Keldysh Functional Integral Theory of Non-equilibrium Kondo Bridge

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We develop a consistent method for calculating non-equilibrium Green’s functions for a nanosized dot coupled to electron reservoirs by tunneling. The leads are generally at different chemical potentials (non-equilibrium), and the dot may be a single molecule characterized by its own vibrational frequency $\omega_{ph}$. We carry out a Keldysh functional analysis of the effective Green’s functions of the local electron in the dot, and also of the vibration mode, in the Kondo regime. Finally, the tunneling current is calculated as a function of bias using non-equilibrium Green’s function. We find stepwise increase of the current when bias exceeds even multiples of the phonon frequency.

I. INTRODUCTION

Observing electron transport through nano-scale structures, often consisting of a single molecule, is an active scientific endeavor nowadays [1–5]. With the ability to fabricate, and to control the conditions of, such small-scale objects, we have the unique opportunity to explore the subtle many-body phenomena under non-equilibrium conditions. A good example of this will be the Kondo phenomenon occurring in a quantum dot flanked by a current source and drain [2–5]. Fixing the leads’ chemical potentials at different values lead to “non-equilibrium Kondo phenomena”.

Unlike the solid-state quantum dot that has been studied extensively in the past few years [4,5], a molecular dot contains a new degree of freedom associated with a conformational change. Such mode can be typically described by an optical phonon of frequency $\omega_{ph}$. As a consequence, the tunneling current exhibits a step-wise increase as the bias voltage passes through an integer multiple of the vibration frequency $\omega_{ph}$ [1]. The coupling of phonon mode to electron transport is an interesting feature absent in a more conventional quantum dot.

It is conceivable that the same electron-phonon coupling takes place in the Kondo regime, i.e. when the electrical transport is carried out by the Abrikosov-Suhl resonance state formed across the dot and the leads. A signature of phonon-assisted Kondo peak has been reported in a recent experiment using $C_{60}$ molecule as a tunneling bridge [3]. On the theoretical side, Lee and Choi considered the modification of the Kondo temperature scale $T_K$ when a phonon mode is present in the dot and found that, due to the decreasing value of effective Hubbard parameter $U$, one should expect increased $T_K$ [6]. Diagrammatic treatment of the Kondo effect in the presence of a.c. perturbation and under non-equilibrium is also present in the literature [7].

Despite these early achievements, more progress can be made to develop easy-to-use techniques for sorting out non-equilibrium many-body phenomena. For example, the essence of Kondo resonance in equilibrium can be obtained straightforwardly in the functional integral formalism developed by Read and Newns (RN) [8]. Here, a slave-boson representation of the free energy of the problem is expressed as an imaginary-time path-integral and subsequently the stationary-phase condition is applied to look for the mean-field state. The mean-field solution precisely corresponds to the Abrikosov-Suhl resonance state. On the other hand, the first pioneering study of the non-equilibrium Kondo physics in the Anderson model taken up by Meir, Wingreen, and Lee used non-equilibrium generalization of the non-crossing-approximation (NCA) and equation-of-motion (EOM) techniques [9]. Aguado and Langreth recently introduced the non-equilibrium generalization of the slave-boson theory of the Kondo resonance in their study of the transport through double quantum dot while avoiding the direct use of the free-energy minimization principle of RN [10].

In this paper, we take the first step towards a consistent generalization of the functional integral theory of RN to the case of non-equilibrium Kondo physics. Instead of the imaginary time integral, we write down the real-time action over the Keldysh contour. Integrating out the lead fermion degrees of freedom, the effective action for the local fermion in the dot is derived that agree with the expressions obtained by earlier authors [9,10]. The method is then applied to study the phonon-coupled Kondo resonance under non-equilibrium. We obtain the linear damping rate of the phonon mode due to coupling to the current at finite bias $V$. Furthermore, current vs. voltage formula is obtained for this case that exhibits the step-wise increase in the current, at even multiples of $\omega_{ph}$, for strong electron-phonon coupling and for a narrow width of the resonance spectrum.

