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Kondo-type transport through a quantum dot: a new finite-U slave-boson mean-field approach

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Abstract

In this paper, we generalize the finite-U slave-boson mean-field theory, provided by Kotliar and Ruckenstein (Kotliar G and Ruckenstein A E 1986 *Phys. Rev. Lett.* **57** 1362), to investigate the Kondo correlation effects on linear and non-linear transport in a quantum dot connected to reservoirs at zero temperature. A comparison between the present formulation and other slave-boson formulations shows that this approach provides a more precise description of Kondo-type transport through quantum dots. In addition, this approach naturally fulfils the Friedel–Langreth sum rule exactly. The numerical results for the linear conductance at zero temperature agree well with experimental data and the numerical renormalization group calculations. The zero-temperature non-linear differential conductance is also discussed for Kondo and non-Kondo systems. A pronounced zero-bias maximum in the Kondo regime and flat zero-bias minimum in the non-Kondo regime are predicted for the zero-temperature differential conductance.

1. Introduction

Recently, due to the rapid development in nanoelectronics, the Kondo effect, which has been studied for magnetic impurity in a metallic host for many years [1], has led to considerable interest in mesoscopic systems. A series of subtly devised experiments made it possible to probe many different regimes of the Kondo effects in semiconductor quantum dot (QD) systems under adjustable conditions [2–9]. So far, the main features of the Kondo effect that have been explored for the quantum dot are Kondo-assisted enhancement of conductance, its specific temperature dependence, a peak splitting in a magnetic field, the zero-bias maximum in the differential conductance in the Kondo regime, and the integer-spin Kondo effect. These effects in QD were successfully proposed in early theoretical work [10–16], which described the electron transport through QD using the well-known impurity Anderson model [17]. This age-old model has been extensively studied for more than thirty years and many numerical and analytical methods have been developed to explore its equilibrium physical properties, such as the Bethe-*ansatz* method [18], the equation-of-motion (EOM) method [19], the second-order perturbation theory (SOPT) for Coulomb interaction U in QD [20], the slave-boson non-crossing approximation (NCA), [21], and the numerical renormalization group (NRG) method [22].

However, the Bethe-*ansatz* and NRG methods cannot be used to study non-linear transport phenomena. Meir *et al* [11] used the EOM method early on to investigate the properties of linear and non-linear transport through QD. Due to the decoupling approximation employed by them, this treatment breaks down at low temperatures because of underestimation of the Kondo correlations. The SOPT has been applied by Hershfield *et al* to explore the Kondo resonance in the finite-U Anderson model out of equilibrium [10], which has been confirmed to be reliable for the symmetric case ($2\varepsilon_d + U = 0$, ε_d being the QD energy level), but fails for asymmetric systems owing to the deviation from the current-conservation and Friedel sum rules. Therefore, a modified SOPT was developed in order to overcome this shortcoming [15, 16]. Craco and Kang [16] employed this modified SOPT to study the transport through QD for the Kondo and non-Kondo regimes in non-equilibrium conditions. They found a zero-bias maximum in the differential conductance for the Kondo system due to the Kondo resonance effect, but a weak zero-bias minimum for the non-Kondo system. Although this approach achieves numerical success in the proper description of the linear and non-linear transport through QD over a wider range of parameters and approximately fulfils the Friedel sum rule, it is evident that it employs an equilibrium density of states (DOS) to study transport properties, which are non-equilibrium phenomena. Consequently, this approach may not predict the splitting of the Kondo-enhanced DOS at the Fermi energy under a finite voltage bias between the left and right leads, in contrast with the quantitative calculation of the EOM in combination with the NCA in the limit of infinite Coulomb interaction $U \to \infty$ [12, 14]. The NCA provides a good description for the investigation of the excitation spectra for QD based on Coleman's slave-boson formulation (Coleman's formulation) [23], but the necessary Fermi liquid behaviour is not reproduced at the low-energy and low-temperature limit. Recently, a slave-boson mean-field theory (SBMFT) has been presented for studying transport through tunnelling-coupled double quantum dots under the same assumption—that the Coulomb interaction $U \to \infty$ [24,25]—for which Coleman's formulation was applied [23]. This scheme transforms the strong-correlation Hamiltonian to an equivalent non-interacting one by introducing several auxiliary boson operators just as the NCA does. It evades the dilemma of how both the Coulomb interaction U and the mixing between the QD and the two leads can be simultaneously treated in deriving the self-energy of the QD. Subsequently, this simple and effective scheme was extended to investigate the Kondo-related transport in hybrid mesoscopic structures, such as normal-metal–QD–superconductor (N–QD–S) [26] and superconductor–QD–superconductor (S–QD–S) systems [27]. All of these investigations have concentrated on the limit of $U \to \infty$. However, the experiments on transport through QD show that the Coulomb interaction U is finite. Therefore, further investigation of the non-equilibrium finite-U Anderson model is necessary.

