 R^2} & \frac{i(B - \mu)q}{\lambda_2 \lambda_3 R}\\ 0 & -\frac{i(B - \mu)q}{\lambda_2 \lambda_3 R} & \frac{M\omega_n^2 + \Delta q^2}{\lambda_2 \lambda_3} \end{pmatrix}.$$
(2.5)

Here  $\epsilon_1^2(q) = v_T^2 q^2$  with  $v_T$  in Eq. (2.2), and

$$\epsilon_{2,3}^2(q) = (\omega_B^2/2)[1 + q^2R^2 \mp E(q)]$$
 (2.6)

with

$$E(q) = [1 + 2q^2R^2(1 - 8B\mu/\Delta^2) + q^4R^4]^{1/2}.$$
 (2.7)

In the long-wavelength limit,  $qR \ll 1$ , further simplifications are possible. Although the theory is valid also for larger qR, we shall make this inessential approximation whenever appropriate. To lowest order in qR, we obtain for the three eigenmodes

$$\epsilon_1^2(q) = v_T^2 q^2, \quad \epsilon_2^2(q) = v_S^2 q^2, \quad \epsilon_3^2(q) = \omega_B^2,$$
 (2.8)

where

$$v_S^2 = 4B\mu/\Delta M, \quad \omega_B^2 = \Delta/MR^2. \tag{2.9}$$

The eigenmodes corresponding to  $\lambda_{1,2,3}$  are the twisting, stretching and breathing phonon modes, respectively. The sound velocities for the twisting and stretching modes are  $v_T$  and  $v_S$ , and the breathing mode frequency is  $\omega_B$ . From Eq. (2.2) we obtain the following estimates

$$v_T = 1.23 \times 10^4 \text{ m/sec},$$

$$v_S = 1.99 \times 10^4 \text{ m/sec},$$

$$\hbar \omega_B = \frac{0.14}{R} \text{ eVÅ}.$$
(2.10)

Note that both  $v_S$  and  $v_T$  are much smaller than the Fermi velocity,  $v_F = 8 \times 10^5$  m/sec. The stretching mode corresponds to the longitudinal acoustic (LA) phonon, while the twisting and breathing ones correspond to transverse acoustic (TA) phonons.

Next we address the coupling of the phonon modes to electrons. The relevant electron states for a metallic SWNT are spinors  $\psi_{p\alpha\sigma}(y)$  [20], where  $p=\pm$  denotes the sublattice (the honeycomb lattice has two basis atoms),  $\alpha=\pm$  labels the two distinct K points, and  $\sigma=\pm$  the spin. Suppressing the  $\alpha,\sigma$  indices, the electron-phonon coupling corresponds to Hamiltonian densities  $\mathcal{H}^{K,K'}_{e-ph}$  for the two K points,

$$\mathcal{H}_{e-ph}^{K} = \begin{pmatrix} V_1 & V_2 \\ V_2^* & V_1 \end{pmatrix}, \quad \mathcal{H}_{e-ph}^{K'} = \begin{pmatrix} V_1 & V_2^* \\ V_2 & V_1 \end{pmatrix}. \quad (2.11)$$

Here the deformation potential is

$$V_1 = g_1(u_{xx} + u_{yy}), (2.12)$$

where  $g_1 \approx 16$  eV in bulk graphite [28]. For a 2D graphite sheet this value should be multiplied by 3/2 [12], and we therefore take the estimate  $g_1 \approx 20 - 30$  eV. The off-diagonal terms in sublattice space arise from a bond-length change,

$$V_2 = g_2 e^{3i\eta} (u_{xx} - u_{yy} + 2iu_{xy}), \tag{2.13}$$

where  $\eta$  is the chiral angle, with  $\eta=0$  for zig-zag tubes and  $\eta=\pi/6$  for armchair tubes. The respective coupling constant is  $g_2\approx 1.5$  eV [12]. Although both the free electron and the free phonon low-energy theory do not depend on chirality, the  $V_2$  term in the electron-phonon coupling does.

# III. INTERACTIONS FROM PHONON EXCHANGE

We can now integrate out the phonons and obtain an effective action for the electrons that includes the phonon-mediated retarded interaction. To that purpose, we evaluate the Gaussian path integral for the phonons,

$$\int \mathcal{D}\mathbf{u} \exp\left\{-\frac{1}{2L} \int [dq] \left[\mathbf{u}^{T}(-\omega_{n}, -q)\underline{A}(\omega_{n}, q)\mathbf{u}(\omega_{n}, q)\right] + 2\mathbf{V}^{T}(-\omega_{n}, -q)\mathbf{u}(\omega_{n}, q)\right]\right\} = e^{-S_{e-ph}},$$
(3.1)

with the notation

$$\int [dq] = \frac{1}{\beta} \sum_{\omega_n} \int_{-\infty}^{\infty} \frac{dq}{2\pi}.$$
 (3.2)

The result  $S_{e-ph}$  defines the phonon-mediated contribution to the electronic action. In Eq. (3.1), we use the vector

$$\mathbf{V}(\omega_{n}, q) = g_{1} \left[ \sum_{\alpha} \rho_{\alpha}(\omega_{n}, q) \right] \mathbf{M}(q)$$

$$+ \frac{g_{2}}{2} e^{3i\eta} [J_{1+}(\omega_{n}, q) + J_{2-}(\omega_{n}, q)] \mathbf{N}_{+}(q)$$

$$+ \frac{g_{2}}{2} e^{-3i\eta} [J_{1-}(\omega_{n}, q) + J_{2+}(\omega_{n}, q)] \mathbf{N}_{-}(q).$$
(3.3)

