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

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We consider a semiconducting carbon nanotube (CNT) lying on a ferromagnetic insulating substrate with one end passing the substrate and suspended over a metallic gate. We assume that the polarized substrate induces an exchange interaction acting as a local magnetic field for the electrons in the nonsuspended 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 localized quantum spin state are possible.

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I. INTRODUCTION

Nanoelectromechanics with suspended carbon nanotubes has evolved rapidly in last few years [1–7]. Recently, Snyman and Nazarov [8] considered a semiconducting carbon nanotube (CNT) lying 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 a homogeneous electric field (see Fig. 1 of Ref. [8]). The mechanical bending of the suspended part of the nanotube then induces 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 and both the elastic potential of the CNT and the quantum rigidity of the electronic wave function makes the mechanical bending and the formation of the localized polaronic state at the movable end of the CNT occur as a first-order phase transition as a function of the electric field. The estimate for the critical field for a realistic experimental setup was predicted in Ref. [8] to be 0.01 $V/\mu m$.

An impressive effort of the nanoelectronics community is currently underway 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_{ex}/μ_B (with μ_B being the Bohr magneton), on the electronic spin is currently being actively investigated [10–13]. More surprisingly, such exchange fields can also have remarkable consequences on the dynamics of a nanomechanical 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 the presence of a magnetic dielectric substrate allows the formation of a localized fully polarized polaronic state. The experimentally observed exchange energy E_{ex} (see Refs. [13,14]) turns out to be as large as tens of K, thus being the same order of magnitude as 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 nonsuspended parts of the CNT (see Fig. 1). As a result, a continuous 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 states of the CNT is thus possible in this system.

This paper is organized as follows: Section II describes the system considered, with the approximations performed to arrive at the Hamiltonian used in the remainder of the paper. Section III considers the case in which the nanotube cannot deflect or the deflection is negligible. The conditions for the formation of a bound state are studied. Section IV deals with the nanomechanical effects by including the deflection of the carbon nanotube in the calculation of the bound-state energy. Section V discuss the typical scale for the mechanical fluctuations and thus the observability of the energy splitting of the electronic bound state. Finally, Sec. VI gives our conclusions.

II. THE SYSTEM

Following Ref. [8], let us consider a CNT lying on a substrate with the suspended part protruding out a length L (see Fig. 1). In Ref. [8] it was shown that the wave function $\psi(x)$ of the electrons in the valence band of the CNT can be described by a standard one-dimensional Schrödinger equation with an effective mass $m^* = 0.6 m_e a_0/r$, where m_e is the electronic mass, a_0 is the Bohr radius, and r is the radius of the CNT. The variable x parametrizes the position along the CNT; its value is zero 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 much larger than L and is taken as infinity for simplicity. Then vanishing boundary conditions apply at $x = L$ and $x = -\infty$. As in Ref. [8], 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

$$IY \int dx [y''(x)]^2/2, \tag{1}$$

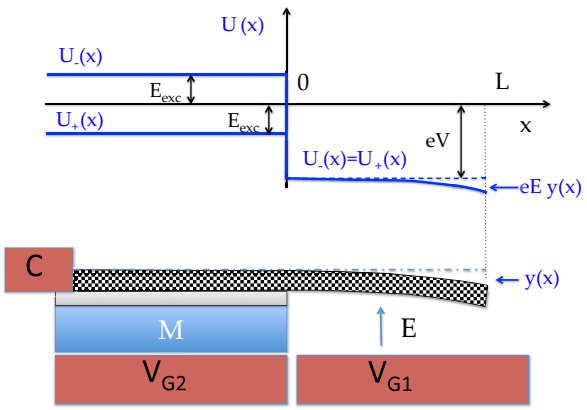

FIG. 1. (Color online) Schematic of the system considered: a CNT lying on a magnetic substrate (M) and protruding out a length L. Two independently adjustable gates (V_{G1} and V_{G2}) are shown, with a contact (C) on the substrate side. The potential for spin up and down (U_+ and U_-) is also sketched above.