More recently, a new SBMFT has been developed to investigate transport through QD with arbitrary strength of the Coulomb interaction under the influence of magnetic fields [28]. This scheme is an extension of the saddle-point approximation to the auxiliary-boson functional integral method for the Anderson models, suggested by Kotliar and Ruckenstein [29] (the KR formulation), to non-equilibrium situations. It has been confirmed that this formulation's simple saddle-point approximation for all Bose fields and Lagrange multipliers introduced is, at zero temperature, equivalent to the results derived from the Gutzwiller variational wave function [29], the well-known analytical approach used for studying strongly correlated fermions. This approach has been applied extremely extensively in the literature and is believed to be a powerful non-perturbative tool for studying strongly correlated fermion systems [30]. To our knowledge, it is the first time that this powerful method has been applied to explore coherent transport through a single Anderson impurity. The purpose of the present paper is to apply this finite-U approach to investigate the linear and non-linear transport through QD.

The remaining parts of the paper are arranged as follows. The detailed formulation will be presented in the second section. In the wide-band limit, we can obtain the linear conductance G of QD, which has the same form as the well-known Breit–Wigner formula, but with the effective energy level and coupling constant instead. Of course, the Friedel sum rule is naturally satisfied within the SBMFT framework. The slave-boson formulation given by us is evidently different from the usual finite-U slave-boson formulation [31], which has been extensively utilized within the diagrammatic NCA. The third section gives a comparison of our KR formulation, in detail, with other finite-U slave-boson formulations at the slave-boson mean-field level, which indicates that our formulation provides a more precise description of the Kondo effects in QD at zero temperature. On the basis of our approach, a numerical investigation and discussion are given for the Kondo effects on linear and non-linear transport through QD in the next section. In the linear case, the conductance G is evaluated and shows good consistency with the experimental data and NRG calculations. Finally, our conclusions are given in section 5.

2. The finite-U slave-boson mean-field approach

Transport through a QD connected to the leads in the presence of an external bias voltage can be described by the Anderson single-impurity model:

$$H = \sum_{\sigma,k_\alpha} \epsilon_{k_\alpha,\sigma} c^\dagger_{k_\alpha,\sigma} c_{k_\alpha,\sigma} + \sum_\sigma \epsilon_{d\sigma} c^\dagger_{d,\sigma} c_{d,\sigma} + U n_{d,\uparrow} n_{d,\downarrow} + \sum_{\sigma,k_\alpha} (V_\alpha c^\dagger_{k_\alpha,\sigma} c_{d,\sigma} + \text{H.c.}) \tag{1}$$