Fourier transforming  $V_1$  and  $V_2$  in Eqs. (2.12) and (2.13) specifies the auxiliary vectors  $\mathbf{M}^T(q) = (0, -iq, 1/R)$ ,  $\mathbf{N}_+^T(q) = (q, iq, 1/R)$ , and  $\mathbf{N}_-(q) = \mathbf{N}_+^*(-q)$ . Using fermionic Matsubara frequencies  $p_n = (2n+1)\pi/\hbar\beta$  and analogous integration measure  $\int [dp]$ , electronic densities are

$$\rho_{\alpha}(\omega_n, q) = \int [dp] \ \overline{\psi}_{\alpha}(p_n, p) \psi_{\alpha}(p_n + \omega_n, p + q).$$

Similarly, electronic currents are defined as

$$J_{\alpha\pm}(\omega_n, q) = \int [dp] \ \overline{\psi}_{\alpha}(p_n, p) \tau_{\pm} \psi_{\alpha}(p_n + \omega_n, p + q).$$
(3.4)

The fermionic (Grassmann) fields represent spinors, where we have suppressed the sublattice and spin indices, and Pauli matrices  $\tau_{\pm} = \tau_1 \pm i\tau_2$  act in sublattice space. The integration over phonons is now straightforward, leading to the phonon-mediated action contribution

$$S_{e-ph} = -\frac{1}{2L} \int [dq] \mathbf{V}^T(-\omega_n, -q) \underline{A}^{-1}(\omega_n, q) \mathbf{V}(\omega_n, q).$$
(3.5)

This form will be analyzed in the remainder of the paper. To make further progress, it is convenient to invoke the Abelian bosonization scheme adapted to SWNTs [20]. To keep the paper self-contained, we briefly review the ingredients needed for our subsequent discussion. This requires first a unitary transformation in sublattice space, which transforms the free-electron Hamiltonian into the standard form containing right- and left-moving fields,  $\psi_{p\alpha\sigma} = \sum_{r=R/L=+} U_{pr} \tilde{\psi}_{r\alpha\sigma}$ , where

$$U = \frac{-e^{-i\pi/4}}{\sqrt{2}} \begin{pmatrix} 1 & 1\\ i & -i \end{pmatrix}.$$

Under the unitary transformation, we have to replace  $\tau_2 \to \tau_3$ ,  $\tau_3 \to \tau_1$ , and  $\tau_1 \to \tau_2$ . We then work in the transformed picture, and omit the tilde in the field operators henceforth. The bosonization formula for the electron operator is [20]

$$\psi_{r\alpha\sigma}(y) = \frac{\eta_{r\alpha\sigma}}{\sqrt{2\pi a}} \exp\{i(rq_F y + \alpha k_F y + r\sqrt{4\pi}\phi_{r\alpha\sigma})\},$$
(3.6)

where  $\eta_{r\alpha\sigma}$  are Klein factors,  $k_F$  is the y-projection of the K point, and  $q_F = |E_F|/v_F$  depends on the doping level  $E_F$ . The chiral fields  $\phi_{r\alpha\sigma}$  are related to a pair of dual nonchiral boson fields,  $\phi_{\alpha\sigma} = \phi_{R\alpha\sigma} + \phi_{L\alpha\sigma}$  and  $\theta_{\alpha\sigma} = \phi_{R\alpha\sigma} - \phi_{L\alpha\sigma}$ . Switching to total/relative charge/spin fields,  $\phi_{c\pm} = \frac{1}{2} \sum_{\sigma} (\phi_{1\sigma} \pm \phi_{2\sigma})$  and  $\phi_{s\pm} = \frac{1}{2} \sum_{\sigma} \sigma(\phi_{1\sigma} \pm \phi_{2\sigma})$ , and similarly for the dual fields, the electronic action including repulsive forward-scattering Coulomb interactions but without phonon exchange is described by a four-channel ( $\lambda = c+, c-, s+, s-$ ) Luttinger liquid [20],

$$S_0 = \sum_{\lambda} \frac{1}{2} \int [dq] \frac{|\phi_{\lambda}(\omega_n, q)|^2}{u_{\lambda}^0 K_{\lambda}^0} (\omega_n^2 + (u_{\lambda}^0)^2 q^2).$$
 (3.7)

We ignore the tiny electron-electron backscattering processes [20] in this paper. The velocities are  $u_{\lambda}^0 = v_F/K_{\lambda}^0$ , where  $K_{\lambda}^0 = 1$  in all neutral channels  $(\lambda \neq c+)$ . For the charged channel,  $u_{c+}^0 = v_F/K_{c+}^0$ , where the Luttinger liquid parameter  $K_{c+}^0$  depends on the electron-electron interaction strength;  $K_{c+}^0 = 1$  for the noninteracting problem. In the presence of unscreened repulsive interactions,  $K_{c+}^0 \approx 0.2$ . In the rest of the paper we shall use the symbols  $u_{\lambda}, K_{\lambda}$  without superscript to denote the values of the effective parameters renormalized by the phonon exchange. After this short review of bosonization for SWNTs, we now analyze the various terms in the phonon-mediated action  $S_{e-ph}$  in Eq. (3.5) using bosonization.

