Auger transitions in one-dimensional metals

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(Dated: February 2, 2008)

We present a dynamical theory of the Auger decay in one-dimensional (1D) metals described by the Tomonaga-Luttinger model. An analytic expression of the Auger current is derived in the framework of the 1-step approach, where the finite lifetime of the initial core-hole and the core-valence interaction are taken into account. This allows to capture typical dynamical features like the shake-down effect, in which the Auger spectrum shows a non-vanishing weight above the 2-step high-energy threshold. The obtained results give also a hint to understand the sizable suppression of Auger spectral weight closed to the Fermi energy recently observed in carbon nanotubes with respect to graphite.

INTRODUCTION

The dynamics of the core-valence-valence (CVV) Auger transitions in strongly correlated solids has been extensively studied during the last three decades\[1\]. However, despite the great interest devoted to this problem, several aspects are still not well understood. The theoretical calculation of the Auger spectrum of correlated solids is a challenging task because, beside the intrinsic difficulty to deal with a many-body interacting system, the creation of the core-hole and the Auger process itself are in principle coherent events, involving virtual Auger transitions and incomplete relaxation phenomena\[2\]. The complete formulation of the theory describing the Auger decays has been provided in 1980 by Gunnarsson and Schönhammer (GS)\[2\]. In the framework of the so-called 1-step approach, they derived a general formula for the Auger current by treating the decay of the initial core-hole to all orders. Unfortunately such formulation cannot be cast in terms of Green’s functions and is of hard implementation for practical purposes. A significant progress can be done within the 2-step approximation, where the photoemission and the Auger decay are considered as independent events. In this framework, Cini\[3\] and Sawatzky\[4\] (CS) proposed a simple and elegant theory able to provide a quantitative understanding of the experimental Auger spectra of transition metals with (almost) closed valence bands. An advantage of such theory is that it also provides a practical scheme to estimate the value of the screened interaction from the experimental spectra\[5, 6, 7\]. This is particularly useful to support LDA+$U$ calculations\[8\]. In the case of open-band systems the CS approach breaks down and no reliable theory is currently available. Very recently Seibold and collaborators\[8\] presented a theory of the dynamical two-particle response function in the 2D Hubbard model based on the time-dependent Gutzwiller approximation. Although important effects are not treated there (e.g., the finite lifetime of the core-hole and the interaction of the core-hole with the valence electrons), the theory provides a novel tool to attack the calculation of the Auger spectrum in correlated open-band systems.

In this paper we develop a dynamical theory of the CVV Auger transitions in an ideal 1D metal. In the CVV Auger decay two holes are left in the valence band after the X-ray photoemission of a deep core-hole. Here assume that the valence electrons form the so-called Luttinger Liquid (LL), described by the Tomonaga-Luttinger model. We also allow for the interaction between the core-hole and the valence electrons and introduce a term responsible for the Auger transition, which destroys the core-hole and creates the Auger electron together with the two valence holes (and viceversa). The corresponding Auger current is calculated analyticly by using the bosonization and equations of motion methods.

The paper is organized as follows. In Section II we describe in detail the model Hamiltonian used in the present work. In Section III we derive a closed analytic expression for the Auger current in framework of the 1-step approach. In Section IV we discuss the relevant features emerging form the obtained formula. In particular we show that the theory exposed here is able to capture some striking features recently observed in the Auger spectra of carbon nanotubes. Finally, a brief summary and the main conclusions are drawn in Section V.