where $\epsilon_{k_\alpha,\sigma}$ represents the conduction electron energy and $c^\dagger_{k_\alpha,\sigma}$ ($c_{k_\alpha,\sigma}$) are the creation (annihilation) operators for electrons in the lead α (=L, R). When an external voltage V is applied between the two leads, their chemical potential difference is $\mu_{\rm L} - \mu_{\rm R} = eV$. The two leads are assumed to be in local equilibrium and their distribution functions are given by the Fermi distribution functions $f_\alpha(\omega) = [1 + \exp{(\omega - \mu_\alpha)/k_B T}]^{-1}$ (α = L or R). $\epsilon_{d\sigma}$ are the discrete energy levels in the QD and only considering the lowest energy level in this model is proven reliable for the present experimental technique. Owing to spin degeneracy, we have $\epsilon_{d\uparrow} = \epsilon_{d\downarrow} = \epsilon_d$. The other parameters U and V_α stand for the Coulomb interaction and the coupling between the QD and the reservoirs, respectively. According to the KR slave-boson representation [29], four auxiliary Bose fields e, p_σ ($\sigma = \pm 1$), and d have been introduced, which act as projection operators respectively onto the empty, singly occupied (with spin up and down), and doubly occupied electronic states of the QD. In order to eliminate additional unphysical states, three constraints have to be imposed on these bosons:

$$\sum_\sigma p^\dagger_\sigma p_\sigma + e^\dagger e + d^\dagger d = 1 \tag{2}$$

$$c^\dagger_{d,\sigma} c_{d,\sigma} = p^\dagger_\sigma p_\sigma + d^\dagger d \qquad \sigma = \pm 1. \tag{3}$$

Equations (2) and (3) are the complete relation and the charge-conservation condition, respectively. In the physical subspace defined by these constraints, the fermion operators $c^\dagger_{d\sigma}$ and $c_{d\sigma}$ for the QD are replaced by

$$z^\dagger_\sigma c^\dagger_{d,\sigma} \qquad c_{d,\sigma} z_\sigma \tag{4}$$

so the matrix elements are the same in the combined fermion–boson Hilbert space as those in the original one, equation (1). Here

$$z_\sigma = (1 - d^\dagger d - p^\dagger_\sigma p_\sigma)^{-1/2} (e^\dagger p_\sigma + p^\dagger_{\bar\sigma} d)(1 - e^\dagger e - p^\dagger_{\bar\sigma} p_{\bar\sigma})^{-1/2}. \tag{5}$$

Therefore, the Hamiltonian (1) can be replaced by the following effective Hamiltonian in terms of auxiliary boson operators:

$$H_{\rm eff} = \sum_{\sigma,k_\alpha} \epsilon_{k_\alpha,\sigma} c^\dagger_{k_\alpha,\sigma} c_{k_\alpha,\sigma} + \sum_\sigma \epsilon_{d\sigma} c^\dagger_{d,\sigma} c_{d,\sigma} + U d^\dagger d + \sum_{\sigma,k_\alpha} (V_\alpha c^\dagger_{k_\alpha,\sigma} c_{d,\sigma} z_\sigma + {\rm H.c.}) + \lambda^{(1)} \left(\sum_\sigma p^\dagger_\sigma p_\sigma + e^\dagger e + d^\dagger d - 1 \right) + \sum_\sigma \lambda^{(2)}_\sigma (c^\dagger_{d,\sigma} c_{d,\sigma} - p^\dagger_\sigma p_\sigma - d^\dagger d). \quad (6)$$

The constraints are incorporated via the three Lagrange multipliers, $\lambda^{(1)}$ and $\lambda^{(2)}_\sigma$. Under the framework of the SBMFT, the four slave Bose fields can be assumed as c-numbers and replaced by their corresponding expectation values.

