Destructive quantum interference in transport through molecules with electron–electron and electron-vibration interactions

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Abstract
We study the transport through a molecular junction exhibiting interference effects. We show that these effects can still be observed in the presence of molecular vibrations if Coulomb repulsion is taken into account. In the Kondo regime, the conductance of the junction can be changed by several orders of magnitude by tuning the levels of the molecule, or displacing a contact between two atoms, from nearly perfect destructive interference to values of the order of $2e^2/h$ expected in Kondo systems. We also show that this large conductance change is robust for reasonable temperatures and voltages for symmetric and asymmetric tunnel couplings between the source–drain electrodes and the molecular orbitals. This is relevant for the development of quantum interference effect transistors based on molecular junctions.

Keywords: Kondo effect, interference, molecules

1. Introduction

Transport properties of single molecules are being extensively studied due to their potential use as active components of new electronic devices [1, 2]. In particular, recent works [3–11] have focused on the possibility of using quantum interference effects present in molecular junctions to control the transport. Level (quasi-)degeneracy is very common to molecular systems [12] providing different pathways for electron to tunnel, and when these levels have opposite parity, there is destructive interference and the conductance is strongly reduced [13, 14]. The proposal of the quantum interference effect transistor (QuIET) [3] for example, is based on exploiting destructive interference (DESINT) and switching on-off the current by introducing-removing decoherence in a controlled manner.

In recent experiments, the position of the highest occupied and lowest unoccupied molecular orbitals with respect to the Fermi level of two different molecules has been shifted using an electrochemically gated, mechanically controllable break junction technique [10, 11]. This permitted to reduce the conductance from values below $10^{-3}G_0$, where $G_0 = 2e^2/h$ is the quantum of conductance to values of the order of $10^{-6}G_0$ with a small change in gating potential. More specifically, a change in voltage by only 17 mV caused a change in one order of magnitude in the conductance [10].

In most of the above mentioned works, the ground state has an even number of electrons and then, the Kondo effect is absent. In addition, the theoretical analysis often neglected electronic correlations, which are essential in the Kondo effect. Due to their small sizes, charging energy in molecules is very
important [15] and configurations with an even or odd number of electrons are separated by a large Coulomb energy. For an odd occupancy, the localized spin of the molecular orbital can be screened by the conduction electrons of the electrodes leading to the Kondo effect. This phenomenon is well known in condensed matter [16] and leads to a peak in the conductance, at zero bias which appears at low temperatures. Signatures of the Kondo effect have been observed in semiconducting [17, 18] as well as in molecular [19–26] quantum dots. The conductance at zero bias reaches a maximum near the quantum of conductance $G_0$, which in non-interacting systems can only be obtained by tuning the energy of one level near the Fermi energy.

In this work we explore the physics of the QuIET in the Kondo regime, where the values of the conductance are near $G_0$, incorporating also the effect of molecular vibrations, which are known to be strongly coupled to electrons, playing a major role in molecular junctions leading for example to finite-voltage replicas of the zero-bias peak of the conductance as a function of bias voltage [22–26]. At temperatures higher than the relevant frequencies, vibrations have been shown to strongly quench DESINT [27, 28]. At small temperatures $T$ the vibrations have been argued to have a small effect [4]. In this work we show that even at $T = 0$ some effects of the vibrations remain (renormalization of the energies and tunnel amplitudes) but DESINT can be restored if the difference between the interference levels can be tuned.

As shown in more detail below (appendix A), in the presence of two quasi-degenerate orbitals of opposite parity, it is known that the Kondo effect is enhanced due to additional degrees of freedom (two possible orbitals and spin up/down). Interference is observed in the Kondo regime and the conductance can be varied from zero, total DESINT, to a high value $\sim G_0$ by breaking the orbital degeneracy [29]. Contrary to the non-interacting case, the levels do not need to be aligned with the Fermi level to lead to a large conductance and the effect relies on the formation of a many-body state at low temperature. However, how this picture of a many-body QuIET changes for asymmetric coupling to the leads and when vibrations are included is not obvious.

In this paper, we generalize previous models describing the effect of interference on molecular transport, to include both Coulomb interaction which leads to the Kondo effect and electron-vibration interaction. Our main result is that by tuning the energy difference between the quasi-degenerate levels $\delta$ (by stretching the device [14, 20] for example), DESINT can be restored even in the presence of vibrations. In contrast to the non-interacting case, we find that almost perfect DESINT persists over a wide range of voltages and temperatures for general tunnel coupling to the electrodes. We show that perfect DESINT is also expected in annulene molecules connected to the leads at an angle of 90 degrees (for example, one lead connected with one C atom and the other between two C atoms, see appendix D), and changing this angle conduction is restored. Our results show that the large tunable change in the conductance could be exploited for a more robust ‘many-body QuIET’ operating in the Kondo regime at low bias voltage.

For symmetric coupling to the leads, the effect can be understood as follows. In absence of electron-vibration interaction (EVI), as discussed in detail below, the model has SU(4) symmetry, and the conductance is zero due to perfect DESINT. This symmetry is broken by the EVI permitting finite conductance. However, in the Kondo regime for a given $\delta$ we obtain the conductance drops to zero within the precision of our results and is very low for a scale of temperatures and voltages below a characteristic SU(4) Kondo scale. This is due to the fact to a very good approximation, the SU(4) symmetry is restored as an emergent one at low energies. For asymmetric coupling to the leads, we find numerically that tuning $\delta$ also the conductance falls to very small values (below $\sim 10^{-6}$), but we cannot support this result with symmetry arguments.

The emergence of SU(4) symmetry at low energies has been recently discussed [30, 31] as an explanation of the observed SU(4) Kondo physics in a transport experiment through a double quantum dot system in spite of the different coupling parameters for both dots [18]. Here we show its relevance for the ‘many-body QuIET’ in presence of EVI.

The paper is organized as follows. In section 2 we describe the model and the formalism used to calculate the conductance. Section 3 contain the main results, and section 4 contains a brief summary and a discussion.

