Decoherence of the Kondo Singlet Caused by Phase-sensitive Detection

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Abstract

We investigate the dephasing effect of the Kondo singlet in an Aharonov-Bohm interferometer with a quantum dot coupling to left and right electrodes. By employing the cluster expansions, the equations of motion of Green functions are transformed into the corresponding equation of motion of connected Green functions, which contains the correlation of two conduction electrons beyond the Lacroix approximation. With the method we show that the Kondo resonance is suppressed by phase-sensitive detection of Aharonov-Bohm interferometer. Our numerical results have provided a qualitative explanation with the anomalous features observed in a recent experiment by Avinun-Kalish et al. [Phys. Rev. Lett. 92, 156801 (2004)].

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Controlled dephasing experiments in mesoscopic devices provide an excellent playground for probing the nature of phase coherence transport and studying the wave-particle duality in quantum mechanics. In the devices, coherence of the quantum dots (QD) was monitored by an Aharonov-Bohm interferometer (ABI), and decoherence was induced by
a quantum point contact (QPC). Initially such experiments were performed in the mesoscopic structures based on QD in the Coulomb blockade regime [1, 2, 3]. Then this kind of experiment was extended to the Kondo regime of QD. In the Kondo regime, a Kondo singlet is formed between the localized spin in a QD and electrons in the electrodes. It was shown that the existence of the QPC plays a role of path-sensitive detector and raises significant suppression of the Kondo resonance [4]. However, properties of the suppression were strongly different from the theoretical prediction of Ref. [5]. The most significant deviation from the theory is that the measured suppression strength of the Kondo resonance is larger 30 times than expected.

Recently, to explain the anomalous features, a theory was proposed by K. Kang [6], in which K. Kang thought that the phase-sensitive detection of the QPC is also an important component for the decoherence of the Kondo singlet. We point out that this treatment is incomplete, because the phase-sensitive detection of the QD is performed mainly by the ABI and not by the QPC. Therefore phase-sensitive detection of the ABI should also be taken into account. One way to prove our proposal is to throw off the QPC from the controlled dephasing devices and only to check the influence of phase-sensitive detection of the ABI, then the controlled dephasing device becomes an Aharonov-Bohm interferometer with a quantum dot coupling to left and right electrodes, which is designed first by Yacoby [7] to measure the phase sensitivity of a QD. It is just the model that we intend to investigate.

In this Letter, we provide a qualitative explanation with the anomalous features observed in a recent dephasing experiment by Avinun-Kalish et al. By employing the cluster expansions, the equations of motion (EOM) of Green’s functions are transformed into the corresponding EOM of connected Green’s functions, which contains the correlation of two conduction electrons beyond the Lacroix approximation. With the method we investigate the Kondo effect in an Aharonov-Bohm interferometer with a quantum dot coupling to left and right electrodes. The differential conductance of the system are calculated to
show that the Kondo resonance is suppressed by phase-sensitive detection of the ABI.
Our numerical results have shown that the theory of K. Kang is incomplete and the phase-sensitive detection of the ABI should also be taken account.

An Aharonov-Bohm interferometer with a quantum dot coupling to left and right electrodes can be modeled by the following Hamiltonian:

$$H = \sum_{\alpha k} \varepsilon_{\alpha k} C_{\alpha k}^\dagger C_{\alpha k} + \sum_\sigma \varepsilon_\sigma d_\sigma^\dagger d_\sigma + \frac{U}{2} \sum_\sigma n_\sigma n_\sigma + \sum_{\alpha k} (V_\alpha d_\sigma^\dagger C_{\alpha k} + V_\alpha^* C_{\alpha k}^\dagger d_\sigma)
+ \sum_{kk'} (T_{LR} C_{Lk}^\dagger C_{Rk'} + T_{LR}^* C_{Rk'}^\dagger C_{Lk}), \quad (1)$$

where $\alpha = L, R$ denotes the left or right electrode, and $\sigma = \uparrow, \downarrow$ denotes spin up or down. The first term describes electrons in the left and the right electrodes, and the second one describes electrons of the quantum dot. The third one corresponds to the on-site Coulomb interactions, and $U$ is the on-site Coulomb repulsion. The fourth one describes the tunneling through the quantum dot, and $V_\alpha$ represents the $s-d$ hybridization. The last one describes the tunneling of electrons between two electrodes via the direct channel, and $T_{LR}$ is the direct electron transmission. The Aharonov-Bohm phase $\phi = 2\pi \Phi \times e/hc$ is included in the tunneling matrices as $V_L T_{LR} V_R = |V_L T_{LR} V_R| e^{i\phi}$. $\Phi$ is the magnetic flux enclosed in the Aharonov-Bohm ring.

