Magnetococonductance through a vibrating molecule in the Kondo regime

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The effect of a magnetic field on the equilibrium spectral and transport properties of a single-molecule junction is studied using the numerical renormalization group method. The molecule is described by the Anderson-Holstein model in which a single vibrational mode is coupled to the electron density. The effect of an applied magnetic field on the conductance in the Kondo regime is qualitatively different in the weak and strong electron-phonon coupling regimes. In the former case, the Kondo resonance is split and the conductance is strongly suppressed by a magnetic field \( g \mu_B B \gtrsim k_B T_K \), with \( T_K \) the Kondo temperature. In the strong electron-phonon coupling regime a charge analog of the Kondo effect develops. In this case the Kondo resonance is not split by the field and the conductance in the Kondo regime is enhanced in a broad range of values of \( B \).

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I. INTRODUCTION

Transport through molecular nanodevices\(^ \text{1}\) has recently been a subject of intense experimental\(^ \text{2,3,4,5,6,7,8,9} \) and theoretical\(^ \text{10,11,12,13,14,15,16,17} \) investigation. These systems are not only of great interest because of their potential for technological applications but they also pose some interesting and challenging theoretical problems. They arise because in molecular nanodevices electron-electron (\( e-e \)) and electron-phonon (\( e-ph \)) interactions are present simultaneously and their interplay may lead to new physics if their strengths are comparable.

Effects of \( e-e \) interactions in single-molecule devices were seen through the observation of Coulomb blockade peaks in the conductance. At these peaks the charge of the molecule changes by one electron while it stays well defined in the valleys between them\(^ \text{6} \).

The Kondo effect\(^ \text{18} \) was also observed in C\(_{60}\) single molecules coupled to metallic\(^ \text{18} \) and ferromagnetic electrodes\(^ \text{18} \). It occurs in the valleys in which the charge of the molecule is close to an odd integer. Its experimental manifestation is an increase of the conductance with decreasing temperature and a zero-bias peak in the differential conductance below a characteristic temperature scale, the Kondo temperature \( T_K \).

Furthermore, some features in the I-V characteristics of a vibrating C\(_{60}\) single-molecule transistor were interpreted as being a manifestation of the effects of the \( e-ph \) interaction\(^ \text{18} \).

It was shown in previous work\(^ \text{15,18} \) that the interplay of \( e-e \) and \( e-ph \) interactions has important effects on the physical properties of the system in the Kondo regime. There are two different cases characterized by the strength of the \( e-ph \) coupling. When the latter is weak (in a sense that will be defined below), the ground state of the isolated molecule in the odd electron number valleys is a spin doublet. Then, the conventional Kondo effect appears when the molecule is coupled to metallic leads. The presence of the \( e-ph \) interaction results in an increase of the spin fluctuation energy and of the amplitude of charge fluctuations. In the strong \( e-ph \) coupling regime, polaronic effects result in an effective attractive interaction \( U_{eff} \) between the electrons and this leads to qualitatively new physics. If the charge in the device is close to an odd integer the ground state of the isolated molecule is a spinless charge doublet. This is the regime in which the charge Kondo effect develops. It differs from the conventional Kondo effect in that the low lying excitations of the system are charge fluctuations whereas spin fluctuations become increasingly stiff as the \( e-ph \) coupling increases. The charge Kondo effect enhances the transport through the molecule and leads to the appearance of a narrow peak in the conductance as a function of the gate voltage.

In this paper we study the properties of the device in an applied magnetic field. We found that these are quite different at weak and strong \( e-ph \) coupling. At weak coupling the system behaves qualitatively as in the absence of the latter\(^ \text{19} \). The magnetic field breaks the spin symmetry of the molecule’s ground state and splits the Kondo peak in the density of states thus suppressing the conductance for fields \( g \mu_B B \gtrsim k_B T_K \). At strong coupling, the molecule’s low lying states are spinless and are thus insensitive to the magnetic field. The Kondo peak is not split by the latter and there is almost perfect transmission at low temperatures for fields \( B \lesssim B_{crit} = |U_{eff}|/g \mu_B \). Furthermore, within this range of field values, the width of the conductance vs. gate voltage peak increases rapidly with \( B \). Beyond \( B_{crit} \) there is level crossing and the conductance peak splits into two peaks that are strongly spin polarized.