where $I = 6.4\pi a_0 r^2$ is the second moment of area of the tube cross section and Y is the CNT Young's 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 restrict ourselves 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 has closely followed Ref. [8]. We now introduce the main difference: We will assume that the substrate is a magnetic insulator that induces an exchange interaction term

$$-E_{\rm ex}\int_{-\infty}^{0} dx\sigma|\psi_\sigma(x)|^2 \tag{2}$$

for the electrons in the CNT over the substrate ($x < 0$). The variable σ indicates the spin projection in the z direction. This creates a spin-dependent potential, so that the spin-up electrons ($\sigma = +$) are attracted in the $x < 0$ region. In order to tune the potential we assume that two different gates are present, one below the magnetic substrate and another one under the suspended part. By changing independently the potentials on the two gates it is possible to modify the electrostatic potential V and the electric field E acting on the electrons on the suspended part (taking the nonsuspended region as a reference for the potential; see Fig. 1). We can then write the full Hamiltonian for the problem as follows (θ_x is the Heaviside function):

$$H = \sum_\sigma \int_{-\infty}^{L} dx \left\{ \frac{\hbar^2}{2m^*}|\partial_x\psi_\sigma(x)|^2 + \frac{IY}{2}\left[\partial_x^2 y(x)\right]^2 - \left[E_{\rm ex}\sigma\theta_{-x} + eV\theta_x - eEy(x)\right]|\psi_\sigma(x)|^2 \right\}. \tag{3}$$

The first term in Eq. (3) gives the quantum kinetic energy, the second gives 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. [8], for $V = 0$ and for $E_{\rm ex} = 0$, it was shown that a critical value of the electric field E_c exists 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 $E_{c1} < E < E_c$. At $E = E_c$ the localization length is thus finite and is 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 progressively delocalize 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 $E_{\rm ex}$ allows us to create a spin-dependent tunable bound state that is associated with a displacement of the CNT tip.

III. ELECTRONIC PROBLEM

Let us begin with the purely electronic problem [$y(x) \equiv 0$ for all x]. The ground state can be found by solving the Schrödinger equation,

$$\left[-\frac{\hbar^2\partial_x^2}{2m^*} - E_{\rm ex}\sigma\theta_{-x} - eV\theta_x\right]\psi_\sigma(x) = \epsilon_\sigma\psi_\sigma(x), \tag{4}$$

for each spin projection. The presence of a bound state is signaled by the existence of a solution of Eq. (4) with $\epsilon_\sigma < -\sigma E_{\rm ex}$ as the bottom of the relative band.

Taking $\epsilon_\sigma < -\sigma E_{\rm ex}$ as a reference in energy, the problem for each spin species reduces to that described by Eq. (4) with $E_{\rm ex} \to 0$ and $eV \to eV - \sigma E_{\rm ex} = U$. The solution can then be found by matching the wave function

$$\begin{aligned} \psi(x) &= Ae^{\kappa x} \quad \text{for } x < 0, \\ \psi(x) &= Be^{ikx} + Ce^{-ikx} \quad \text{for } x > 0 \end{aligned} \tag{5}$$

at $x = 0$ by solving for the continuity of the wave function and of its derivative. The boundary conditions lead to the eigenvalue equation

$$e^{-2ikL} = -(ik + \kappa)/(ik - \kappa), \tag{6}$$

with

$$\kappa L = [-2m^*\epsilon_b/\hbar^2]^{1/2}, \quad kL = [2m^*(U + \epsilon_b)/\hbar^2]^{1/2}, \tag{7}$$

and $\epsilon_b < 0$ being the bound-state energy. At the threshold $\epsilon_b \to 0^-$, κ vanishes, and the eigenvalue equation reduces to $e^{-2ikL} = -1$. This gives $kL = \pi/2$, and the threshold value for the potential

$$U_t = (\pi/2)^2 E_K, \tag{8}$$

with $E_K = \hbar^2/(2m^*L^2)$ being the kinetic energy scale. For $U - U_t \ll E_K$ the localization length

$$\kappa^{-1} = 2LE_K/(U - U_t) \tag{9}$$

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, we can continuously change the energy difference of the up and down bound states. The bound-state energy for each spin state reads

$$\epsilon_\sigma = -\sigma E_{\rm ex} + \epsilon_b(eV - \sigma E_{\rm ex}), \tag{10}$$

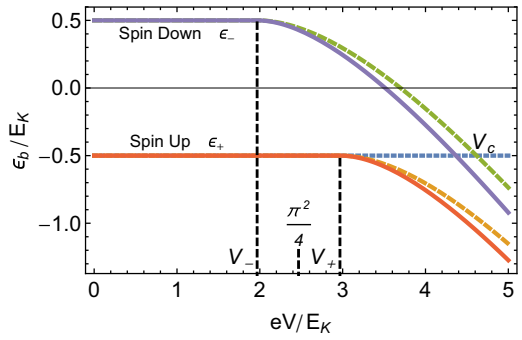

FIG. 2. (Color online) Dependence on the gate voltage V of the two spin-projection bound-state energies ϵ_σ for $E_{ex}/E_K = 0.5, \alpha = 0$ (i.e., $E = 0$, dashed lines) and $\alpha = 50$ (solid lines). The bottom of the lower electronic band (spin up) is shown as a short-dashed line.