THE MODEL

The LL is the prototype of interacting electrons confined in one spatial dimension, characterized by striking phenomena such as the so-called spin-charge separation and the power-law dependence of observables in proximity of the Fermi energy\[10, 11, 12, 13, 14, 15\]. In $H_{\text{Lutt}}$, the electrons have a linear dispersion relation around positive (Right) and negative (Left) Fermi points and the electron-electron (e-e) interactions act only between Right/Left electron densities. The model is exactly solvable by means of the bosonization technique, which allows to write the electron Hamiltonian in terms of bo-
son operators $b^\dagger_s$:

$$H_{\text{Lutt}} = \frac{v_F}{2} \sum_{q \neq 0, \sigma} |q| \left[ b^\dagger_\sigma(q) b_\sigma(q) + b_\sigma(q) b^\dagger_\sigma(q) \right],$$

$$+ \sum_{q \neq 0, \sigma} \frac{g_s}{4\pi} |q| \left[ b^\dagger_\sigma(q) b_\sigma(q) + b_\sigma(q) b^\dagger_\sigma(q) \right],$$

$$+ b^\dagger_\sigma(q) b_{-\sigma}(q) + b_\sigma(q) b^\dagger_{-\sigma}(q),$$

$$- \sum_{q \neq 0, \sigma} \frac{g_s}{4\pi} |q| \left[ b^\dagger_\sigma(q) b^\dagger_\sigma(-q) + b_\sigma(q) b_\sigma(-q) \right]$$

$$+ b^\dagger_\sigma(q) b^\dagger_{-\sigma}(-q) + b_\sigma(q) b_{-\sigma}(-q),$$

where $\sigma = \uparrow, \downarrow$ is the spin index, $[b_\sigma(q), b^\dagger_{\sigma'}(q')] = \delta_{\sigma,\sigma'} \delta_{q,q'}$, $v_F$ is the Fermi velocity, $g_s$ is the interaction parameter between Right-Right (positive $q$) and Left-Left (negative $q$) electron densities, while $g_s$ is the interaction parameter between Left-Right densities.

The key point of the bosonization is that it is possible to express the fermion fields in terms of boson fields. Here it is useful to introduce a chirality index $\nu = R, L$ to distinguish between Right and Left electron modes. For instance the $\nu = R$ fermion field is given by:

$$\psi_{\sigma,R}(x) = \frac{\eta_{R,\sigma}}{(2\pi\alpha)^{1/2}} e^{i\Phi_{\sigma,R}(x)},$$

where $\eta_{R,\sigma}$ is an anticommuting Klein factor and

$$\Phi_{\sigma,R}(x) = \sum_{q > 0} \left( \frac{2\pi}{qL} \right)^{1/2} e^{-\alpha q/2} \left[ b^\dagger_\sigma(q) e^{-iqx} + b_\sigma(q) e^{iqx} \right]$$

$$+ \varphi_{0,R} + 2\pi x N_{R}/L,$$

where $N_R$ is the total number of Right-electrons, $[\varphi_{0,R}, N_R] = i$ and $L$ is the length of the system. $\alpha$ is a short-distance cutoff that must be introduced in order to have converging integrals. In principle the bosonization provides exact results in the limit $\alpha \to 0$, however for practical purposes it is useful to take a non-zero (small) $\alpha$ which introduces a finite effective bandwidth $\gamma = v_F/\alpha$ in the system.

By doing this we have to bare in mind that such procedure gives an accurate physical description only in the low-energy part of the spectrum.

The coupling of valence electrons to the core-hole is given by

$$H_\lambda = \sqrt{\frac{2\pi}{L}} \sum_{q \neq 0} \lambda(q) [b^\dagger_\sigma(q) + b_\sigma(q)](1 - n_c),$$

where $\lambda(q)$ is the core-valence coupling constant, $L$ is the volume of the system, $c^{(1)}_c$ is the annihilation (creation) operator of the core-electron, whose occupancy and energy are $n_c = c^\dagger_c c_c$ and $\varepsilon_c$ respectively. In the following we will take $\lambda(q) \equiv \lambda$.

The term responsible for the Auger decay is more conveniently expressed in the fermionic representation and reads:

$$H_A = c^\dagger_p c^\dagger_c A + \text{h.c.}, \quad A = V \psi_i(0) \psi_i(0),$$

where $c_p^{(1)}$ destroys (creates) the Auger electron and

$$\psi_\sigma = \psi_{\sigma,R} + \psi_{\sigma,L}.$$

$V$ is the so-called Auger matrix element, which here is taken as a constant. Here we are assuming for simplicity that the CVV decay leaves the two final holes in the origin of the system in a singlet configuration. This reflects the local nature of the Auger process; however such assumption is not essential and could be relaxed.

