Topologically protected, correlated end spin formation in carbon nanotubes

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For most chiralities, semiconducting nanotubes display topologically protected end states of multiple degeneracies. We demonstrate using density matrix renormalization group based quantum chemistry tools that the presence of Coulomb interactions induces the formation of massive end spins. These are the close analogues of ferromagnetic edge states emerging in graphene nanoribbon. The interaction between the two ends is sensitive to the length of the nanotube, its dielectric constant, as well as the size of the end spins: for $S = 1/2$ end spins their interaction is antiferromagnetic, while for $S > 1/2$ it changes from antiferromagnetic to ferromagnetic with increasing nanotube length. The interaction between end spins can be controlled by changing the dielectric constant of the environment, thereby providing a possible platform for two-spin quantum manipulations.

Introduction – Topological insulators represent unique states of matter, and besides their theoretical appeal, they hold the promise to revolutionize quantum computation, spintronics and thermal electrics [1–3]. While their insulating bulk does not differ significantly from that of a simple band insulator, their topological character is manifested by the appearance of emergent surface and edge states, frequently exhibiting unusual physical properties. Probably the best known incarnation of a topological state is the edge state in the Su-Schrieffer-Heeger (SSH) model [4], describing the dimerization of polyethylene. In this case, the dimerized phase is a topological band insulator, and correspondingly, at the edges of the polyethylene chain or at topological defects separating different dimerized phases, mid-gap bound states and corresponding local spin excitations emerge [5, 6].

Surprisingly, it has been discovered only a few years ago that most insulating carbon nanotubes also belong to the class of topological systems. As a consequence, they should possess mid-gap states [7–10], quite similar to those found in the SSH model. Quite astonishingly, as we discuss below, the number and character of these mid-gap states is exclusively determined by the chirality of the nanotube, and in most nanotubes, several end states are predicted to appear at each end of the tube. However, in a neutral and non-interacting nanotube, all these states would be almost degenerate, and therefore they are expected to be most sensitive to interaction effects.

In this work, we focus our attention to these interaction effects, and demonstrate that — in the presence of interactions — these topologically protected end states behave in many ways as spontaneously formed quantum dots. In particular, interactions lead to spin formation and tend to align spins ferromagnetically at each end of the nanotube [11–14], thereby producing end spins of size $S_1 = S_2 = N_{\text{edge}}/2$, (1) with $N_{\text{edge}}$ denoting the total number of topologically protected mid-gap states at each end (see Fig. 1.(a)). Depending on chirality, $N_{\text{edge}}$ can be quite large for many nanotubes, so that these states are expected to be very sensitive to interaction effects.

![FIG. 1. (a) Topologically protected spins are formed at both edges of most semiconducting nanotubes. (b) Band structure of a semiconducting nanotube in the absence of interactions. Topological end states (red lines) appear in the gap. (c) Many-body spectrum at finite interaction. For ferromagnetic end spin coupling, the ground state has a total spin $S_T$, equal to the number of edge states $N_{\text{edge}}$. Spin excitations appear at low energies due to coupling between end spins.](attachment:image.png)
nanotubes, implying the appearance of surprisingly large end spins, parallel in many ways ferromagnetic edge states observed in graphene nanoribbons [15–20]. The two end spins then couple to each other via an exchange interaction which, in the absence of spin-orbit coupling, takes on a simple form:

\[ H_{\text{exch}} = \frac{1}{2} J_{\text{eff}} S_1 S_2 . \] (2)

The sign and strength of the exchange interaction here turns out to depend sensitively on the length of the nanotube as well as on its chirality and the dielectric constant of its environment.

Hamiltonian. In this work, we use a tight binding approach to describe interacting nanotubes, and express the Hamiltonian as

\[ H = -\sum_{s} \sum_{r,r'} t(r-r') c_{s}^\dagger(r) c_{s}(r') + \frac{1}{2} \sum_{r,r'} V(r-r') : n(r) :: n(r') : , \] (3)

Here \( c^\dagger_{s}(r) \) creates an electron with spin \( s \) at the \( p_z \) orbital of a carbon atom at a position \( r \). The hopping matrix elements \( t(r-r') \) describe hopping between nearest neighbour and next nearest neighbour orbitals. They incorporate curvature effects [21], and also can be generalized to include spin-orbit effects neglected here [22].