with the threshold value for V:

$$eV_\sigma = U_t + \sigma E_{ex}\,. \tag{11}$$

A typical picture of the eV dependence of the two bound states for $E = 0$ is shown as dashed lines in Fig. 2. For $V_- < V < V_+$ a unique bound state exists for spin down. Let's define V_c as the value for which the spin-down energy crosses the spin-up bottom band:

$$\epsilon_-(V = V_c) = -E_{ex}\,. \tag{12}$$

For $V_+ < V < V_c$ two bound states exist, but only the lowest one (spin up) is stable since the spin down lies 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 $L \gg 1$ nm. This fact allows the formation of a controllable single-electron fully spin polarized state at the protruding part of the CNT.

IV. NANOMECHANICAL EFFECTS

We now consider how the system behaves when we let the CNT bend. It is no longer possible to find the ground-state energy analytically; we will thus closely follow the variational method used in Ref. [8], to which we refer for more details. We introduce the dimensionless variables

$$z = x/L, \quad h = H/E_K, \quad f = yYI/eEL^3, \quad \phi_\sigma = \psi_\sigma\sqrt{L} \tag{13}$$

and the coupling parameter

$$\alpha = (eE)^2L^3/(YIE_K). \tag{14}$$

The problem can then be completely determined by giving only three independent coupling parameters: α, $\mu = E_{ex}/E_K$, and $\nu = eV/E_K$. The functional to be minimized reads

$$h = \int_{-\infty}^{1} dz\left[{\phi_\sigma}''^2 + \alpha\left(f\phi_\sigma^2 + \frac{f''^2}{2}\right) - (\mu\sigma\theta_{-z} + \nu\theta_z)\phi_\sigma^2\right]. \tag{15}$$

By writing

$$\phi(z) = \begin{cases} \sum_{n=1}^{M} a_n(1-z)^n & \text{for } z > 0, \\ \sum_{n=1}^{M} a_n z^n e^{\kappa z} & \text{for } z < 0, \end{cases} \tag{16}$$

and

$$f(z) = \sum_{n=1}^{M} b_n z^{n+1}, \tag{17}$$

one can enforce the boundary conditions and numerically minimize the functional in order to find the parameters $\{a_n, b_n, \kappa\}$ and thus the ground-state energy ϵ_σ with explicit expressions for the bending and the wave function. The charge accumulated on the suspended part of the CNT in the 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, the exchange interaction favors a stronger localization of the wave function on the tip (measured by κ^{-1}). For $E_{ex} = eV = 0$ in Ref. [8] 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 wave function 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 tip 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. (15), one has for the part proportional to α

$$h_\alpha = \alpha\left(2a^2 + n\frac{a}{3}\right); \tag{18}$$

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 in the value of n, which cannot be larger than 1.

We present in 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

$$n_\sigma = \int_0^1 dz\phi_\sigma^2 \tag{19}$$

as 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_σ 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].

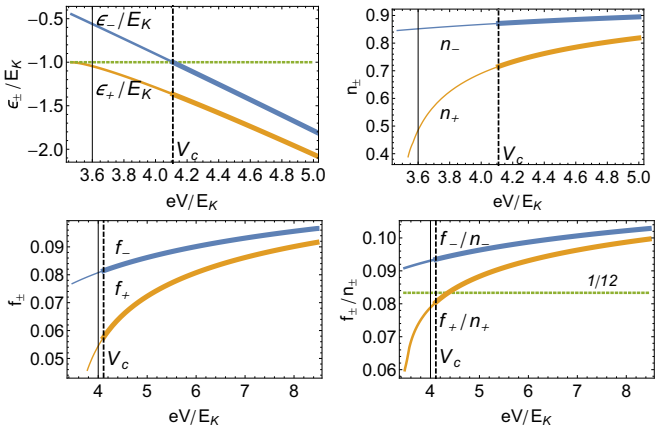

FIG. 3. (Color online) For $E_{ex} = E_K$ and $\alpha = 175$ gate voltage dependence of (top left) the bound-state energies, (top right) the fraction of localized charge or spin, (bottom left) deflection of the tip, and (bottom right) the ratio of deflection to localized charge.