In order to determine these unknown parameters, we start from the constraints (2), (3) and deduce the equation of motion of the slave-boson operators from the Hamiltonian (6), yielding the following equations within the SBMFT [25, 28]:

$$\sum_\sigma |p_\sigma|^2 + |e|^2 + |d|^2 = 1 \quad (7)$$

$$|p_\sigma|^2 + |d|^2 - \langle c^\dagger_{d,\sigma} c_{d,\sigma} \rangle = 0 \qquad \sigma = \pm 1 \quad (8)$$

$$\sum_{k_\alpha,\sigma} V_\alpha \left(\frac{\partial z_\sigma}{\partial e} \langle c^\dagger_{k_\alpha,\sigma} c_{d,\sigma} \rangle + \frac{\partial z^\dagger_\sigma}{\partial e} \langle c^\dagger_{d,\sigma} c_{k_\alpha,\sigma} \rangle \right) + \lambda^{(1)} e = 0 \quad (9)$$

$$\sum_{k_\alpha} V_\alpha \left(\frac{\partial z_\sigma}{\partial p_\sigma} \langle c^\dagger_{k_\alpha,\sigma} c_{d,\sigma} \rangle + \frac{\partial z^\dagger_\sigma}{\partial p_\sigma} \langle c^\dagger_{d,\sigma} c_{k_\alpha,\sigma} \rangle \right) + (\lambda^{(1)} - \lambda^{(2)}_\sigma) p_\sigma = 0 \quad (10)$$

$$\sum_{k_\alpha,\sigma} V_\alpha \left(\frac{\partial z_\sigma}{\partial d} \langle c^\dagger_{k_\alpha,\sigma} c_{d,\sigma} \rangle + \frac{\partial z^\dagger_\sigma}{\partial d} \langle c^\dagger_{d,\sigma} c_{k_\alpha,\sigma} \rangle \right) + \left(U + \lambda^{(1)} - \sum_\sigma \lambda^{(2)}_\sigma \right) d = 0. \quad (11)$$

In these equations, calculations of statistical expectations can be expressed in terms of the Fourier transforms of the non-equilibrium correlation Green functions (GFs):

$$G^<_{d\sigma,k_\alpha\sigma}(t,t') \equiv {\rm i}\langle c^\dagger_{k_\alpha,\sigma}(t') c_{d,\sigma}(t) \rangle \qquad G^<_{k_\alpha\sigma,d\sigma}(t,t') \equiv {\rm i}\langle c^\dagger_{d,\sigma}(t') c_{k_\alpha,\sigma}(t) \rangle.$$

With the effective Hamiltonian (6), these correlation GFs can be readily related to the Fourier transforms of the retarded (advanced) GF:

$$G^{r\,(a)}_{d\sigma}(t,t') \equiv \pm {\rm i}\theta(\pm t \mp t') \langle \{ c_{d,\sigma}(t), c^\dagger_{d,\sigma}(t') \} \rangle$$

and the correlation GF:

$$G^<_{d\sigma}(t,t') \equiv {\rm i}\langle c^\dagger_{d,\sigma}(t') c_{d,\sigma}(t) \rangle$$

for the QD by applying the Langreth analytic continuation rules [32]. Finally, these equations (7)–(11) can be closed in terms of the QD's correlation GF $G^<_{d\sigma}$ in Fourier space:

$$\frac{1}{2\pi {\rm i}} \int {\rm d}\omega\, G^<_{d\sigma}(\omega) = |p_\sigma|^2 + |d|^2 \quad (12)$$

$$\frac{1}{2\pi {\rm i}} \sum_\sigma \frac{\partial \ln z_\sigma}{\partial e} \int {\rm d}\omega\, G^<_{d\sigma}(\omega)(\omega - \tilde\epsilon_{d\sigma}) + 2\lambda^{(1)} e = 0 \quad (13)$$

$$\frac{1}{2\pi {\rm i}} \sum_{\sigma'} \left(\frac{\partial \ln z_{\sigma'}}{\partial p^\dagger_\sigma} + \frac{\partial \ln z_{\sigma'}}{\partial p_\sigma} \right) \int {\rm d}\omega\, G^<_{d\sigma'}(\omega)(\omega - \tilde\epsilon_{d\sigma'}) + 2(\lambda^{(1)} - \lambda^{(2)}_\sigma) p_\sigma = 0 \quad (14)$$

$$\frac{1}{2\pi {\rm i}} \sum_\sigma \frac{\partial \ln z_\sigma}{\partial d} \int {\rm d}\omega\, G^<_{d\sigma}(\omega)(\omega - \tilde\epsilon_{d\sigma}) + 2\left(U + \lambda^{(1)} - \sum_\sigma \lambda^{(2)}_\sigma \right) d = 0. \quad (15)$$