Before we go into the details of the result it is worthwhile to note a similar effort by Komnik and Gogolin, who combined effective action approach with the Keldysh technique to work out the mean-field theory of the Anderson impurity model under non-equilibrium condition [11].

The following sections are organized as follows. Section II introduces the main formalism through discus-
II. NON-EQUILIBRIUM KONDO RESONANCE

We consider the simplest non-equilibrium case of two leads with chemical potentials $\mu_L$ and $\mu_R$, connected by tunneling to a quantum dot. We employ the model Hamiltonian $H = H_L + H_R + H_d + H_T$ where

$$H_L(R) = \sum_{k\sigma}(\epsilon_k - \mu L(R))c_{L(R)k\sigma}^\dagger c_{L(R)k\sigma},$$

$$H_d = -\epsilon_d n_d + U n_d(n_d - 1)$$

$$H_T = V_L \sum_{k\sigma} (c_{L\kappa\sigma}^\dagger d_{\sigma} + d_{\sigma}^\dagger c_{L\kappa\sigma}) + (L \to R),$$

(2.1)

to study such system. We denote the local fermion occupation by $n_d = \sum_{\sigma} d_{\sigma}^\dagger d_{\sigma}$. There is no notion of well-defined set of eigenstates for a non-equilibrium problem such as this one. Consequently, one is unable to write down the free energy for the problem according to the textbook recipe. This is why, we believe, naively writing down the imaginary-time action for $\mu_L \neq \mu_R$ leads to incorrect results. Instead, we write down the Lagrangian density in real-time coordinate along the Keldysh contour $[t_i, t_f] \times [t_f, t_i]$ with $t_f - t_i = T$. Eventually we take $t_i \to -\infty$, and $t_f \to \infty$. First, the Lagrangian density for the Kondo problem, Eq. (2.1), in the slave-boson representation $(U \to \infty)$ is written down:

$$S = \int dC \mathcal{L}(t).$$

From this we isolate the dynamics of the dot by integrating out the lead electrons $c_{L\kappa\sigma}, c_{R\kappa\sigma}$.

$$\mathcal{L}_{\text{eff}} = -\sum_{\sigma} b^\dagger \sum_k G_{Lk} + V_L^2 \sum_k G_{Rk} b^\dagger f_{\sigma}$$

$$+ f_{\sigma}^\dagger (i\partial_t + \epsilon_d) f_{\sigma} + b^\dagger i\partial_t b - \lambda (f_{\sigma}^\dagger f_{\sigma} + b^\dagger b - 1).$$

(2.3)

The self-energy part is defined over the double Keldysh contour $\int_C dC dt'$. The remaining terms are over a single contour, $\int_C dt$. Green’s functions for the lead electrons are given by $G_{L(R)k} = (i\partial_t - \epsilon_k + \mu L(R))^{-1}$. At this stage, we take the mean-field ansatz, $b(t) = b$ and $\lambda(t) = \lambda$, over the entire contour $C$. When this is done, in fact the $\lambda(b^+ b - 1)$ part drops out from the Lagrangian because the forward and backward integrals cancel out. We thus have the effective action ($G_L = \sum_k G_{Lk}, G_R = \sum_k G_{Rk}, \lambda' = \lambda - \epsilon_d, V_L$).

$$S_{\text{eff}} = \int_C dt f_{\sigma}^\dagger(t) (i\partial_t - \lambda') f_{\sigma}(t)$$

$$- \int_C dtdt' f_{\sigma}^\dagger(t) [V_L^2 G_L(t, t') + (L \to R)] f_{\sigma}(t').$$

(2.4)