Finally, the bottom right panel shows that the ratio $f_\pm/n_\pm$ is actually close to the rough estimate of $1/12$.

Figure 3 shows that a particularly important quantity is the value of the physical parameters (ϵ_σ, n_σ, and f_σ) 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 thus gives a very good indication of the range in which the state can be accessible. We thus show in Fig. 4, as a function of α and for different values of μ, the threshold V_c, the energy splitting $\epsilon_- - \epsilon_+$, the difference in the occupation $n_- - n_+$, and the difference in the deflection $f_- - f_+$. As expected, the critical voltage V_c decreases as a function of α, and in particular, for sufficiently small μ, it vanishes when α approaches the critical value α_c. The bound-state energy splitting is monotone in α since the electric field increases the localization of the bound state and thus reduces the difference of the two states.

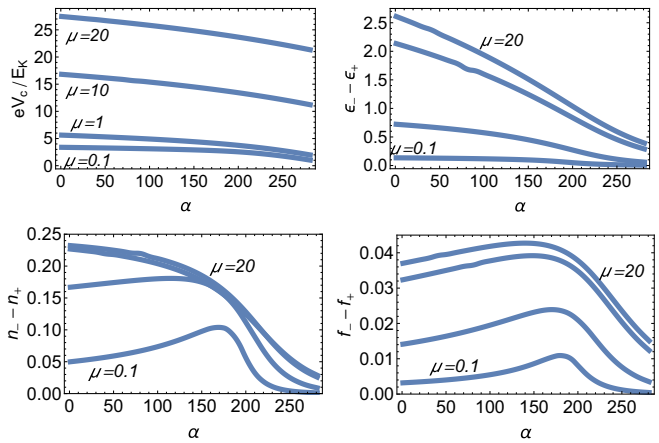

FIG. 4. (Color online) (top left) The critical gate voltage value V_c, (top right) the energy splitting of the two bound states $\epsilon_- - \epsilon_+$, (bottom left) the difference in the fraction of localized charge $n_+ - n_-$, and (bottom right) the difference of the CNT tip deflection $f_- - f_+$ as a function of α for $\mu = 0.1$, 1., 10, and 20; the last three quantities are calculated at $V = V_c$.

Its α dependence is rather weak. Even for $\mu \gg 1$ the energy splitting remains of the order of E_K, which 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 μ as a function of the electric field. This is due to the fact that the transition region is approached at different values of α for each spin state. A similar behavior is observed in $f_- - f_+$. One can conclude that the optimal value of α to observe a well-defined bound state is between 100 and 200.

V. ESTIMATES

In order to consider the possibility of observing the two bound states we discuss the typical scales of the problem. Expressing the radius in nanometers and the length in microns, $E_K \approx 13.9(r/L^2)$ mK. The typical value of L ranges between 0.1 and 1 μm, leading to a range for E_K between a few K and tens of mK, which is thus always accessible with standard cryogenics. The thermal and quantum fluctuations of the displacement of the tip also play an important role since they define the distinguishability of the displacement of the two bound states. From Eq. (18) one can write an approximate potential for the tip displacement $\delta f = f(1) - f_0$ (with $f_0 = n/12$ the equilibrium value):

$$h_\alpha = 2\alpha(\delta f)^2. \tag{20}$$

The equipartition theorem then gives for the thermal fluctuations

$$\delta f_T = [k_B T/(4\alpha E_K)]^{1/2}. \tag{21}$$

Quantum fluctuations δf_Q have the same expression with $k_B T \to \hbar\omega_m$. Since $\hbar\omega_m/E_K = 0.0332$ independently of L or r [8,18], $\delta f_Q = 0.09/\sqrt{\alpha}$. Expressing, as above, T in mK, L in microns, and r in nanometers,

$$\delta f_T = 0.13L[T/(r\alpha)]^{1/2}. \tag{22}$$

Those values have to be compared with $f_- - f_+$ that are, at best, 0.04. f_Q is thus 5 times smaller than this value already for $\alpha = 100$, while in order to keep δf_T small, one needs $T \ll 0.09r\alpha/L^2$. This is realizable by, for instance, choosing $L = 0.5$ μm, $r = 2$ nm, and $\alpha = 200$ and working at temperatures $T \approx 20$ mK (E_K is 111 mK in this case).

VI. CONCLUSIONS

We have shown that by 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 effective manipulation of such spin-polaron states offering a controllable magnetoelectromechanical transduction with single-electronic charge and spin sensitivity involving subnanometer mechanical displacement.

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