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Two-level physics in a model metallic break junction

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We consider a model inspired by a metal break junction hypothetically caught at its breaking point, where the nonadiabatic center-of-mass motion of the bridging atom can be treated as a two-level system. By means of numerical renormalization group (NRG) we calculate the influence of the two-level system on the ballistic conductance across the bridge atom. The results are shown to be fully consistent with a conformal field theory treatment. We find that the conductance calculated by coupling Fermi-liquid theory to our NRG is always finite and fractional at zero temperature but drops quite fast as the temperature increases.

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I. INTRODUCTION

A number of transport measurements on organic and inorganic molecules bridged between metallic leads has recently succeeded in revealing signatures of the molecular vibrational and motional degrees of freedom in the inelastic tunneling spectrum and raised interesting theoretical issues. Most notably, since in these nanosized devices the time scales of the nuclear dynamics may be comparable to those involved in the electron tunneling, nonadiabatic quantum effects become not negligible. This question has been the subject of extensive theoretical activity over the past years, mostly concerned with the vibrational effects, for which we refer to a recent review[1] and to references therein. The role of the center-of-mass oscillations of a bridging site between the two leads has been well addressed mainly via generalized master equations in the context of nanoelectromechanical quantum-shuttle devices. On the contrary, the low-temperature quantum-coherent regime has been only slightly touched and with rather controversial results. For instance, Al–Hassanieh *et al.*[2] made use of exact diagonalization procedure supplemented by a Dyson-equation embedding to conclude that conductance should be suppressed in resonance conditions for arbitrary coupling strength between the center-of-mass motion and the hybridization with the leads and both at finite and vanishing charging energies. This result was questioned by Mravlje *et al.*[3] who found, by a variational procedure and for finite charging energy, that the center-of-mass motion does not affect perfect transmission at resonance.

In this paper we address the same class of questions, concerning the role of the center-of-mass motion at low temperature, in a different type of systems, namely, metallic break junctions (BJ).[4] In a BJ the metal bridge or neck, initially forming a single solid body strongly bonded with the leads, is mechanically broken apart typically at criogenic temperatures. The conductance drops, prior to breaking, typically take place through a sequence of plateaus corresponding to thinning of the neck, down the ultimate monatomic contact, whose conductance is of the order of the conductance quantum $G_0=2e^2/h$, where e and h are the electron charge and Planck's constant, respectively. These plateaus are interpreted in terms of ballistic conductance which, in the adiabatic Landauer-Buettiker linear-response theory,[5,6] is controlled by the few residual one-electron conduction channels and by their respective transmittivity. The moment when the left and the right leads are separating, the physical bridge between the two is, as a rule, a single metal atom as indicated by the last conductance plateau.[4] Here, nonadiabatic effects could in principle be caught right at the moment of separation. The bridge atom, initially strongly attached to both leads, eventually detaches from one of them to remain after separation exclusively attached to the other. In the process, the atom coordinate will move for a while in a double-well effective potential. Therefore, between the initial solid metal-metal nanocontact, held together by a strong bond and with electrical properties governed by ordinary ballistic conductance, and the broken contact, there is a room for a transient state where a new regime involving double-well tunneling may be relevant. As the double well initially develops out of a flat single well, the two well minima can (to a good accuracy) be considered equivalent; moreover, the barrier separating them is initially very weak, which calls for quantum tunneling even when the atom mass is not small. A schematic sketch of this system is shown in Fig. 1. If the mechanical breaking takes place slowly enough in time, the dynamics of the bridge atom nucleus tunneling in the double well may be approximated by that of a two-level system (TLS), whereas the electronic level of the bridge atom, assumed to be non-

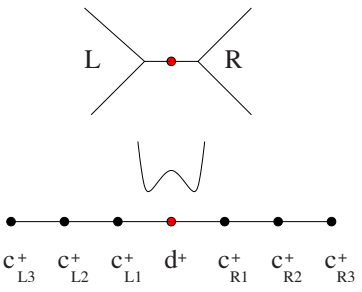

FIG. 1. (Color online) Sketch of a mechanical break junction.

degenerate, gives rise to a resonant electronic level.

Within these assumptions, the physics might be assimilated to that of conduction electrons scattering off TLSs in bulk metals proposed by Vladar and Zawadowski[7] as a possible realization of a two-channel Kondo (2CK) model.[8] This idea recurred several times in recent years in the context of a variety of phenomena in metals[9–14] although again rather controversial. According to Aleiner *et al.*,[15] in fact, the appropriate high-energy cutoff of a TLS coupled to conduction electrons is not the electron bandwidth but rather the oscillation frequency within each potential well since above this energy the conduction electrons follow adiabatically the motion of the atom. Since the Kondo temperature T_K is typically exponentially smaller than the high-energy cutoff, the conclusion of Aleiner *et al.* is that T_K is too small to be relevant. The BJ problem proposes now a new interesting physical situation which we treat here in a slightly different model, arriving at interesting conclusions about the zero-temperature conductance and its temperature evolution.

By means of the numerical renormalization group (NRG),[16] we calculate the influence of the two-level system on the ballistic conductance across the bridge atom. We find that the zero-temperature zero-voltage conductance is always finite and fractional. However it is found to drop quite fast to zero as the temperature increases.