# IV. ATTRACTIVE INTERACTIONS AND WENTZEL-BARDEEN SINGULARITY

To begin with, there is a dominant forward-scattering term coupling to the total electronic density, which in bosonized form reads  $\rho(y) = (2/\sqrt{\pi})\partial_y\phi_{c+}$ . The respective contribution to Eq. (3.5) is

$$S_f = -\frac{g_1^2}{2L} \int [dq] \ \rho(-\omega_n, -q) D_f(\omega_n, q) \rho(\omega_n, q), \quad (4.1)$$

with the inverse propagator

$$D_f(\omega_n, q) = \mathbf{M}^T(-\omega_n, -q)\underline{A}^{-1}(\omega_n, q)\mathbf{M}(\omega_n, q)$$
$$= \frac{M\omega_n^2(1 + q^2R^2) + 4\mu q^2}{\lambda_2 \lambda_3 R^2}.$$

This is the only phonon exchange contribution of order  $g_1^2$ . Due to the large deformation potential [as compared to the coupling  $g_2$ ], it is indeed expected to be the dominant one.

Notice that the twisting mode, corresponding to the eigenvalue  $\lambda_1$ , does not contribute to  $D_f$ . In order to make explicit the contributions from the other two phonon branches, we can rewrite  $D_f$  as follows,

$$D_f(\omega_n, q) = \frac{1}{MR^2} \left[ \frac{Z_2(q, \mu)}{\omega_n^2 + \epsilon_2^2(q)} + \frac{Z_3(q, \mu)}{\omega_n^2 + \epsilon_2^2(q)} \right], \quad (4.2)$$

where we use the functions

$$Z_{2,3}(q,\Lambda) = \pm \frac{R^2}{\Delta E(q)} \left[ -(1+q^2R^2)M\epsilon_{2,3}^2(q) + 4\Lambda q^2 \right];$$
(4.3)

E(q) is defined in Eq. (2.7). The contribution (4.1) thus only operates in the charged channel, there is no effect on neutral channels. Including the action  $S_0$  in Eq. (3.7), the electronic action in the charged channel then takes the form

$$S[\phi_{c+}] = \frac{1}{2v_F} \int [dq] |\phi_{c+}(\omega_n, q)|^2 \left[ \omega_n^2 + (u_{c+}^0)^2 q^2 - (4.4)^2 \right] - \gamma q^2 \left( \frac{Z_2(q, \mu)}{\omega_n^2 + \epsilon_2^2(q)} + \frac{Z_3(q, \mu)}{\omega_n^2 + \epsilon_3^2(q)} \right),$$

where

$$\gamma = 2v_F g_1^2 / \pi^2 \hbar M R^3. \tag{4.5}$$

The term related to  $Z_2$  is due to the stretching mode, while the term related to  $Z_3$  comes from the breathing mode. As pointed out above, the twisting mode drops out in this forward-scattering phonon exchange term, despite its importance for transport coefficients like the high-temperature conductivity [14]. Notice that the retarded phonon exchange contribution comes with a minus sign, indicating attractive interactions.

Further simplifications in Eq. (4.4) are then possible in the long-wavelength limit. To lowest order in qR, Eq. (4.3) gives  $Z_3(q,\Lambda)=1$  and  $Z_2(q,\Lambda)=\Lambda v_S^2 q^2/(\Delta-\Lambda)\omega_R^2$ , so that

$$\frac{Z_2(q,\mu)}{\omega_p^2 + \epsilon_2^2(q)} = \frac{\mu v_S^2 q^2 / B \omega_B^2}{\omega_p^2 + v_S^2 q^2},\tag{4.6}$$

$$\frac{Z_3(q,\mu)}{\omega_n^2 + \epsilon_3^2(q)} = \frac{1}{\omega_n^2 + \omega_R^2}.$$
 (4.7)

The forward scattering due to the stretching mode does not create a significant attractive interaction since it is suppressed by a factor  $(v_S/v_F)^2$  due to the linear dispersion of this phonon mode [11]. A significant attractive interaction can only be expected from the breathing mode. Since  $\omega_B$  corresponds to room temperature for SWNT radius  $R\approx 4$  Å, see Eq. (2.10), we neglect retardation effects from the breathing mode in what follows. This approximation can be justified using the two-cutoff scheme of Ref. [19]. Putting  $\omega_n^2 + \omega_B^2 \to \omega_B^2$  in Eq. (4.7), interactions mediated by the breathing mode then simply renormalize parameters in the effective LL picture. Concerning the stretching mode, see Eq. (4.6), we make no such approximation, and keep its influence on the WB singularity exactly.

Straightforward algebra then leads to exactly the action studied before in Ref. [21],

$$S[\phi_{c+}] = \int [dq] \frac{|\phi_{c+}(\omega_n, q)|^2}{2u_{c+}K_{c+}} \left[ \omega_n^2 + u_{c+}^2 q^2 - \frac{b^2 q^4}{\omega_n^2 + v_S^2 q^2} \right],$$
(4.8)

with the parameter identifications

$$u_{c+}^{2} = (u_{c+}^{0})^{2} - \gamma/\omega_{B}^{2},$$

$$b^{2} = \gamma \mu v_{S}^{2}/B\omega_{B}^{2}.$$
(4.9)

The corresponding LL parameter  $K_{c+}$  is then given by  $K_{c+} = v_F/u_{c+}$ , leading directly to Eq. (1.1) with the radius  $R_B$  defined as

$$R_B = \frac{2g_1^2}{\pi^2 \hbar v_F \Delta} = 2.4 \pm 0.9 \text{ Å}.$$
 (4.10)

The uncertainty in the estimate for  $R_B$  largely results from uncertainties about the value for  $g_1$ , see above. For this action (plus the standard free boson action for the neutral modes), all correlation functions have been worked out in Ref. [21], and one can simply adapt their results to the four-channel case encountered here.

