Tunable spin-polaron state in a singly clamped semiconducting carbon nanotube

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We consider a semiconducting carbon nanotube (CNT) laying on a ferromagnetic insulating substrate with one end depassing the substrate and suspended over a metallic gate. We assume that the polarised substrate induces an exchange interaction acting as a local magnetic field for the electrons in the non-suspended CNT side. Generalizing the approach of I. Snyman and Yu.V. Nazarov [Phys. Rev. Lett. 108, 076805 (2012)] we show that one can generate electrostatically a tunable spin-polarized polaronic state localized at the bending end of the CNT. We argue that at low temperatures manipulation and detection of the localised quantum spin state is possible.

Nanoelectromechanics with suspended carbon nanotubes evolved rapidly in last few years [1—7]. Recently I. Snyman and Yu.V. Nazarov [8] considered a semiconducting CNT laying on an insulating substrate with one end of it suspended. A metallic gate below both the insulating substrate and the suspended part of the CNT generates an homogeneous electric field (cf. Fig. 1 of Ref. [8]). The mechanical bending of the suspended part of the nanotube induces then a spatial inhomogeneity of the electrostatic potential along the CNT forming a minimum at the deformable end of the wire. The competition between such an electrostatic bending with both the elastic potential of the CNT and the quantum rigidity of the electronic wave function makes the mechanical bending as well as the formation of the localized polaronic state at the movable end of the CNT to occur as a first order phase transition as a function of the electric field. The estimate for the critical field for a realistic experimental set up was predicted in Ref. [8] to be 0.01 V/µm.

An impressive effort of the nanoelectronics community is currently deployed to manipulate and exploit the electronic spin degrees of freedom in transport devices (spintronics) [9]. In this context the possibility of magnetic gating, i.e., the use of ferromagnetic leads inducing magnetic exchange fields \( E_{\text{ex}}/\mu_B \) (with \( \mu_B \) the Bohr magneton) on the electronic spin is currently actively investigated [10—13]. More surprisingly such exchange fields can have remarkable consequences also on the dynamics of a nano-mechanical system for which dynamical (shuttle) instabilities, strong spin-polarized currents, and cooling have been predicted [14—16].

In this paper we show that the system discussed by Snyman and Nazarov [8] in presence of a magnetic dielectric substrate allows the formation of a localized fully polarized polaronic state. The experimentally observed exchange energy \( E_{\text{ex}} \) (see Ref. [13, 14]) turns out to be as large as tens of Kelvins, thus being of the same order of magnitude of the localization energy for an electron in a CNT on the scale of the micrometer. This allows for a high tunability of the polaronic state by means of two electric gates, below the suspended and non-suspended part of the CNT (see Fig. 1). As a result a continous electrostatic tuning of the localization length and the bound state energy can be achieved, forming a stability diagram of spin-up and spin-down polaronic states. Detection of the state of the system can be envisaged by use of a nearby single-electron transistor, for which the CNT tip acts as a gate [17]. Fully electric manipulation of the mechanical and electronic spin state of the CNT is thus possible in this system.

The system. Following Ref. [8] let us consider a CNT laying on a substrate with a suspended part protruding out of a length \( L \). Two independently adjustable gates \( (V_{G1} \text{ and } V_{G2}) \) are shown and a contact \( (C) \) on the substrate side. The potential for spin up and down \( (U_+ \text{ and } U_-) \) is also sketched above.

FIG. 1. Schematic of the system considered: a CNT laying on a magnetic substrate \((C)\) and protruding out of a length \( L \). Two independently adjustable gates \((V_{G1} \text{ and } V_{G2})\) are shown and a contact \((C)\) on the substrate side. The potential for spin up and down \((U_+ \text{ and } U_-)\) is also sketched above.
value is 0 at the edge of the substrate and \( L \) on the tip of the suspended part. The length of the CNT on the substrate is supposed to be \( \gg L \), and is taken infinity for simplicity. Then vanishing boundary conditions apply at \( x = L \) and \( x = -\infty \). As in Ref. [3] the CNT can bend with a displacement \( y(x) \) (for \( 0 < x < L \)) in the direction orthogonal to the substrate. The elastic energy cost reads \( IY \int dx \left| y''(x) \right|^2 / 2 \), where \( I = 6.4 \pi a_0 r^2 \) is the second moment of area of the tube cross section and \( Y \) the CNT Young modulus (of the order of 1.2 TPa). Single clamping implies that \( y(0) = y'(0) = 0 \) and \( y''(L) = y'''(L) = 0 \). In this paper we will restrain to the classical description of the deflection. The tip of the CNT on the substrate is in tunneling contact with a metal whose chemical potential can be tuned close to the valence band of the CNT by adjusting the electric potential. Up to now the description followed closely Ref. [8].