The paper is organized as follows. In Sec. II we introduce the model Hamiltonian and discuss the parameters chosen. In Sec. III we first solve some limiting cases by mean of analytical methods. In Sec. IV we study the low-energy properties of our model by mean of NRG. We show that conformal field theory (CFT) provides a strikingly direct interpretation of the low-lying spectrum obtained by NRG. In Sec. V by using both our NRG routine and a Fermi-liquid theory we give an estimate of the conductance of our model. In Sec. VI we finally summarize and comment our results.

II. MODEL HAMILTONIAN

The physics and language of our model is inspired by a bridge atom suspended between two one-dimensional metallic leads moving quantum mechanically in a symmetric double-well potential, although the model could be equally describing other pseudospin variables coupled to a ballistic conductance channel. As a simplification we will assume that the dynamics of the atom nuclear coordinate is that of a TLS.

Indeed, we neglect the role of the excited states of the double well, which has been analyzed in detail in Ref. 15 in a slightly different model.

We introduce a pseudospin variable τ_z identifying the atom's positions $\tau_z=1$ and -1 when the atom is in the minimum close to the right (R) and left (L) lead, respectively. With this definition, assuming the bridge atom wave function to be real,[7] the quantum tunneling operator between the two wells corresponds to the Pauli matrix τ_x.

The right and left metal leads are modeled as semi-infinite chains (site label $n=1,\ldots,\infty$) with nearest-neighbor hopping, amplitude $-t$, and creation (annihilation) operators $c^{\dagger}_{\alpha n\sigma}$ ($c_{\alpha n\sigma}$), where $\alpha=\mathrm{R},\mathrm{L}$ and the spin $\sigma=\uparrow,\downarrow$. The bridge atom is endowed with a single nondegenerate electronic orbital (the bridge level) and with creation and annihilation operators $d^{\dagger}_{\sigma}$ and d_{σ}, respectively, constituting the ballistic conducting channel. The electron hopping amplitude from the leads to the bridge level is assumed to depend explicitly on τ_z. When the atom is in the right well ($\tau_z=+1$), the level is more coupled to the R chain with amplitude $-t_0(1+\gamma)$, where $0\leq\gamma\leq 1$ than to the L chain with amplitude $-t_0(1-\gamma)$ and vice versa when the atom is in the left well ($\tau_z=-1$). Therefore the model Hamiltonian reads

$$\mathcal{H}_0 = -t\sum_{\alpha=\mathrm{R},\mathrm{L}}\sum_{\sigma}\sum_{n=1}^{\infty} c^{\dagger}_{\alpha n\sigma}c_{\alpha n+1\sigma} + \mathrm{H.c.} - t_0\sum_{\sigma}(1+\gamma\tau_z) \times (c^{\dagger}_{\mathrm{R}1\sigma}d_{\sigma} + \mathrm{H.c.}) - t_0\sum_{\sigma}(1-\gamma\tau_z)(c^{\dagger}_{\mathrm{L}1\sigma}d_{\sigma} + \mathrm{H.c.}) - \Delta_x\tau_x - V_x\tau_x\sum_{\sigma} d^{\dagger}_{\sigma}d_{\sigma}. \quad (1)$$

The last term represents the electron-assisted tunneling of the bridge atomic nucleus arising from the influence of the atom's state of charge on the height of the barrier of the double-well tunneling potential.[7] In principle this type of assisted tunneling process includes other possible operators that couple the bridge level and the nuclear pseudospin coordinate provided that (given our assumption of a symmetric double well and equivalent leads) they are equal even under reflection with respect to the center of the double well (we will call this even parity). The last term in Eq. (1) is therefore just one of the operators that presumably might possess a large matrix element involving the bridge level charge occupancy. In later calculations below we will actually consider more general assisted tunneling operators too. The electron-electron interaction is neglected here.

One can note at the outset that model (1) is closely related to a 2CK model with the role of the spin being played by the lead labels R and L for the conduction electrons and by the pseudospin $\vec{\tau}$ that identifies the TLS, while the role of the silent channels is played by the real spin σ. An alternative way of writing Eq. (1), which may be convenient in some cases, is by introducing the even (e) and odd (o) combinations

$$c_{en+1\sigma} = \sqrt{\frac{1}{2}}(c_{Rn\sigma} + c_{Ln\sigma}), \quad (2)$$

$$c_{on\sigma} = \sqrt{\frac{1}{2}}(c_{Rn\sigma} - c_{Ln\sigma}), \quad (3)$$

and formally defining

$$c_{e1\sigma} = d_{\sigma}$$

through which the model (1) is rewritten as

$$\mathcal{H} = -t \sum_{\alpha=e,o} \sum_{\sigma} \sum_{n=1}^{\infty} c^{\dagger}_{\alpha n\sigma} c_{\alpha n+1\sigma} + \text{H.c.} - (V_e - t) \times \sum_{\sigma} (c^{\dagger}_{e1\sigma} c_{e2\sigma} + \text{H.c.}) - V_o \tau_z \sum_{\sigma} (c^{\dagger}_{o1\sigma} c_{e1\sigma} + \text{H.c.}) - V_x \tau_x \sum_{\sigma} (c^{\dagger}_{e1\sigma} c_{e1\sigma} - \xi c^{\dagger}_{o1\sigma} c_{o1\sigma} + \eta c^{\dagger}_{e2\sigma} c_{e2\sigma}) - \Delta_x \tau_x, \tag{4}$$