The rest of this paper is organized as follows. In Section \( \text{II} \) we present the model Hamiltonian and some general considerations that follow from exact Fermi liquid relationships at \( T = 0 \). In Section \( \text{III} \) we present Numerical Renormalization Group results for the spin resolved spectral densities and conductance in the presence of a local magnetic field at finite temperature and as a function of gate voltage. A summary and our concluding remarks are presented in Section \( \text{IV} \).
II. MODEL HAMILTONIAN

We consider a model of a molecule with a single relevant electronic level coupled to left (L) and right (R) metallic electrodes and a vibrational mode of frequency \( \omega_0 \) linearly coupled to the charge fluctuations of the molecule. The Hamiltonian of the system is

\[
H = H_M + H_E + H_{\text{M} - \text{E}} + H_{\text{MF}},
\]

where the first three terms describe the isolated molecule, the electrodes and their coupling, respectively. The last term is the coupling of the spin of the molecule to an external magnetic field acting only on the molecule. We have

\[
H_M = \varepsilon_d \hat{n}_d + U \hat{n}_d \hat{n}_d^\dagger - \lambda (\hat{n}_d - 1) \left( a + a^\dagger \right),
\]

\[
H_E = \sum_{k, \sigma, \alpha = \{L, R\}} \varepsilon_{\sigma \alpha} (k) \hat{c}_{k \sigma \alpha}^\dagger \hat{c}_{k \sigma \alpha},
\]

\[
H_{\text{M} - \text{E}} = \sum_{k, \sigma, \alpha = \{L, R\}} V_{k \sigma \alpha} \left( \hat{d}_{k \sigma}^\dagger \hat{c}_{k \sigma \alpha} + \hat{c}_{k \sigma \alpha} \hat{d}_{k \sigma} \right),
\]

\[
H_{\text{MF}} = g \mu_B B \hat{S}_{z}^d.
\]

Here, \( \hat{n}_d = \sum \sigma d_{\sigma}^\dagger d_{\sigma} \) and \( \hat{S}_{z}^d = \frac{1}{2}(d_{\uparrow}^\dagger d_{\downarrow} - d_{\downarrow}^\dagger d_{\uparrow}) \) are the charge and spin operators of the molecule, respectively. The position of the electronic molecular level relative to the Fermi level of the electrodes is denoted by \( \varepsilon_d \) and \( U \) is the Coulomb repulsion between two electrons that occupy the same molecular level. Finally, \( a^\dagger \) is the creation operator of a phonon of frequency \( \omega_0 \) and \( \lambda \) is the \( e \)-\( ph \) coupling constant. We consider for simplicity the case of identical electrodes with dispersion \( \varepsilon_R(k) = \varepsilon_L(k) = \varepsilon(k) \) and a \( k \)-independent tunnelling matrix element. We further assume that the conduction band is symmetric around the chemical potential and denote its half-width by \( D \). In the following we use units such that \( k_B = D = g \mu_B = 1 \).