The second term in Eq. (3) accounts for the long-ranged Coulomb interaction between local charge fluctuations on the nanotube

\[ V(r) = \frac{e^2}{\epsilon} \frac{1}{\sqrt{r^2 + \alpha^2}} , \] (4)

with \( U_0 = 11.3 \text{eV} \) and \( \alpha \approx 0.127 \text{nm/} \epsilon \) a short distance cut-off, and \( \epsilon \) the dielectric constant [23]. Densities in Eq. (3) appear in a normal ordered form, : \( n(r) : = \sum_{s} (c^\dagger_{s}(r) c_{s}(r) - 1/2) \), thereby measuring deviations from half filling. In the following, we shall determine and analyze the many-body ground state and excitation spectrum of this Hamiltonian.

Non-interacting nanotubes and topological end states. Nonotubes are classified by their chirality, \( \chi = (n,m) \), i.e. the lattice vector \( \mathbf{C} = n \mathbf{a}_1 + m \mathbf{a}_2 \), along which a graphene sheet needs to be rolled up to form the nanotube. In this work, we focus on semiconducting nanotubes with \( (n-m) \text{ mod } 3 = \pm 1 \).

For topological considerations, it is most useful to consider a perfect and infinite nanotube, and use a so-called helical construction [24, 25]. Similar to graphene, the nanotube possesses two sublattices, \( A \) and \( B \). In the helical construction, one introduces a helical vector \( \mathbf{H} \) within the graphene sheet, and lines up all atoms of the nanotube along just \( d \) spirals along the direction \( \mathbf{H} \), with \( d \) defined as the greatest common divisor of \( n \) and \( m \) (see supplemental material [26] for details).

FIG. 2. (a) Mapping of an infinite carbon nanotube to an effective 1D ladder-like lattice model with \( d \) decoupled chains, for a chirality \( \chi = (6, 2) \) and \( d = 2 \). Arrows indicate hoppings between carbon atoms. (b) The number of edge states, \( N_{\text{edge}} \), as a function of the chirality \( \chi = (n, m) \). (c) Band structure and the corresponding winding numbers for a (6, 2) nanotube.

Clearly, an infinite nanotube possesses a discrete \( d \)-fold rotational symmetry around the axis of the tube, \( C_d \), and a 'gliding' (helical) translational symmetry along the chain, as generated by the helical vector \( \mathbf{H} \). Correspondingly, single particle (but also many-body) states can be labeled by their ”angular momentum” \( \mu = 0, \ldots, d - 1 \) and a quasimomentum \( k \) along the chain, and are organized into \( 2d \) bands, \( \epsilon^{(\mu)}(k) \), the band index \( \pm \) originating from the sublattice structure of the nanotube, and referring to bonding (valance) and anti-bonding (conduction) bands. Within the tight binding scheme used here, these bands are associated with \( d \) independent one dimensional chains, each giving rise to one conduction and one valence band, and describing the motion of electrons with a given ‘angular momentum’ \( \mu \) (see Fig. 2(c) and Ref. [26] for details). Interestingly, each of these bands possesses a topological winding number [9],

\[ w_{\pm}^{(\mu)} = \frac{1}{2\pi i} \int dk \langle \psi_{\pm}^{(\mu)} (k) | \partial_k \psi_{\pm}^{(\mu)} (k) \rangle \] (5)

with \( |\psi_{\pm}^{(\mu)} (k) \rangle \) the corresponding eigenstates and the integral running over the band. Non-zero winding numbers imply the presence of topologically protected end states [27]. Remarkably, we can express the total number of end states at each end of a semiconducting tube in a closed form, just in terms of the nanotube's chirality,
where $\Theta(x) = (x+1) \mod 3 - 1$ is a modified modulo function taking values 0 and $\pm 1$, and $[\ldots]$ denotes the floor function. In Fig. 2, (b), we display $N_{\text{edge}}$ as a function of the chirality of the nanotubes. White squares indicate metallic tubes, while colored ones refer to semiconducting tubes. Clearly, most of the tubes are semiconducting, and the vast majority of semiconducting tubes possess topological end states, typically several ones. For zigzag tubes with chirality $(n,0)$, e.g., the number of end states increases linearly with the circumference of the tube, $N_{\text{zig-zag}} \approx n/3$.

Remarkably, as our tight binding calculations also demonstrate, in contrast to the SSH model, these end states are rather robust and insensitive to the form of ending of the nanotube as well as lattice defects. This is due to the fact that in the effective one dimensional model, carbon atoms are connected with many neighbors. Therefore removing some of the atoms or adding a few atoms to the end of the tube will break the $C_3$ symmetry and therefore mix the mid-gap states, but does not remove them.