The Green’s function $G_{L(R)}(t, t')$ may be labeled $(+), (+), (-), (-)$ depending on whether the time arguments $t, t'$ are on the upper $(+)$ or lower $(-)$ branch of the contour. In turn, we can associate each Green’s function with $G_T$, $G^<$, $G^>$ and $G_T^\dagger$ that are commonly used in the non-equilibrium theory as

$$G^{++}(t - t') = G_T(t - t') = -i\langle T\psi(t)\overline{\psi}(t')\rangle$$

and

$$G^{--}(t - t') = G^T(t - t') = -i\langle T\overline{\psi}(t)\psi(t')\rangle.$$

In addition retarded and advanced Green’s function may be obtained readily by $G^R = G^T - G^<, G^A = G^T - G^>$. We must also distinguish the fermion operators defined in the upper and lower branches separately, as $F_{\sigma} = \left< f_{\sigma}^+ \right>$. In Fourier space, the effective action of Eq. (2.4) becomes

$$\sum_{\omega} F^{++}_{\sigma}(\omega) \left( \omega + \lambda' - \Sigma^{++, \pm} \Sigma^{+, -} \right) F_{\sigma}(\omega),$$

where we introduced the simplifying notation $\Sigma^{ab} = (V_L^2 G_{ab} + V_R^2 G_{ab})$, $a, b = +, -, \sum_\omega = \int \frac{d\omega}{2\pi}$. The inverse of the $2 \times 2$ matrix in the above effective action is the Green’s function for the local fermion. Lead Green’s functions are readily obtained

$$\left( \begin{array}{cc} G_T^+ & G_T^- \\ G_T^- & G_T^+ \end{array} \right) = -i\pi\rho \left( \begin{array}{cc} \text{sgn}(\omega - \mu_L) & -2\theta(\mu_L - \omega) \\ 2\theta(\omega - \mu_L) & \text{sgn}(\omega - \mu_L) \end{array} \right),$$

(2.5)

assuming a constant density of states $\rho$. Similar definitions apply for the electrons in the right lead. We assume that the left/right leads have the same density of states. On inverting the matrix, we get for the local fermion Green’s function
where $\Gamma_L = \pi \rho V_L^2$, $\Gamma_R = \pi \rho V_R^2$ and $\Gamma = \Gamma_L + \Gamma_R$. The non-equilibrium Green’s functions obtained in this way are identical to those obtained by earlier authors [9,10]. However, we argue that the present method is much simpler in the sense that only the Gaussian integration is involved in evaluating the effective Green’s function. One should introduce two species of fermions, for the upper/lower branches of the contour, but can otherwise proceed with the usual theory of integration over quantum fields. The retarded Green’s function is given by $G_f^R = G_f^T - G_f^G = 1/(\omega - \lambda' + i\Gamma)$. The spectral function, given as the imaginary part of $G_f^G$, indicates the formation of a resonance state of width $\Gamma$, centered at the energy $\lambda'$.

Determination of the precise value of $\lambda'$ is hampered by the lack of precise definition of the free energy at hand, as discussed at the beginning of this section [12]. How to obtain a suitable generalization of the free energy minimization principle for non-equilibrium is outside the scope of the present paper. Instead, we resort to ref. [10] to conclude $\lambda' \approx (\mu_L + \mu_R)/2$. Therefore, a slave-boson theory in non-equilibrium predicts a single Kondo resonance peak centered half-way between the chemical potentials of the leads as noted earlier [10].

### III. PHONON-COUPLED KONDO RESONANCE AT NON-EQUILIBRIUM

A molecular structure placed between the metallic leads, as well as serving as a bridge for electrons to hop over, may vibrate thermally, or quantum-mechanically in response to interaction with the passing electrons. Such phonon signature in the $I-V$ characteristics has been first detected in the tunneling experiment with the $C_{60}$ molecule. In this experiment, the observed phonon mode is that of the center-of-mass displacement of the molecule as a bridge [1]. A schematic drawing of the experimental setup is shown in Fig. 1.

