Information transfer via electronic wavepackets in single-walled carbon nanotubes

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Extending the results recently reported in [1], we show that in metallic single-walled carbon nanotubes[2] (SWNTs) spatially localized electronic wavepackets travel maintaining their shapes essentially unaltered, even in the presence of electron-phonon scattering (see Fig. 2). This property has a remarkable impact in nanoelectronics, where generating sequences of wavepackets that propagate coherently without overlapping to each other is a crucial requirement to find electronic alternatives to photon-based quantum information processing.

In materials characterized by a parabolic-like electron spectrum, such as quantum wires or semiconducting SWNT, an electron wavepacket is well known to experience a fast spatial broadening, even in the absence of any scattering mechanisms (see Fig. 1a). In contrast, metallic SWNTs are characterized by a linear spectrum, where the group velocity is independent of the magnitude of the wavevector. This causes an initial wavepacket to split into two identical distributions moving unaltered, in the absence of scattering mechanisms, in opposite directions (see Fig. 1b). A similar behavior is in principle expected in graphene as well, although in two-dimensions the initial wavepacket would propagate radially, and the spatial distribution would progressively decrease in amplitude.

Although the linearity of the spectrum plays a crucial role under ideal scattering-free conditions, implementation in realistic devices requires to determine the impact of scattering mechanisms. In particular, at intermediate and room temperature, electron-phonon processes are indicated by experiments as the main source of scattering[3]. In order to account for these effects, the main difficulty is to provide a correct description of the interplay between coherence, without which no spatial localisation could be possible, and scattering-induced dissipation/decoherence. To this purpose here we adopt a recently proposed non-linear Lindblad-based density-matrix approach (LBA) [4], which overcomes the limitations of oversimplified dephasing models like the Relaxation Time Approximation (RTA), and is numerically much more performant than non-Markovian density matrix approaches, such as the Quantum-Montecarlo technique or Quantum kinetics treatments.

The main result of our work is a detailed analysis of the evolution of a spatially localized electronic distribution in a realistic nanomaterial, i.e. in the presence of electron-phonon scattering, and is shown by the solid line of Fig. 2. Comparing these results with the scattering-free evolution (dashed line in Fig. 2), we find that in metallic SWNTs scattering processes do not significantly alter the shape of a wavepacket, so that the transmission is essentially dispersionless up to the micrometric scale already at room temperature, and even less dispersive at lower temperatures (i.e. at 77K the signal attenuation is less than 1% over more than one micron). Such strong suppression of the phonon-induced dissipation predicted by our LBA is mainly due to cancellations between forward processes (i.e., those which preserve velocities), although their electron-phonon couplings are a priori one order of magnitude bigger then the backward ones[5]. In sharp contrast, the oversimplified RTA strongly overestimates the phonon-induced dissipation, due to its inability to distinguish between forward and backward processes, as shown by the dash-dotted line of Fig.2. Notice that, while semiclassical approaches show a somehow similar forward-scattering suppression,

here the off-diagonal nature of the density matrix makes such phenomena highly nontrivial: in fact, contrary to the Boltzmann Equation, in our LBA the cancellations take place only for those forward processes which are mediated by phonons with small-enough wavevectors. Finally, we observe that the spatial localization of the initial electron distribution is given by interstate coherences (i.e. polarizations), which may, in principle, be generated experimentally via a properly tailored optical excitation. We thus expect these results will pave the way for advanced optoelectronics with metallic SWNTs.

References

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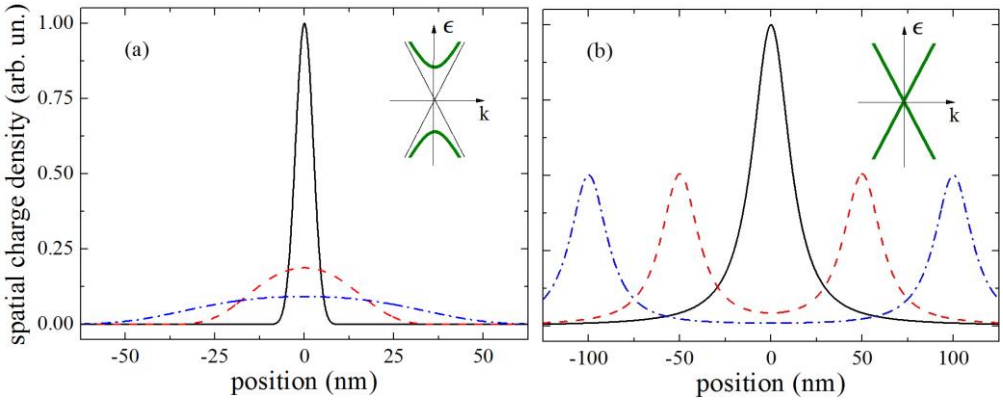

Figure 1: Room-temperature scattering-free evolution in (a) a semiconducting (10, 0) and (b) a metallic (12, 0) SWNT of a localized electronic wavepacket as a function of the position along the SWNT axis at t=0 fs (solid), t=50 fs (dashed), and t=100 fs (dashed-dotted).

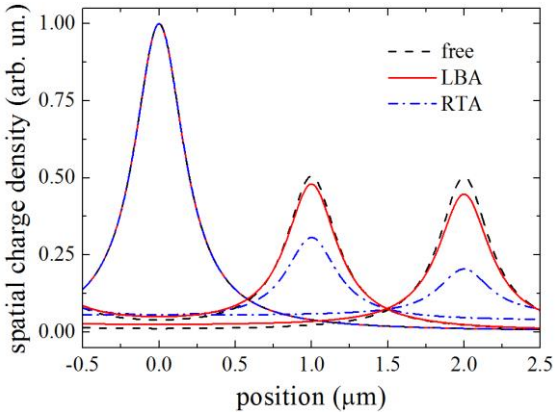

Figure 2: Room-temperature evolution of an electronic wavepacket in a metallic (12, 0) SWNT as a function of the position along the SWNT axis, at three different times: t=0 ps (left peaks), t=1 ps (central peaks), and t=2 ps (right peaks), as predicted by our LBA (solid lines), by the RTA (dotted-dashed lines) and in the absence of scattering mechanisms (dashed lines).