2. Model and formalism

The minimal electronic model for total DESINT consist of two degenerate levels of opposite parity, one coupled to both conducting leads with hybridization $V$ and the other with matrix elements $V$ and $-V$ respectively [27, 29] (see the inset of figure 1). Annulene molecules with contacts at 90 degrees are described by this model (see [7, 8] and appendix D). To include the effect of vibrations in this minimal model we consider an extension to two levels of the Anderson–Holstein
Hamiltonian [32–41] in which a spin-1/2 doublet is connected to two metallic reservoirs and coupled to a phonon mode of energy \( \Omega \), through the electron–phonon interaction \( \lambda \). It is also an extension of the model proposed by of H"{a}rtle et al [27] to include Kondo physics and general couplings to the leads.

The Hamiltonian is

\[
H = \sum_{\sigma} \left[ (E_d + \delta)n_{1\sigma} + E_{d\sigma}n_{2\sigma} \right] + U \sum_{\sigma \neq \sigma'} n_{\sigma\sigma'} n_{\sigma'\sigma'} + \sum_{i, \sigma} \varepsilon_i^c c_{i\sigma}^{\dagger} c_{i\sigma} + \sum_{i, \sigma} \left( V_{d\sigma}^{\dagger} d_{i\sigma}^{\dagger} c_{i\sigma} + \text{H.c.} \right) + \Omega a^{\dagger}a + \sum_{\sigma} \lambda (a^{\dagger} + a)n_{\sigma\sigma},
\]

where \( a^\dagger \) creates the Holstein phonon mode, \( n_{\sigma\sigma'} = d_{i\sigma}^{\dagger}d_{i\sigma} \), \( d_{i\sigma}^\dagger \) \((i = 1, 2)\) creates an electron with spin \( \sigma \) at the molecular state \( i \), \( c_{i\sigma}^{\dagger} \) creates a conduction electron at the left \((\nu = L)\) or right \((\nu = R)\) lead, and \( V_{d\sigma} \) describe the hopping elements between the leads and the molecular states. As in [27], we only couple level 1 with the vibration (this is justified by the strong variation of the EVI depending on the electronic level and the vibrating mode [12]), and assume that level 1 is even and level 2 is odd (the choice of level is irrelevant). We take the limit of very large Coulomb repulsion \( U \to \infty \).

For \( \delta = \lambda = 0 \), a unitary transformation (see appendix A) maps the electronic part of the model into another one with SU(4) symmetry. This means that the Hamiltonian is invariant under a unitary change of basis in the 4-dimensional space of orbital and spin degrees of freedom. The conductance vanishes in this limit reflecting perfect DESINT [29].

We calculate the conductance \( G(V_b, T) = dI/dV_b \) by numerical differentiation of the current \( I \) with respect to the bias voltage \( V_b \). The expression of the current is given by [8]

\[
I = \frac{2ie}{h} \int d\omega \text{Tr}[(\Gamma^L f_L(\omega) - \Gamma^R f_R(\omega))G^R_\sigma(\omega)] + (\Gamma^L (1 - f_L(\omega)) - (1 - f_R(\omega)))G^L_\sigma(\omega),
\]

where the two \( 2 \times 2 \) matrices \( \Gamma^\nu \), \( \nu = L, R \) are defined by the matrix elements \( (\Gamma^\nu)^{ij}_{\sigma\sigma'} = \pi \sum_{k} V_{ik}^\nu V_{kj}^{\dagger \sigma}(\omega - \varepsilon_k^\nu) \), assumed independent of \( \omega \) and \( G^R_\sigma(\omega) \) and \( G^L_\sigma(\omega) \) are \( 2 \times 2 \) matrices that correspond to the lesser \( G^R_\sigma(\omega) \) and greater \( G^L_\sigma(\omega) \) Green functions, calculated in the Keldysh formalism within the noncrossing approximation (NCA) [42, 43]. We assume \( \mu_L = eV_b/2 \) and \( \mu_R = -eV_b/2 \). Our conclusions do not depend on this assumption. This approach has been successfully applied to a variety of problems [8, 21, 29, 30, 32, 33, 44, 45], in particular to one magnetic level interacting with phonons [32, 33] and two interfering magnetic levels without phonons [8, 29]. The observed scaling with temperature of the satellite peaks of the main Kondo peak due to electron vibration interaction [25], is correctly reproduced by the theory [33]. While the extension of the NCA formalism to the full problem: interference + Kondo + vibrations is rather straightforward, the physics of the complete system is much richer, as we show below. Alternative treatments for non-equilibrium problems such as renormalized perturbation theory [46–48] are difficult to generalize for the two-level case.

![Figure 2](image.png)

**Figure 2.** Spectral density of the two levels for \( \lambda = \sqrt{10} \times 10^{-4}, \Delta = 0.05, \delta = 0.009/3 \) and \( T = 0.17T_K^{SU(4)} \) with \( T_K^{SU(4)} = 7.5 \times 10^{-4} \). Other parameters as in figure 1. The left inset includes in dashed-dots–dot line the case \( \lambda = \delta = 0 \) for comparison. The right inset shows the temperature dependence of the occupations \( \langle n_{\sigma\sigma'} \rangle \).

We define \( \Delta'_i = \pi \sum_k |V_{ik}^\nu|^2 \delta(\omega - \varepsilon_k^\nu) \) assumed independent of energy and \( \Delta_i = \Delta_{i\sigma} + \Delta_{i\sigma'} \). We take a flat band of conduction states extending from \(-D < \omega < D\), chosen as the unit of energy. We also fix \( \Omega = 0.1, E_d = -0.4 \) and vary the other parameters. For \( D = 1 \) eV, the values of \( \Omega \) and \( \lambda \) that we use are typical [27], while the Kondo temperature \( T_K \) depends on the particular system (for example it varies between 1.1 and 210 K in [20]).

**3. Results**

**3.1. Renormalization of \( \delta \) by the EVI**

We start by first discussing the simplest case of symmetric coupling to the leads so that \( V_{ik}^L = V_{ik}^R = \lambda = -V_{ik}^L \) (see the inset in figure 1). Later we will change the magnitude of the hoppings but not the relative signs. Without vibrations \((\lambda = 0)\), the model for \( \delta = 0 \) is equivalent to the SU(4) impurity Anderson model in the Kondo limit (see appendix A). The total DESINT is reflected as a zero conductance, as shown in figure 1 with black squares. As the level detuning \( \delta \) increases from zero, orbital symmetry is lost and the conductance increases.