The eigenstates of the Hamiltonian \( H_M + H_{\text{MF}} \) of the isolated molecule are direct products of electronic states (denoted by a subscript \( e \)) and oscillator states. The eigenfunctions and their energies can be written explicitly:

\[
|0, m\rangle = |\tilde{U}^- |0\rangle_e |m\rangle,
\]

\[
|\sigma, m\rangle = |\sigma\rangle_e |m\rangle,
\]

\[
E_m^\sigma = -\frac{\lambda^2}{\omega_0} + m \omega_0,
\]

\[
|2, m\rangle = |\tilde{U}^+ |1\rangle_e |m\rangle,
\]

\[
E_m^2 = -\frac{\lambda^2}{\omega_0} + 2 \varepsilon_d + U + m \omega_0,
\]

where \( \tilde{U}^\pm = \exp \left[ \pm \lambda / \omega_0 \left( a^\dagger - a \right) \right] \), \( |m\rangle \) is the \( m \)-th excited state of the harmonic oscillator and \( \sigma = \pm 1/2 \). The ground state energies of the empty and doubly occupied electronic states are reduced by the polaronic shift \( \lambda^2 / \omega_0 \).

At zero field the differences between the occupied and empty states \( E_m^\sigma = E_m^\sigma - E_m^0 \) and \( E_m^2 - E_m^0 \) are \( E_m^\sigma = \varepsilon_d + \lambda^2 / \omega_0 \) and \( E_m^2 - \varepsilon_d + U \), respectively. The effective interaction between two electrons occupying the same state is thus \( E_m^2 - 2E_m^\sigma = U - 2\lambda^2 / \omega_0 \approx U_{\text{eff}} \).

The sign of this quantity determines the low energy physics of the system and its response to an applied field. For positive \( U_{\text{eff}} \), the ground state of the isolated molecule is a spin doublet and the Kondo effect occurs at low temperatures when the molecule is coupled to the leads. For negative \( U_{\text{eff}} \) the ground state of the isolated molecule is either empty, doubly occupied or a charge doublet. In the latter case the coupling of the molecule to the leads generates the charge Kondo effect with an anisotropic Kondo (AK) exchange coupling \( -\frac{\lambda}{\omega_0} \).

In this paper we only study the case of paramagnetic contacts and, therefore, we set \( \Gamma_{\sigma L}(\omega) = \Gamma_{\sigma R}(\omega) \equiv \frac{\lambda}{\omega_0} \Gamma(\omega) \), where \( \Gamma(\omega) \equiv 2\pi \sum_k \delta (\omega - \varepsilon(k)) V_k^2 \).

The spin resolved conductance of the molecular junction at zero bias \( \frac{G}{G_0} = 2 \cos^2 (\pi n_{da}) \),

\[
G_{\sigma} = \frac{e^2}{h} \pi \int_{-\infty}^{\infty} d\omega \left( \frac{\partial f(\omega)}{\partial \omega} \right) \rho_{da}(\omega) \Gamma(\omega),
\]

where \( \rho_{da}(\omega) = -\pi^{-1} \text{Im} G_{da}(\omega) \), \( G_{da}(\omega) \) is the retarded electronic Green function of the molecule in the presence of the leads and \( f(\omega) \) is the Fermi distribution.

At zero temperature, in the wideband limit, the dimensionless conductance satisfies the Fermi liquid relationship

\[
g \equiv \frac{G}{G_0} = \pi \sum_{\sigma} \rho_{da}(0) = \pi \sum_{\sigma} \sin^2 (\pi n_{da}),
\]

where \( G_0 = e^2/h \) is the quantum of conductance, \( n_{da} = \langle \hat{n}_{da} \rangle, \Gamma = \Gamma(0) \), and the second equality follows from Luttinger’s theorem generalized to the case in which \( e \)-\( ph \) interactions are present.

Consider first the case \( \sum_{\sigma} n_{da} = 1 \) corresponding to the electron-hole symmetric situation \( \varepsilon_d = -U/2 \). The conductance in zero field is then \( g = 2 \). In the presence of the applied field \( B \) the molecule acquires a magnetization \( m_d = \frac{1}{2} (n_{dl} - n_{dl}) \) and Eq. (5) becomes

\[
g = \sum_{\sigma} \sin^2 [\pi(1/2 - 2\sigma m_d)] = 2 \cos^2 (\pi m_d).
\]

In the low field limit we have,

\[
g \approx 2(1 - \pi^2 m_d^2) \approx 2(1 - \pi^2 \chi_d^2 B^2),
\]

were \( \chi_d = \partial m_d / \partial B \) is the local spin susceptibility. In the large field limit we have \( m_d \rightarrow 1/2 \) and the conductance vanishes. The characteristic field beyond which the conductance is suppressed is \( B^* \sim \chi_d^{-1} \).