where

$$V_e = \sqrt{2} t_0, \quad V_o = \sqrt{2} t_0 \gamma. \tag{5}$$

In $\mathcal{H}$ of Eq. (4) we in fact included additional assisted tunneling operators with coupling constants parametrized by η and ξ, which are missing in Eq. (1). In the *even-odd* formulation, the analogy with a 2CK model is much more explicit especially once we rotate the pseudospin by $\pi/2$ around the y axis with even e and odd o labels playing the role of spin up ($\Uparrow$) and down ($\Downarrow$). A similar model was recently proposed by Zarand[17] in the context of TLSs in metals. According to him the presence of the resonant level may push the equivalent 2CK model into a strong-coupling regime with a large Kondo temperature of the same order as the high-energy cutoff.[18] For comparison, we may also write the conventional two-channel flavor-Kondo model (after a $\pi/2$ rotation around the y axis of the flavor pseudospin)

$$\mathcal{H}_{2\text{CK}} = -t \sum_{\alpha=e,o} \sum_{\sigma} \sum_{n=1}^{\infty} c^{\dagger}_{\alpha n\sigma} c_{\alpha n+1\sigma} + \text{H.c.} + J_x \tau_x T^x_1 + J_y \tau_y T^y_1 - J_z \tau_z T^x_1, \tag{6}$$

where

$$T^a_n = \frac{1}{2} \sum_{\alpha\beta=e,o} \sum_{\sigma} c^{\dagger}_{\alpha n\sigma} \sigma^a_{\alpha\beta} c_{\beta n\sigma}, \tag{7}$$

are the local generators of the flavor $SU(2)$ with σ^a as the Pauli matrices.

Our model $\mathcal{H}$ in Eq. (4) differs from the anisotropic 2CK model (6) since:

(1) the even ($\Uparrow$) chain has one more site than the odd one ($\Downarrow$),

(2) in the even ($\Uparrow$) chain the hopping between sites 1 and 2 differs from the others, and

(3) a local magnetic field Δ_x acts on the pseudospin.

In addition, V_x in Eq. (4) is generally coupled to an operator more complicated than T^x_1 unlike J_x in Eq. (6). This difference has no effect when $\Delta_x = 0$. In that case our model (4) will display the conventional 2CK behavior but plays an important role when a finite Δ_x drives the model away from the 2CK fixed point. Specifically, we found that models with different ξ and η in Eq. (4) may fall into two different classes:

(i) if $\eta = 0$ and $\xi = 1$, the assisted tunneling term $V_x \tau_x$ in Eq. (4) is proportional to T^x_1 or, more generally, if

$$\xi = 1 + \eta, \tag{8}$$

then an intermediate 2CK crossover regime should survive in the presence of a small but finite Δ_x and

(ii) if Eq. (8) is not satisfied, then this crossover regime is likely to be absent for any $\Delta_x \neq 0$. In this case the model with $\xi = \eta = 0$ can be taken as representative of all the others.

We note that the condition (8) means simply that the assisted tunneling operator

$$\sum_{\sigma} c^{\dagger}_{e1\sigma} c_{e1\sigma} - \xi c^{\dagger}_{o1\sigma} c_{o1\sigma} + \eta c^{\dagger}_{e2\sigma} c_{e2\sigma}$$

is orthogonal to the local charge density

$$\sum_{\sigma} c^{\dagger}_{e1\sigma} c_{e1\sigma} + c^{\dagger}_{o1\sigma} c_{o1\sigma} + c^{\dagger}_{e2\sigma} c_{e2\sigma} = \sum_{\sigma} d^{\dagger}_{\sigma} d_{\sigma} + c^{\dagger}_{\text{R}1\sigma} c_{\text{R}1\sigma} + c^{\dagger}_{\text{L}1\sigma} c_{\text{L}1\sigma}.$$

The fact that such a property discriminates between two quite distinct classes of behaviors suggests that the charge degrees of freedom play, in this problem, an active role unlike in conventional Kondo models as we are going to discuss in what follows.

III. PRELIMINARY ANALYSIS OF THE MODEL

Simplifying the double-well dynamics of the bridge atom to a TLS form permits a numerical analysis of the original model $\mathcal{H}_0$ (1). We performed an analysis by means of the numerical renormalization group[16] and the results will be presented and discussed later. Prior to doing this we can, exploiting the analogy with a 2CK problem, discuss first some instructive limiting cases of Eq. (1) that can be easily understood.

First, if $\Delta_x = V_x = 0$ the model describes a conventional electron hopping across the bridge level with inequivalent leads because of $\gamma \neq 0$. In particular, for any value of τ_z, the zero-temperature differential conductance in units of $G_0 = 2e^2/h$ is readily found to be[19]

$$\frac{G}{G_0} = \frac{1 - \gamma^2}{1 + \gamma^2}. \tag{9}$$

If $\gamma = 0$ with finite Δ_x and V_x, it is more convenient to use the even-odd representation in which the conductance is

$$\frac{G}{G_0} = \sin^2(\delta_e - \delta_o), \tag{10}$$

where δ_e and δ_o are the phase shifts at the chemical potential in the even and odd channels, respectively, determined by coupling of the leads to the bridge level. By solving the one-dimensional scattering problem and choosing for simplicity $\eta = \xi = 0$, we find that

$$\delta_e = \frac{\pi}{2} + \frac{t V_x}{2 t_0^2} \tau_x,$$

$$\delta_o = 0,$$

so that

$$\frac{G}{G_0} = \frac{4t_0^4}{4t_0^4 + t^2 V_x^2} \tag{11}$$

is always finite.