Following Zubarev [8], the retarded Green’s function $\langle\langle A(t); B(t') \rangle\rangle$ is defined as

$$\langle\langle A(t); B(t') \rangle\rangle = -i\theta(t - t')\langle[A(t), B(t')]\rangle. \quad (2)$$

By the Fourier transformation of the time variable, the retarded Green’s function satisfies the following equation:

$$\omega \langle\langle A; B \rangle\rangle = \langle[A, B]_\pm \rangle + \langle\langle [A, H]; -; B \rangle\rangle. \quad (3)$$

Eq. (3) is named as the equation of motion (EOM) of Green’s function for the Hamiltonian (1), which can be expressed specifically as follows:

$$\omega \langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle = 1 + \varepsilon_\sigma \langle\langle d_\sigma; d_\sigma^\dagger \rangle\rangle + \sum_{\alpha k} V_\alpha \langle\langle C_{\alpha k}; d_\sigma^\dagger \rangle\rangle + U \langle\langle n_\sigma d_\sigma; d_\sigma^\dagger \rangle\rangle. \quad (4)$$
\[ G_{\alpha\sigma}(\omega) = \langle \langle d_{\sigma}; d_{\sigma}^{\dagger} \rangle \rangle \] is the Green’s function of the QD, and for the high-order Green’s function

\[
\omega\langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle = n_\sigma + (\varepsilon_{d_\sigma} + U)\langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle + \sum_{ak} V_\alpha \langle\langle n_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle + \sum_{ak} V_\alpha \langle\langle d_\sigma^{\dagger} C_{ak\sigma} d_\sigma; d_\sigma^{\dagger} \rangle \rangle - \sum_{ak} V_\alpha^* \langle\langle C_{ak\sigma} d_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle,
\]

(5)

instead of employing directly Lacroix decoupling scheme [9, 10], we make use of a cluster expansions to separate the connected part of the Green’s function. As an example, the high-order Green’s function \( \langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle \) is expressed as follows:

\[
\langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle = \langle\langle d_\sigma; d_\sigma^{\dagger} \rangle \rangle + \langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c,
\]

where \( \langle\langle \cdot \cdot \cdot \rangle \rangle_c \) represents a connected Green’s function and it is straightforward to derive the EOM. We write down the EOM of the connected Green’s function \( \langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c \) as follows:

\[
(\omega - \varepsilon_{d_\sigma} - U(1 - n_\sigma))\langle\langle n_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c = U n_\sigma(1 - n_\sigma)\langle\langle d_\sigma; d_\sigma^{\dagger} \rangle \rangle + \sum_{ak} V_\alpha \langle\langle n_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c + \sum_{ak} V_\alpha^* \langle\langle C_{ak\sigma} d_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c.
\]

(6)

It is not difficult to obtain the EOM of the other connected Green’s function such as \( \langle\langle n_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \), \( \langle\langle d_\sigma^{\dagger} C_{ak\sigma} d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c \), \( \langle\langle C_{ak\sigma} d_\sigma d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c \), \( \langle\langle d_\sigma^{\dagger} C_{ak\sigma} C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \), \( \langle\langle C_{ak\sigma} d_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \), and \( \langle\langle C_{ak\sigma}^\dagger d_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \). In order to truncate the EOM, if let \( \langle\langle d_\sigma^{\dagger} C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \), \( \langle\langle C_{ak\sigma} d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c \), and \( \langle\langle C_{ak\sigma}^\dagger d_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \) involving with the correlation of two conduction electrons to be zero, one reaches Lacroix approximation.