For \( U_{\text{eff}} \) large and positive \( \chi_d^{-1} \sim T_K \) and increases slowly with increasing \( \chi_d \). Therefore, \( B^* \sim T_K \) is small in the limit \( U_{\text{eff}} \gg \Gamma \). For \( B \geq B^* \) the conductance at \( \varepsilon_d \sim -U/2 \) is thus suppressed and \( g \) acquires a double-peak structure as a function of the gate voltage. The zero temperature conductance at the positions of the peaks is \( g = 1 \).

For \( U_{\text{eff}} \) large and negative \( \chi_d^{-1} \sim |U_{\text{eff}}| \) and \( B^* \) is thus large. In this case, a single conductance peak with \( g = 2 \) is expected in a broad range of magnetic fields.
In zero field but off electron-hole symmetry, \( \epsilon_d = -U/2 + \delta \varepsilon_d \), we have:

\[
g \approx 2 \left( 1 - \pi^2 \delta n_d^2 / 4 \right) \approx 2 \left( 1 - \pi^2 \chi_c^2 \delta \varepsilon_d^2 / 4 \right),
\]

where \( \chi_c = -\partial n / \partial \varepsilon_d \) is the charge susceptibility and \( \delta n_d = \sum_{\sigma} n_{d\sigma} - 1 \). The width \( \delta \varepsilon_d^* \) of the conductance peak is \( \sim \chi_c^{-1} \sim T_{AK} \), the Kondo temperature of the effective anisotropic Kondo model that is small for very large \( |U_{\text{eff}}| \), \( \delta \varepsilon_d^* \sim \exp \left| - \left( \pi |U_{\text{eff}}|^2 / 4 \Gamma \omega_0 \right) \right| \). In the same limit the field-dependence of \( \delta \varepsilon_d^* \) can also be evaluated analytically (see Eqs. 13 and 14 below). We find

\[
\frac{\delta \varepsilon_d^*(B)}{\delta \varepsilon_d^*(0)} \sim \exp \left[ \pi B^2 / (16 \Gamma \omega_0) \right].
\]

The width of the conductance peak thus increases exponentially with \( B^2 \) in the strong coupling limit.

**III. NUMERICAL RESULTS**

In this section we present numerical results for the spin resolved spectral density \( \rho_{d\sigma}(\omega) = -\pi^{-1} \text{Im} \mathcal{G}_{d\sigma}(\omega) \) and conductance obtained using the Numerical Renormalization Group method (NRG) \(^{26,27}\) modified to include e–ph coupling \(^{28}\) and to calculate accurately the spectral density \( \rho_{d\sigma}(\omega) \) using the method of Ref. \(^{29}\).

Figure 1 represents the total spectral density in zero field (full line) and its spin resolved components (dotted and dashed lines) in the presence of a small magnetic field \( B \sim T_K \) for a case with \( U_{\text{eff}} > 0 \). Parameters are \( \epsilon_d = -0.04, \Gamma = 0.00393, U = 0.1, \omega_0 = 0.05 \), and \( U_{\text{eff}} = 0.0375 \). Full line: total spectral density for \( B = 0 \). Dotted and dashed lines: spin down and spin up components, respectively, for \( B \sim T_K \). Inset: structure of the Kondo peak. Full thick and thin lines: total spectral density for \( B = 0 \) and \( B \sim T_K \), respectively. Dotted and dashed lines: majority and minority spin components of the spectral density, respectively.