It is clear that for the effective Hamiltonian (6) the retarded (advanced) and correlation GFs $G^{r,a,<}_{d\sigma}(\omega)$ can be written as

$$G^{r\,(a)}_{d\sigma}(\omega) = \frac{1}{\omega - \tilde{\epsilon}_{d\sigma} \pm \mathrm{i}\tilde{\Gamma}} \tag{16}$$

$$G^{<}_{d\sigma}(\omega) = \frac{\mathrm{i}\tilde{\Gamma}[f_{\mathrm{L}}(\omega) + f_{\mathrm{R}}(\omega)]}{(\omega - \tilde{\epsilon}_{d\sigma})^2 + \tilde{\Gamma}^2} \tag{17}$$

which are formally the same as those for non-interacting electrons, except with the effective energy level $\tilde{\epsilon}_{d\sigma} = \epsilon_{d\sigma} + \lambda^{(2)}_{\sigma}$ and the effective coupling constant $\tilde{\Gamma} = (\Gamma_{\mathrm{L}} + \Gamma_{\mathrm{R}})|z_\sigma|^2/2$ (where $\Gamma_\alpha = 2\pi \sum_{k_\alpha} |V_\alpha|^2 \delta(\omega - \epsilon_{k_\alpha,\sigma})$ is the strength of coupling between the QD level and the lead α). Therefore, these equations (7) and (12)–(15) together with the definition of the correlation GF, equation (17), form a closed self-consistent set of equations, which can define the seven parameters, and thus describe linear and non-linear transport through QD under finite external voltage bias.

According to the treatment of reference [33], we can write the current per spin I_σ between the QD and the lead α as

$$I = \sum_\sigma I_\sigma = \frac{2\mathrm{e}}{\hbar} \sum_\sigma \int \mathrm{d}\omega\, \Gamma' |z_\sigma|^2 \{f_{\mathrm{L}}(\omega) - f_{\mathrm{R}}(\omega)\}\, \rho_\sigma(\omega) \tag{18}$$

where $\Gamma' = \Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}/(\Gamma_{\mathrm{L}} + \Gamma_{\mathrm{R}})$. In the present paper, we focus our attention on the symmetric systems with $\Gamma_{\mathrm{L}} = \Gamma_{\mathrm{R}} = \Gamma$. In the wide-band limit of the reservoirs, the coupling strength Γ can be taken as a constant and it is chosen as the energy unit throughout the paper. $\rho_\sigma = -(1/\pi)\,\mathrm{Im}\, G^{r}_{d\sigma}(\omega)$ is the spectral DOS of the electron in the QD. Utilizing equation (18), the linear conductance G_σ for electrons with spin σ in the limit of zero bias voltage can be obtained:

$$G_\sigma = \left.\frac{\mathrm{d}I_\sigma}{\mathrm{d}V}\right|_{V=0} = \frac{e^2}{h} \frac{1}{(\tilde{\epsilon}_{d\sigma}/\tilde{\Gamma})^2 + 1} \tag{19}$$

at absolute zero temperature. The total conductance G is $G = \sum_\sigma G_\sigma$. Clearly, the conductance G_σ has the same form as the Breit–Wigner formula for non-interacting electron tunnelling. The Coulomb correlation is reflected only through the effective energy level and coupling constant within the present theoretical framework. Consequently, it is evident that transport through QD can be fully characterized by the seven factitiously introduced parameters e, p_σ, d, $\lambda^{(1)}$, and $\lambda^{(2)}_\sigma$ under the SBMFT.