The first term in Eq. (1) gives the quantum kinetic energy, the second the elastic energy, and the third is a sum of three parts: the exchange energy, the electrostatic potential and its variation induced by the deflection \( [y(x)] \) of the CNT. In Ref. [3], for \( V = 0 \) and for \( E_{\text{ex}} = 0 \), it has been shown that it exists a critical value of the electric field \( E_c \) for which the ground state is an electronic localized state on the CNT suspended part. The formation of the bound state is a first order transition: the CNT starts to bend only for \( E > E_c \) and a metastable bound state exists for \( E_{\text{ex}1} < E < E_c \). At \( E = E_c \) the localization length is thus finite and typically much shorter than \( L \). In order to have a tunable bound state it is necessary to have a smooth transition from the delocalized to the localized state. This is actually the typical case in quantum mechanics, by decreasing the depth of a potential well that allows a bound state one can delocalize progressively the wave function. The bound-state radius then diverges at the threshold for its appearance. We will thus see that the presence of \( V \) and \( E_{\text{ex}} \) allows to create a spin-dependent tunable bound state, that is associated to a displacement of the CNT tip.

**Electronic problem.** Let us begin with the purely electronic problem \([y(x) \equiv 0 \text{ for all } x]\). The ground state can be found by solving the Schrödinger equation:

\[
\left[ -\frac{\hbar^2}{2m^*} \nabla^2 - E_{\text{ex}} \sigma \theta_x - eV \theta_x \right] \psi_\sigma(x) = \epsilon_\sigma \psi_\sigma(x)
\]

for each spin projection. The presence of a bound state is signaled by the existence of a solution of Eq. (2) with \( \epsilon_\sigma < -\sigma E_{\text{ex}} \) the bottom of the relative band. Taking \( \epsilon_\sigma < -\sigma E_{\text{ex}} \) as a reference in energy the problem for each spin species reduces to that described by Eq. (2) with \( E_{\text{ex}} \to 0 \) and \( eV \to eV - \sigma E_{\text{ex}} = U \). The solution can then be found by matching the wave function \( \psi(x) = Ae^{ikx} + Ce^{-ikx} \) for \( x > 0 \) and \( \psi(x) = Be^{ikx} + Ce^{-ikx} \) for \( x < 0 \). At \( x = 0 \) the boundary condition is that the wave function and its derivative are continuous. The boundary conditions lead to the eigenvalue equation \( e^{-2ikL} = -(ik + \kappa)/(ik - \kappa) \) with \( \kappa L = [-2m^*_b/e^2L^2]^{1/2} \). To ensure that \( \epsilon_b < 0 \) the bound state energy. At the threshold \( \epsilon_b \to 0^+ \), thus there \( \kappa \) vanishes and the eigenvalue equation reduces to \( e^{-2ikL} = -1 \). This gives \( kL = \pi/2 \) and the threshold value for the potential \( U_0 = (\pi/2)^2E_K \). With \( E_K = h^2/(2m^*L^2) \) the kinetic energy scale. For \( U - U_0 \ll E_K \) the localization length \( \kappa^{-1} = 2LE_K/(U - U_0) \) and diverges as anticipated. By changing \( U \) it is then possible to adjust the spread of the wave function on the magnetic substrate. Since the two spin species feel a different potential only on the substrate, this allows to change continuously the energy difference of the up and down bound states. The bound state energy for each spin state reads:

\[
\epsilon_\sigma = -\sigma E_{\text{ex}} + \epsilon_b(eV - \sigma E_{\text{ex}})
\]