Interacting nanotubes.— To perform numerical calculations, we first construct a finite nanotube, and diagonalize the noninteracting part of the Hamiltonian Eq. (3) to find its eigenstates $\phi_n(r)$ and the corresponding eigenenergies, $\epsilon_n$, and express the interaction term within this basis. Normal ordering needs to be treated with special care in this process (see [26]). To treat nanotubes of reasonable length, $L \approx 40$ nm, we restrict the many-body calculations to just about a hundred active states from the valence and conduction bands with energies $|\epsilon_n| < \Lambda \approx 5\Delta$, with $\Delta$ the band gap of the noninteracting infinite nanotube. Then we apply a density matrix renormalization group (DMRG) based approach adopted to Hamiltonians with arbitrary long-ranged two-body interactions [28–30] to determine the ground state and low lying excitations of the nanotube. In this procedure, we use $U(1) \times U(1)$ symmetries, i.e. we fix the excess charge $Q$ on the nanotube and the $z$ component of the total spin, $S_T^z$. In practice, the computational basis is further optimized using fermionic mode transformation[31].

As sketched in Fig. 1, end spins manifest in the form of low energy sub-gap excitations, which can be described by the effective Hamiltonian, Eq. (2). The many-body spectra observed reveal consistently the formation of end spins with $S_{1,2} = N_{\text{edge}}/2$, coupled to each other. In the absence of spin-orbit coupling, this interaction is $SU(2)$ symmetrical, and the many-body spectrum consists of multiplets with total spin $S_T = 0, \ldots, N_{\text{edge}}$.

The alignment and size of the electron spins at the ends of the nanotubes can be easily understood. In a topological nanotube, $2N_{\text{edge}}$ spin degenerate states are split from the conduction and valance bands, and form the mid-gap states, and are therefore populated by $2N_{\text{edge}}$ electrons in a neutral (half-filled) tube. End states are thus half-filled in a neutral nanotube. The spatial extension of these localized end states states is roughly $\xi_0 \approx \hbar c/\Delta \sim R$, with $c$ the Fermi velocity and $R$ the radius of the nanotube. Electrons confined on these states interact therefore strongly with each other, and moving one electron from one end of the tube to the other would cost an energy $\sim E_C \sim c^2/(\epsilon_0 \xi_0) \sim c^2/(\epsilon R)$. Therefore, to minimize their Coulomb energy, $N_{\text{edge}}$ electrons go to each end of the tube. Moreover, since all these single particle levels are degenerate, and wave functions on one end overlap with each other, electrons at one end follow Hund’s rule, and align their spins to minimize their interaction, thereby yielding a composite spin, $S_{1,2} = N_{\text{edge}}/2$, Eq. (1).

We have analyzed the excitation spectra of dozens of nanotubes, and verified Eq. (1) numerically in the presence of Coulomb interaction for all nanotubes listed in Fig. 2.b. In these simulations, we have observed end spins as large as $S_{1,2} = 5/2$, and corresponding ground state spins as large as $S_T = S_1 + S_2 = 5$. According to Eqs. (1) and (6), for appropriate chiralities and larger nanotube radii, the total emergent spin can largely exceed these values. The ground state spin of the nanotube is determined by the exchange coupling $J_{\text{eff}}$ between the end spins. Be-

![FIG. 3. Effective exchange interaction $J_{\text{eff}}$ between the localized spins at the two ends of the nanotube as function of its length. When $N_{\text{edge}}=1$, $J_{\text{eff}}$ is always positive indicating an antiferromagnetic exchange, while for $N_{\text{edge}} \geq 2$ an antiferromagnetic to ferromagnetic transition occurs. As the inset shows, for appropriate nanotube length, the sign of the interaction can be changed by changing the dielectric constant of the environment.](image-url)
ing generated by tunneling between the topological end states, this coupling is expected to fall off exponentially with the length of the nanotube. The coupling $J_{\text{eff}}$ can be readily extracted from the spin excitation spectrum, and is displayed for two particular nanotubes as a function the nanotube length $L$ in Fig. 3. On top, we show the results for a $(7, 5)$ nanotube with $N_{\text{edge}} = 1$, and corresponding spin $S = 1/2$'s at the edges. The coupling is antiferromagnetic, and therefore $S_F = 0$ in this case, irrespective of the length of the nanotube. As expected, the coupling $J_{\text{eff}}$ decays exponentially with $L$, reflecting the exponentially localized nature of the end states.