The geometrical distance between the molecule and the lead varies as the center-of-mass position, denoted by $x$, swings back and forth. The tunneling amplitude, being proportional to the overlap of the wavefunctions in the lead and the molecule, becomes dependent on $x$. The tunneling Hamiltonian will be accordingly modified:

$$H_T = V_L(x) \sum_{k\sigma} c_{Lk\sigma}^+ d_\sigma + V_R(x) \sum_{k\sigma} c_{Rk\sigma}^+ d_\sigma + h.c. \quad (3.1)$$

The motion of the molecule itself is modeled with a harmonic oscillator of frequency $\omega_{ph}$. In this section, we discuss how the phonon mode is damped due to interaction with the electrons that form the resonance. The influence of phonons on the electronic sector has been considered in detail in Ref. [6]. Hereafter we adopt the term “phonon-Kondo model” to describe the situation we are interested in.

![FIG. 1. Schematic setup of the phonon-coupled Kondo model.](image)

The phonon-Kondo model may be written in real-time,}

$$\mathcal{L}(t) = \sum_{k\sigma} c_{Lk\sigma}^+ (i\partial_t - \epsilon_k + \mu_L) c_{Lk\sigma} - bV_L(x) \sum_{k\sigma} \left[c_{Lk\sigma}^+ f_\sigma + f_\sigma^+ c_{Lk\sigma}\right] + (L \to R)$$

$$\quad + f_\sigma^+ (i\partial_t - \lambda') f_\sigma + \frac{1}{2\omega_{ph}} [(\partial_t x)^2 - \omega_{ph}^2 x^2]. \quad (3.2)$$

We anticipate the mean-field condition $b(t) = b, \lambda(t) = \lambda$ in writing down the above Lagrangian. Getting rid of the lead fermions as before, the effective action becomes

$$S_{eff} = -\int_C dt_1 dt_2 f^+_\sigma (t_1) [V_L^x(x(t_1))G_L(t_1, t_2) V_L^x(x(t_2))] f_\sigma (t_2) + (L \to R)$$

$$\quad + \int_C dt f^+_\sigma (t) (i\partial_t - \lambda') f_\sigma (t) + \frac{1}{2\omega_{ph}} \int_C dt [(\partial_t x)^2 - \omega_{ph}^2 x^2]. \quad (3.3)$$
We have once again introduced the simplifying notation $V'_f(x) = bV_L(x)$. The two remaining dynamical modes in the above effective action are the local fermions and the phonon. We now integrate out the local fermions to derive the effective dynamics of the phonons, in part to demonstrate the utility of the Keldysh technique in describing the boson dynamics in non-equilibrium. We treat $V'_f(x) \approx V'_0 - V'_1 x$, $V'_R(x) \approx V'_0 + V'_1 x$, and expand the effective action to quadratic order in $x$. In particular we have the bosonic part of the action

$$L_{\text{eff}} \approx \frac{1}{2 \omega_{ph}} [(\partial_t x)^2 - \omega_{ph}^2 x^2] + 2iV'_1^2 \text{Tr}[\mathcal{G}_f x \mathcal{G}_e x]. \quad (3.4)$$

Here $G_f$ refers to the inverse of $[i\partial_t - \lambda - V'_0 G_e]$, derived in Eq. (2.6) of the previous section, and $G_e = G_L + G_R$ (See Eq. (2.5)). The self-energy portion of Eq. (3.4) can be written out also in the form

$$2iV'_1^2 \int_C dt \text{d}t' X(t) \left( K^{++} + K^{+-} \right) (t-t')X(t'), \quad (3.5)$$

where we introduced $X = (x_+ x_-)$, and

$$D(\nu) = \begin{bmatrix} D^T & D^< \\ D^> & D^\tau \end{bmatrix} = \frac{1}{(\nu^2 - \omega_{ph}^2)^2 + V'_1^4 (K^{++} - K^{--})^2} \begin{bmatrix} \frac{\nu^2 - \omega_{ph}^2}{2 \omega_{ph}} & -2iV'_1^2 K^{--} \\ 2iV'_1^2 K^{++} & \frac{\nu^2 - \omega_{ph}^2}{2 \omega_{ph}} - 2iV'_1^2 K^{++} \end{bmatrix}. \quad (3.7)$$

