Theory for transport through a single magnetic molecule: Endohedral N@C$_{60}$

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We consider transport through a single N@C$_{60}$ molecule, weakly coupled to metallic leads. Employing a density-matrix formalism we derive rate equations for the occupation probabilities of many-particle states of the molecule. We calculate the current-voltage characteristics and the differential conductance for N@C$_{60}$ in a break junction. Our results reveal Coulomb-blockade behavior as well as a fine structure of the Coulomb-blockade peaks due to the exchange coupling of the C$_{60}$ spin to the spin of the encapsulated nitrogen atom.

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I. INTRODUCTION

The rapid progress of miniaturization of electronic devices has led to chip features smaller than 100 nm, for which standard semiconductor technology reaches its limit. One proposed solution is a transistor consisting of a single molecule. In recent years transport through single molecules has been studied quite extensively$^{1,2,3,4,5,6,7,8,9}$—for example, in break junctions$^{10}$—Inelastic transport occurs due to the interaction of electrons with internal vibrational or magnetic degrees of freedom of the molecules. Transport through magnetic molecules$^{11,12}$ is particularly interesting also from the point of view of spintronics—i.e., the idea of exploiting the electron spin in electronic devices. While most molecules are normally nonmagnetic, there are exceptions such as endohedral N@C$_{60}$—i.e., a nitrogen atom encapsulated in a C$_{60}$ cage$^{13}$ It is known that the encapsulated atom retains its $p$ electrons, leading to a localized spin $S_N = 3/2$. There are fascinating ideas of employing this spin in a quantum computer.$^{14}$

In this paper we propose to measure the current through a single N@C$_{60}$ molecule in a break junction and we calculate the current-voltage ($I$-$V$) characteristics and the differential conductance $dI/dV$. Since transport through a single C$_{60}$ molecule has been demonstrated$^{15}$ and the synthesis of endohedral fullerenes is also feasible,$^{13}$ such an experiment is possible with present-day apparatus. Besides the typical Coulomb-blockade behavior we predict a characteristic fine structure of the Coulomb-blockade peaks in $dI/dV$ due to the exchange coupling of the C$_{60}$ spin to the spin $3/2$ of the encapsulated nitrogen atom. It should be mentioned that the discussion of transport through P@C$_{60}$ proceeds quite analogously and yields qualitatively identical results.

II. THEORY

In our model the N@C$_{60}$ molecule is treated as a quantum dot and the leads, labeled as L (left) and R (right), as macroscopic charge reservoirs. Relaxation in the leads is assumed to be sufficiently fast so that the electron distributions in the leads can be described by Fermi functions. As C$_{60}$ generally prefers to be singly or doubly negatively charged$^{15,16,17,18,19}$ we assume that electronic transport through the molecule involves only the threefold-degenerate LUMO (lowest unoccupied molecular orbital)$^{20}$ Since we concentrate on the fine structure of the differential conductance close to degeneracy points, we assume that the fivefold-degenerate HOMO (highest occupied molecular orbital), which lies about 7.5 eV below the LUMO,$^{21}$ remains fully occupied, whereas the threefold-degenerate LUMO+1, about 1.7 eV above the LUMO,$^{18}$ remains empty.$^{21}$ Charge transfer from the nitrogen atom to the fullerene cage is assumed to be negligible. When the LUMO is partially occupied, the net spin of the electrons in the LUMO, $S_{C_{60}},$ couples to the spin $3/2$ of the nitrogen atom, $S_N,$ and the total spin of the molecule is $S = S_{C_{60}} + S_N.$ The exchange interaction can be written in the simple form $-J S_{C_{60}} \cdot S_N$ due to Hund’s first rule: Note that the three LUMO’s and the three nitrogen $p$ orbitals both have odd parity with a single nodal plane each, which can be chosen as the $xy$, $yz$, or $zx$ plane. Consequently, there is only a significant exchange interaction between any LUMO and the $p$ orbital of the same symmetry. The exchange interaction can thus be written as a sum of terms for the three pairs of orbitals. However, due to the strong Hund’s-rule coupling, the $p$ orbital spins combine to $S_N = 3/2$; i.e., they are all parallel. Then the spin of each $p$ orbital is $S_N/3,$ as can be proved by projecting the spins onto the $S_N = 3/2$ subspace. Thus the exchange terms can be combined to the simple scalar product. The full Hamiltonian of the system then reads $H = H_d + H_{\text{leads}} + H_t,$ where