A completely different behavior is observed, however, for an $(8, 3)$ nanotube with $N_{\text{edge}} = 2$, as displayed on the bottom of Fig. 3. Here we observe an antiferromagnetic coupling in very short nanotubes with $L \lesssim 5$ nm, while in longer tubes the interaction becomes ferromagnetic and decays exponentially, as expected.

The behavior shown in Figs. 3 appears to be generic: we have studied a great number of nanotubes with different chiralities, and in all nanotubes with $N_{\text{edge}} = 1$ we find an antiferromagnetic coupling, while all nanotubes with $N_{\text{edge}} \geq 2$ exhibit an exchange interaction that changes from antiferromagnetic to ferromagnetic with increasing nanotube length. As demonstrated in the lower panel, the precise location of the sign change is sensitive to the dielectric constant, $\epsilon$, and by appropriate engineering of $\epsilon$, one can even completely decouple the two end spins. This mechanism provides a tool to perform quantum manipulations with the end spins.

Charging the end states.— As discussed above, a topological nanotube behaves to a large extent as a self-organized double quantum dot system. Whether one can charge these topological quantum dots or not and observe the end states in a direct spectroscopic (tunneling) experiment, depends largely on screening, i.e., the value of $\epsilon$. Placing an additional electron to the topological states costs a Coulomb energy of the order of $E_C \sim e^2/(\epsilon R)$, while adding a delocalized particle to the valence band needs an energy $\Delta \sim \hbar c/R$. Therefore, for each chirality, there is a critical value $\epsilon_C \sim e^2/(\hbar c)$ of the dielectric constant. For dielectric constants larger than $\epsilon_C$ (strong screening), electrons and holes added to a neutral nanotube localize at the end and the topological quantum dots can be charged, while for smaller dielectric constants (weak screening) they must go directly to the conduction or valence band, and delocalize along the nanotube.

According to our calculations, this transition happens at around $\epsilon \approx 3$, as is displayed in Fig. 4. The inset of Fig. 4 shows the spatial location of an electron added to the nanotube in terms of the position $\xi$ along the helix. Clearly, the added particle is localized on sublattice $A$ at one end, while it localizes on sublattice $B$ at the other end (in close similarity with the SSH model). As shown in the main panel, the localization length of the added particle, $\xi$ is strongly influenced by Coulomb interactions, and diverges as one approaches the critical value of $\epsilon$. This localization length should not be confused with that of the end spins, which remains of the order of $R$. Close to $\epsilon \gtrsim \epsilon_C$, the delocalized charges can create a glue between the end spins.

Closing observations and conclusions.— As we demonstrated in this work, most carbon nanotubes are topological, and all topological nanotubes possess interaction induced end spins, residing at the edges of the tube, and localized within a distance $\approx \xi_0 \sim R$. Being protected by topology, these naturally formed end spins are robust, are typically larger than spin $S = 1/2$, and couple to each other exponentially weakly in longer nanotubes (longer than a few nanometers). Their presence may provide a natural explanation for the intrinsic spin formation observed a long time ago in encapsulated nanotubes (pea pods) [32], and simple model calculations support that an exponentially weak ferromagnetic exchange quite naturally explains the super-Curie behavior reported earlier [33].

The large end spins demonstrated here are the nanotube analogues of ferromagnetic edge states appearing in graphene nanoribbons [15, 17–20, 34]. Indeed, selecting any topologically non-trivial chirality $(p, q)$ with $p$ and $q$ being relative primes, we can think of nanoribbons of width $W$ as nanotubes with chirality $(n, m) \equiv (r p, r q)$ and length $L = W$, with $r$ taken to infinity. In this limit, the length of the nanotube remains finite while its radius $R$ is taken to infinity, thereby yielding nanoribbons closed into a cylinder. In this limit, $d \to \infty$, yielding...
a proliferation of topological end states, thus forming a dispersionless band, and therefore subject to Stoner ferromagnetism. The sign change of $J_{\text{eff}}$ observed has also its counterpart in nanoribbons: in close analogy with the sign change of $J_{\text{eff}}$ observed here, the coupling between ferromagnetic edge states is observed to change sign, too, from being antiferromagnetic to ferromagnetic as a function of $W$ [19].