As long as the interactions do not depend on spin, $H_{\text{Lutt}}$ can be diagonalized by introducing charge and spin boson operators: $b_c^{(1)}(q) = [b^\dagger_\uparrow(q) \pm b^\dagger_\downarrow(q)]/\sqrt{2}$ and performing a Bogoliubov transformation in the charge sector: $b_c(q) = \cosh \varphi_c(q) + \sinh \varphi_c(q)$, $b^\dagger_c(q) = \sinh \varphi_c(q) - \cosh \varphi_c(q)$ with $\tan 2\varphi = (g_s/\alpha)/v_F + g_s/\pi$ and renormalized velocity $v = [(v_F + g_s/\pi)^2 - (g_s/\pi)^2]^{1/2}$. In the next Section we use the bosonization scheme sketched above compute the Auger spectrum of a 1D metal described within the Luttinger liquid theory.

**CALCULATION OF THE AUGER SPECTRUM**

The 1-step formulation of the the Auger processes has been provided by GS\[2\] who showed that the Auger current is given by the following correlator:\[2\][22]:

$$j(\omega) = \frac{\pi\alpha^2}{2} \int_0^\infty dt \int_0^\infty dt' e^{i\omega(t-t')} f(t, t')$$

where the factor $\pi\alpha^2/2$ is chosen in order to have a normalized spectrum and

$$f(t, t') = \langle g| e^{iH[0]t} | f \rangle e^{iH[1](t-t')} A c^\dagger_c e^{-iH[0]t} c_c | g \rangle.$$

In the above expression $|g\rangle$ is the ground state before the X-ray photoemission, $H[0,1]$ is the Hamiltonian of the system $H = H_{\text{Lutt}} + \varepsilon_c(1 - n_c) + H_\lambda$ with $n_c = 0, 1$ respectively, and $\Gamma$ is an effective optical potential describing virtual Auger transitions and relaxation processes. In order to proceed we make the following approximation:

$$f(t, t') \approx \langle g| e^{iH[0]t'} A^\dagger e^{iH[1](t-t')} A e^{-iH[0]t} | g \rangle$$

$$\times e^{-\varepsilon_c(t-t')} e^{-\Gamma(t+t')}$$

$$\equiv C(t, t') \times e^{-\varepsilon_c(t-t')} e^{-\Gamma(t+t')}$$

where the second line of the above equation is the core-hole Green’s function with lifetime $1/\Gamma$ which is a c-number. $|g\rangle$ denotes the ground state of $H_{\text{Lutt}}$ (whose elementary excitations are created by $b^\dagger_c$ and $b^\dagger_c$), describing
the valence band in the initial state, and \( \tilde{H}[0] \equiv H[0] - \varepsilon_c \).

As noticed by GS\[2\], the strength of the effective optical potential is proportional to the square of the Auger matrix element, and hence we can replace \( V^2 \) by \( \Gamma \). \( C(t, t') \) can be calculated exactly by using the bosonization formulas in Eqs.\[3\] and the equations of motion method. After some algebra one gets a compact expression by introducing new variables \( \tau = t - t' \) and \( T = (t + t')/2 \):

\[
C(\tau, T) = \frac{\Gamma}{2\pi} \left[ \frac{\alpha e^{\phi(\tau, T)}}{(-i\tau\nu + \alpha)^g} + \frac{\alpha^{l+1} e^{\psi(\tau, T)}}{(-i\tau\nu + \alpha)^l(-i\tau\nu F + \alpha)} \right],
\]

where we have defined \( \phi = 2(\cosh^2\varphi + \sinh^2\varphi) \) and \( \psi = (\cosh \varphi + \sin \varphi)^2 \). The complex functions \( h(\tau, T) \) and \( k(\tau, T) \) are reported in Appendix A. Finally the Auger current reads

\[
j(\omega - \varepsilon_c) = \int_{-\infty}^{\infty} d\tau \int_0^\infty dT \ e^{i\omega T} e^{-2\Gamma T} C(\tau, T),
\]

where we refer the kinetic energy of the Auger electron \( \omega \) with respect to the core-level energy \( \varepsilon_c \). Eqs.\[10\] and \[11\] constitute the main finding of the present work. In the next Section we discuss the most relevant features emerging from Eqs.\[10\] and \[11\], which give a hint to understand the physics of the Auger transitions in 1D systems.