$$H_d = (\varepsilon - eV) n_d + \frac{U}{2} n_d(n_d - 1) - J S_{C_{60}} \cdot S_N$$

represents the molecular quantum dot,

$$H_{\text{leads}} = \sum_{\alpha = \text{L,R}} \sum_{\kappa \sigma} \varepsilon_{\alpha \kappa} a_{\alpha \kappa \sigma}^{\dagger} a_{\alpha \kappa \sigma}$$

represents the leads, and

$$H_t = \sum_{\alpha = \text{L,R}} \sum_{\kappa \kappa' \sigma} (t_{\alpha \kappa \sigma} c_{\alpha \kappa \sigma}^{\dagger} c_{\alpha \kappa' \sigma} + t_{\alpha \kappa' \sigma}^{*} c_{\alpha \kappa' \sigma}^{\dagger} c_{\alpha \kappa \sigma})$$

describes the tunneling between the dot and the leads, which is assumed to be weak compared to typical excitation energies of the molecule. Here, the operator $c_{\alpha \kappa \sigma}^{\dagger}$ creates an elec-
tron with spin $\sigma$ in the molecular orbital $n$, while $a_{\alpha k\sigma}^\dagger$ creates an electron in lead $\alpha$ with spin $\sigma$, momentum $k$, and energy $\epsilon_{\alpha k}$ relative to the Fermi energy. $n_{\alpha k} = \sum_n c_{\alpha k}\sigma^\dagger c_{\alpha k}\sigma$ and $S_{C_{60}} = \sum_{\alpha k} c_{\alpha k}\sigma^\dagger c_{\alpha k}\sigma$ are the number and spin operators of electrons on the dot, respectively. Electron-electron interaction is taken into account by the local Coulomb repulsion $U$ and the exchange interaction with the nitrogen spin by the exchange coupling $J$. The values of $\varepsilon$, $U$, and $J$ are not well known at present. 

Ab initio calculations indicate that $C_{60}^-$ is the ground state, whereas $C_{60}^+$ has a slightly higher energy. This is in agreement with the experimental observation of a very long-lived metastable $C_{60}^-$ (Ref. 15). However, there are recent contradicting ab initio results predicting $C_{60}^2^-$ to be slightly bound relative to $C_{60}^-$ (Ref. 15). For our numerical calculations we use $\varepsilon = -2.75$ eV and $U = 2.84$ eV in accordance with Ref. 17. $J$ appears to be ferromagnetic. We take $J = 1$ meV from ab initio calculations of Udvardi. This relatively strong exchange coupling is consistent with the absence of electron-paramagnetic-resonance (EPR) signals for N@C$_{60}$ anions with charges $-1$ through $-5$, while the signal is present for the neutral molecule and the hexa-anion. Note that the exchange coupling is significantly smaller than the energy of relevant vibrational modes. The oscillations of the molecule as a whole have an energy of the order of $5$ meV. The oscillations of the nitrogen atom within the C$_{60}$ have an energy of $13$ meV whereas the modes of the C$_{60}$ cage lie at much higher energies.

We next derive rate equations for this model starting from the equation of motion for the density matrix $\rho$.

$$\frac{d\rho(t)}{dt} = -i [H_{\text{tot}}, \rho(t)] + \sum_{\alpha n k} |t_{\alpha}|^2 \left\{ f(\epsilon_{\alpha k}) e^{i\epsilon_{\alpha k}t'} c_{\alpha n}\sigma e^{-iH_{\text{tot}}t'} c_{\alpha n}\sigma^\dagger \rho(t) + \text{H.c.} \right\} \sum_{\alpha n k} \left( \frac{H_{\text{tot}}}{2} \right)^2.$$  

(8)