Much of the physics of the problem can be understood by looking at the spectral density, which is involved in the determination of the transport properties. The spectral density in the SU(4) case, \( \rho_{\sigma\sigma'}(\omega) \), shows a peak near the Fermi energy (dashed-dots–dot line in the left inset of figure 2) [49, 50]. The half width at half maximum of this peak is of the order of the Kondo temperature for the SU(4) model \( T_K^{SU(4)} \), and its center is at \( \omega \sim T_K^{SU(4)} \), where \( \omega = 0 \) is the Fermi energy. For \( \delta \neq 0 \)
the model has only spin SU(2) symmetry, but the changes in different quantities are not significant until $|\delta| > T_K^{SU(4)}$ [29]). For $\delta > T_K^{SU(4)}$, the spectral densities split and the peak in $\rho_{\sigma \sigma}(\omega)$ for the level $i$ of lower energy narrows and displaces towards the Fermi level as $|\delta|$ increases, while the other is near $\omega = \delta$. The half width at half maximum of the former peak represents the Kondo temperature $T_K$ of the system and lies between $T_K^{SU(4)}$ for $\delta = 0$ to the usual (much lower) one-level Kondo temperature $T_K^{SU(2)}$ of the SU(2) case for $\delta \rightarrow \infty$.

The crossover $SU(4) \rightarrow SU(2)$ is reflected in transport as an increase in conductance from zero at $\delta = 0$ to a larger value as $\delta > T_K^{SU(4)}$ (illustrated by squares in figure 1). For $\delta = 0$, the conductance $G(V_b, T) = 0$ for any bias voltage $V_b$ and temperature $T$ due to DESINT [29]. At $T = 0$, Fermi liquid relationships imply (see appendix C)

$$G(0, 0) = \frac{e^2}{h} \sum_{\sigma} \sin^2 \left[ \pi \left( n_{2\sigma} - n_{1\sigma} \right) \right],$$

which depends on the mean occupations of the levels. For $\delta = 0$, these occupations are the same and therefore, $G$ goes to zero. The dependence of $G(0, 0)$ on $\delta$ is illustrated by squares in figure 1. For small $\delta$, $G(0, 0) > 0$ but very small, and $G(0, T)$ has the temperature dependence characteristic of SU(4) systems [29, 51] while for $\delta > T_K^{SU(4)}$, $G(0, T)$ approaches that of the one-level SU(2) case [29].

Next, we note some basic results of the Anderson–Holstein model for one level [32-41]. As also showed in the experiments [25], satellites of the Kondo peak appear at energies shifted from it in integers of $\Omega$. Moreover, the temperature dependence of the satellites follow the universal one of the main Kondo peak [33] for $\Omega \gg T_K$. The energy level is shifted by an amount $\delta_0$ which for small hybridization is $-\lambda^2/\Omega$ (in general $-\lambda^2/\Omega < \delta_0 < 0$), and the effective hybridization is reduced [32]. This can be understood qualitatively using a Lang–Firsov canonical transformation [27, 28]. However, decoupling electrons and phonons after this transformation, predicts that the Kondo temperature changes exponentially with the electron–phonon coupling $\lambda$, which is actually not the case [32, 35, 36, 40].

In figure 1 we show the effect of this renormalization. Here we compare $G(0, T \rightarrow 0)$ with and without electron-phonon interaction as a function of $\delta$. The temperature is low enough so that the conductance is saturated to the zero-temperature value [44]. As stated above, for $\delta = \lambda = 0$ there is perfect DESINT and the conductance vanishes. Keeping $\delta = 0$ and turning on EVI, a sizable value of the conductance, of the order of 40% of the ideal one $G_0 = 2e^2/h$ is obtained (circles in figure 1). Interestingly, increasing $\delta$ a situation with total DESINT is restored for a new value of $\delta$, which we denote as $\delta_{\text{res}}$ (numerically $G < 3 \times 10^{-3}G_0$ for $\delta = \delta_{\text{res}} = 0.005$). This indicates that the primary effect of the EVI is just a downward correction of the energy of the corresponding level $\delta_\lambda \gtrsim -\lambda^2/\Omega = -0.006$ which can be compensated in the model by a positive shift $\delta_{\text{res}} = +|\delta_\lambda|$ of the bare energy, and total DESINT is obtained again. This can be understood in a Fermi liquid description: at temperatures below all relevant energy scales in the model, phonons can be integrated out and the low-energy physics can be described by a purely electronic weakly interacting system with effective parameters, retaining the symmetry of the problem. This leads to equation (3) for the conductance at $T = 0$ and changing $\delta$, one can render $(n_{2\sigma} - n_{1\sigma}) = 0$ and then $G(0, 0) = 0$. Note that for these parameters, the occupancies behave in the same way as a system with SU(4) symmetry, although (as we shall show) small deviations with temperature and in other properties indicate that the actual symmetry is still SU(2). As we show below (section 3.3), this phenomenon of (approximate) symmetry restoration is more robust than in a non-interacting system and relies on the formation of a many-body Kondo state at low temperatures.