FIG. 1: Total and spin-resolved spectral densities at \( T = 0 \) for \( U_{\text{eff}} > 0 \). Parameters values are \( \epsilon_d = -0.04, \Gamma = 0.00393, U = 0.1, \omega_0 = 0.02 \), and \( U_{\text{eff}} = 0.0375 \). Full line: total spectral density for \( B = 0 \). Dotted and dashed lines: spin down and spin up components, respectively, for \( B \sim T_K \). Inset: structure of the Kondo peak. Full thick and thin lines: total spectral density for \( B = 0 \) and \( B \sim T_K \), respectively. Dotted and dashed lines: majority and minority spin components of the spectral density, respectively.

FIG. 2: Zero temperature spectral density in the region of the Kondo peak and conductance as a function of temperature and magnetic field at the electron-hole symmetric point.

In all cases \( \epsilon_d = -0.05, \Gamma = 0.01 \), and \( \omega_0 = 0.05 \). (a): Zero temperature spectral density for \( U_{\text{eff}} = 0.051 \) and three values of the magnetic field. \( T_K = 0.004 \) (b) Zero temperature spectral density for \( U_{\text{eff}} = -0.044 \) and three values of the magnetic field. \( T_{AK} = 1.1 \times 10^{-4} \). (c) Conductance as a function of the magnetic field and temperature for \( U_{\text{eff}} = 0.051 \). Temperatures are \( T = 0 \) (top curve) and \( T = 0.006 \times 2^{-N}, N = 0,1,2,\ldots,5 \) (from bottom to top).

(c) Conductance as a function of the magnetic field and temperature for \( U_{\text{eff}} = -0.044 \). Temperatures are as in (b) with \( N = 0,1,2,\ldots,9 \).

The vertical lines in Fig. 1 represent the positions of the poles of \( G_{d\sigma}^{\ast} \) given in Eq. (15) of Reference \(^{28}\). It can be seen that they are in fairly good agreement with the positions of the peaks observed away from the Kondo feature in Fig. 1.

The presence of a field \( B \sim T_K \) has drastic effects on the spin resolved spectral spectral function. Due to the high magnetic susceptibility of the molecule (\( \chi \sim 1/T_K \)) the latter acquires a large magnetization. Most of the electron density is composed of majority spins (down spins) and the population of the minority spins (up spins) is small. The spectral function of the majority spins (represented by dotted lines) is thus large for \( \omega < 0 \) whereas that of
the minority spins (represented by dashed lines) is large for $\omega > 0$.

The inset to the figure shows in detail the effect of the magnetic field on the Kondo peak. The thick and thin full lines represent the total spectral function in the central region in zero field and for $B \sim T_K$, respectively. It can be seen that the Kondo peak splits and its amplitude is reduced anticipating the suppression of the Kondo effect at higher fields. The dotted and dashed lines represent the spin down and spin up components of $\rho_d(\omega)$, respectively. It is seen that position of the two Kondo peaks shift in opposite directions by an amount $\sim \pm B|U_d|$.

Figure 4 displays the spin resolved spectral density at $T = 0$ for three values of the magnetic field (a,b), and the conductance as a function of magnetic field and temperature (c,d) at the electron-hole symmetric point. The parameters are $\Gamma = 0.01$, $U = 0.1$, and $\omega_i = 0.05$. We only show the minority-spin spectral density $\rho_{\uparrow}(\omega)$ since electron-hole symmetry and spin reversal invariance lead to the relationship $\rho_{\downarrow}(\omega) = \rho_{\uparrow}(\omega)$.

It can be seen that the Kondo peak behaves differently in a magnetic field in the cases shown in Fig. 2(a) ($U_{\text{eff}}(\omega) = 0.051 > 0$) and Fig. 2(b) ($U_{\text{eff}}(\omega) = -0.044 < 0$). Whereas in the former case the Kondo peak shifts and its height decreases upon applying a small magnetic field, in the latter case, for fields $B < |U_{\text{eff}}|$, its position and height remain unchanged. Note that the shape of the peak is asymmetric and its width increases sharply upon applying the field. The spectral asymmetry is due to the decrease of the density of minority spins in the presence of the field as discussed above. The field-dependence of the width of the Kondo peak will be discussed below.