**DISCUSSION**

We first observe that despite the LL nature of the valence electrons, the correlator \( C(\tau, T) \) does not obey a power-law, which is spoiled by the interaction \( \lambda \) between the valence electrons and the core-hole. It is also interesting to study the relationship of our solution with the 2-step approach. This is done in the limit \( \Gamma \to 0 \). As discussed by GS, if such limit exists, one should recover the well-known 2-step solution since the Auger transition happens after the complete relaxation of the initial state. Such limit is carried out by observing that

\[
\lim_{\Gamma \to 0} 2\Gamma \int_0^\infty dT e^{-2\Gamma T} e^{z(\tau, T)} = \lim_{T \to \infty} e^{z(\tau, T)},
\]

with \( z = h, k \). We note that for any finite \( \lambda \) the limit on the r.h.s. does not exist because for large \( T \) we have \( h(\tau, T) \sim k(\tau, T) \sim (\lambda/v)^2 i\nu \tau \ln(\nu T/\alpha) \). This is a remarkable result, showing that the 2-step approach is not justified if the valence band is described by the LL. On the other hand if we set \( \lambda = 0 \) the 1-step and 2-step solutions do coincide because the 2-step spectrum is obtained from the 2-particle Green’s function describing the valence electrons (holes) in the ground state of \( H_{\text{sat}} \). The 2-step approach is often employed in typical Auger calculations and therefore it is instructive to compare it with our 1-step solution. The 2-step Auger current is readily obtained by setting \( \lambda = 0 \) and results

\[
j_{2\text{-step}}(\omega - \varepsilon_c) = \int_{-\infty}^{\infty} d\tau \ e^{i\omega \tau} \frac{\alpha e^{h(\tau, T)}}{4\pi} \left[ \frac{\alpha}{(-i\tau\nu + \alpha)^g} + \frac{\alpha^{l+1}}{(-i\tau\nu + \alpha)^l(-i\tau\nu F + \alpha)} \right],
\]

which recovers the characteristic power law suppression at \( \omega \approx 0 \). The comparison between the Auger spectra calculated with \( j(\omega - \varepsilon_c) \) and \( j_{2\text{-step}}(\omega - \varepsilon_c) \) is shown in Fig.\[1\]  As discussed above, it is seen that \( j \) does not approach \( j_{2\text{-step}} \) for small \( \Gamma \) (compared to \( \gamma \)). In particular we note that for \( \Gamma = 0 \) the center-of-gravity \( \varepsilon_g \) of \( j \) (blue and violet curves) is shifted towards lower kinetic energies with respect to the center of gravity of \( j_{2\text{-step}} \) (black curve) with a logarithmic dependence \( \varepsilon_g \propto \lambda^2 \ln(\Gamma a/v) \).

Another interesting case is obtained in the limit \( \Gamma \to \infty \), that is for very short core-hole lifetime. In this case \( 2\Gamma e^{-2\Gamma T} \) produces a Dirac delta in the \( T \)-integration:

\[
\lim_{\Gamma \to \infty} 2\Gamma \int_0^\infty dT e^{-2\Gamma T} e^{z(\tau, T)} = e^{z(\tau, 0)},
\]