### 3.2. Renormalization of $\Delta_1$ and its effect on the DESINT

However, the effect of vibrations at low temperatures is more involved than just to replace $\delta$ by $\delta - \delta_{\text{res}}$. The reduction of the hybridization of the level coupled to the phonons, also plays a significant role. Moreover, it is not clear a priori if perfect DESINT for some $\delta$ can persist for $T \neq 0$ or $V_b \neq 0$, where the Fermi liquid results cease to be valid. To show this effect more clearly, we have considered a larger $\lambda (-\lambda^2/\Omega = -0.01)$ and smaller $\Delta_1$ to increase the relative importance of EVI $^4$. In figure 2 we show both spectral densities $\rho_{\sigma \sigma}(\omega)$ for these new parameters and $\delta = \delta_{\text{res}} = 0.00903$ adjusted so that they look very similar near the Fermi energy. The spectral density of the level coupled to phonons $\rho_{\sigma \sigma}(\omega)$ shows satellites of the Kondo peak at $\omega \pm \Omega$ (as discussed for example in [32]). Small satellites at $\omega \pm 2\Omega$ can also be noticed. The spectral density of level 2, $\rho_{2\sigma}(\omega)$ does not have these satellites. However, strikingly, the Kondo peaks for both $\rho_{\sigma \sigma}(\omega)$ are very similar and recall the corresponding result for SU(4) symmetry, although contrary to the Kondo peak of the SU(4) case $\delta = \lambda = 0$ they are narrower (dashed-dot–dot line in the left inset). This can be interpreted as follows: in addition to a downward shift in $E_1$, the EVI causes also a downward renormalization of the magnitude of the coupling $\Delta_1$ [32, 52]. Recent results [30, 31] show that even if the couplings $\Delta_1$ are different, breaking SU(4) symmetry, this symmetry can be restored to a very good approximation as an emergent low-temperature symmetry by adjusting $\delta$. The resulting Kondo temperature corresponds to the geometrical average of both $\Delta_1$. In our case in which the effective $\Delta_1$ is reduced, one expects a lower Kondo temperature for the restored SU(4) case than to the bare one. In fact, by direct comparison with the spectral density without vibrations, for the parameters of figure 2, we find that $\Delta_1$ is reduced by a factor 0.941. The effects of the EVI on the DESINT can be counterbalanced by an appropriate shift in $\delta$. In particular, $G(0, 0) = 0$ by tuning $\delta$ in such a way that $\langle n_{2\sigma} \rangle = \langle n_{1\sigma} \rangle$. Moreover, the occupancies have a very weak

$^4$For these parameters $\lambda = \sqrt{10}$ and $\Delta = 0.05$, the non-equilibrium calculations turned out to be very cumbersome. Then we have calculated only equilibrium properties. They suffice to show the effects on the EVI on $T_K$.
temperature dependence (see right inset of figure 2 in semi-log scale), indicating that the SU(4) symmetry restoration continues to be a very good approximation. The deviation between the occupancies of both levels is below 5% in a range of two orders of magnitude in temperature.

3.3. Comparison with the noninteracting case

The restoration of the SU(4) symmetry, and with it of the DESINT, is a robust effect that relies on the spectral densities being almost identical close to the Fermi level. This is very different to what can be obtained in a non-interacting case (without Coulomb interaction and without EVI). The appropriate way to compare both situations is the following: we consider the interacting case for \( \lambda = 0 \) with the same parameters of figure 2 but include the non-trivial renormalization of the hybridization \( \Delta_1 = 0.941 \Delta_2 \). The \( \Delta \) is adjusted, as for figure 2, to get identical occupations of both levels at low temperatures. The situation we want to compare is for the non-interacting case with the same \( \Delta_1 \). In this case, for \( \Delta_1 \neq \Delta_2 \), tuning both \( E_i \) one can also fix the two mean occupations \( \langle n_{\text{res}} \rangle = 1/4 \) and obtain at \( V_b = T = 0 \) perfect DESINT. Since the non-interacting spectral densities are just Lorentzian functions it turns out that \( \langle n_{\text{res}} \rangle = 1/4 \) implies \( E_i = \Delta_e \). Following known equations for the non-interacting case [53], we obtain

\[
G = \frac{e^2}{h} \int d\omega \left( -\frac{\partial}{\partial \omega} [f_L(\omega) - f_R(\omega)] \right) g(\omega),
\]

\[
g(\omega) = \sum_i \frac{\Delta_i^2}{(\omega - \Delta_i)^2 + \Delta_i^2} - \frac{\Delta_1 \Delta_2 h(\omega)}{\hbar^2(\omega) + (\Delta_1 - \Delta_2)^2 \omega^2},
\]

\[
h(\omega) = (\omega - \Delta_1)(\omega - \Delta_2) + \Delta_1 \Delta_2,
\]

where \( f_L(\omega) = f(\omega - \mu_L) \) and \( f(\omega) \) is the Fermi function.

The transport properties for the non-interacting and Kondo cases are compared in figure 3. The conductance at low temperatures in the interacting case (black thick) and the non-interacting case (blue circles) is shown as a function of the bias voltage scaled with the relevant scale in each case: the Kondo temperature \( T_K \) in the former and the hybridization \( \Delta_2 \) in the latter. In the non-interacting case, with this tuning of both energies, we realize a situation where the device can be operated as a QuIET: changing \( E_2 - E_1 \) by a quantity larger than \( \Delta_1 \), a conductance of the order of \( G_0 \) can be reached. However, since the spectral densities are different, there is no emergent symmetry, perfect DESINT is rapidly lost for small \( V_b \sim \Delta_2 \) as shown in figure 2. Instead, in the interacting Kondo case, the regime to operate the 'many-body QuIET' is found tuning just one energy \( E_1 \) and perfect DESINT is obtained with a total occupancy near 1, more robust under \( V_b \). The conductance remains small even for \( V_b \sim T_K \) and \( T \sim 5T_K \). This is expected because the spectral densities of both levels are very similar, as shown in figure 2.

![Figure 3. Conductance as a function of bias voltage for \( \lambda = 0 \), \( E_d = -0.4 \Delta_2 = 0.05 \) and \( \Delta_1 = 0.941 \Delta_2 \), \( \delta = 0.001499 \) and several temperatures. The resulting Kondo temperature is \( T_K = 8 \times 10^{-4} \). Blue circles indicate the non-interacting result at \( T = 0 \) for \( E_d = \Delta_2 \) and \( \delta = \Delta_1 - \Delta_2 \) as a function of \( V_b/\Delta_2 \).](image)

![Figure 4. Kondo temperature as a function of \( \delta \). Other parameters as in figure 2.](image)

3.4. Effect of \( \delta \) on \( T_K \)

To discuss in more detail the width of the Kondo peak (which is of the order of \( 2T_K \)), we represent \( T_K/\text{SU}(4) \) as a function of \( \delta \) in figure 4. \( T_K^{\text{SU}(4)} \) is the Kondo temperature of the pure SU(4) case \( \delta = \lambda = 0 \). For practical purposes, we have calculated \( T_K \) from the temperature dependence of the conductance \( G_e(T) \) of an equivalent model for an SU(4) system under a symmetry breaking field. Specifically \( T_K \) is determined from \( G_e(T_K) = G_M/2 \), where \( G_M \) is \( G_e(0) \) for a total occupation of one electron in the dot (\( G_M \) is the maximum possible value of the conductance that can be obtained in the model for fixed coupling to the leads, changing the other parameters, see appendix B). This definition is more precise than the width of the spectral density or the peak in \( G(V_b) \) because they depend...
on details of the fit and the proximity of the charge-transfer peak [48]. We have checked that the ratio $T_K/\lambda_{SU(4)}$ calculated in this way or from the width at half maximum of the Kondo peak are practically the same. The maximum $T_K$ is about 17% below $T_{K_{SU(4)}}$ due to EVI. Note that this maximum is reached for a value $\delta = \delta_m$ slightly larger than $\delta_{\text{res}}$, indicating again that the emergent SU(4) symmetry is approximate and depends on the property studied. As $\delta$ deviates from $\delta_m$, $T_K$ decreases, and more strongly for $|\delta - \delta_m| > T_{K_{SU(4)}}$.