It is worth noting that equation (12) gives the occupation number of electrons per spin in the QD: $n_\sigma = |p_\sigma|^2 + |d|^2$. In the linear case, we can easily deduce the following formula:

$$n_\sigma = \frac{1}{2} - \frac{1}{\pi} \arctan\left(\frac{\tilde{\epsilon}_{d\sigma}}{\tilde{\Gamma}}\right) \tag{20}$$

at zero temperature. Explicitly, the SBMFT perfectly satisfies the famous Friedel–Langreth sum rule [34]:

$$G_\sigma = \frac{e^2}{h} \sin^2(\pi n_\sigma). \tag{21}$$

Note that such agreement could not be yielded by the EOM method and the NCA. In the linear limit the transmission $t_{d\sigma} = -G^{r}_{d\sigma}$ and its phase shift $\phi_{d\sigma} = \pi n_\sigma$.

In the present paper, we limit our attention to the spin-degenerate case and assume that the energy levels in the QD are equal for electrons with spin up and down (the Kondo effect in the presence of magnetic fields has been investigated in our recent paper, in which the energy levels for spin up and down are separated by the Zeeman energy [28]). As a consequence, we have

$p_\uparrow = p_\downarrow = p$, $z_\uparrow = z_\downarrow$, and thus $\lambda_\uparrow^{(2)} = \lambda_\downarrow^{(2)} = \lambda^{(2)}$, $n_\uparrow = n_\downarrow = n_d$, and $G_\uparrow = G_\downarrow$. Moreover, it is easily found from equation (11) that $d = 0$ in the limit of infinite Coulomb interaction $U \to \infty$. This means that no doubly occupied state is permitted due to the infinite on-site Coulomb repulsion interaction. Then the set of self-consistent equations can be simplified to four equations.

3. Comparison with other slave-boson formulations

It is well known that there is a different version of the finite-U slave-boson formulation, which has been extensively utilized to investigate the single-impurity Anderson model by means of the diagrammatic NCA, even in the presence of magnetic fields [31]. Nevertheless, we argue in the following that, within the slave-boson mean-field framework, this formulation is just not appropriate for this problem.

Two auxiliary Bose fields have been induced in the usual slave-boson formulation: b the empty-state boson operator and $d_{\sigma\bar{\sigma}}$ the doubly occupied-state boson operator, which has the property $d_{\sigma\bar{\sigma}} = -d_{\bar{\sigma}\sigma}$. Only one constraint

$$\sum_\sigma c_{d,\sigma}^\dagger c_{d,\sigma} + b^\dagger b + d_{\sigma\bar{\sigma}}^\dagger d_{\sigma\bar{\sigma}} = 1 \tag{22}$$

is needed to guarantee that the transformed boson–fermion mixed Hamiltonian equation (23) is equivalent to the original one, equation (1). Following reference [31], the transformed Hamiltonian equation (1) can be written as

$$\begin{aligned} H_{\mathrm{eff}} = &\sum_{\sigma,k_\alpha} \epsilon_{k_\alpha,\sigma} c_{k_\alpha,\sigma}^\dagger c_{k_\alpha,\sigma} + \sum_\sigma \epsilon_{d\sigma} c_{d,\sigma}^\dagger c_{d,\sigma} + (U + \epsilon_{d\sigma} + \epsilon_{d\bar{\sigma}}) d_{\sigma\bar{\sigma}}^\dagger d_{\sigma\bar{\sigma}} \\ &+ \sum_{\sigma,k_\alpha} (V_\alpha c_{k_\alpha,\sigma}^\dagger b^\dagger c_{d,\sigma} + \mathrm{H.c.}) + \sum_{\sigma,k_\alpha} (V_\alpha c_{k_\alpha,\sigma}^\dagger c_{d,\bar{\sigma}}^\dagger d_{\sigma\bar{\sigma}} + \mathrm{H.c.}) \\ &+ \lambda\left(\sum_\sigma c_{d,\sigma}^\dagger c_{d,\sigma} + b^\dagger b + d_{\sigma\bar{\sigma}}^\dagger d_{\sigma\bar{\sigma}} - 1\right) \end{aligned} \tag{23}$$