Retarded Green’s function for non-equilibrium is the difference

$$D^R = D^T - D^< = \frac{2\omega_{ph}}{\nu^2 - \omega_{ph}^2 + 2i\omega_{ph}V'_1^2 (K^{++} - K^{--})}, \quad (3.8)$$

using the relation $2(K^{++} - K^{--}) = K^{+-} - K^{-+}$. Straightforward calculation yields $K^{+-} - K^{-+} = \rho \left( \tan^{-1} \left( \frac{\mu_L + \nu - \lambda}{\Gamma} \right) - \tan^{-1} \left( \frac{\mu_L - \nu - \lambda}{\Gamma} \right) \right) + \rho \left( \tan^{-1} \left( \frac{\mu_R + \nu - \lambda}{\Gamma} \right) - \tan^{-1} \left( \frac{\mu_R - \nu - \lambda}{\Gamma} \right) \right)$

$$\approx \left( \frac{2\rho \Gamma}{(\mu_L - \lambda)^2 + \Gamma^2} + \frac{2\rho \Gamma}{(\mu_R - \lambda)^2 + \Gamma^2} \right) \nu \quad (3.9)$$

for a pair of chemical potentials $\mu_L$ and $\mu_R$ of the leads and for low frequency $\nu$. Mean-field condition sets $|\mu_L - \lambda| \approx |\mu_R - \lambda| \approx V/2$ without the phonon coupling. We do not expect much modification of this conclusion with the phonon coupling turned on, since the strength of the electron-phonon coupling is significantly reduced to $V'_1 = bV_1 \ll V_1$ after the Kondo resonance is established. We then get the linear damping coefficient for the phonon

$$K^{++}(t) = [G_f^T(t)G_f^T(-t) + G_f^T(-t)G_f^T(t)]/2$$

$$K^{+-}(t) = -[G_f^T(t)G_f^T(-t) + G_f^T(-t)G_f^T(t)]/2$$

$$K^{-+}(t) = -[G_f^T(t)G_f^T(-t) + G_f^T(-t)G_f^T(t)]/2$$

$$K^{--}(t) = [G_f^T(t)G_f^T(-t) + G_f^T(-t)G_f^T(t)]/2. \quad (3.6)$$

A product of Green’s functions has the following identities

$$G_f^T(t)G_f^T(-t) = \theta(t)G_f^T(t)G_f^T(-t) + \theta(-t)G_f^T(t)G_f^T(-t)$$

$$G_f^T(t)G_f^T(-t) = \theta(t)G_f^T(t)G_f^T(-t) + \theta(-t)G_f^T(t)G_f^T(-t)$$

that one can use to show, in Fourier components, $K^{++} = K^{--} = \frac{1}{2}(A + B + C + D)$, $K^{+-} = \frac{1}{2}(A - B)$, $K^{-+} = \frac{1}{2}(C + D)$ where $A = \sum \omega G_f^T(\omega)G_e^T(\omega - \nu)$, $B = \sum \omega G_f^T(\omega)G_e^T(\omega + \nu)$, $C = \sum \omega G_f^T(\omega)G_e^T(\omega - \nu)$, $D = \sum \omega G_f^T(\omega)G_e^T(\omega + \nu)$. By using Eqs. (2.5) and (2.6) one can readily calculate $A, B, C,$ and $D$ and all the kernels in Eq. (3.6).

On inserting the self-energy expression back into Eq. (3.4) and inverting the matrix, a remarkably simple expression of the phonon Green’s function emerges:

$$\gamma(V) = \frac{4\rho V'_1^2}{(V/2)^2 + \Gamma^2}. \quad (3.10)$$

Interestingly, we find the damping rate that is independent of the renormalization factor $b^2$ at zero-bias, $\gamma(V = 0) = (4/\pi) V'_1^2/(V'_1^2 + V'^2_0)$. Finite $V$ surprisingly reduces the damping of the phonons.