A. Asymptotic solution for strong electron-nucleus coupling: $\gamma=1$

The parameter γ in Eq. (1) measures the strength of "electron-phonon" coupling between the bridge atom and the leads. When the bridge atom double well is tiny, the two minima are close and γ will be small; in a wide double well, with the bridge atom very close to either R or L lead, γ will be large (while Δ_x will correspondingly be small). The upper limit for γ is $\gamma=1$, when the bridge atom in the left (right) only couples well to the left (right) lead. As it turns out, this limit is interesting by itself.

Since the bare electron hopping t_0 is of the order of electron volt, which is many orders of magnitude larger than both Δ_x and V_x, one can safely treat the latter terms perturbatively within the path-integral formalism originally developed by Yuval and Anderson[20] and by Hamann[21] for the single-channel Kondo and Anderson-impurity models, respectively. This approach had in turn been built by extending the Nozières-De Dominicis solution[22] of the x-ray edge singularity to a succession of emission-absorption processes. In our problem, because of the presence of the silent spin-channel and of the bridge level, it is necessary to resort to a multichannel extension of the Anderson-Yuval formalism,[23,24] where the perturbation expansion consists of a series of pseudospin flips induced by the operator τ_x. What is important in the calculation is the phase-shift difference suffered by each channel at any pseudospin flip. In the present case the most convenient representation is in terms of R and L leads. We do not present details of the calculations since as it turns out the final result can be inferred by very simple arguments. Because as was said when $\gamma=1$ and $\tau_z=+1$, only the R lead is hybridized with the level, while the L lead is untouched. R acquires a phase shift $\delta_{\mathrm{R}}^{+}=\pi/2$, corresponding to a resonant-level model, while for the left lead L, $\delta_{\mathrm{L}}^{+}=0$. Vice versa, for $\tau_z=-1$, it is only the L lead that is coupled; hence, $\delta_{\mathrm{R}}^{-}=0$ while $\delta_{\mathrm{L}}^{-}=\pi/2$. Therefore the phase-shift differences in the pseudospin flip from $\tau_z=-1$ to $+1$ are $\delta_{\mathrm{R}}=\delta_{\mathrm{R}}^{+}-\delta_{\mathrm{R}}^{-}=\pi/2$ and $\delta_{\mathrm{L}}=\delta_{\mathrm{L}}^{+}-\delta_{\mathrm{L}}^{-}=-\pi/2$ for each spin σ, which here plays the role of a silent channel. This is exactly the location of the so-called Emery-Kivelson point,[25] which also coincides with the intermediate coupling fixed point of the 2CK model.[24,26] Interesting enough, this situation should also correspond to the maximum Kondo temperature attainable,[18] confirming Zarand's expectation.[17] We find that, at equilibrium, the perturbative expansion of the partition function coincides with that of the generalized resonant-level model

$$\mathcal{H}_* = \mathcal{H}_0[\psi_f, \psi_{sf}] - \Delta_x \sqrt{\frac{2v}{\Gamma}}[\psi_f^\dagger(0) f + f^\dagger \psi_f(0)] - V_x \sqrt{\frac{2v}{\Gamma}}(f^\dagger - f)[\psi_{sf}^\dagger(0) + \psi_{sf}(0)], \tag{12}$$

where $\Gamma=4t_0^2/t$ is the hybridization width of the d level, which plays the role of the high-energy cutoff and $\mathcal{H}_0[\psi_f, \psi_{sf}]$ is the continuum limit of a noninteracting Hamiltonian on a closed chain for two different chiral Fermi fields $\psi_f(x)$ and $\psi_{sf}(x)$ that move with Fermi velocity v,[25] namely,

$$\mathcal{H}_0[\psi_f, \psi_{sf}] = iv \sum_{a=f,sf} \int dx\ \psi_a^\dagger(x) \partial_x \psi_a(x),$$

and, finally, f and $f^\dagger$ are the annihilation and creation operators of an auxiliary fermion satisfying $f^\dagger f - 1/2 = \tau_z$.

Here we labeled the fields following Emery and Kivelson[25] to stress the fact that the role of spin s (here the real spin σ) and of flavor f (here the R and L leads) are interchanged in our model with respect to the conventional 2CK model.

Unlike the Emery-Kivelson Hamiltonian[25] for the 2CK model, in our case, a pseudospin field Δ_x is present, which spoils the anomalous 2CK behavior.[27] For any finite Δ_x, the spectrum of the Hamiltonian (12) is Fermi-liquid-type, corresponding in fact to a 2CK model in the presence of a magnetic field applied to the impurity—a case studied by Affleck *et al.*[26] We further note that the original Hamiltonian (4) is invariant under a generalized parity operator

$$\mathcal{P} = \tau_x (-1)^{N_o}, \tag{13}$$

where N_o is the total number of electrons in the odd channel. Since a Fermi-liquid spectrum implies that the TLS (the Kondo impurity) asymptotically dissolves into the conduction bath, it follows that the value on each state of the generalized parity operator (13) turns effectively into the "Fermi-liquid" parity $(-1)^{N_o}$. This observation implies a zero-bias conductance dictated by the form (10) in the low-energy spectrum.