At first sight, when the radius R reaches the critical value  $R_c = (K_{c+}^0)^2 R_B$ , a singularity is found, which corresponds to the WB singularity associated with the breathing phonon mode. However, due to the additional retarded interaction mediated by the stretching mode, i.e. the term  $\sim b^2$  in Eq. (4.8), this singularity is reached at an even larger radius. Following Ref. [21], the condition for the WB singularity is  $b/v_S = u_{c+}$ , leading to a critical radius  $R_c = (K_{c+}^0)^2 R_0$  with

$$R_0 = (\Delta/B)R_B = 3.6 \pm 1.4 \text{ Å}.$$
 (4.11)

The unexpectedly large value predicted for  $R_0$  suggests that it may be possible to reach this elusive singularity in practice. This may come as a surprise, since standard reasoning tells us that a small ratio between sound and Fermi velocity implies negligible effects due to acoustic phonon exchange, and this ratio is rather small in SWNTs. However, the effective phonon exchange at work here involves two phonon branches, namely the stretching mode with  $\epsilon_2(q) = v_S|q|$  and the breathing mode,  $\epsilon_3(q) = \omega_B$ . These two modes reinforce each other in driving the system towards the WB singularity. In addition, in SWNTs one has a very strong deformation potential that provides very efficient electron-phonon coupling.

An important conclusion in the context of nanotube superconductivity is that this forward-scattering phonon exchange process is very efficient in inducing attractive electron-electron interactions. To judge the importance of the stretching mode, we compare the scaling dimensions of various order parameters computed (i) under a non-retarded Luttinger liquid description with LL parameters  $u_{c+}$  and  $K_{c+}$  given in Eqs. (4.9) and (1.1), i.e., neglecting the stretching mode altogether, and (ii) keeping both the breathing mode and the retarded stretching mode, i.e. the action in Eq. (4.8), using a straightforward generalization of exact results from Ref. [21]. Focussing on the scaling dimensions for charge density wave (CDW) and singlet superconductivity (SC) order parameters [20], this comparison is shown in Fig. 1. Remarkably, concerning SC there is practically no difference at all. For the CDW order parameter, a significant difference is observed only in the close vicinity of the WB singularity. Sufficiently far away from the WB singularity, it is therefore possible to neglect the stretching mode and describe the electronic system as a Luttinger liquid with (possibly) attractive interactions. The stretching mode then only affects the location of the WB singularity but

not the magnitude of the non-retarded attractive interactions. The LL interaction strength (including Coulomb interactions and phonon exchange) is determined by the parameter  $K_{c+}$ , which describes attractive interactions for  $K_{c+} > 1$ . With Eq. (1.1), we provide an estimate for  $K_{c+}$  as a function of the tube radius R, the interaction strength parameter  $K_{c+}^0$ , and various material parameters.

### V. OTHER PHONON EXCHANGE CONTRIBUTIONS AND PEIERLS TRANSITION

Let us now consider the remaining terms in the phonon-mediated action (3.5). First we combine the  $J_{\alpha\pm}$  defined in Eq. (3.4), with  $\alpha=1,2=\pm$  labeling the two K points, as  $J_{1+}+J_{2-}=iJ_{c-}+J_{CDW}$  and  $J_{1-}+J_{2+}=-iJ_{c-}+J_{CDW}$ . Here  $J_{c-}=\int [dp]\sum_{\alpha}\overline{\psi_{\alpha}}\tau_{2}\psi_{\alpha}$  and  $J_{CDW}=\int [dp]\sum_{\alpha}\overline{\psi_{\alpha}}\tau_{1}\psi_{\alpha}$ . The reason for these definitions becomes clear once we transform these operators back to real space and transform from sublattice to chiral space. In bosonized form,  $J_{c-}(y)=(2/\sqrt{\pi})\ \partial_{y}\theta_{c-}$  and

$$J_{CDW}(y) = \frac{4}{\pi a} \Big( \cos(2q_F y + \sqrt{\pi}\phi_{c+}) \cos(\sqrt{\pi}\phi_{c-}) + \sin(\sqrt{\pi}\phi_{s+}) \sin(\sqrt{\pi}\phi_{s-}) + [\sin\leftrightarrow\cos] \Big).$$
 (5.1)

These expressions show that  $J_{c-}$  is just the current density in the c- channel, whereas  $J_{CDW}$  is the intersublattice CDW order parameter [20]. Phonon interactions involving  $J_{CDW}$  are therefore important in relation to the Peierls transition and describe phonon backscattering processes.

From Eq. (3.5), we then obtain several other contributions in addition to the  $g_1^2$  term in Sec. IV, namely S' and S'' due to the  $g_2^2$  and  $g_1g_2$  terms, respectively. Let us start with  $S' = S'_{c-} + S'_{CDW}$ , where

$$S'_{c-} = -\frac{g_2^2}{L} \int [dq] |J_{c-}(\omega_n, q)|^2 \times \left[\sin^2(3\eta)D_+(\omega_n, q) + \cos^2(3\eta)D_-(q)\right], \quad (5.2)$$

and

$$S'_{CDW} = -\frac{g_2^2}{L} \int [dq] |J_{CDW}(\omega_n, q)|^2 \times \left[\cos^2(3\eta)D_+(\omega_n, q) + \sin^2(3\eta)D_-(q)\right].$$
 (5.3)