The probability of the dot being in the many-particle state $|n\rangle$ in $P_n = \langle n| \rho(t) |n\rangle$. Introducing the overlap matrix elements $C_{mn}^\sigma = \langle m| c_{\sigma n}^\dagger |n\rangle$ and $C_{mn}^\sigma = \langle m| \sum_{\sigma} c_{\sigma n}^\dagger |n\rangle$ and identifying the integrals in Eq. (8) as $\delta$ functions we can write Eq. (5) as a set of rate equations

$$\frac{dP_n}{dt} = \sum_{m \neq n} P_m R_{m\rightarrow n} - P_n \sum_{m \neq n} R_{n\rightarrow m},$$  

(9)

with transition rates

$$R_{n\rightarrow m} = \sum_{\alpha} 2\pi |t_{\alpha}|^2 D_{\alpha} f(\epsilon_{\alpha}^m - \epsilon_{\alpha}^n - \mu_{\alpha}).$$  

(10)

Here, $\epsilon_{\alpha}^m$ is the energy of the many-particle state $|m\rangle$ of the dot and $D_{\alpha}$ denotes the density of states per spin species in lead $\alpha$, which we take to be constant and equal for both leads. The matrix elements $C_{mn}^\sigma$ ($C_{mn}^\sigma$) can only be finite if the electron number of state $|n\rangle$ is larger (smaller) by 1 than the electron number of state $|m\rangle$. We are interested in the stationary state, which corresponds to $dP_n/dt = 0$ for all states $|n\rangle$.

In deriving Eq. (9) we have assumed that the density matrix $\rho_{\text{tot}}$ is completely diagonal. This assumption requires some thought since many of the eigenstates of our molecular quantum dot are degenerate so that one might expect finite off-diagonal components even in the stationary state. However, this is not the case: Let $U$ be a unitary matrix that leaves the dot Hamiltonian $H_{\text{tot}}$ invariant. With any stationary density matrix $\rho_{\text{tot}}$, $U \rho_{\text{tot}} U^\dagger$ is another solution. Now suppose that there exists a stationary solution $\rho_{\text{tot}}$ that is not diagonal within a block of degenerate states. Then one can choose $U$ so that $U \rho_{\text{tot}} U^\dagger$ is diagonal since the nonzero off-diagonal components have been assumed to connect degenerate states (we exclude the case of accidental degeneracy). But then $U \rho_{\text{tot}} U^\dagger$ has unequal diagonal components—i.e., probabilities $P_{nm}$ for symmetry-related states. This is clearly unphysical. On
the other hand, if $\rho_{d}$ is already diagonal with degenerate dot states having equal diagonal components, any allowed transformation $U$ leaves $\rho_{d}$ invariant.

The current operator for lead $\alpha = L, R$ reads[26]

$$I_{\alpha} = i [H, N_{\alpha}] = -i \sum_{n,k\sigma} \left( t_{\alpha} c_{n\sigma}^\dagger a_{nk\sigma} - t_{\alpha}^* a_{nk\sigma}^\dagger c_{n\sigma} \right), \quad (11)$$

where $N_{\alpha}$ is the number operator for electrons in lead $\alpha$. Tracing out the leads we arrive at an expression for the expectation value of the current:

$$\langle I_{\alpha} \rangle = 2\pi D_{\alpha} |t_{\alpha}|^2 \sum_{m,l,\sigma} \left( f(\epsilon_m^d - \epsilon_l^d - \mu_{\alpha}) |C_{m|l\sigma}|^2 
- \left[ 1 - f(\epsilon_m^d - \epsilon_l^d - \mu_{\alpha}) \right] |C_{m|l\sigma}|^2 \right) P^{m}.$$  

We here consider the symmetric case $t_{L} = t_{R}$ and $\mu_{L} = -\mu_{R} = V/2$.

As there are ($L_1$) possible ways of filling the threefold-degenerate $C_{60}$ LUMO with $i$ electrons according to the Pauli principle and as the nitrogen atom possesses a spin $3/2$, solving the rate equations and calculating the current reduces to an eigenvalue problem of dimension $4 \times 6 = 256$.