in which λ is the Lagrange multiplier which induces the constraint (22). Within the SBMFT these slave-boson fields can be replaced with their corresponding expectation values. Note that $d_{\sigma\bar{\sigma}} = -d_{\bar{\sigma}\sigma} = d$. Just as was done in the above section, the corresponding self-consistent equations are given from the constraint (22) and the equation of motion of the slave-boson operators. Here, in order to obtain those statistical expectations utilized in the self-consistent equations, we have to solve the 2×2 matrix correlation GF $\mathbf{G}_{d\sigma}^<(t, t')$:

$$\mathbf{G}_{d\sigma}^<(t, t') = \mathrm{i}\begin{pmatrix} \langle c_{d,\sigma}^\dagger c_{d,\sigma}\rangle & \langle c_{d,\bar{\sigma}} c_{d,\sigma}\rangle \\ \langle c_{d,\sigma}^\dagger c_{d,\bar{\sigma}}^\dagger\rangle & \langle c_{d,\bar{\sigma}} c_{d,\bar{\sigma}}^\dagger\rangle \end{pmatrix}. \tag{24}$$

By employing the Dyson equation, we can easily obtain the Fourier transform of the correlation GF $\mathbf{G}_{d\sigma}^<(t, t')$, for the non-interacting Hamiltonian (23), as

$$\mathbf{G}_{d\sigma}^<(\omega) = \mathrm{i}\Gamma_u \begin{pmatrix} \dfrac{f(\omega - \mu_{\mathrm{L}}) + f(\omega - \mu_{\mathrm{R}})}{(\omega - \tilde{\epsilon}_{d\sigma})^2 + (\Gamma_u)^2} & 0 \\ 0 & \dfrac{f(\omega + \mu_{\mathrm{L}}) + f(\omega + \mu_{\mathrm{R}})}{(\omega + \tilde{\epsilon}_{d\sigma})^2 + (\Gamma_u)^2} \end{pmatrix} \tag{25}$$

with $\Gamma_u = \Gamma(|b|^2 + |d|^2)$ and $\tilde{\epsilon}_{d\sigma} = \epsilon_{d\sigma} + \lambda$.

Finally, following the same procedure as was used above, from the KR formulation, one can write the set of self-consistent equations in terms of the correlation GF $\mathbf{G}_{d\sigma}^<(\omega)$ as

$$\frac{1}{\pi \mathrm{i}} \int \mathrm{d}\omega\, [\mathbf{G}_{d\sigma}^<(\omega)]_{11} + |b|^2 + |d|^2 = 0 \tag{26}$$

$$\frac{1}{\pi \mathrm{i}} \int \mathrm{d}\omega\, [\mathbf{G}^{<}_{d\sigma}(\omega)]_{11}(\omega - \tilde{\epsilon}_{d\sigma}) + \frac{1}{\pi \mathrm{i}} \int \mathrm{d}\omega\, [\mathbf{G}^{<}_{d\sigma}(\omega)]_{22}(\omega + \tilde{\epsilon}_{d\sigma}) + \lambda(|b|^2 + |d|^2) = 0 \qquad (27)$$

$$\frac{1}{\pi \mathrm{i}} \int \mathrm{d}\omega\, [\mathbf{G}^{<}_{d\sigma}(\omega)]_{11}(\omega - \tilde{\epsilon}_{d\sigma}) + \frac{1}{\pi \mathrm{i}} \int \mathrm{d}\omega\, [\mathbf{G}^{<}_{d\sigma}(\omega)]_{22}(\omega + \tilde{\epsilon}_{d\sigma}) + 4(U + \epsilon_{d\sigma} + \epsilon_{d\bar{\sigma}} + \lambda)(|b|^2 + |d|^2) = 0. \qquad (28)$$