The inverse propagators are  $D_{-}(q) = q^2/\lambda_1$  and

$$D_{+}(\omega_{n}, q) = \frac{M\omega_{n}^{2}(1 + q^{2}R^{2}) + 4Bq^{2}}{\lambda_{2}\lambda_{3}R^{2}}$$

$$= \frac{1}{MR^{2}} \left[ \frac{Z_{2}(q, B)}{\omega_{n}^{2} + \epsilon_{2}^{2}(q)} + \frac{Z_{3}(q, B)}{\omega_{n}^{2} + \epsilon_{3}^{2}(q)} \right].$$
(5.4)

The functions  $Z_{2,3}$  were defined in Eq. (4.3). In principle, there is another contribution to S' from mixed terms

involving the product of  $J_{c-}$  and  $J_{CDW}$ . However, such terms vanish for a doped SWNT by virtue of momentum conservation. In real space, this is reflected by the oscillatory  $\cos(2q_Fy)$  factor appearing in  $J_{CDW}$ . Since this factor is absent in  $J_{c-}$ , we ignore the mixed terms in what follows. The second contribution to the action reads

$$S'' = \frac{g_1 g_2}{L} \sin(3\eta) \int [dq]$$

$$\times \rho_{c+}(-\omega_n, -q) D_m(\omega_n, q) J_{c-}(\omega_n, q),$$

$$(5.5)$$

with

$$D_{m}(\omega_{n}, q) = \frac{M\omega_{n}^{2}(1 - q^{2}R^{2})}{\lambda_{2}\lambda_{3}R^{2}}$$

$$= \frac{1}{MR^{2}} \left[ \frac{\tilde{Z}_{2}(q)}{\omega_{n}^{2} + \epsilon_{2}^{2}(q)} + \frac{\tilde{Z}_{3}(q)}{\omega_{n}^{2} + \epsilon_{3}^{2}(q)} \right] ,$$
(5.6)

where  $\tilde{Z}_{2,3}(q) = \mp (1 - q^2 R^2) M R^2 \epsilon_{2,3}^2(q) / \Delta E(q)$ , with E(q) given in Eq. (2.7). At long wavelengths, this yields  $\tilde{Z}_2(q) = -v_S^2 q^2 / \omega_B^2$  and  $\tilde{Z}_3(q) = 1$ . Then Eq. (5.6) simplifies to

$$D_m(\omega_n, q \ll R^{-1}) = \frac{\omega_n^2 / \Delta}{\omega_n^2 + v_S^2 q^2}.$$
 (5.7)

Again, there is in principle another contribution that arises from mixing  $\rho_{c+}$  with  $J_{CDW}$ . However, this contribution also vanishes by virtue of momentum conservation and is disregarded.

Next, we analyze these additional terms using bosonization, starting with the forward-scattering term  $S'_{c-}$ , which can be treated along the same lines as the forward-scattering term in the c+ channel, see Sec. IV. Neglecting retardation in the breathing mode as above, the long-wavelength action for the bosonic field  $\theta_{c-}$  including  $S'_{c-}$  is

$$S[\theta_{c-}] = \frac{1}{2v_F} \int [dq] |\theta_{c-}(\omega_n, q)|^2 \left\{ \omega_n^2 + v_F^2 q^2 - \gamma' q^2 \right\}$$

$$\times \left[ \sin^2(3\eta) \left( \frac{1}{\omega_B^2} + \frac{4B^2 q^2 R^2 / \Delta^2}{\omega_n^2 + v_S^2 q^2} \right) + \cos^2(3\eta) \frac{q^2 R^2}{\omega^2 + v_S^2 q^2} \right] \right\},$$
(5.8)

with the parameter  $\gamma'=2v_Fg_2^2/\pi^2\hbar MR^3$ . Amusingly, the contributions of different phonon modes are weighted by chirality-dependent factors. In particular, for zigzag tubes  $(\eta=0)$  only the twisting mode contributes, whereas for armchair tubes  $(\eta=\pi/6)$  only breathing and stretching modes do. Again we obtain a WB singularity but now in the c- channel at a corresponding critical radius  $R_0'=2g_2^2/\pi^2\hbar v_F\mu$ . Inserting the parameter values given above, due to the small ratio  $g_2/g_1$ , the critical radius is exceedingly small,  $R_0'\approx 0.02$  Å. Using

the same reasoning as in Sec. IV, the effect of  $S'_{c-}$  again leads to a LL action in the c- channel, with a renormalization of  $u_{c-}$  and  $K_{c-}$ . However, such renormalizations amount to tiny changes of the order  $10^{-3}$  even for very thin SWNTs. Therefore  $S'_{c-}$  does not imply observable consequences and is omitted henceforth.

Next we focus on S'', which mixes the c+ and c- sectors and constitutes another forward scattering mechanism. First, we observe that this term vanishes for zigzag tubes ( $\eta = 0$ ). Neglecting again retardation in the breathing mode and keeping only terms to lowest order in qR, we find from Eq. (5.7)

$$S'' = \epsilon \kappa \int [dq] \phi_{c+}(-\omega_n, -q) \theta_{c-}(\omega_n, q) \frac{\omega_n^2 q^2}{\omega_n^2 + v_S^2 q^2}, \quad (5.9)$$

with  $\epsilon = g_2/g_1$  and  $\kappa = \sin(3\eta)v_F R_B/\hbar R$ . Introducing the notation  $\Phi^T = (\phi_{c+}, \theta_{c+}, \phi_{c-}, \theta_{c-})$ , the total action [including Eq. (4.8) and S''] can be written as

$$S = \frac{1}{2} \int [dq] \Phi^T [\underline{S}_0 + \epsilon \underline{S}_1] \Phi, \qquad (5.10)$$

where  $\underline{S}_0$  is a block-diagonal matrix in (c+,c-) space, and  $\underline{S}_1$  contains the mixing term due to S''. Since  $\epsilon \ll 1$ , we proceed by expanding to first order in  $\epsilon$ . This allows the explicit calculation of scaling dimensions of all order parameters of interest. Details about this calculation are contained in an appendix, and the main results are shown in Fig. 2. Clearly, the effect of S'' is also very tiny, even for very thin tubes. Neglecting this term, only the term  $S'_{CDW}$  describing backscattering phonon exchange remains.