We conclude by briefly discussing the other limit $\Delta_x=0$, when the bridge atom is so heavy, or the barrier so large, that the double-well tunneling is suppressed. Here the model flows to the 2CK fixed point, and here it is well known that the elastic-scattering S matrix at the chemical potential is zero.[28] Since the even and odd channels in our model correspond to the spin-up and -down channels in the 2CK problem, both have vanishing S matrix; hence, the conductance is zero. For an infinitesimally small magnetic field acting on the impurity spin, it was shown in Ref. 26 that a Fermi-liquid behavior is recovered with a phase-shift difference of $\pi/2$ between the two spin channels. The translation of this result in our case is not so straightforward since, in the absence of any coupling to the TLS, i.e., $V_o=V_x=0$, the even and odd phase shifts are finite unlike the conventional 2CK. Actually, since the even chain has one more site, the "bare" phase-shift difference is already $\pi/2$. One possibility appears to be that the $\pi/2$ phase-shift difference acquired by switching on an infinitesimal Δ_x at the 2CK fixed point adds to the bare value to give a total difference of zero modulo π. This would imply zero conductance for $\Delta_x \ll V_x$, raising to nonzero by increasing Δ_x. We shall see that this is actually what happens if Eq. (8) is satisfied, namely, if the assisted tunneling does not involve charge degrees of freedom. In the opposite case, the conductance behavior is more complicated.

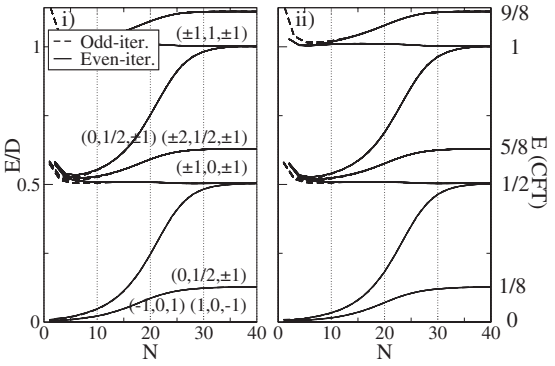

FIG. 2. NRG flow of lowest eigenvalues for the model in Eq. (4) with $\Delta_x=0$. Case (i) is analyzed in the left panel and case (ii) in the right one.

IV. NUMERICAL RESULTS

We address the spectrum of the model Hamiltonian $\mathcal{H}$ of Eq. (4) by standard NRG,[16] whose results we are going to present in this section. Tentative values of the Hamiltonian parameters which we adopted are a conduction bandwidth $2D_0 \sim 2$ eV, the attempt frequency $D \sim 10^{-2}$ eV,[15,17] $V_e \simeq V_o \sim 0.2$ eV, and $V_x \simeq \Delta_x \sim 10^{-3} V_e$. As discussed previously, only the conduction electrons with energy smaller than the attempt frequency are involved in the pseudospin screening. In order to enforce this condition, we take a flat conduction-electron density of states of bandwidth 2 eV (the chemical potential is zero), but we assume that only the conduction electrons with energy $-D \leq \epsilon \leq D$ are coupled to the local degrees of freedom. Consequently, we perform the NRG procedure only on these electrons, which amounts to assume an effective bandwidth $2D \sim 2 \times 10^{-2}$ eV, yet with a flat density of states equal to the original one, namely, $0.5\ \text{eV}^{-1} = 0.5 \times 10^{-2}/D$. Using the attempt frequency D as our energy unit, the net result in the Wilson chain[16] is a renormalization of

$$V_{e(o)} \to \sqrt{\frac{D}{D_0}} V_{e(o)} = \frac{V_{e(o)}}{\sqrt{D D_0}} D = 2,$$

which keeps the d-level hybridization width at the chemical potential invariant, while V_x and Δ_x rescale trivially into themselves,

$$V_x \to \frac{V_x}{D} D, \quad \Delta_x \to \frac{\Delta_x}{D} D,$$

implying $V_x \simeq \Delta_x \sim 10^{-2} V_e$,[29] which are the values we assume throughout. Moreover, to better identify each state of the spectrum, in the numerical calculations, we implemented the spin SU(2) symmetry, the charge U(1) symmetry and the discrete parity defined by Eq. (13).

Following the discussion of Sec. II, we ran NRG calculations for the two different implementations of the electron-charge-assisted tunneling, i.e., case (i), in which Eq. (8) holds with $\eta=0$ and $\xi=1$ and case (ii) with $\eta=\xi=0$. In Fig. 2 we show the NRG flow for the Hamiltonian in Eq. (4) for both cases (i) and (ii) above with $\Delta_x=0$ and with $V_e=V_o=2$ and $V_x=10^{-2}V_e$. The energy of the lowest-lying eigenvalues is plotted as a function of the number N of NRG iterations corresponding to an energy (temperature) scale $\omega_N = D\Lambda^{-N/2}$ where Λ is the Wilson discretization parameter (we henceforth set $\Lambda=2$). At large N, the spacing between the levels, their degeneracy and the disappearance of any difference between even and odd iterations N (see for instance Ref. 27), is typical of a 2CK. These results are summarized in Table I and are consistent with the conformal field theory prediction[30,31] for the 2CK.

TABLE I. Lowest-energy NRG spectrum of the Hamiltonian $\mathcal{H}$ of Eq. (4) for $\Delta_x=0$. The energies E(NRG) are given in units of the fundamental level spacing and compared with the conformal field theory prediction E(CFT). For each eigenvalue we indicate its degeneracy (deg) together with its quantum numbers Q (charge), S (spin), and parity P defined in Eq. (13).