with \( z = h, k \). In this limit the Auger transition occurs when the initial state is still excited, since \( e^{-iH[0]t}\vert \tilde{g} \rangle \) is not an eigenstate of \( H[1] \). As a consequence the excitations created on emission of the initial core-electron transfer their energy to the Auger electron, which then has a kinetic energy exceeding the high-energy threshold \( \varepsilon_c \) in the 2-step model [see Eq.\[13\] and Fig.\[1\] (black curve)]. This phenomenon, known as shake-down, is a typical example of qualitative departures from the predictions of the 2-step model.
Finally, we show that our theory provides an explanation of the sizable suppression of CVV Auger spectral weight closed to the Fermi energy observed in carbon nanotubes with respect to graphite. This is a striking trend, since the structure of the one-particle density of states (1PDOS) of the two carbon structures would predict the opposite behavior. In fact, while in metallic nanotubes the 1PDOS at the Fermi energy is finite due to the 1D linear dispersion, in graphite it is vanishing, due to the 2D conical dispersion. Therefore we expect that correlation effects have to be invoked in order to revert the one-particle scenario.

Metallic carbon nanotubes are believed to be rather good (although approximate) realizations of LL since in normal conditions the main correlation effects come from the long-range part of the Coulomb repulsion. In nanotubes with radius $R$, the back-scattering interactions with large momentum transfer suffer a $1/R$ suppression. Therefore we believe that typical metallic (10,10) nanotubes are well described by the present theory. Concerning graphite, we use the CS approach, which is known to give the Auger spectrum in excellent agreement with experimental one. In order to employ the CS approach we must compute the 2-particle valence Green’s function within the bare ladder approximation. This is accomplished starting from the non-interacting valence 1PDOS

$$\rho^{2D}_0(\omega) = \gamma^{-2}\theta(-\omega)|e^{-|\omega|/\gamma}|,$$

which is obtained by imposing the 2D linear spectrum $\varepsilon(k_x, k_y) = v_F(k_x^2 + k_y^2)^{1/2}$ and the momentum cutoff $1/\alpha$. We note en passing that $\rho^{2D}_0$ vanishes linearly at $\omega = 0$, as it should. The corresponding non-interacting 2-particle Green’s function $G_{0}^{2D}$ is obtained by self-folding $\rho^{2D}_0$ and by Hilbert transforming:

$$G_{0}^{2D}(\omega) = \frac{1}{2\sqrt{\pi}}\frac{(\omega - \varepsilon_F)^2}{\sqrt{-\omega}}\frac{1}{\sqrt{\omega}}\frac{1}{\sqrt{\omega}},$$

where $\Gamma(x, y)$ is the incomplete gamma function. Thus the Auger spectrum of graphite according to CS theory is

$$j^{2D}_{CS}(\omega - \varepsilon_c) = -\frac{1}{\pi} \text{Im} \left[ \frac{G_{0}^{2D}(-\omega + i0^+) - U G_{0}^{2D}(-\omega - i0^+)}{U G_{0}^{2D}(-\omega + i0^+)} \right],$$

where $U$ is the short-range screened repulsion felt by the two valence holes in the final state. It is worth to recall that our model is suitable to represent the π electrons of nanotubes and graphite, which are the ones involved in proximity of the Fermi level (placed at $\omega = 0$). Therefore only the low-energy portion of the experimental Auger spectra can be addressed within the present framework, while the high-energy spectral region, corresponding to deep $\sigma_u$ and $\sigma_g$ states, cannot be described here. A complete analysis including the missing $\sigma_u$ and $\sigma_g$ states can be found in Ref. However, in that paper the suppression of the Auger spectrum of nanotubes closed to the Fermi energy was reproduced by including some phenomenological form factors which have been fitted with the experimental data. Conversely in the present work the problem is treated starting form a fully microscopic theory with no adjustable parameter.