As a consequence of a coherent superposition of spin flip cotunneling events, the forming of the Kondo resonance are inevitably involved with the correlation of two conduction electrons. Therefore the Lacroix approximation must be improved in order to discus the electron transport properties of the single-impurity Anderson model. To surpass Lacroix approximation it is necessary to consider the EOM of the connected Green’s functions of \( \langle\langle d_\sigma^{\dagger} C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \), \( \langle\langle C_{ak\sigma}^\dagger d_\sigma C_{ak\sigma}; d_\sigma^{\dagger} \rangle \rangle_c \), and \( \langle\langle C_{ak\sigma}^\dagger C_{ak\sigma} d_\sigma; d_\sigma^{\dagger} \rangle \rangle_c \) involving the corre-
lation of two conduction electrons, and to assume higher-order correlation Green’s functions to be zero. After a lengthy but direct calculation, in the limit of \( U \to \infty \), \( \langle \{ d_\sigma; d_\sigma^\dagger \} \rangle \) is obtained finally as

\[
G_{d\sigma} = \frac{1 - n_\sigma - \sum_{ak} \frac{V_\alpha C_{ak\sigma}}{\omega - \varepsilon_{ak}} - \frac{V_\sigma^2}{n_\sigma} \sum_{ak} \frac{C_{ak\sigma}}{\omega - \varepsilon_{ak}} \sum_{ak'} \frac{C_{ak'\sigma}}{\omega - \varepsilon_{ak'}}}{\omega - \varepsilon_{d\sigma} - \sum_{ak} \frac{V_\sigma^2}{\omega - \varepsilon_{ak}} + \sum_{ak} \frac{V_\sigma^2}{\omega - \varepsilon_{ak}} \sum_{ak'} \frac{V_\alpha C_{ak\sigma}}{\omega - \varepsilon_{ak}} + \sum_{ak} \frac{V_\alpha V_{LR} C_{ak\sigma}}{\omega - \varepsilon_{ak}} + \delta}.
\]

where

\[
\delta = \frac{V_\sigma^2}{n_\sigma} \sum_{ak'} \frac{\langle d_\sigma C_{ak'\sigma} C_{ak\sigma} \rangle - \langle d_\sigma C_{ak'\sigma}^\dagger d_\sigma C_{ak\sigma} \rangle}{\omega - \varepsilon_{ak}} + \frac{V_\sigma^2}{n_\sigma} \sum_{ak'} \frac{\langle \hat{n}_\sigma C_{ak'\sigma}^\dagger C_{ak\sigma} \rangle - \langle d_\sigma C_{ak\sigma} \rangle \langle C_{ak'\sigma}^\dagger d_\sigma \rangle}{\omega - \varepsilon_{ak}}
\]

and

\[
\sum_{ak'} + \frac{V_\sigma^2}{n_\sigma} \sum_{ak'} \frac{\langle d_\sigma C_{ak'\sigma} C_{ak\sigma} \rangle - \langle d_\sigma C_{ak'\sigma}^\dagger d_\sigma C_{ak\sigma} \rangle}{\omega - \varepsilon_{ak}} - \frac{V_\sigma^2 T_{LR}}{n_\sigma} \sum_{ak'} \frac{\langle d_\sigma C_{ak\sigma} \rangle \langle C_{ak'\sigma}^\dagger C_{ak'\sigma} \rangle}{\omega - \varepsilon_{ak}} + \frac{\langle \hat{n}_\sigma C_{ak'\sigma} \rangle \langle C_{ak\sigma} \rangle}{\omega - \varepsilon_{ak}} (\omega - \varepsilon_{ak})^{2}\]

\[
= \frac{1}{\pi} \int f(\omega) \text{Im} \langle \{ C_{ak\sigma}; d_\sigma^\dagger \} \rangle,
\]

\[
= \frac{1}{\pi} \int f(\omega) \text{Im} \langle \{ C_{ak\sigma}; C_{ak'\sigma}^\dagger \} \rangle,
\]

where \( f(\omega) = 1/[\exp((\omega - E_F)/T) + 1] \) is the Fermi-distribution function. The EOM of the corresponding Green’s functions read

\[
(\omega - \varepsilon_{ak}) \langle \{ C_{ak\sigma}; d_\sigma^\dagger \} \rangle = (V_\alpha - \frac{V_\alpha T_{LR}}{\omega - \varepsilon_{ak}}) G_{d\sigma}(\omega),
\]

\[
(\omega - \varepsilon_{ak}) \langle \{ C_{ak\sigma}; C_{ak'\sigma}^\dagger \} \rangle = (\delta_{ak'k'} - \frac{V_\alpha V_{\alpha}^*}{\omega - \varepsilon_{ak}} + \frac{V_\alpha V_{\alpha}^* T_{LR}}{\omega - \varepsilon_{ak}}) G_{d\sigma}(\omega).
\]