### III. RESULTS AND DISCUSSION

The $I$-$V$ characteristics plotted in Fig. 1 show a conductance gap for $|V| < 0.18 V$ due to Coulomb blockade. Our numerical results show that the current $I$ is symmetric with respect to the applied source-drain voltage $V$ in accordance with the high symmetry of the fullerene molecule. Each step in the main $I$-$V$ curve corresponds to the opening of additional current channels. Simultaneously, the average occupation $\langle n \rangle$ of the dot changes. For the parameters chosen above, the $C_{60}$ state is the ground state. At the first step, the potential drop becomes large enough to allow transitions between the nearly degenerate charge states $-1$ and $-2$, as the chemical potential $\mu_{L} = V/2$ reaches the value assumed for the ionization energy $E(C_{60}^2-)$ where $E(C_{60}^-) \equiv \varepsilon + U = 0.09 eV$. At the second step, transitions between the charge states $-1$ and 0 become possible, etc.

Our results for the occupation probabilities reveal that detailed balance is satisfied for the broad plateaus in Fig. 1, i.e., $P^{m} R_{n \rightarrow m} = P^{m} R_{m \rightarrow n}$. As a consequence, the dot occupation probabilities $P^{m}$ for all occupied states are identical in the limit $T \rightarrow 0$, as the transition rates $R_{n \rightarrow m}$ are symmetric for each pair $n, m$ of occupied states. This also accounts for the fact that the average occupation $\langle n \rangle$ is exactly unity for $V = 0 V$, increases to $(24 \times 1 + 60 \times 2)/(24 + 60) = 12/7 \approx 1.71$ at the first step, when the molecule is in one of 24 singly charged or 60 doubly charged states with equal probability, and decreases to $(4 \times 0 + 24 \times 1 + 60 \times 2)/(4 + 24 + 60) = 15/11 \approx 1.36$ at the second step, when 4 additional neutral states become available, etc. Furthermore, we find that each Coulomb-blockade step shows a characteristic fine structure, which we discuss below.

The calculation of the differential conductance $dI/dV$ as a function of source-drain voltage $V$ and gate voltage $V_{g}$ shows the usual Coulomb diamonds; see Fig. 2. Close to the degeneracy points between different charge states we observe a relatively complex fine structure, corresponding to the steps in the inset of Fig. 1. We assume very low temperatures, $k_{B} T \ll J$, to exhibit the structure more clearly. At higher temperatures the peaks in $dI/dV$ are thermally broadened. In the following, we briefly explain the physics behind the fine structure, taking Fig. 2(a) as an example.

Since the $C_{60}$ spin $S_{C_{60}}$, the spin of the nitrogen atom, $S_{N}$, and the total spin $S$ (where $S = |S_{C_{60}} - S_{N}|, ..., S_{C_{60}} + S_{N}$) are good quantum numbers, the exchange energy is

$$E_{\text{exc}} = -J/2 \left[ S(S+1) - S_{C_{60}}(S_{C_{60}}+1) - S_{N}(S_{N}+1) \right]. \quad (13)$$

which leads to the level splitting illustrated in Fig. 3. The structure in Fig. 2(a) arises from transitions between charge states $-1$ and $-2$, taking spin excitations into account. In equilibrium ($V = 0 V$) only the ground state of the dot is occupied, which is the $C_{60}^{-}$ state with $S_{C_{60}} = 1/2$ and $S = 2$ for $V_{g}$ smaller than the degeneracy point $V_{g}^{0}$ and the $C_{60}^{-2}$ state with $S_{C_{60}} = 1$ and $S = 5/2$ for $V_{g} > V_{g}^{0}$; cf. Fig. 3(a). For $V_{g} < V_{g}^{0}$ the first peak in $dI/dV$ at nonzero $V$ originates from the transition with $S_{C_{60}} = 1/2 \rightarrow 1$ and $S = 2 \rightarrow 5/2$, corresponding to a gain of exchange energy of $\Delta E_{\text{exc}} = -0.75 \text{ meV}$. The second peak results from a transition with $S_{C_{60}} = 1/2 \rightarrow 0, S = 2 \rightarrow 3/2$, and $\Delta E_{\text{exc}} = +0.75 \text{ meV}$. Simultaneously, the transitions with $S_{C_{60}} = 1/2 \rightarrow 0, S = 1 \rightarrow 3/2$, and $\Delta E_{\text{exc}} = -1.25 \text{ meV}$ and $S_{C_{60}} = 1/2 \rightarrow 1, S = 1 \rightarrow 3/2$, and $\Delta E_{\text{exc}} = -0.25 \text{ meV}$ are enabled [dashed lines in Fig. 3(a)]. Although energetically possible, these transitions are not excited at lower source-drain voltages, because the lower levels are unoccupied. The last two peaks belong to transitions with
$S_{C_{60}} = 1/2 \rightarrow 1, S = 1 \rightarrow 1/2, \text{ and } \Delta E_{\text{exc}} = +1.25 \text{ meV}$ and $S = 1/2 \rightarrow 1, S = 2 \rightarrow 3/2, \text{ and } \Delta E_{\text{exc}} = +1.75 \text{ meV}$. Note that the values of $\Delta E_{\text{exc}}$ account for the level spacing.