E(CFT)	E(NRG)	Q	S	P	Deg
0	0.0000	−1	0	−1	1
0	0.0000	1	0	1	1
1/8	0.1246	0	1/2	±1	4
1/2	0.4999	+1	0	−1	2
1/2	0.4999	−1	0	+1	2
1/2	0.4999	+1	1	+1	3
1/2	0.4999	−1	1	−1	3
5/8	0.6290	0	1/2	±1	4
5/8	0.6290	±2	1/2	±1	8
1	1.0230	−1	1	+1	6
1	1.0230	1	1	−1	6

The numerical results clearly show that, whatever the form of electron-assisted tunneling is, the system has a 2CK behavior at low temperatures. The Kondo temperature T_K is conventionally estimated as $D\Lambda^{-(N_c-1)/2}$ with N_c as the NRG iteration at which, e.g., the first-excited state is 10% off its asymptotic value.[18,27] We find that, while cases (i) and (ii) have roughly the same N_c, the latter is strongly influenced by V_o/V_e. In particular $V_o/V_e \simeq 1$, namely, $\gamma \simeq 1$ is an optimal choice that minimizes $N_c \sim 25$ consistently with the previous analysis and corresponds to a temperature of few hundredths of a Kelvin. Remarkably, even and odd iterations are hardly distinguishable after very few iterations. That seems to be a property of the 2CK model right at its fixed point, the fixed point with the highest $T_K \sim D$,[18,27] which would imply that the above estimate of T_K is a strong underestimation of the real one. However, we cannot exclude the possibility that the even-odd collapse of the energy levels might simply indicate a preliminary crossover to a regime where the effects of V_e and V_o are fully established while those of V_x are still negligible.

We note that, although the level spacings and degeneracies are those of the conventional 2CK model (6), the quantum numbers of each eigenvalue differ substantially from that model. In the flavor 2CK model, labeling states with Q and S and the flavor T [see Eq. (7)], one expects the lowest-energy spectrum of Table II. This spectrum is determined within conformal field theory[30,31] by the so-called fusion of the free-electron spectrum, top in Table II, with the flavor primary field with $T=1/2$.

TABLE II. Lowest-energy spectrum of the 2CK model (6) for $V_a=0$ (top table) and $V_a\neq 0$ (bottom table) as expected by conformal field theory.

E(CFT)	Q	S	T	Deg
0	0	0	0	1
1/2	±1	1/2	1/2	4
1	0	1	1	9
1	±2	1	0	6
1	±2	0	1	6

E(CFT)	Q	S	T	Deg
0	0	0	1/2	2
1/8	±1	1/2	0	2
1/2	0	1	1/2	6
1/2	±2	0	1/2	4
5/8	±1	1/2	1	12
1	±2	1	1/2	12

By contrast, we found that the NRG spectrum, Table I, can be obtained starting from the 2CK one in Table II in the following way:

(1) First we decompose the flavor $SU(2)\rightarrow U(1)\times Z_2$, where $U(1)$ stands for the free bosonic theory that represents the z component of the flavor field and Z_2 is an Ising conformal field theory (see Sec.18.5 in Ref. 32). This decomposition leads to the spectrum in Table III.[33]

(2) Next we shift the charge Q and z component of the flavor T_z by +1.[33] This corresponds to the fact that the even chain has one more site. In this way we obtain the spectrum in Table IV which coincides with that one in Table I including the degeneracy of each eigenvalue.

We note that, if we recombine the charge $U(1)$ with the Ising to form an isospin (charge) $SU(2)$ theory, the spectrum becomes equal to the conventional 2CK one in Table II with the role of Q played by T_z and that of T played by the isospin. In other words, it seems that, although the original model is not invariant under isospin $SU(2)$ symmetry, the fixed point does in fact recover that symmetry. This unexpected result is confirmed by the spectrum calculated during the renormalization-group procedure. Indeed, after very few iterations, the ground state becomes and stays for all $N>1$ doubly degenerate with quantum numbers $(Q,S)=(+1,0),(-1,0)$.

TABLE III. Lowest-energy spectrum of the 2CK model upon decomposing the flavor $SU(2)$ into $U(1)\times Z_2$. T_z is the quantum number that defines the $U(1)$ theory, while Z_2 corresponds to the coset theory, which is an Ising one.

E(CFT)	Q	S	T_z	Z_2
0	0	0	±1	σ
1/8	±1	1/2	0	I
1/2	0	1	±1	σ
1/2	±2	0	±1	σ
5/8	±1	1/2	0	ϵ
5/8	±1	1/2	±2	I
1	±2	1	±1	σ
9/8	±1	1/2	±2	ϵ

TABLE IV. Lowest-energy spectrum obtained from the one in Table III upon shifting Q and T_z by +1.

E(CFT)	Q	S	T_z	Z_2
0	±1	0	0	σ
1/8	0	1/2	±1	I
1/2	±1	1	0	σ
1/2	±1	0	±2	σ
5/8	±2	1/2	±1	I
5/8	0	1/2	±1	ϵ
1	±1	1	±2	σ
9/8	±2	1/2	±1	ϵ

The above observation also clarifies why the charge degrees of freedom play an important role once Δ_x is turned on. As said, a finite Δ_x is equivalent in the 2CK language to a magnetic field on the impurity site, which is known to be a relevant symmetry-breaking perturbation destroying the anomalous 2CK behavior.[26] Indeed, we find that, as soon as $\Delta_x\neq 0$, the spectrum flows to a Fermi-liquid one that can be interpreted as independent even and odd electron channels suffering from different phase shifts δ_e and δ_o.