### 3.5. Asymmetric case

Having demonstrated that perfect DESINT, destroyed after including vibrations, can be restored tuning $\delta$ for symmetric leads ($V_{Lk} = V_{Rk}$ and $V_{L2k} = -V_{R2k}$), one would like to know to what extent this is true for strongly asymmetric leads. A situation that is commonly found in molecular junctions. From the transformations shown in appendix C.1, we know that $G(0, 0) = 0$ if $\lambda = \delta = 0$ and $V_{Lk}^L = V_{Lk}^R > V_{Rk}^L > -V_{Rk}^R > 0$. This model describes in particular annulene molecules (such as 18-annulene [4]) with contacts at 90 degrees, one of then in contact with a C atom and the other in between two C atoms (see appendix D). This perfect DESINT is lost for $\lambda > 0$.

To study the effect of a finite $\lambda$ we have taken $\Delta_{x}^{L} = 30\Delta_{x}^{R}$, keeping the ratios of $V_{k}^L$ as above. This large value is chosen to have a great contrast to the symmetric case. In addition, large asymmetry of the coupling is the general case in molecular quantum dots [21]. In figure 5 we show a similar comparison to that of figure 1 of the conductance calculated with and without phonons in this asymmetric situation. As shown in the inset, for $\lambda = 0$ the conductance $G = 0$ for $V_b = 0$ at low temperatures in agreement with our analytic calculations (appendix C.1). As shown by the numeric results this continues to be true for $V_b \neq 0$. In the inset we also show $G(V_b)$ for $\delta = 0.01$. This curve shows a marked asymmetric behavior and a peak for $eV_b = -T_K$.

This can be understood as follows. For an asymmetry greater than a factor 10 between left and right couplings, $G(V_b)$ and the spectral densities $\rho_{se}(\omega)$ are quite similar to those for the dot considered at equilibrium with the lead with larger coupling [48] (left in our case). The conductance is then similar to that in scanning tunneling spectroscopy experiments, with the right lead playing the role of the tip with the difference that in our case half of the (instead of the whole) voltage falls between the molecule and the right lead giving rise to capacitance effects [54]. For $eV_b = -T_K$, the potential of the left lead is at $\mu_L = -T_K/2$. For the SU(4) Kondo effect, the Kondo peak in $\rho_{se}(\omega)$ is $\sim T_K$ above the Fermi level (see the inset in figure 2). Then for this nonequilibrium case the peak lies at $\mu_L + T_K = T_K/2$, which is precisely $\mu_K$, leading to a maximum in $G(V_b)$.

For other values of $\delta$ and $\lambda$, the shape of $G(V_b)$ is practically the same, but the overall magnitude changes reflecting the different degree of DESINT. In particular, for $\lambda = \sqrt{10} \times 10^{-2}$ and $\delta = 0.007$, we find $G(V_b) < 10^{-6}G_0$ for $|eV_b| < 4T_K$.

As expected, the perfect DESINT’ leading to $G = 0$ for $\delta = V_b = T = 0$ is destroyed as the EVI is tuned on (black squares for $\lambda \neq 0$). However, consistent with our previous findings, tuning $\delta = \delta_{\text{res}}$ the conductance can be made to vanish within numerical precision, although in this case we could not prove analytically that $G(0, 0) = 0$. For $\lambda$ such that $\lambda^2/\Omega = 0.01$, $\delta_{\text{res}} = 0.007$ and we find $G(V_b) < 10^{-6}G_0$ for $|eV_b| < 4T_K$. When $\delta$ is changed by values higher than $T_K$ the conductance reaches high values which for the asymmetry ratio chosen (30/1) are of the order of 0.125$G_0$. This should be compared with values below $2 \times 10^{-6}$ that we obtain for the conductance in the range $-5T_K < V_b < 5T_K$ and $T < T_K$.

### 4. Summary and discussion

In summary, we have calculated the conductance through a molecular junction showing interference effects in the presence of electron-vibration and strong electron–electron interactions, in the Kondo regime. We have shown that for temperatures and voltages such that $k_BT$ and $eV_b$ are below the relevant vibration energies (in particular below the lowest one with important electron–phonon interaction), the vibrations have two effects: (i) a renormalization of the energy level most strongly coupled to the mode and (ii) a non-trivial renormalization of the coupling to the leads. These effects break the SU(4) symmetry of the simplest interference model and therefore, they are expected to cancel the effects of destructive interference and lead to a sizable conductance. This is the case in the non-interacting system. However in the interacting case for an odd occupancy of the molecule (Kondo regime), and symmetric coupling to the leads, tuning the difference between the interacting levels $\delta$, the destructive interference can be restored to a large extent due to a subtle many-body effects.
effect leading to an emergent SU(4) symmetry. For large asymmetric coupling to the leads we find a similar result for the destructive interference, although in this case, the result seems to be not directly related with approximate SU(4) symmetry.

We obtain that for temperature or voltage ranging from 0 to a few times the Kondo temperature $T_K$, destructive interference is almost perfect for a fixed value of the energy difference between the levels $\delta$. Changing $\delta$ by an amount larger than $T_K$ the conductance increases by more than three orders of magnitude reaching values of the order of the quantum of conductance $2e^2/h$. Our results show the robustness of the ‘many-body QuIET’ which works in the Kondo regime (for values of the on-site energies $-E_d \gg \Delta$). To obtain similar large changes in the conductance in a non-interacting system it is necessary that the system is in the intermediate valence regime $|E_d| \sim \Delta$. Moreover for a non-interacting system the destructive interference is more fragile under application of small bias voltages and temperatures due to the lack of emergent SU(4) symmetry.