For the sake of simplicity, we have considered the nonmagnetic case, i.e., \( n_{d\uparrow} = n_{d\downarrow} = n/2 \), which \( n \) is total \( d \) electron number

\[
n = 2n_\sigma = \int f(\omega') \rho(T, \omega') d\omega',
\]
Figure 1: DOS of quantum dot for $T_{LR} = 0.01$. The position of the Kondo resonance peak is labeled by the arrow.

where $\rho(T, \omega) = -(1/\pi) Im G_d(\omega)$ is the density of states with finite temperature. Equations (7)-(12) constitute a closed set of equations, which can be solved self-consistently and numerically.

In the following we calculate the density of states (DOS) of the QD in the Kondo regime by $\rho(T, \omega) = -(1/\pi) Im G_{d\sigma}(\omega)$. Because only the conduction electrons near the Fermi level $\varepsilon_F$ participate in the transport current, the DOS for conduction electrons is taken to be a constant $\rho(\varepsilon) = 1/(2D)$ as $-D < \varepsilon < D$, and the quantum dot level broadening is given by $\Delta = \pi |V_\alpha|^2 \rho(\varepsilon) \Gamma$. The Fermi energy $\varepsilon_F$ (meV) is reference mark of the unit of energy [7]. The parameters are considered in the following. The hopping matrix element $V_\alpha$ between the quantum dot and the electrodes is taken to be 0.1, and the tunneling matrix element $T_{LR}$ is taken to be 0.01, which describes the electron direct transmission between two electrodes via direct channel. The total number of the $d$ electron is taken to be 0.8, which determines self-consistently the chemical potential and the numerical value can ensure that the relative position of the level $\Delta \varepsilon = \varepsilon_F - \varepsilon_d$ lies in the Kondo regime. The half width $D$ is assumed to be 1, which defines the energy scale.
The $d$ electron level $\varepsilon_d$ is taken to be 0. The magnetic flux $\Phi$ enclosed in the ring is taken to be $0.5hc/e$ and the virtual dot level broadening $\Delta = 0.01D$. Figure 1 presents the DOS at the very low temperature ($T = 10^{-5}\Delta$ which is lower than Kondo temperature $T_k = (D\Delta)^{1/2} \exp(\pi(\varepsilon_d - \varepsilon_F)/(2\Delta))$ [12]). The Lorentzian resonance peak, which is the broadened quantum dot level, is slightly shifted away from zero. At the Fermi level a Kondo resonance peak is observed.

The current from the left to the right electrode can be calculated from the time evolution of the occupation number of the left electrode:

$$J_L(t) = -e\langle \frac{dN_L}{dt} \rangle = -\frac{ie}{\hbar} \langle [H, N_L] \rangle. \quad (14)$$

where $N_L = \sum_{k,\sigma} C_{kL,\sigma}^\dagger C_{kL,\sigma}$, Using the Green function of the Keldysh type $G_{dLk\sigma}^{<}(t,t)$ and $G_{CLk\sigma,CRk'}^{<}(t,t)$ corresponding to the states at the dot and in the left electrode and the states in both the electrodes respectively, the current can be expressed as

$$I_L = \langle J_L(t) \rangle = -\frac{2e}{\hbar} \text{Re}\left[\sum_{k,\sigma} V_L G_{dLk\sigma}^{<}(t,t) + \sum_{k'k\sigma} T_{LR} G_{CLk\sigma,CRk'}^{<}(t,t)\right]. \quad (15)$$

According to the Langreth’s rule and using steady-state condition $I = \frac{I_L - I_R}{2}$, the current can be expressed as

$$I = \frac{2e}{\hbar} \Gamma \int d\omega \rho(\omega)[f_R(\omega) - f_L(\omega)] \text{Im}G_{d\sigma}(\omega), \quad (16)$$

where $\Gamma = \pi(|V_L|^2 + |T_{LR}|^2)$. For the zero bias voltage we find the conductance

$$G = -\frac{2e^2}{\hbar} \Gamma \int d\omega \rho(\omega) \frac{\beta e^{\beta(\omega - \varepsilon_F)}}{[e^{\beta(\omega - \varepsilon_F)} + 1]^2} \text{Im}G_{d\sigma}(\omega). \quad (17)$$