In Fig. 3 we show the NRG flow of the low-energy spectrum for $\Delta_x=10^{-4}V_x$ for the two cases (i) and (ii). The asymptotic spectrum can be straightforwardly interpreted using the single-particle spectrum of Fig. 4 and combining all possible single excitations. In particular, we find that, for very small $\Delta_x\ll V_x$, $\delta_e-\delta_o=0$ for case (i) and $\delta_e-\delta_o=\pi/4$ for case (ii). A difference between the two cases is apparent also in the way they approach to the asymptotic behavior. In fact, for the same values of $\Delta_x\ll V_x$, a crossover region with a $\Delta_x=0$ spectrum is still visible in case (i) but not at all in case (ii) (see Fig. 3). This different low-energy behavior has its counterpart on the conductance behavior as will be discussed in Sec. V.

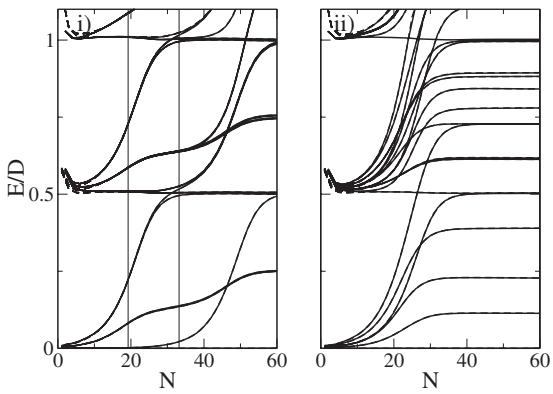

FIG. 3. NRG flow of the lowest eigenvalues for the model in Eq. (4) with $\Delta_x=10^{-4}V_x$. Case (i) in left panel and case (ii) in right panel. Even and odd iterations correspond to solid and dashed lines, respectively.

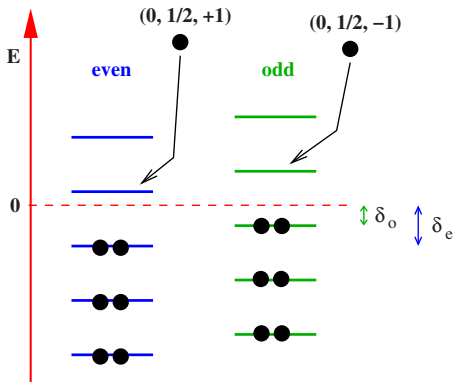

FIG. 4. (Color online) Graphical representation of the Fermi-liquid spectrum for $\Delta_x \neq 0$. The even (odd) single-particle energy levels are equidistant; however, the even spectrum is shifted with respect to the odd one. The ground state is obtained by filling each level below the chemical potential, $E=0$ in the figure, and has quantum numbers $(Q,S,P)=(-1,0,+1)$. All possible excitations can be generated by combining single-particle excitations. We show for instance the two lowest-energy excitations that amounts to adding one electron either even $(0,1/2,+1)$ or odd $(0,1/2,-1)$, which we use to evaluate the phase-shift difference $\delta_e - \delta_o$.

We conclude this part by emphasizing that for realistic $\Delta_x \simeq V_x$ no crossover is visible in the spectrum, which might suggest the absence of any intermediate temperature regime dominated by the singular behavior of the 2CK fixed point. However, this statement should be taken with caution since, as discussed above, the flow, even at $\Delta_x=0$, is quite atypical and does not allow for a precise determination of T_K. Indeed, for $\Delta_x \neq 0$, it remains true that the spectra of even and odd iterations collapse very fast. However, unlike the case $\Delta_x=0$, the levels at even and odd iterations with equal energy have opposite charge Q and parity P. This compares well with the role of a local magnetic field in the 2CK at its fixed point. Levels at even and odd iterations with opposite spin quantum number S_z collapse.[27] Therefore, although we tend to believe that the above estimate of $T_K \sim 10^{-4}D$ is correct, we cannot exclude that the actual value could be much larger.

V. CONDUCTANCE

We mentioned earlier that the zero-bias conductance in the 2CK state $\Delta_x=0$ is zero because the scattering matrix of both the even and the odd channels is zero.[28] For finite Δ_x, the recovery of Fermi-liquid behavior allows us to estimate the conductance by the difference $\delta_e - \delta_o$ [see Eq. (10)], which can be extracted by the spectrum, for instance by calculating the energy difference between the two lowest-energy states with $(Q,S,P)=(0,1/2,1)$ and $(0,1/2,-1)$ in units of the level spacing,

$$\delta_e - \delta_o = \pi(E_{(0,1/2,1)} - E_{(0,1/2,-1)}).$$

These two energies correspond to the cost of adding an even electron $(Q,S,P)=(0,1/2,1)$ or an odd one $(Q,S,P)=(0,1/2,-1)$ to the ground state, which has quantum numbers $(-1,0,1)$, see Fig. 4.