For even larger fields, $B > |U_{\text{eff}}|$, there is a level crossing and the charge doublet is no longer the ground state of the isolated molecule. The charge Kondo effect can not take place and the associated peak in the density of states disappears.

The dependence of the conductance on field and temperature for the cases of positive and negative $U_{\text{eff}}$ is shown in Figs. 2(c) and 2(d), respectively.

For positive $U_{\text{eff}}$, the field-induced suppression of spectral weight at the Fermi level seen in Fig. 2(a) translates into a suppression of the zero temperature conductance as can be seen in Fig. 2(c). As a function of field this quantity exhibits a peak of width $\sim T_K$, as expected from Eq. (11). With increasing temperature the conductance decreases further.

The case of negative $U_{\text{eff}}$ is shown in Fig. 2(d). At temperatures much lower than the zero-field value of $T_K$ we observe a wide plateau of width $\sim 2|U_{\text{eff}}|$. The region of the plateau is that in which charge Kondo effect exists as discussed above and this leads to a high conductance. With increasing temperature the conductance first decreases in the central region where $T_K$ is the lowest (see below).

At high temperatures, two peaks are seen at $B \sim \pm |U_{\text{eff}}|$. These peaks are associated to the crossing of the levels of the isolated molecule [cf. Eq. (10)] for $|B| > |U_{\text{eff}}|$

the ground state of the molecule is either $|\downarrow, 0\rangle$ or $|\uparrow, 0\rangle$, depending on the sign of the field. For $|B| < |U_{\text{eff}}|$, instead, the ground state of the molecule is spinless. These peaks are thus the analogs of the familiar Coulomb blockade peaks that appear for positive $U_{\text{eff}}$ upon varying the charge. For negative $U_{\text{eff}}$ and in the electron-hole symmetric situation that we are discussing the charge is fixed, however, and it is the spin of the molecule that changes at the peaks by an amount $\Delta S_z = 1/2$ when the magnetic field varies.

We now discuss the spin resolved conductance at $T = 0$ as a function of gate voltage (i.e., of $\varepsilon_d$) for the case $U_{\text{eff}} < 0$ and several values of the magnetic field. Figure 3(a) shows the conductance at zero field. When the molecular level departs from the symmetric position, the molecule charge–polarizes and the conductance decreases according to Eq. (11). As a consequence, the conductance exhibits a narrow peak of width $\sim T_K$

When a small magnetic field is applied, $T_K$ increases as mentioned above and the peak in the conductance broadens accordingly [cf. Fig. 3(b)]. There is also a spin polarization of the current that changes sign at the symmetric point. This can be understood as follows: for negative but small $\delta \varepsilon_d$ the charge of the molecule increases and the current is dominated by charge fluctuations between the states $|2, 0\rangle$ and $|1, 0\rangle$. This leads to a predominantly spin-up current. For positive but small $\delta \varepsilon_d$ the charge in the molecule decreases and the relevant fluctuations are now those between $|0, 0\rangle$ and $|1, 0\rangle$ and the spin-polarization of the current is reversed.

The width of the conductance peak further increases with the magnetic field but the peak height remains unchanged as seen in Fig. 3(c). Notice the strong spin-polarization of the current reflected in the strong asymmetry of the peaks in the spin resolved con-

\[ G(\varepsilon, B = 0) = \frac{2 e^2}{h} \left( \frac{\Delta S_z}{2} \right) \]
In this regime the device acts as a very effective spin filter and the spin polarization can be reversed by a small change in the gate voltage. For magnetic fields larger than the spin gap $B \gtrsim |U_{\text{eff}}|$, the ground state of the isolated molecule changes as mentioned above and the total conductance shows a two-peak structure. The heights of these are reduced by half as shown in Fig. 3(d). These peaks are located at $\delta \varepsilon_d \sim \pm (B - |U_{\text{eff}}|)/2$ where there is a level crossing of the molecular states. The conductance peaks are almost fully spin-polarized in this limit.