**IV. NON-EQUILIBRIUM TUNNELING CURRENT**

A step-wise jump in the tunneling current when measured as a function of the bias voltage was observed in the experiment using the C$_{60}$ molecule as a bridge connecting the leads $[1]$. The cause of the jump is the opening up of an additional conducting channel as the bias voltage exceeds integer multiples of the vibration frequency $\omega_{ph}$ of the intermediate molecule. While theory of the conductance through a vibrating molecule has been worked out earlier by several groups $[13–15]$, none addressed the issue using the non-equilibrium Green’s function technique advocated in this paper, nor in the Kondo regime as we do now. We show here that the pronounced features of
the experiment can indeed be shown to follow from our formalism.

To this end, we consider the non-equilibrium Anderson-Holstein model defined by the Hamiltonian consisting of the left/right leads, at different chemical potentials $\mu_L$ and $\mu_R$, the hybridization between the dot and the lead with the tunneling element $V_L$ and $V_R$, now taken as constants, and the dot+phonon Hamiltonian given by $H = -eN_{q+d} + U N_{d(n_d-1)} + \omega_{ph} b^+ b + g \omega_{ph} (n_d - 1)/(b^+ b)$. A well-known Lang-Firsov canonical transformation of the operators, $\hat{O} \rightarrow e^{\hat{S} \hat{O} e^{-\hat{S}}}$, $\hat{S} = \gamma_n (b^+ - b)$, transforms $U$ into $-2g^2 \omega_{ph}$, and the tunneling Hamiltonian becomes

$$V_L \sum_k \langle c_{Lk\sigma}^+ X d_{\sigma} + h.c. \rangle + (L \rightarrow R) \quad (4.1)$$

where $X = e^{g(b^+ b)} - e^{-g^2/2} e^{-gb^+ b} e^{gb}$. At the same time, the local electron operator assumes a composite form $d_{\sigma} \rightarrow Xd_{\sigma}$. Original electron-phonon coupling term has been removed in the transformed Hamiltonian. We further re-write the $d_{\sigma}$ operator in the slave-boson form $b^+ f_{\sigma}$ assuming that the effective Hubbard parameter $U - 2g^2 \omega_{ph}$ is large enough to prohibit double occupation of the dot.

In the Hamiltonian after the Lang-Firsov transformation, electron-phonon coupling takes place through the $X$-operators appearing in Eq. (4.1). When the phonon relaxation is fast, i.e. any change in the phonon numbers caused during the electron tunneling process is relaxed fast, phonon number distribution will be given by the equilibrium value. In this case one can replace $X \approx \langle X \rangle_{\text{equil}} \approx e^{-g^2/2}$. The last equality holds at zero temperature. Now we have achieved complete separation of the phonon and the electron dynamics in the transformed Hamiltonian and the electron-phonon coupling provides only the renormalization of the tunneling amplitudes, $V_{L(R)} \rightarrow e^{-g^2/2} V_{L(R)}$. This is not to say that phonons have no effect on the dynamics of the local electrons. Rather, the electron Green’s function, being a product of the phonon and the transformed local fermion Green’s functions, will depend on the dynamics of both quantities.

We proceed to calculate the Green’s functions for each operator. The Keldysh action one obtains from Lang-Firsov-transformed Hamiltonian will consist of separate pieces for the phonon and the fermion degrees of freedom according to the simplification of the previous paragraph. Therefore, the local electron Green’s function is calculated as $-i (d_{\sigma}(t) d_{\sigma}^+ (t) \langle X(t) \rangle_{\text{equil}} = -ib^2 \langle X(t) X^+ \rangle \langle f_{\sigma}(t) f_{\sigma}^+ \rangle = b^2 \langle X(t) X^+ \rangle G_f^R (t)$, where $G_f^R$ refers to the Green’s function of the Lang-Firsov-transformed fermions. The correlation function for $X$ is obtained straightforwardly from the harmonic oscillator algebra: $\langle X(t) X^+ \rangle = \exp \left[ -i \omega_t - 1 \right]$. After Fourier transform, a simple expression for $G_f^R$ emerges: $G_f^R (\omega) = b^2 e^{-g^2} \sum_{n=0}^{\infty} \frac{1}{n!} 2^n G_f^R (\omega - 2 \omega_{ph})$. In a similar manner we find $G_f^R (\omega) = b^2 e^{-g^2} \sum_{n=0}^{\infty} \frac{1}{n!} 2^n G_f^R (\omega + 2 \omega_{ph})$.