Topological nanotubes spontaneously form double dot devices, which may provide a platform for quantum computation. As we demonstrated, local probes such as scanning tunneling microscopy (STM) can be used to observe these ‘topological quantum dots’, however, to charge them, the effective dielectric constants must be increased over some critical value. Therefore, rather than using suspended nanotubes, nanotubes layed over some tunable dielectrics would be the most promising candidates for a direct experimental observation by tunneling spectroscopy. Local optical spectroscopy may also provide a tool to detect these topologically protected subgap states.

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SUPPLEMENTAL INFORMATION

Effective 1D lattice model

In this section, we describe how to construct the effective Hamiltonian. Our starting point is the quadratic tight binding Hamiltonian describing the underlying graphene sheet

$$H_0 = - \sum_{x, x', s} t(x - x') c_s^\dagger(x) c_s(x'),$$

(7)

where $c_s(x)$ denotes the annihilation operator of an electron at site $x$ and with spin $s = \{\uparrow, \downarrow\}$, while $t(x - x')$ represents the hopping integral between lattice sites $x$ and $x'$. In our calculations, we also include second nearest neighbor hoppings to account for curvature effects [35] (see Fig. 5(b)).

A single wall carbon nanotube is characterized by its chirality $\chi = (n, m)$, where $n$ and $m$ are integers. These specify the chirality vector, $C$, and the helical vector, $H$, as

$$C = n a_1 + m a_2, \quad H = p a_1 + q a_2.$$  

(8)

Here $p$ and $q$ are two integers that satisfy the relation $mp - nq = d$, with $d = \gcd(n, m)$ the greatest common divisor of $n$ and $m$.

The nanotube is obtained by rolling up a graphene sheet along $C$ (see Fig. 5). As explained in the main text, the rolled up tube is invariant under $C_d$ rotations (corresponding to translations by a lattice vector $C/d$ of the graphene sheet) as well as under gliding rotations along the tube (generated by translations with $H$). As illustrated in Fig. 5, atoms forming the tube can correspondingly be organized into $d$ helices of atoms $A$ and $d$ helices of atoms $B$.

Atoms on the nanotube are located at some physical positions $r$. These positions can easily be expressed in terms of the atoms original position $x$ before the roll-up, expressed as

$$x = \begin{cases} \frac{2}{3} C + \ell H & \text{if in } A, \\ \frac{2}{3} C + \ell H + \frac{a_1 + a_2}{3} & \text{if in } B, \end{cases}$$

(9)

with the integer $\nu = \{0, 1, \cdots, d-1\}$ specifying the helix, and $\ell$ the location along this helix. Notice that periodic boundary conditions are used within the graphene plane, i.e., graphene atoms with coordinates $x$ and $x + C$ are considered to be identical, and neighbors are identified accordingly. In our numerics, we use this helical construction, i.e., we specify atoms on the nanotube by the quantum numbers $\nu, \ell$, and the sublattice label $\tau = A$ or $B$.

The integer label $\ell$ can also be thought of as an indicator of the lattice position along the nanotube in units of

$$a_z = \frac{T}{N/d},$$

(10)

which is the shortest distance between two consecutive atoms along one helix, as projected to the axial direction (see Fig. 5(b)). Here $T = a \sqrt{3(n^2 + m^2 + nm)}/\gcd(2n + m, 2m + n)$, is the length of the translation vector (lattice constant) defining the conventional unit cell of the nanotube, and $N = 2(n^2 + m^2 + nm)/d_d$ denotes the total number of $A$ ($B$) atoms in the conventional 1D nanotube unit cell [21].

Having constructed the positions $r = r(x) = r(\nu, \ell, \tau)$, as well as the tunneling matrix elements, $t(r, r') = t(x - x')$, we can construct and diagonalize the non-interacting part of the Hamiltonian (3), and obtain the corresponding eigenfunctions $\phi_\alpha(r) \equiv \phi_\alpha(\nu, \ell, \tau)$, and rewrite the noninteracting part of the Hamiltonian as

$$H_0 = \sum_{\alpha, s} \epsilon_\alpha c^\dagger_\alpha s c_\alpha s.$$  

(11)
Next, we express the interaction in this basis as

\[
H_{\text{int}} = \frac{1}{2} \sum_{s_1 s_2} \sum_{\alpha \beta \gamma \delta} V_{\alpha \beta; \gamma \delta} c_{\alpha s_1}^{\dagger} c_{\gamma s_2}^{\dagger} c_{\beta s_2} c_{\delta s_1} \\
+ \sum_{s} \sum_{\alpha, \beta, \eta} \left( V_{\alpha \eta; \beta \eta} c_{\alpha s}^{\dagger} c_{\beta s} - V_{\alpha \beta; \eta s} c_{\alpha s} c_{\beta s} \right),
\]