with the threshold value for \( V \): \( eV_0 = U_0 + \sigma E_{\text{ex}} \). A typical picture of the \( eV \) dependence of the two bound states for \( E = 0 \) is shown dashed in Fig. 2. For \( V_- < V < V_+ \) a unique bound state exists for spin down. Let’s define \( V_c \) the value for which the down-spin energy crosses the up-spin bottom band: \( \epsilon_- (V = V_c) = -E_{\text{ex}} \). For \( V_+ < V < V_0 \) two bound states exist, but only the lowest one (spin up) is stable, since the spin-down lays above the bottom of the spin-up band, and any spin-flip perturbation allows its decay into the spin-up continuum. Finally for \( V > V_c \) two stable bound states exist. Their energy splitting has a maximum at \( V_c \) and then monotonically decreases as a function of \( V \). This is due to the reduction of the localization length reducing the effect of the exchange interaction that acts only for \( x < 0 \). Although both spin-up and spin-down polaronic states are stable at \( V > V_c \) only one of them can be occupied due to the Coulomb blockade, whose repulsion energy turns out to be much larger than the polaronic bound state energy (\( \sim E_K \)) at \( L \gg 1 \). This fact allows the formation of
a controllable single-electron fully spin polarized state at the protruding part of the CNT.

**Nanomechanical effects.** We now consider how the system behaves when we let the CNT bend. It is not possible any more to find the ground state energy analytically, we will thus follow closely the variational method used in Ref. [3] to which we refer for more details. We introduce the dimensionless variables \( z = x/L \), \( h = H/E_K \), \( f = yYl/eEL^2 \), \( \phi_\sigma = \psi_\sigma \sqrt{T} \), and the coupling parameter \( \alpha = (eE)^2L^3/(YlE_K) \). The problem can then be completely determined by giving only three independent coupling parameters: \( \alpha, \mu = E_{ex}/E_K \), and \( \nu = eV/E_K \).

The functional to be minimized reads:

\[
h = \int_{-\infty}^{1} dz \left[ \phi_\sigma'^2 + \alpha \left( f \phi_\sigma'^2 + \frac{f\mu^2}{2} - (\mu\sigma\theta_z + \nu\theta_z) \phi_\sigma'^2 \right) \right] .
\]

By writing \( \phi(z) = \sum_{n=1}^{M} a_n (1-z)^n \) for \( z > 0 \) and \( \sum_{n=1}^{M} a_n z^n e^{\kappa z} \) for \( z < 0 \), and \( f(z) = \sum_{n=1}^{M} b_n z^n + 1 \) one can enforce the boundary conditions and minimize numerically the functional in order to find the parameters \( \{a_n, b_n, \kappa\} \) and thus the ground state energy \( \epsilon_\sigma \) with explicit expressions for the bending and the wavefunction. The charge accumulated on the suspended part of the CNT in presence of an electric field induces a force that bends the tip of the CNT. The effective electronic potential deepens and bending lowers the bound state energy. In particular it favors a stronger localization of the wave function on the tip (measured by \( \kappa^{-1} \)). For \( E_{ex} = eV = 0 \) in Ref. [3] it is shown that the bound state forms with a first order phase transition for \( \alpha > \alpha_c = 312.03 \). In order to keep a smooth transition we will consider the case \( \alpha < \alpha_c \) and investigate the dependence of the bound state energy and wavefunction on \( eV/E_K \) for given values of \( E_{ex}/E_K \).

Before considering the results of the numerical calculation it is useful to estimate analytically the typical range of the displacement of the CNT tip induced by the localization of the charge. Let us assume that the fraction \( n < 1 \) of an electron charge is accumulated on the CNT uniformly. A simple ansatz for the displacement is \( f(z) = az^2 \). It satisfies both the boundary conditions and the Euler equation \( f''' = 0 \). Substituting it in Eq. (4) one has for the part proportional to \( \alpha \):

\[
h_\alpha = \alpha \left( 2a^2 + \frac{a}{3} \right) \]

this functional has a minimum at \( a = -n/12 = f(1) \). It gives a rough estimate of the dimensionless displacement of the tip by taking into account only the competition between the electric field and the elastic stiffness. The effect of the other two parameters is hidden into the value of \( n \), that cannot be larger than 1.

We present on Fig. 3 the numerical results for \( \alpha = 175 \) and \( \mu = 1 \). One can see that the energy splitting of the two spin states is of the order of \( E_K = E_{ex} \) (top-left panel). Defining \( n_\sigma = \int_0^1 dz \phi_\sigma' \) the fraction of charge (and spin) localized on the suspended part of the CNT one finds that for \( V = V_c \) both bound states present a finite value of \( n_\sigma \) and \( n_- - n_+ \approx 0.17 \). The difference is slowly reduced for larger values of the gate voltage. The same can be said for the deflection of the tip of the CNT \( f_\sigma = f(1) \) for each spin state, bottom-left panel). Finally the bottom-right panel shows that the ratio \( f_\pm/n_\pm \) is actually close to the rough estimate \( 1/12 \).