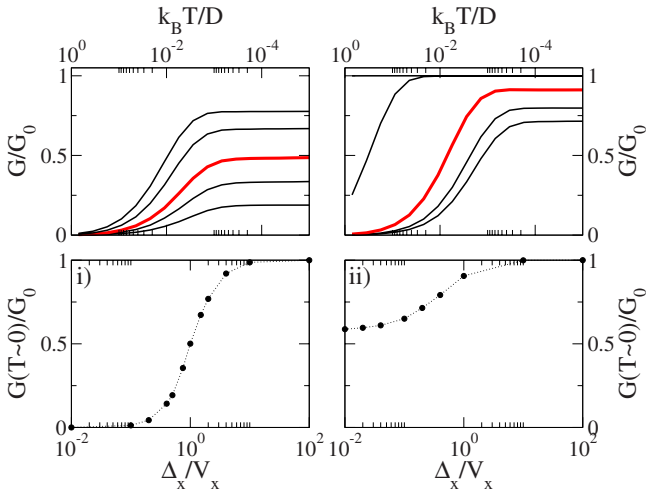

FIG. 5. (Color online) Top panels: Conductance in units of the conductance quantum G_0 as a function of temperature for different values of $\Delta_x/V_x \sim 1$ for case (i) (left panel) and (ii) (right panel). Bottom panels: Zero-temperature conductance as a function of the ratio Δ_x/V_x for cases (i) (left panel) and (ii) (right panel).

We calculate this phase shift, and hence the zero-bias conductance, as a function of the temperature T (extracted from the NRG iterations) for different values of the ratio Δ_x/V_x. We note however that, while we are quite confident about the values at low temperatures, those at high temperatures must be taken with caution since the spectrum is still far from a Fermi-liquid one. The results are shown in the top panels of Fig. 5 for case (i) and case (ii) and realistic values of $\Delta_x/V_x \sim 1$ (red-bold curves). In both cases there is a significant thermal crossover with very small conductance before the asymptotic low-temperature regime is reached. At zero temperature, the conductance is zero if $\Delta_x=0$. However, as soon as an infinitesimal Δ_x is turned on, the zero-temperature conductance stays zero in case (i) but jumps to $G_0/2$ in case (ii) (see bottom panels of Fig. 5). For realistic values of $\Delta_x \simeq V_x$, the zero-temperature conductance is in all cases finite, $G \sim (0.5\text{–}0.9)G_0$, and smaller than the unitary value.

VI. DISCUSSION AND CONCLUSIONS

In summary, we have discussed the influence in the transport across a bridge atom of its quantum-mechanical center-of-mass motion, whose dynamics in the double-well case is approximated as a two-level system.[7] In this regime, the two equilibrium positions of the bridge atom play the role of a pseudospin, whose dynamics is influenced by the electron hopping from the contacts into its valence orbital. This realizes effectively the same physics of a magnetic atom or a quantum dot bridging between two leads with the role of spin played by the position of the atom and the real spin playing the role of an additional flavor index. It is speculated that this hypothetical situation might be applicable to a metal break junction caught right at the breaking point when the central atom bridging the two contacts develops, although for a very short time interval, a double-well potential before collapsing finally onto one of the two.

We find that, as long as the atom can tunnel between the two contacts, the zero-bias conductance at zero temperature is finite, although smaller than its value in the solid metal-metal nanocontact, with a single well for the bridge atom. This finite conductance seems at variance with the earlier result by Al–Hassanieh *et al.*[2] according to which the zero-temperature conductance at resonance should vanish at zero bias when the center-of-mass motion modulates the hopping amplitude into the leads. The discrepancy might be due to our two-level-system approximation or, more likely, to the different low-energy accuracy of NRG with respect to the numerical technique employed by Al–Hassanieh *et al.*[2] Indeed, we find that the finite-temperature conductance, which should correspond to the effective zero-temperature value obtained with less low-energy accuracy, decreases quite rapidly toward zero with increasing temperature.

In the limiting (and unrealistic) case of a vanishing spontaneous tunneling $\Delta_x=0$, in spite of a finite-assisted one $V_x \neq 0$, the model displays a two-channel-Kondo behavior again with vanishing zero-temperature conductance. For finite $\Delta_x \ll V_x$, the zero-temperature conductance is found either to remain zero or to jump to 1/2 of the unitary limit (the conductance quantum) $G=0.5G_0=e^2/h$ depending on the form of the assisted tunneling. On the contrary, for realistic values of $\Delta_x \simeq V_x$, the conductance is always finite, $G \sim (0.5–0.9)G_0$.

In break junctions it is very difficult to apply gate voltages to change the energy of the atomic orbital. Indeed the large amount of metal around the contacted object and the large distance to the substrate give rise to an almost complete screening of the gate electric field. However, assuming that a gate voltage could be applied, we find that its role is very critical at low temperatures. Depending on whether the sign of the voltage gate is positive or negative, the conductance is strongly enhanced or suppressed. However in both cases, by raising the temperature, the conductance goes to zero.

A critical aspect of the model is that, with the realistic parameters used, distinct signatures of the two-level-system dynamics could be hard to observe at temperatures around 4 K, which is commonly used in metal break junction experiments.[4] Even harder could be the detection of possible manifestations of two-channel-Kondo anomalies. Cooling to lower temperature would offer the possibility to observe these effects. Time-resolved conductance experiments could show the tunneling regime as a transient just before breaking and a coherent Kondo-type regime could be reached for light-mass shuttling centers, for instance hydrogen atoms or molecules moving onto and into mechanically controllable break junctions (see, e.g., Refs. 34–36). In that case, the conductance plateaus found below the unitary limit could be ascribable to the two-level-system dynamics similar to that found in our model (see Fig. 5), which is now shifted to higher-temperature scales. A possible realization could be a metal contact bridged by a malone aldehyde molecule, where a hydrogen bond is known to shuttle quantum mechanically between two equivalent positions.[37]

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