At finite temperatures the zero bias conductance $G$ can be calculated numerically through the Green function $G_{d\sigma}(\omega)$ of the QD. The relative position of the level $\Delta \varepsilon = \varepsilon_F - \varepsilon_d$ can be varied by the gate voltage applied to the QD. The temperature $T$ is taken to be $10^{-5}\Delta$ lower than the Kondo temperature. The hopping matrix element $V_a$ is taken to
Figure 2: Zero bias conductance as a function of $\Delta \varepsilon$ for $T_{LR} = 0.01$. The asymmetry line-shape comes from Fano effect.

be 0.1 and the magnetic flux $\Phi$ enclosed in the ring is taken to be $0.5hc/e$. Figure 2 presents the zero bias conductance $G$ as a function of $\Delta \varepsilon$ for $T_{LR} = 0.01$. The position of maximum conductance is slightly away from $\Delta \varepsilon = 0$, which comes from the Kondo effect. The asymmetry line-shape comes from the Fano effect. By employing the cluster expansions, the EOM of Green’s functions are transformed into the corresponding EOM of connected Green’s functions. With the method under the Lacroix approximation, we have calculated the DOS of the QD and the zero conductance of the system, in which the Kondo resonance and the Fano effect have been shown. It indicates our numerical method is reasonable.

In a similar way we calculate the source-drain voltage properties of the device. It was assumed that the potential $V$ is applied to the left electrode and at the right electrode the potential is kept zero. The relative position of the level $\Delta \varepsilon = \varepsilon_F - \varepsilon_d$ is hold at 0.04, which lies in the Kondo regime. The hopping matrix element $V_a$ is taken to be 0.1 and the magnetic flux $\Phi$ enclosed in the ring is taken to be $0.5hc/e$. The temperature $T$ is taken to be $10^{-5}\Delta$ lower than the Kondo temperature. Figure 3 presents the differential
Figure 3: Differential conductance for $T_{LR} = 0$ (solid line) and $T_{LR} = 0.01$ (dotted line). Conductance $dI/dV$ as a function of $V$ at the different direct tunneling matrix elements $T_{LR}$. The case for the pure quantum dot ($T_{LR} = 0$) is shown by solid line. Because the relative position $\Delta \varepsilon$ of the level of the quantum dot lies in the Kondo regime, the differential conductance curve shows a very narrow peak at low voltage, which is just the Kondo resonance observed experimentally as reported in Ref.[14, 15]. The broad maximum seen in Fig. 3 comes from the Lorentzian resonance tunneling when the chemical potential $\varepsilon_F + eV$ approaches $\varepsilon_d$. The influence of the direct channel is shown by dotted line. The direct electron transmission ($T_{LR} = 0.01$) enhances the differential conductance but suppresses the Kondo resonance peak. It shows the existence of the direct channel induces the decoherence of the Kondo singlet. However this is only a phenomenon. Its essence lies in the phase-sensitive detection of the ABI because the states of the direct channel decides whether the ABI possesses a phase-sensitive detection function or not. When the direct channel is not zero, even though the phase of the QD is not measured, the ABI possesses a potential phase-sensitive detection function and a strong dephasing of the Kondo singlet is induced. The results of Fig. 3 provide a qualitative explanation with the anomalous features observed in a recent experiment by Avinun-Kalish et al. [Phys.
Rev. Lett. 92, 156801 (2004)] and indicates that the theory [5] of K. Kang is incomplete and the dephasing effect of the phase-sensitive detection of the ABI should also be taken account.

In conclusion, by employing the cluster expansions, the EOM of Green’s functions are transformed into the corresponding EOM of connected Green’s functions. With the method under the Lacroix approximation, we have calculated the DOS of the QD and the zero bias conductance of the system, in which the Kondo resonance and the Fano effect are shown. It indicates our numerical method is reasonable. In a similar way we have calculated the differential conductance and shown that the Kondo assisted transport is suppressed by the phase-sensitive detection of the ABI. Our numerical results have provided a qualitative explanation about the anomalous features observed in a recent dephasing experiment by Avinun-Kalish et al. We have also pointed out that the theory of K. Kang is incomplete and the dephasing effect due to the phase-sensitive detection of the ABI should also be taken account.

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