Let us then study the  $S'_{CDW}$  term. As this describes an effective interaction involving  $J_{CDW}$ , this part monitors the possibility of a Peierls transition. In order to keep the discussion transparent, we focus on the static limit. Then Eq. (5.3) reduces to

$$S'_{CDW} = -\frac{g_2^2}{\mu L} \int [dq] |J_{CDW}(\omega_n, q)|^2.$$
 (5.11)

Transforming to real space, using the bosonized expression of  $J_{CDW}$  in Eq. (5.1), we find a term involving  $4q_F$  oscillatory contributions that violate momentum conservation and average to zero, and in addition a tiny renormalization of the LL parameters  $u_{\lambda}$  and  $K_{\lambda}$ . This renormalization represents a direct generalization of the one/two-channel theory of Voit and Schulz [11] to the four-channel case of interest here. We do not give any details here, since the relevant dimensionless coupling constant is  $R'_0/\pi^3 R$ , and the resulting renormalizations are again of order  $10^{-3}$ , i.e. unobservable. Nevertheless, we confirm the finding of Ref. [15] that the relevant Peierls distortion mode for armchair SWNTs is given by a twist distortion, see Eq. (5.3). For arbitrary chiral angle  $\eta$ , however, the relevant distortion involves a linear

combination of all three phonon modes. Finally, we mention that on half-filling, the oscillatory contribution could survive. However, its scaling dimension suggests that this term is strongly irrelevant unless electron-electron backscattering gaps out the neutral channels. For very thin tubes, these gaps may be sufficiently pronounced [20] to allow for Eq. (5.11) to be a relevant perturbation. Provided  $K_{c+} < 2$ , one could possibly expect a small (twist) Peierls gap in this nearly commensurate situation, see Ref. [15]. However, this would require a detailed analysis of additional phonon exchange processes neglected above due to incommensurability. Away from half-filling, we do not see a possibility for this gap to survive.

#### VI. DISCUSSION AND CONCLUSIONS

In this paper, we have studied acoustic phonon exchange mechanisms operating in an individual metallic SWNT. The description of phonons within an elastic continuum model allows for explicit analytical progress, and we have shown that integrating out the phonon system can produce very substantial attractive electron-electron interactions. For sufficiently large tube radius, the system can be described by a standard Luttinger liquid theory, where the interaction parameter  $K_{c+}$  is renormalized away from the value  $K_{c+}^0 \leq 1$  describing the theory without phonons but fully taking into account Coulomb interactions. We have shown that  $K_{c+} > 1$  corresponding to attractive interactions is possible, in particular once the Coulomb interactions are externally screened. These attractive interactions are basically mediated via a breathing phonon mode. For thin SWNTs, one also has to take into account a retarded branch describing a stretching mode. The combined effect of the stretching and the breathing mode then produces a Wentzel-Bardeen singularity at a critical radius  $R_0 \approx 3.6$  Å. Nanotubes may then offer the possibility to reach this singularity in experiments. Remarkably, all other mechanisms, e.g. backscattering phonon exchange, turn out to be remarkable inefficient in mediating effective electron-electron interactions. In particular, based on our analysis, it should be extraordinarily difficult to observe traces of the Peierls transition. As our treatment is essentially exact, we believe that this also invalidates some earlier theories that were mainly based on mean-field approximations.

As mentioned in the introduction, the phonon-mediated attractive interaction can only drive the system into a true superconducting phase if inter-tube couplings are taken into account. This will be studied in detail elsewhere [23]. In order to gain preliminary insights about inter-tube phonon exchange effects in a rope of SWNTs or a multi-wall nanotube, let us briefly contemplate a simplified model of two parallel SWNTs and study phonon exchange in the presence of elastic couplings between both tubes. We shall focus on the breathing mode

alone, which will produce the most important effects. In the long-wavelength limit, it can be approximated as a dispersionless mode, leading to the free-phonon action

$$S = \frac{M}{2L} \int [dq] \sum_{i,j=1,2} u_i(-\omega_n, -q) A_{ij}(\omega_n) u_j(\omega_n, q),$$

where  $u_i$  is the radial component  $(u_z)$  of the displacement field on tube i,

$$A_{ij}(\omega_n) = \begin{pmatrix} \omega_n^2 + \omega_B^2 (1 + \alpha_l) & -\alpha_t \omega_B^2 \\ -\alpha_t \omega_B^2 & \omega_n^2 + \omega_B^2 (1 + \alpha_l) \end{pmatrix},$$

and  $\alpha_t, \alpha_l$  are dimensionless parameters. While one can compute these parameters from a microscopic force-constant model, here we take them simply as phenomenological parameters. On general grounds, they must obey  $0 \le \alpha_{t,l} \le 1$ , where  $\alpha_{t,l} = 0$  in the absence of intertube couplings. With total electronic densities  $\rho_i$  on tube i = 1, 2, the dominant electron-phonon interaction is due to the deformation potential (3.3), producing a contribution