The presence of the Kondo effect and nearly degenerate levels of opposite parity is very common in molecular systems. If the difference between the energy of these levels $\delta$ can be controlled, the corresponding two-level Kondo effect that we have described seems promising for a quantum interference effect transistor, operating at low bias voltage and hence with low power dissipation. In fact mechanically controllable break junctions have shown a great tunability of several parameters, like the relative position of the Fermi level [10, 11] and a Kondo temperature ranging from near 1 to 200 K [20]. It is natural to expect that stretching the device, as done for example in [20], $\delta$ can also be varied. Another possibility is to control the angle at which the leads are connected to an annulene molecule, as described in appendix D.

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Appendix A. Equivalence of the interference model and transport through an SU(4) QD under a magnetic field

The model for destructive interference (DESINT) is like equation (1) of the main text without phonons (last line of equation (1)): 

$$H = \sum_{i,\sigma} E_d n_{i\sigma} + \delta \sum_{\sigma} n_{1\sigma} + \sum_{\nu,\sigma} \epsilon^{\nu,\sigma}_{c,\nu,\sigma} c^\dagger_{\nu,\sigma} c_{\nu,\sigma} + \sum_{\nu,\sigma} (V^{\nu}_{ik} d^\dagger_{i,\sigma} c_{\nu,\sigma} + \text{H.c.}) + U \sum_{i,\sigma \neq \nu,\sigma'} n_{i\sigma} n_{i\sigma'}.$$ 

(A.1)

We assume identical left and right leads with equal coupling to the two levels, and one symmetric and one antisymmetric molecular level with splitting $\delta$. Specifically $V^{R}_{ik} = V^{L}_{ik}$, and $V^{R}_{ik} = -V^{L}_{ik}$. A schematic representation of the model is in figure A1.

Transport through a nanotube quantum dot (QD) [51] or a Si QD in a Si fin-type field effect transistors [45] is characterized by a valley (or pseudospin) degree of freedom in addition to the spin one. The spin and pseudospin degrees of freedom can be interchanged, so that the Zeeman splitting can be replaced by a pseudospin splitting. The model that describes the system differs from the above one not only in the symmetry of the levels, but also in the presence of the pseudospin index in the leads:

$$H = \sum_{i,\sigma} E_d n_{i\sigma} + \delta \sum_{\sigma} n_{1\sigma} + \sum_{\nu,\sigma} \epsilon^{\nu,\sigma}_{c,\nu,\sigma} c^\dagger_{\nu,\sigma} c_{\nu,\sigma} + \sum_{\nu,\sigma} (V^{\nu}_{ik} d^\dagger_{i,\sigma} c_{\nu,\sigma} + \text{H.c.}) + U \sum_{i,\sigma \neq \nu,\sigma'} n_{i\sigma} n_{i\sigma'}.$$ 

By symmetry, the matrix elements $V^{R}_{ik}$ should be independent of pseudospin index, but we allow for different matrix elements for the two levels. The same model describes a system with two dots capacitively coupled [18]. This model is represented in figure A2.

While there are four spin degenerate bands of mobile electrons in the leads, depending on valley index $i$ or position with respect to the quantum dot (left or right), for each energy $\epsilon^{\nu}_{k}$ for which there are states at the left and the right leads, only the linear combination $f^{\dagger}_{ik} = (V^{L}_{ik} d^\dagger_{i,\sigma} c_{\nu,\sigma} + V^{R}_{ik} c^\dagger_{\nu,\sigma} 1_{ik,\nu,\sigma})/\tilde{V}_k$ hybridizes with the state $d^\dagger_{i,\sigma}$ while the orthogonal one decouples. The normalization factor is

$$\tilde{V}_k = [(V^{L}_{ik})^2 + (V^{R}_{ik})^2]^{1/2}. \quad (A.3)$$

Then, the model equation (A.2) reduces to

$$H = \sum_{i,\sigma} E_d n_{i\sigma} + \delta \sum_{\sigma} n_{1\sigma} + \sum_{i,\sigma} \epsilon^{\nu}_{i,\sigma} f_{ik} c^\dagger_{\nu,\sigma} + \sum_{\nu,\sigma} (f^{\dagger}_{ik} d_{i,\sigma} c_{\nu,\sigma} + \text{H.c.}) + U \sum_{i,\sigma \neq \nu,\sigma'} n_{i\sigma} n_{i\sigma'}.$$ 

(A.4)

When $\delta = 0$ and $\tilde{V}_k$ is independent of $i$, the model reduces to the SU(4) impurity Anderson model.
For the model equation (A.1) we can define
\[ f_{1k\sigma}^\dagger = \frac{1}{\sqrt{2}} \left( c_{Lk\sigma}^\dagger + c_{Rk\sigma}^\dagger \right), \]
\[ f_{2k\sigma}^\dagger = \frac{1}{\sqrt{2}} \left( -c_{Lk\sigma}^\dagger + c_{Rk\sigma}^\dagger \right), \]
(A.5)
and the model takes the same form as equation (A.4) with \( \tilde{V}_k = \sqrt{2}V_{ik}^r \).

### Appendix B. Conductance for the SU(4) QD with symmetry reduced to SU(2)

For the model equation (A.2) it is reasonable to assume couplings \( \Delta_i^r = \pi \sum_i |V_{ik}^r|^2 \delta(\omega - \epsilon_i^c) \) independent of energy. Then, the total current is given by the sum of four independent contributions for each spin and pseudospin \( I = \sum_{i\sigma} I_{i\sigma} \).