where the last terms originate from normal ordering, and \(V_{\alpha \beta; \gamma \delta}\) denotes the two-body interaction element,

\[
V_{\alpha \beta; \gamma \delta} = \sum_{a, a'} \phi_a^* (a) \phi_{a'} (a) V (r_a - r_{a'}) \phi_{a'}^* (a') \phi_a (a').
\]

Here, for compactness, we have introduced the composite label, \(a = (\nu, \ell, \tau)\). For effective Coulomb interaction we use the so-called Ohno potential [23],

\[
V (r_1 - r_2) = \frac{e^2}{\epsilon_r} \frac{1}{\sqrt{(r_1 - r_2)^2 + \alpha^2}},
\]

with \(\alpha = \frac{Q}{Q_{\text{cut}}^2}\), and \(U_0 = 11.3\) eV for the \(\pi\)-orbital [23].

To perform density matrix renormalization group (DMRG) calculations, we now assume that quantum fluctuations only influence the occupation of levels not far from the Fermi energy, \(|\epsilon_a| < \Lambda\), with \(\Lambda\) an energy cut-off introduced. However, in doing so, we must treat occupied 'core' levels and normal ordering carefully. In practice, we do that by adding the truncated normal ordered part of the interactions to the kinetic energy, and thereby renormalizing the non-interacting part as

\[
H_0 \rightarrow \tilde{H}_0 = \sum_s \sum_{|r_a|,|s|<\Lambda} T_{\alpha \beta} c_{\alpha s}^{\dagger} c_{\beta s},
\]

with the single particle matrix elements defined as

\[
T_{\alpha \beta} = \epsilon_a \delta_{\alpha \beta} + \sum_{|\epsilon_\gamma|<\Lambda} \left( V_{\epsilon_\gamma; \epsilon_\gamma} - V_{\epsilon_\alpha; \epsilon_\gamma} \right),
\]

while interactions are restricted to active orbitals,

\[
H_{\text{int}} \rightarrow \tilde{H}_{\text{int}} = \frac{1}{2} \sum_{s_1 s_2} \sum_{\alpha, \beta, \gamma, \delta} V_{\alpha \beta; \gamma \delta} c_{\alpha s_1}^{\dagger} c_{\gamma s_2}^{\dagger} c_{\beta s_2} c_{\delta s_1}.
\]

Here the tilde sign indicates restriction to active orbitals. A delicate and important feature of the cut-off construction above is that it preserves electron-hole symmetry even for the interacting spectrum, in case we have only nearest neighbor hopping, as readily verified by explicit analytical calculations as well as by our numerics.

**DMRG calculations with long range Coulomb interactions**

For our DMRG calculations we employ the two-site variant of DMRG, as first introduced by White [28]. We compute the ground state energy as well as the energy of a few excited states above the ground state. In practice, the performance of the DMRG can be boosted significantly by optimizing the computational basis using fermionic mode transformation [31].

The local electron density for the effective 1D lattice model is then easily expressed in terms of the reduced (spin traced) density matrix \(\varrho_{\alpha \beta} \equiv \sum_s (c_{\alpha s}^{\dagger} c_{\beta s})\) as

\[
n(\nu \ell \tau) = \sum_{\alpha \beta} \varrho_{\alpha \beta} \phi_a^* (\nu \ell \tau) \phi_a (\nu \ell \tau) + n_{\text{core}} (\nu \ell \tau),
\]

with \(n_{\text{core}} (\nu \ell \tau)\) the electron charge of the completely occupied core states. A summation over the helix label \(\nu\) yields the total density of atoms \(A\) or \(B\) at a helix position \(\ell\),

\[
n^A (\ell) \equiv \sum_\nu n(\nu \ell). \quad (17)
\]

Computing then the excess charge density, \(\Delta n^A (\ell) \equiv n_{\ell=1}^A (\ell) - n_{\ell=0}^A (\ell)\), induced upon adding one electron to the nanotube, allows us, for example, to explore the localization and spin structure of the edge states and to estimate their extension in real space, as presented in Fig. 4 of the main text.