$$(g_1/2\pi R^2) \int [dq] \sum_{i=1,2} \rho_i(-\omega_n, -q) u_i(\omega_n, q)$$

to the action. We can diagonalize this action by introducing symmetric and antisymmetric combinations,  $u_{s/a} = (u_1 \pm u_2)/\sqrt{2}$  and  $\rho_{s/a} = (\rho_1 \pm \rho_2)/\sqrt{2}$ . Integrating out the phonons, the forward-scattering contribution in the c+ channel leads to a Luttinger liquid, but with renormalized parameters,

$$S[c+] = \frac{1}{2} \sum_{j=s,a} \int [dq] \frac{|\phi_{j,c+}|^2}{u_{j,c+} K_{j,c+}} \left[ \omega_n^2 + (u_{j,c+})^2 q^2 \right],$$
(6.1)

where  $u_{s/a,c+} = v_F/K_{s/a,c+}$ . The interaction parameters are

$$K_{s/a,c+} = \frac{K_{c+}^0}{\sqrt{1 - (K_{c+}^0)^2 R_B / f_{s/a} R}},$$
 (6.2)

where  $f_{s/a} = 1 + \alpha_l \mp \alpha_t$ .

There are now two types of superconducting order parameters. Focusing on the most important singlet superconducting fluctuations, there is one operator describing a Cooper pair on the same tube,  $\mathcal{O}_{SSC0}^{\text{intra}}$ , and another one where the electrons forming the Cooper pair reside on different tubes,  $\mathcal{O}_{SSC0}^{\text{inter}}$ , with explicit form

$$\mathcal{O}_{SSC0}^{\text{intra}} \sim \sum_{r\alpha\sigma} \sigma \psi_{1,r\alpha\sigma} \psi_{1,-r-\alpha-\sigma},$$

$$\mathcal{O}_{SSC0}^{\text{inter}} \sim \sum_{r\alpha\sigma} \sigma \psi_{1,r\alpha\sigma} \psi_{2,-r-\alpha-\sigma},$$

where  $\psi_{1/2,r\alpha\sigma}$  is the electron spinor on tube 1/2. From Eq. (6.1), the scaling dimensions of these operators follow as

$$\Delta_{SSC0}^{\text{intra}} = \frac{1}{8} \left( 6 + \frac{1}{K_{s,c+}} + \frac{1}{K_{a,c+}} \right), \tag{6.3}$$

$$\Delta_{SSC0}^{\text{inter}} = \frac{1}{8} \left( 6 + \frac{1}{K_{s,c+}} + K_{a,c+} \right). \tag{6.4}$$

Two conclusions can be drawn from the inspection of these scaling dimensions. First, for inter-tube couplings with  $\alpha_t$  sufficiently larger than  $\alpha_l$ , attractive interactions within a given tube are increased. Second, whenever  $K_{a,c+} > 1$ , which holds true in the absence of Coulomb interactions, the intra-tube superconducting order parameter is always more relevant than the inter-tube one. In other words, we expect that Cooper pairs predominantly form on a given tube but not across different tubes. Remarkably, this conclusion does not depend on the values of  $\alpha_{l,t}$ . Clearly, this finding will be important in the theoretical analysis of experiments on SWNT ropes and related systems.

Finally, we briefly address the role of electron-electron backscattering that has been neglected in our study. From Ref. [20], backscattering is expected to open tiny gaps that depend exponentially on the radius R. While for R > 5 Å, the gap is extremely small and of no relevance in practice, for ultrathin tubes  $(R \approx 2 \text{ Å})$  the gaps may be more important. However, in this limit also the bandstructure may change in a profound way due to hybridization of  $\pi$  and  $\sigma$  orbitals, and the analysis of Ref. [20] cannot simply be taken over. In addition, the presence of the Wentzel-Bardeen singularity poses an intrinsic lower limit to the validity and self-consistency of our effective low-energy approach. With the predicted value  $R_0 \approx 3.6$  Å, we therefore do not expect that backscattering leads to dramatic changes to the picture put forth in this paper.

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### APPENDIX A: PERTURBATIVE TREATMENT OF S'

In this appendix, we briefly describe some details concerning the perturbative treatment of S', see Eq. (5.9), in Sec. V. With the notation  $\Phi^T = (\phi_{c+}, \theta_{c+}, \phi_{c-}, \theta_{c-})$ , the full action in the total/relative charge channels is Eq. (5.10) with the block-diagonal matrix  $\underline{S}_0 = \operatorname{diag}(\underline{A}_{c+}, \underline{A}_{c-})$ , where

$$\begin{split} \underline{A}_{c+} &= \begin{pmatrix} \frac{u_{c+}^2}{v_F} q^2 - \frac{b^2 q^4 / v_F}{\omega_n^2 + v_S^2 q^2} & -i \omega_n q \\ -i \omega_n q & v_F q^2 \end{pmatrix}, \\ \underline{A}_{c-} &= \begin{pmatrix} v_F q^2 & -i \omega_n q \\ -i \omega_n q & v_F q^2 \end{pmatrix}. \end{split}$$