Assuming also
\[ V_{ik}^L/V_{ik}^R = V_{ik}^L/V_{ik}^R, \]  
(B.1)
which implies \( \tilde{V}_k \) independent of \( i \) (see equation (A.3)) and therefore SU(4) symmetry for \( \delta = 0 \), for each of the four channels one can use the expression of Meir and Wingreen, [53] leading to
\[ I_{i\sigma}(V) = \frac{\pi e}{\hbar} \Delta_i^L \Delta_i^R \int d\omega \rho_{i\sigma}(\omega) \left( f(\omega - \mu_L) - f(\omega - \mu_R) \right), \]
(B.2)
where \( \Delta_i = \Delta_i^L + \Delta_i^R \), \( \rho_{i\sigma}(\omega) \) is the spectral density of states of level \( i \) with spin \( \sigma \), \( f(\omega) \) is the Fermi distribution and \( \mu_L - \mu_R = eV_b \), where \( V_b \) is the applied bias voltage. For \( V_b \rightarrow 0 \) the contribution to the conductance \( G_{i\sigma}(V_b) = dI_{i\sigma}(V_b)/dV_b \) is
\[ G_{i\sigma}(0) = \frac{\pi e}{\hbar} \Delta_i^L \Delta_i^R \int d\omega \left( -\frac{\partial f(\omega)}{\partial \omega} \right) \rho_{i\sigma}(\omega). \]
(B.3)

At zero temperature, it is known that the system is a Fermi liquid and since spin and pseudospin are conserved, \( \rho_{i\sigma}(\omega) \) can be related to the phase shift \( \delta_{i\sigma} \) ([55], [56]). For constant density of states of the leads, the generalized Friedel sum rule, for the case in which SU(4) symmetry is reduced only to SU(2), [55] gives
\[ \rho_{i\sigma}(\omega) = \frac{1}{\pi \Delta_i} \sin^2(\delta_{i\sigma}), \]
(B.4)
where
\[ \delta_{i\sigma} = \pi \langle n_{i\sigma} \rangle, \]
(B.5)
so that at \( T = 0 \)
\[ G(0) = \sum_{i\sigma} G_{i\sigma}(0) \]
(B.6)
\[ G_{i\sigma}(0) = \frac{e^2}{\hbar} \sin^2(\pi \langle n_{i\sigma} \rangle). \]

In the Kondo limit for \( U \rightarrow \infty \), one has in the SU(4) case \( \langle n_{i\sigma} \rangle \rightarrow 1/4 \), and therefore \( G(0) = 2e^2/\hbar \). We define the Kondo temperature \( T_K \) as the temperature at which the conductance \( G(V_b, T) \) at \( V_b = 0 \) falls to half of the \( T = 0 \) value, i.e.
\[ G(0, T_K) = e^2/\hbar. \]
(B.7)

The resulting value of \( T_K \) is similar (and in general more reliable [48]) to other possible definitions of \( T_K \), such as the width of the peak nearer to the Fermi energy in the total spectral density, [29] as we have verified explicitly in our case. Since the models equations (A.1) and (A.2) are equivalent, we can use this definition of \( T_K \) also for DESINT in spite of the fact that the conductance for the model equation (A.1) vanishes for some parameters (see next section).

### Appendix C. Conductance at \( T = 0 \) for the interference problem

While for arbitrary temperatures, a full non-equilibrium calculation is necessary to compute the conductance of the interference model, equation (A.1), at \( T = V_b = 0 \) we can derive the conductance using the Fermi liquid properties discussed in appendix B for the equivalent problem equation (A.4).

We know the scattering matrix \( S^{\sigma\sigma'} \) in the basis of the states corresponding to the \( f_{ik\sigma}^\dagger [57, 58] \)
\[ S^{\sigma\sigma'} = \begin{pmatrix} \exp(2i\delta_{\sigma\sigma'}) & 0 \\ 0 & \exp(2i\delta_{2\sigma\sigma'}) \end{pmatrix}, \]
(C.1)
and we also know from equation (A.5) the transformation matrix to left and right leads
\[ U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \]
(C.2)
so that
\[ S^{\sigma\sigma'} = US^{\sigma\sigma'}U^\dagger. \]
(C.3)
The conductance at \( T = V_b = 0 \) is given by the off-diagonal element of \( S^{\sigma\sigma'} [57, 58] \)
\[ G = \frac{e^2}{\hbar} \sum_{i\sigma} |S_{iRi\sigma}|^2, \]
(C.4)
which using the above expressions and some algebra takes the form
\[ G = \frac{e^2}{\hbar} \sum_{\sigma} \sin^2(\pi \langle n_{i\sigma} \rangle), \]
(C.5)
and \( \delta_{i\sigma} \) are given by equation (B.5).

#### C.1. Case \( \delta = 0 \) and arbitrary constant couplings

Here we generalize the above result for \( \delta = 0 \) and \( V_{ik}^r = V_{ik}^f \) independent of \( k \) but otherwise arbitrary. The independence of \( k \) is usually well justified because the range of energies that determine \( T_K \) is much smaller than that of the variation of \( V_{ik}^f \). The model is appropriate for annulene molecules in which the
relevant configuration with odd number of particles has orbital degeneracy, with two states of opposite angular momenta [7]. One example is benzene [8]. The hybridization term in equation (A.1) is
\[ H_V = \sum_{k\sigma} H_{k\sigma} H_{k\sigma} = \sum_{i\nu} (V_i^\dagger d_{i\sigma} c_{i\nu\sigma} + \text{H.c.}) \] (C.6)
Then
\[ \left[ H_{k\sigma}, d_{i\sigma}^\dagger \right] = \sum_{\nu} V_i^\dagger V_{i\nu} d_{i\sigma}^\dagger, \]
\[ \left[ H_{k\sigma}, d_{j\sigma}^\dagger \right] = \sum_{\nu} V_i^\dagger V_{i\nu} d_{j\sigma}^\dagger. \] (C.7)
Now we look for new operators \( \tilde{d}_{i\sigma}^\dagger \), linear combinations of \( d_{i\sigma}^\dagger \) and \( d_{j\sigma}^\dagger \) such that
\[ \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right] = \tilde{V}_{i\sigma}^\dagger. \] (C.8)
Clearly, the problem is equivalent to diagonalize the quadratic form \( \sum_{ij} V_i^\dagger V_{j\sigma} \tilde{d}_{i\sigma}^\dagger \). The corresponding matrix is Hermitian, so that it can always be diagonalized. Furthermore, it can be easily checked that the matrix is positive definite, so that \( \Lambda \geq 0 \). We denote the two eigenvalues as \( (\tilde{V}_i)^2 \) with \( \tilde{V}_i \geq 0 \). Clearly the operators that result from the diagonalization satisfy canonical anticommutation rules \( \{ \tilde{d}_{i\sigma}^\dagger, d_{j\sigma} \} = \delta_{ij} \).