The situation is different for $V_g$ significantly larger than $V_0^0$, where we observe only two peaks; cf. Fig. 2(a). As soon as the transition from the $C_{60}^{-}$ ground state into the lowest $C_{60}^{-}$ state with $S_{C_{60}} = 1 \rightarrow 1/2, S = 5/2 \rightarrow 2, \text{ and } \Delta E_{\text{exc}} = +0.75 \text{ meV}$ becomes possible, the transitions corresponding to $\Delta E_{\text{exc}} = -0.75 \text{ meV}, -1.75 \text{ meV}, +0.25 \text{ meV}, \text{ and } -1.25 \text{ meV}$ [dashed lines in Fig. 2(b)] are also enabled. Again the latter four would be energetically possible at lower $V$, but do not appear as peaks of $dI/dV$, since the corresponding lower levels are unoccupied. In the vicinity of $V_0^0$ we find that the slope of several lines abruptly changes sign. This corresponds to the situation where two levels connected in Fig. 2 by a transition cross as $V_g$ is varied. The fine structure in Fig. 2(b) can be discussed analogously. The structure is different for all degeneracy points and can thus serve as a fingerprint of the particular charge transition. This should be useful since the zero of the $V_g$ axis is often shifted significantly from one experiment to the next.

Selection rules for single-electron tunneling require that $\Delta S_{C_{60}} = \pm 1/2 \text{ and } \Delta S = \pm 1/2$. The different brightness of the peaks in Fig. 2(b) is correlated with the number of transitions that are possible at a given source-drain voltage. Each allowed transition may be thought of as one current channel.

Experimentally, the magnetic origin of the fine structure is most conclusively tested by observing the behavior in a magnetic field. For ionized $C_{60}$ in lattices and in solution, the orbital moment is quenched.\textsuperscript{27,28} We assume that the fields generated by the electrodes in a break junction are also sufficiently strong to quench the orbital moment. Then the molecule couples to a magnetic induction $B$ only through the spin moments, described by the new Hamiltonian

$$H' = H - g \mu_B B S_{C_{60}}^z - g \mu_B B S_N^z = H - g \mu_B B S^z. \quad (14)$$

Here, $\mu_B$ is the Bohr magneton and $g$ is the $g$ factor, which is $g \approx 2$ for both the nitrogen spin $S_N$ and the $C_{60}$ spin. We choose a many-particle basis of simultaneous eigenstates of $n_{C_{60}}, S_{C_{60}}$, $S$, and $S^z$. Then the only difference is that additional Zeeman energies appear in our expression for the transition rates, Eq. (10). In Figs. 2(c) and 2(d) we show $dI/dV$ for the same parameters as in Figs. 2(a) and 2(b) but with $B = 2 \text{T}$. As expected, the peaks split, but in addition several peaks are absent since they are not allowed by the selection rules. For example, for $V_g > V_0^0$ the first peak is due to a transition with $S_{C_{60}} = 1 \rightarrow 1/2, S = 5/2 \rightarrow 2$, and $N = 2 \rightarrow 1$. Since the initial state has all spins aligned in parallel, one electron tunneling out of the dot can only reduce $S^z$ so that there is only a single peak in $dI/dV$.

To summarize, we have presented a theory for transport through a single $N@C_{60}$ molecule weakly coupled to metallic electrodes. Our results for the differential conductance $dI/dV$ as a function of the source-drain and gate voltages show Coulomb-blockade and exhibit a characteristic fine structure.
of the Coulomb-blockade peaks due to the coupling of the C$_{60}$ spin to the spin of the encapsulated nitrogen atom.

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