Furthermore, the mixing term leads to a matrix  $\underline{S}_1$ , whose only non-zero entry is

$$(\underline{S}_1)_{14} = (\underline{S}_1)_{41} = \kappa \omega_n^2 q^2 / (\omega_n^2 + v_S^2 q^2),$$

where  $\kappa$  is defined immediately after Eq. (5.9). We then expand to first order in  $\epsilon$ ,

$$(\underline{S}_0 + \epsilon \underline{S}_1)^{-1} = \underline{S}_0^{-1} - \epsilon \underline{S}_0^{-1} \underline{S}_1 \underline{S}_0^{-1} + \mathcal{O}(\epsilon^2)$$
$$= S_0^{-1} - \epsilon \kappa \begin{pmatrix} 0 & \underline{H} \\ \underline{H}^T & 0 \end{pmatrix}.$$

Some algebra yields for the matrix  $\underline{H}$  the following result:

$$\underline{H} = \left( \begin{array}{cc} (iv_F \omega_n/q) \mathcal{P} & v_F^2 \mathcal{P} \\ \mathcal{P}' & (iv_F \omega_n/q) \mathcal{P} \end{array} \right),$$

where

$$\mathcal{P} = \sum_{\beta = \pm, i} \frac{F_{\beta} Q_i^{\beta}}{\omega_n^2 + v_{i\beta}^2 q^2}, \quad \mathcal{P}' = \sum_{\beta = \pm, i} \frac{v_{i\beta}^2 F_{\beta} Q_i^{\beta}}{\omega_n^2 + v_{i\beta}^2 q^2}.$$

Here i=0,1,2 and we denoted  $v_{1\pm}=v_S,v_{2\pm}=v_F$ . The velocities  $v_{0\pm}\equiv v_{\pm}$  and the coefficients  $F_{\beta},C_{\beta}$  are given in Ref. [21]:

$$\begin{split} 2v_{\pm}^2 &= u_{c+}^2 + v_S^2 \mp \sqrt{(u_{c+}^2 - v_S^2)^2 + 4b^2}, \\ F_{\beta} &= \frac{v_{\beta}^2 - v_S^2}{v_{\beta}^2 - v_{-\beta}^2}, \\ C_{\beta} &= \frac{u_{c+}}{v_{\beta}} \frac{v_{\beta}^2 - v_S^2 + b^2/u_{c+}^2}{v_{\beta}^2 - v_{-\beta}^2}. \end{split}$$

Finally, the coefficients  $Q_i^{\beta}$  are defined by

$$Q_0^{\pm} = \frac{-v_{\pm}^2}{(v_{\pm}^2 - v_S^2)(v_{\pm}^2 - v_F^2)},$$

$$Q_1^{\pm} = \frac{-v_S^2}{(v_S^2 - v_F^2)(v_S^2 - v_{\pm}^2)},$$

$$Q_2^{\pm} = \frac{-v_F^2}{(v_F^2 - v_S^2)(v_F^2 - v_{\pm}^2)}.$$

With this, it is straightforward to compute correlation functions for the bosonic field. The T=0 equal-time correlation functions  $\langle \Phi_i(x)\Phi_i(0)\rangle$  are given by

$$\langle \Phi_i(x)\Phi_j(0)\rangle = -\frac{G_{ij}}{4\pi} \ln([x^2 + a^2]/L_0^2),$$

where a and  $L_0$  are UV and IR cutoff lengths. The only non-zero entries of  $G_{ij}$  are  $G_{33} = G_{44} = 1$  and

$$\begin{split} G_{11} &= \sum_{\beta} v_F F_{\beta}/v_{\beta}, \\ G_{14} &= -\epsilon \kappa v_F^2 \sum_{\beta,i} F_{\beta} Q_i^{\beta}/v_{i\beta}, \\ G_{22} &= \sum_{\beta} u_{c+} C_{\beta}/v_F, \\ G_{23} &= -\epsilon \kappa \sum_{\beta,i} v_{i\beta} F_{\beta} Q_i^{\beta}. \end{split}$$

With this, the scaling dimension of any operator  $\exp[i\alpha^T\Phi(x)]$  is found as  $\alpha^T\underline{G}\alpha/4\pi$ .

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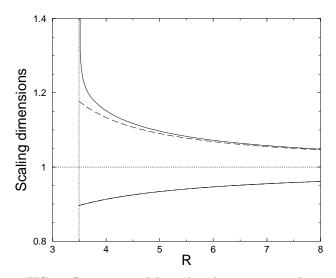


FIG. 1. Comparison of the scaling dimensions as a function of radius R (in Å) for SC (lower curves) and CDW (upper curves) order parameters. Here we take the deformation potential coupling constant  $g_1=25$  eV. The dashed curves give the non-retarded LL prediction, while the solid curves rely on Eq. (4.8). The dotted vertical line denotes the location of the WB singularity. In the case of the SC order parameter, the dashed and the solid curves cannot be distinguished.

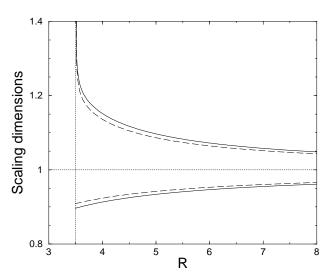


FIG. 2. Comparison of the scaling dimensions as a function of radius R (inÅ) for the SC (lower curve) and the CDW (upper curve) order parameter, computed with  $\epsilon=0$  (dashed curves) and  $\epsilon=0.06$  (solid curves). The calculation employs Eq. (4.8). Taking  $g_1=25$  eV, the value  $\epsilon=0.06$  corresponds to  $g_2=1.5$  eV. We consider the case of an armchair tube  $(\eta=\pi/6)$ , where the effect of S'' is most pronounced.