In order to compare with the experiment, we use the following realistic values for graphite and (10,10) metallic nanotubes: $v_F \approx 10^6 m/s$, $\alpha$ such that $\gamma = v_F/\alpha \approx 10 eV$, $\Gamma \approx 0.2 eV$, $g_1 = 0.02$, $g_2 = 2e^2/\kappa$, $\alpha \approx 1 A$, $U \approx 2 eV$, and leaving the adimensional ratio $\lambda/\sqrt{\alpha \gamma}$ as free parameter. In Fig.2 we see that the inclusion of e-e correlations in carbon nanotubes according to the LL theory within the 2-step approach (black solid line) is not enough to reproduce the suppression of $j$ vs $E^{2D}_{CS}$ closed to $\omega \approx 0$. On the other hand the full 1-step theory with finite $\lambda/\sqrt{\alpha \gamma}$ provides results in qualitative agreement with the experimental trend. This is a quite reasonable finding, considering that the core-valence repulsion is larger than (but of the same order of) the valence-valence repulsion.

**SUMMARY AND CONCLUSIONS**

Traditional photoemission and inverse photoemission experiments which probe one-particle dynamical responses provide a well-established tool for the understanding of strongly correlated 1D systems. A great amount of theoretical work devoted to this problem has been published in the past, enlightening the role of the LL concept to explain several features.
Surprisingly the study of the 1D Auger transitions, which are related to the two-particle dynamics, has been only poorly addressed. On the other hand the Auger spectroscopy is a powerful experimental technique which permits the characterization of the correlations in solids and therefore is of crucial importance in the study of strongly correlated systems.

In the present work we have developed a dynamical theory of the Auger processes in 1D metals described within the LL theory. Our theory includes the finite core-hole lifetime, the valence-valence and the core-valence interactions as well. A typical 1-step feature is observed in the limit of small core-hole lifetime, in which the valence electrons cannot relax before the Auger transition, and the shake-down phenomenon occurs. Remarkably it is shown that the 2-step approximation is not valid for any finite core-valence interaction, which also spoils the low-energy power-law behavior typically expected in the LL. Only for vanishing core-valence interaction the power-law is recovered. Finally we have shown that our 1-step theory is able to reproduce the low-energy suppression of Auger spectral weight observed in carbon nanotubes with respect to graphite.

The author kindly acknowledges M. Cini for helpful discussions.

**APPENDIX A: THE FUNCTIONS $h(\tau,T)$ AND $k(\tau,T)$**

The final expression for $C(t,t')$ in Eq. (10) has been obtained by employing the bosonization formulas in Eqs. (223) and the equations of motion method. In order to perform the sum over $q$ we used that $q = 2\pi n/L$ and took the large-$L$ limit. When doing this, it is useful to set $L = aN$ where $N$ is the number of sites of the 1D system and $a$ is the lattice constant, and send $N \to \infty$. The functions $h(\tau,T)$ and $k(\tau,T)$ obtained in this way read

$$h(\tau,T) = -\frac{\lambda}{v} 2i\sqrt{\pi} (\cosh \varphi - \sinh \varphi)$$

and

$$k(\tau,T) = \left(\frac{\lambda}{v}\right)^2 \left[ -4 \alpha \ln \left(\frac{2\alpha}{a}\right) + 2(2\alpha - iv\tau) \ln \left(\frac{2\alpha - iv\tau}{a}\right) \right]$$

with $\lambda = \lambda \sqrt{2}(\cosh \varphi - \sinh \varphi)$.