We conclude by discussing in detail the field-dependence of the charge Kondo temperature $T_{\text{AK}}$. As shown in Reference 16, the low-energy effective model for the charge fluctuations in the strong $e$–$ph$ coupling case is the anisotropic Kondo model with couplings $J_{||}$ and $J_{\perp}$ and Kondo temperature $^{30,31}$

$$T_{\text{AK}} \sim \left(J_{\perp}/J_{||}\right)^{1/2}.$$  

(13)

In the present case, in the presence of a magnetic field, the coupling constants are $^{16}$

$$J_{||} = J_0 \sum_{m,\sigma=\pm1/2} \frac{e^{-(\lambda/\omega_0)^2/2 \lambda^2/\omega_0^2 U - 1 - 2\sigma B/U + 2m\omega_0/U}}{2\lambda^2/\omega_0^2 U - 1 - 2\sigma B/U + 2m\omega_0/U}, \quad J_{\perp} = J_0 \sum_{m,\sigma=\pm1/2} (-1)^m e^{-(\lambda/\omega_0)^2/2 \lambda^2/\omega_0^2 U - 1 - 2\sigma B/U + 2m\omega_0/U}$$  

(14)

where $J_0 = 8 \Gamma/(\pi U \rho_0)$.

For very large $e$–$ph$ coupling the expressions above can be evaluated analytically leading to the result quoted in Eq. (12) in Sec. II. In the numerical calculations reported here we used moderate values of $\lambda$ and the expressions for the couplings in Eq. (14) must be evaluated numerically.

Figure 4 represents the field dependence of $T_{\text{AK}}$ for the same parameters as in Fig. 3. It can be seen that in this regime $T_{\text{AK}}$ still increases exponentially with $B$.

IV. CONCLUSIONS AND SUMMARY

We analyzed the equilibrium transport and spectral properties of a model molecular transistor when the spin symmetry is broken by applying an external magnetic field. For weak $e$–$ph$ coupling, in zero field, the conductance shows the well known Coulomb blockade peaks at high temperature and the enhancement of the conductance due to the Kondo effect at low temperatures. An external magnetic field $B \gtrsim T_K$ suppresses the conductance as a result of the splitting of the Kondo peak. The properties of the conductance at zero bias are qualitatively the same as those found in the case in which there is no $e$–$ph$ coupling but with a set of phonon renormalized parameters. The spectral density, however, presents a set of additional peaks separated by the phonon energy $\omega_0$, that can be understood analyzing the level structure of the isolated molecule. The properties of the spectral density are experimentally accessible in transport experiments at finite but small source-drain voltages or in scanning tunneling microscopy (STM) experiments for molecules on surfaces.

In the strong $e$–$ph$ coupling regime the behavior of the system is qualitatively different. The odd Coulomb blockade valleys are completely suppressed and the low temperature physics is dominated by charge fluctuations instead of spin fluctuations. In a small range of gate voltages the charge Kondo effect takes place and results in an enhancement of the conductance at low temperatures. In contrast with the previous case, the Kondo peak is not split by a magnetic field. Instead, for a broad range of magnetic fields, it broadens as the latter increases. For large enough fields or temperatures a spin blockade regime is observed.

The magnetic field dependence of the conductance of a molecular transistor with strong $e$–$ph$ coupling resembles in many ways the gate voltage dependence of the conductance of a device with weak $e$–$ph$ coupling in zero field. The two cases are related to each other through the transformation $\langle S^z_d \rangle \rightarrow \langle \hat{n}_d \rangle$ and $B \rightarrow V_g$. This transformation is not an exact one because the symmetries in the spin and charge sectors of the Hilbert space are different.
but it gives a good qualitative physical picture.

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