We now define new conduction operators by
\[ \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right] = \tilde{V}_{i\sigma}^\dagger. \] (C.9)
If for one \( l, \tilde{V}_i = 0 \), the corresponding \( f_{i\sigma} \) is defined by orthonormality \( \{ f_{i\sigma}, f_{2\sigma} \} = 0 \) and normalization \( \{ f_{i\sigma}, f_{i\sigma} \} = 1 \). In general one has
\[ \tilde{V}_i \tilde{V}_j \{ f_{i\sigma}, f_{j\sigma} \} = \left\{ \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right], \tilde{d}_{j\sigma}, H_{k\sigma} \right\} \]
\[ = \left[ H_{k\sigma}, \tilde{d}_{j\sigma}^\dagger \right] (\tilde{d}_{j\sigma} H_{k\sigma} - H_{k\sigma} \tilde{d}_{j\sigma}) \]
\[ + (\tilde{d}_{j\sigma} H_{k\sigma} - H_{k\sigma} \tilde{d}_{j\sigma}) \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right] \]
\[ = -\tilde{d}_{j\sigma} \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right] H_{k\sigma} - \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right] \tilde{d}_{j\sigma} \]
\[ + \tilde{d}_{j\sigma} \tilde{d}_{j\sigma} \left[ H_{k\sigma}, \tilde{d}_{i\sigma}^\dagger \right] + \tilde{d}_{j\sigma} \tilde{d}_{j\sigma} \left[ H_{k\sigma}, \tilde{d}_{j\sigma}^\dagger \right] \]
\[ = \tilde{V}_i^2 \{ \tilde{d}_{i\sigma}^\dagger, \tilde{d}_{j\sigma} \} = (\tilde{V}_i)^2 \delta_{ij}. \] (C.10)
Then if both \( \tilde{V}_i > 0 \), \( \{ f_{i\sigma}, f_{j\sigma} \} = \delta_{ij} \) automatically.
Clearly in the new basis
\[ H_{k\sigma} = \sum_i (\tilde{V}_i \tilde{d}_{i\sigma}^\dagger f_{i\sigma} + \text{H.c.}). \] (C.11)
Then, for \( \delta = 0 \), the Hamiltonian takes the same simple form as equation (A.4) but with different localized operators \( \tilde{d}_{i\sigma}^\dagger \) instead of \( d_{i\sigma}^\dagger \). This transformation can greatly simplify the treatment of annulene molecules at arbitrary temperatures. In particular, in the calculation of the conductance [8] off-diagonal elements and complex numbers disappear.

The unitary matrix that changes the basis from the \( f_{i\sigma}^\dagger \) to the \( c_{i\nu\sigma} \) has the general form
\[ U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}. \] (C.12)
Then, using equations (B.5), (C.1), (C.3), and (C.4) we obtain
\[ G = 4|\alpha \beta|^2 \frac{e^2}{h} \sum_{\sigma} \sin^2 \left[ \pi \left( \langle \tilde{n}_{2\sigma} \rangle - \langle \tilde{n}_{1\sigma} \rangle \right) \right], \] (C.13)
where the occupancies \( \tilde{n}_{\sigma} = \tilde{d}_{\sigma}^\dagger \tilde{d}_{\sigma} \).

**Appendix D. Kondo effect and destructive interference in transport through annulene molecules**

In this section, we show that the minimal model describing \( \pi \) orbitals for annulenes connected to conducting leads at appropriate places, and for one electron added or removed from the neutral configuration (so that the ground state has an odd number of electrons and Kondo effect becomes possible), corresponds to the model described above, with perfect destructive interference for \( \delta = 0 \).

The model that describes the \( \pi \) orbitals is a Hubbard or Pariser–Parr–Pople model [7] in a ring of \( N = 4n \) or \( N = 4n + 2 \), with \( N \pm 1 \) electrons. The ground state is doubly degenerate, with wave vectors \( K_2 = -K_1 \). We assume that one of the leads (the left one) is connected to site \( j_L \). Without loss of generality, changing the phases of the states 1 and 2 if necessary, one can take that the couplings of these states to the leads are real and positive and by symmetry \( V_1^\dagger = V_2^\dagger = 0 \). Using symmetry arguments, for the right lead connected at site \( j_R \), the matrix element of the hybridization between both states of the molecule and the right lead are [7, 8]
\[ V_R^\dagger = t_R \exp[-iK_2(j_R - j_L)], \] (D.1)
where \( t_R > 0 \). For symmetric coupling to the leads \( t_R = V_R^\dagger \).

For \( N = 4n \), \( K_3 = \pm \pi/2 \). Changing the phase of the conduction electrons at the right lead one can fix \( V_R^\dagger \) to be real and positive and then using equation (D.1)
\[ V_2^\dagger = V_1^\dagger \exp[-i(K_2 - K_1)(j_R - j_L)] = (-1)^{j_R-j_L}, \] (D.2)
so that for odd differences between the position of the leads one has perfect DESINT according to the results of the previous section (the sum and difference of the states 1 and 2 diagonalize the matrix \( \sum_{ij} V_i^\dagger V_j^\dagger d_{i\sigma}^\dagger d_{j\sigma} \)).

For \( N = 4n + 2 \), the last occupied electrons have wave vectors \( \pm \pi/(2n + 1) \) and the first unoccupied ones \( \pm (n + 1)\pi/(2n + 1) \). Therefore we take \( K_1 = m\pi/(2n + 1) \), with \( m = n + 1 \) for one added hole (electron) and choose the situation with \( m \) odd. We propose to connect the right lead at 90 degrees with respect to the left one, so that the former is equally coupled at the sites \( j_R = n \) and \( j_R + n + 1 \). Then equation (D.1) should be replaced with
\[ V_R^\dagger = 2t_R \cos(K_1/2) \exp[-iK_1(n + 1)/2]. \] (D.3)
As before one can change the phases of the right lead so that \( V_R^2 \) is real and positive, what leads to
\[
V_R^2 = 2t_R \cos (K_r / 2), \\
V_R^2 = V_R^2(-1)^m, 
\]
so that again there is perfect DESINT for odd \( m \).

It is easy to see that changing the angle between the leads allows for large conductance again, as in the case of benzene in the ortho or meta positions [8].

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