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[1] For a review, see e.g. C. Verdoesii, M. Cini and A. Marini, J. Electron Spectroscopy and Rel. Phen. 117, 41 (2001).
[2] O. Gunnarsson and K. Schönhammer, Phys. Rev. B 22, 3710 (1980).
[3] M. Cini, Sol. State Commun. 24, 681 (1977).
[4] G.A. Sawatzky, Phys. Rev. Lett. 39, 504 (1977).
[5] P. Bennett, J. C. Fuggle, F. Ulrich Hillebrecht, A. Lenselink and G. A. Sawatzky, Phys. Rev. B 27, 2194 (1983).
[6] R. Lof, M. A. van Veenendaal, B. Koopmans, H. T. Jonkman and G. A. Sawatzky, Phys. Rev. Lett. 68, 3924 (1992).
[7] K. Maiti, D. D. Sarma, T. Mizokawa and A. Fujimori, Phys. Rev. B 57, 1572 (1998).
[8] V. I. Anisimov, F. Aryasetiawan and A. I. Lichtenstein, J. Phys.: Cond. Matt. 9, 767 (1997).
[9] G. Seibold, J. Lorenzana and F. Becca, arXiv:0706.1424 (unpublished).
[10] F.D.M. Haldane, J. Phys. C: Solid State Phys. 14, 2585 (1981).
[11] H.J. Schulz, J. Phys.: Sol. St. Phys. 16, 6769 (1983).
[12] T. Giamarchi and H. J. Schulz, Phys. Rev. B 39, 4620 (1989).
[13] K. Schönhammer and V. Meden, Phys. Rev. B 47, 16205 (1993).
[14] J. Voit, Rep. Prog. Phys. 58, 977 (1995).
[15] V. Meden, Phys. Rev. B 60, 4571 (1999).
[16] J. González, M. A. Martín-Delgado, G. Sierra and M. A. H. Vozmediano, Quantum Electron Liquids and High-\textit{T}c\ Superconductivity, Chap. 4, Springer-Verlag, Berlin (1995).
[17] A. Luther and I. Peschel, Phys. Rev. B 9 2911 (1974).
[18] J. Voit, J. Phys.: Cond. Matt. 5, 8305 (1993).
[19] K.D. Schotte and U. Schotte, Phys. Rev. 182, 479 (1969).
[20] K.D. Schotte and U. Schotte, Phys. Rev. 185, 509 (1969).
[21] O. Gunnarsson and K. Schönhammer, Surf. Sci. 89, 575 (1979).
[22] V. Drchal and M. Cini, J. Phys. C: Condens. Matter 6, 8549 (1994).
[23] A. P. Dementjev, K. I. Maslakov, A. V. Naumkin, Appl. Surf. Sci. 245, 128 (2005).
[24] E. Perfetto, M. Cini, S. Urgenti, P. Castrucci, M. Scarselli, M. De Crescenzi, F. Rosé and M. A. El Khakani, Phys. Rev. B 76, 233408 (2007).
[25] B. Gao, A. Komnik, R. Egger, D. C. Glattli and A. Bachtold, Phys. Rev. Lett. 92 216804 (2004).
[26] Z. Yao, H. W. Ch. Postma, L. Balents and C. Dekker, Nature 402, 273 (1999).
[27] M. Bockrath, D. H. Cobden, J. Lu, A. G. Rinzler, R. E. Smalley, L. Balents and P. L. McEuen, Nature 397, 598 (1999).
[28] R. Egger and A. O. Gogolin, Phys. Rev. Lett. 79, 5082 (1997); Eur. Phys. J. B 3, 281 (1998).
[29] C. Kane, L. Balents, and M. Fisher, Phys. Rev. Lett. 79, 5086 (1997).
[30] J. E. Houston, J. W. Rogers, R. R. Rye, F. L. Hutson and D. E. Remaker, Phys. Rev. B 34, 1215 (1986).
[31] In Eq.(17) we use $G^D_\omega (-\omega+i\eta^+) = G^D_\omega (\omega+i\eta^+)$ because CS theory is formulated in terms of binding energy while in the present paper we use the kinetic energy scale.
[32] A. Goldoni, R. Larciprete, L. Gregoratti, B. Kaulich, M. Kiskinova, Y. Zhang, H. Dai, L. Sangaletti, F. Parmigiani, Appl. Phys. Lett. 80, 2165 (2002).
[33] $\kappa \approx 2$ is the dielectric constant of carbon nanotubes, see e.g. Ref.[28].
[34] S. Bellucci, J. González and P. Onorato, Phys. Rev. Lett 95, 186403 (2005).
[35] In order to compare the low-energy part of Fig.2 with the experiment reported in Ref.[24] one has to shift the energy scale $\omega$ of 284.6eV, which is the $1s$ core-hole binding energy in the two carbon structures.