In calculating the current through the dot, we invoke the Meir-Wingreen formula [9] that requires the knowledge of the tunneling density of states $\rho_d(\omega)$. A short manipulation gives $\rho_d(\omega) = (i/2\pi) [G_f^R (\omega) - G_f^R (\omega)]$. Current at zero-temperature is proportional to the integral of $\rho_d(\omega)$ in the energy window $\mu_R \leq \omega \leq \mu_L$, assuming $\mu_L - \mu_R = V > 0$. We find, up to a proportionality constant, the current

$$2 \tan^{-1} \left( \frac{V}{2\Gamma} \right) + \sum_{n=1}^{\infty} \frac{g^{2n}}{n!} \theta (\omega - n \omega_{ph}) \times \left\{ \tan^{-1} \left( \frac{V}{2\Gamma} \right) + \tan^{-1} \left( \frac{V - 2n \omega_{ph}}{2\Gamma} \right) \right\} \quad (4.2)$$

In obtaining this expression we used the mean-field result, $X \approx (\mu_L + \mu_R)/2$, valid in the Kondo regime. The current formula depends on the combined broadening parameter $\Gamma = \Gamma_L + \Gamma_R$.

Plot of the current vs. voltage for several values of broadening parameter $\Gamma$ and electron-phonon coupling strength $g$ is shown in Fig. 2. It shows that the step-wise behavior is most pronounced for small values of $\Gamma$ and for large $g$. In this regard, the Kondo resonance regime may be an excellent venue for the observation of the phonon-assisted steps because of the small $\Gamma$ value of the Abrikosov-Suhl state. Interestingly, the steps occur at even multiples of the phonon frequency, and are absent for odd integer multiples of $\omega_{ph}$. This is to be distinguished from the steps at both even/odd integer multiples of $\omega_{ph}$ observed in $C_{60}$ experiment. The difference is due to the nature of the energy level of the Kondo resonance state. In a resonant-tunneling model the energy level of the dot is fixed regardless of the bias. In the Kondo regime, however, the resonance is located at midway between the chemical potentials of the leads, hence it “floats” as the average $(\mu_L + \mu_R)/2$ is varied. Effectively, the relative energy difference between a lead and the dot level is half the overall bias applied.

![FIG. 2. Tunneling current vs. bias voltage (in units of $\omega_{ph}$)](image)

We have demonstrated that such non-equilibrium phenomena as the phonon-assisted steps in the I-V characteristics can be consistently derived using the formalism.
developed here.

V. SUMMARY AND OUTLOOK

In this paper, we considered some theoretical aspects of transport through a prototype single-molecule device, as experimentally realized recently. A formalism has been developed that extrapolate smoothly between equilibrium and non-equilibrium situations. In summary, our method is based on writing down the real-time action over the Keldysh contour and integrating out the lead electrons’ degree of freedom. This leaves us with the effective dynamics of the localized electron in the dot, or for the phonon-coupled case, the dynamics of the oscillatory motion of the dot. For example, we have obtained the linear damping rate of the phonon mode in interaction with the tunneling electrons in the Kondo regime. The tunneling current through the phonon-coupled dot has been calculated as well; it shows step-like increase in the current vs. voltage behavior.

Although the Kondo regime has been assumed through the discussion of this paper, it is clear that our technique can be applied to any out-of-equilibrium, resonant-level model. This work demonstrates the utility and simplicity of the Keldysh functional integral approach for dealing with non-equilibrium transport phenomena.

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