The plots of Fig. 3 show that a particularly important quantity is the value of the physical parameters \( (\epsilon_\sigma, n_\sigma, f_\sigma) \) at the threshold \( V_c \). The dependence on \( V \) is always monotonic and the maximum or minimum values are observed at \( V_c \). In view of manipulating the spin state, the value at \( V_c \) gives thus a very good indication of the range in which the state can be accessible. We thus show in Fig. 4 as a function of \( \alpha \) and for different values of \( \mu \) the threshold \( V_c \), the energy splitting \( \epsilon_- - \epsilon_+ \), the difference in the occupation \( n_- - n_+ \), and in the deflection \( f_- - f_+ \). As expected the critical voltage \( V_c \) decreases as a function of \( \alpha \), and in particular, for sufficiently small \( \mu \), it vanishes when \( \alpha \) approaches the critical value \( \alpha_c \). The
the difference in the fraction of localized charge $n_0$ and the main energy scale of the problem. Quite surprisingly the $E_f$ (bottom-right); the last three quantities calculated at $\mu = 20$ the critical gate voltage value $V_c$ (top left), the electric field $\alpha$ that the optimal value of bound state is between 100 and 200. A similar behavior is observed in $\mu$ that $\alpha \gg 1$ the energy splitting remains of the order of $E_K$, that thus sets the main energy scale of the problem. Quite surprisingly the difference in the fraction of localized charge $n_+ - n_-$ (bottom left), and the difference of theCNT tip deflection $f_- - f_+$ (bottom-right); the last three quantities calculated at $V = V_c$.

bound-state energy splitting is monotone in $\alpha$, since the electric field increases the localization of the bound state, and thus reduces the difference of the two states. Its $\alpha$-dependence is rather weak. Even for $\mu \gg 1$ the energy splitting remains of the order of $E_K$, that thus sets the main energy scale of the problem. Quite surprisingly the difference in the fraction of localized charge $(n_- - n_+)$ is not monotonic for small $\mu$ as a function of the electric field. This is due to the fact that the transition region is approached at different values of $\alpha$ for each spin state. A similar behavior is observed in $f_- - f_+$. One can conclude that the optimal value of $\alpha$ to observe a well defined bound state is between 100 and 200.

Estimates. In order now to consider the possibility to observe the two bound states we discuss the typical scales of the problem. Expressing the radius in $nm$ and the length in $\mu m E_K \approx 13.9(r/L^2)$ mK. The typical value of $L$ ranges between 0.1 and 1$\mu m$, leading to a range for $E_K$ between few K to tens of mK, thus always accessible with standard cryogenics. The thermal and quantum fluctuations of the displacement of the tip plays also an important role, since they define the distinguishability of the displacement of the two bound states. From Eq. (5) one can write an approximate potential for the tip displacement $\delta f = f(1) - f_0$ (with $f_0 = n/12$ the equilibrium value): $h_\alpha = 2\alpha(\delta f)^2$. The equipartition theorem then gives for the thermal fluctuations $\delta f_T = \left[k_B T/(4\alpha E_K)\right]^{1/2}$. Quantum fluctuations $\delta f_Q$ has the same expression with $k_B T \to \hbar \omega_m$. Since $\hbar \omega_m/E_K = 0.0332$ independently of $L$ or $r$ then $\delta f_Q = 0.09/\sqrt{\alpha}$. Expressing as above $T$ in mK, $L$ in $\mu m$, and $r$ in $nm$ $\delta f_T = 0.13L[T/(\alpha r)]^{1/2}$. Those values have to be compared with $f_- - f_+$ that are at best 0.04. $f_Q$ is thus 5 times smaller of this value already for $\alpha = 100$, while in order to keep $\delta f_T$ small one needs $T < .09\alpha r/L^2$. This is realizable for instance choosing $L = 5\mu m$, $r = 2nm$, $\alpha = 200$ and working at temperatures $T \approx 20$ mK ($E_K$ is 111 mK in this case).

Conclusions. We have shown that combining electrostatic and magnetic gating the formation of a spin-polaronic state in a singly clamped CNT becomes possible. Electric, magnetic, and mechanical tuning provides an effective manipulation of such spin-polaron states offering a controllable magneto-electro-mechanical transduction with single electronic charge and spin sensitivity involving sub nanometer mechanical displacement. 

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