Therefore, one can solve the set of equations (26)–(28) to define the three unknown parameters b, d, and λ and then determine properties of transport through QD under finite external voltage. Unfortunately, this set of equations is not solvable mathematically because these equations contain the two parameters b and d only in the combined form $|b|^2 + |d|^2$. Thus, from these equations one cannot obtain a rational expectation value for the doubly occupied slave-boson operator d. In addition, in the special $U \to \infty$ limit, these equations cannot reduce to those originally derived from the infinite-U formulation (Coleman's formulation; see the following) [24, 25]. These are two severe objections to the application of this formulation at the mean-field level.

In contrast, the KR formulation is especially designed for the purpose of application of the slave-boson mean-field method, and can give qualitatively rational parameters e^2, p^2, and d^2 for the whole range of the energy level ϵ_d. In figure 1(b) we show the expectation values of the slave-boson operators e^2, p^2, and d^2 calculated from our formulation versus the discrete energy level of the QD with $U = 7$. When the energy level of the QD is far below the Fermi energy of the two leads (we assume $\mu_{\mathrm{L}} = \mu_{\mathrm{R}} = 0$ in the calculation), electrons can be filled into both of the two energy levels ϵ_d and $\epsilon_d + U$ of the QD, which naturally means that $d^2 = 1$ and $e^2 = p^2 = 0$. As the energy level ϵ_d increases, d^2 is evidently reduced, and the singly occupied-state number p^2 starts to increase and we obtain a maximum at the symmetric point $\epsilon_d = -U/2$. Subsequently, with further increase of the energy level, there are no electrons residing simultaneously in the two energy levels, and d^2 tends to zero. Also p^2 begins to reduce. Finally, when the energy level is far away from the Fermi energy of the two leads again, there are no electrons occupying the QD, i.e., $e^2 = 1$ and $p^2 = d^2 = 0$. It is clear that our numerical results for these expectation values of slave-boson operators meet the physical requirements very well.

On the other hand, we should point out that our results in the limit of $U \to \infty$ are also different from those derived from the infinite-U Coleman formulation [23]. The Coleman Hamiltonian can be obtained by setting $d_{\sigma\bar{\sigma}} = d = 0$ in the effective Hamiltonian (23). Clearly, the set of self-consistent equations can be readily derived and the correlation GF is equal to $[\mathbf{G}^{<}_{d\sigma}(\omega)]_{11}$ with $\Gamma|b|^2$ instead of Γ_u in equation (25). Likewise, from the KR formulation for the case of $U \to \infty$, the set of equations derived in the above section can determine the unknown parameters e^2, p^2, $\lambda^{(1)}$, and $\lambda^{(2)}$, and then provide a definition of the occupation number n_σ and conductance G of QD. For the sake of comparison, we calculate them numerically and plot them in figure 2 as functions of the discrete energy level of the QD. We can explicitly establish, from our formulation, that the conductance shows strong enhancement at $\epsilon_d \lesssim -0.5$ and reaches unity at about $\epsilon_d \approx -2$; these findings show good consistency with experimental results [3, 4, 8]. In contrast, from Coleman's formulation at the mean-field level, one finds that the Coulomb interaction does not enhance the conductance until $\epsilon_d \approx -2.5$. In view of these findings, we can state that the SBMFT in the KR formulation describes the Kondo-type transport through QD more precisely than the old version of the SBMFT. In our opinion, both approaches are actually variational methods. So, the present SBMFT formulation describing the Kondo-type transport through QD better than the previous version of the SBMFT can be understood on the basis of the fact that there are two slave-boson-operator-related parameters e^2 and p^2 ($d^2 = 0$ in the limit $U \to \infty$) in the present

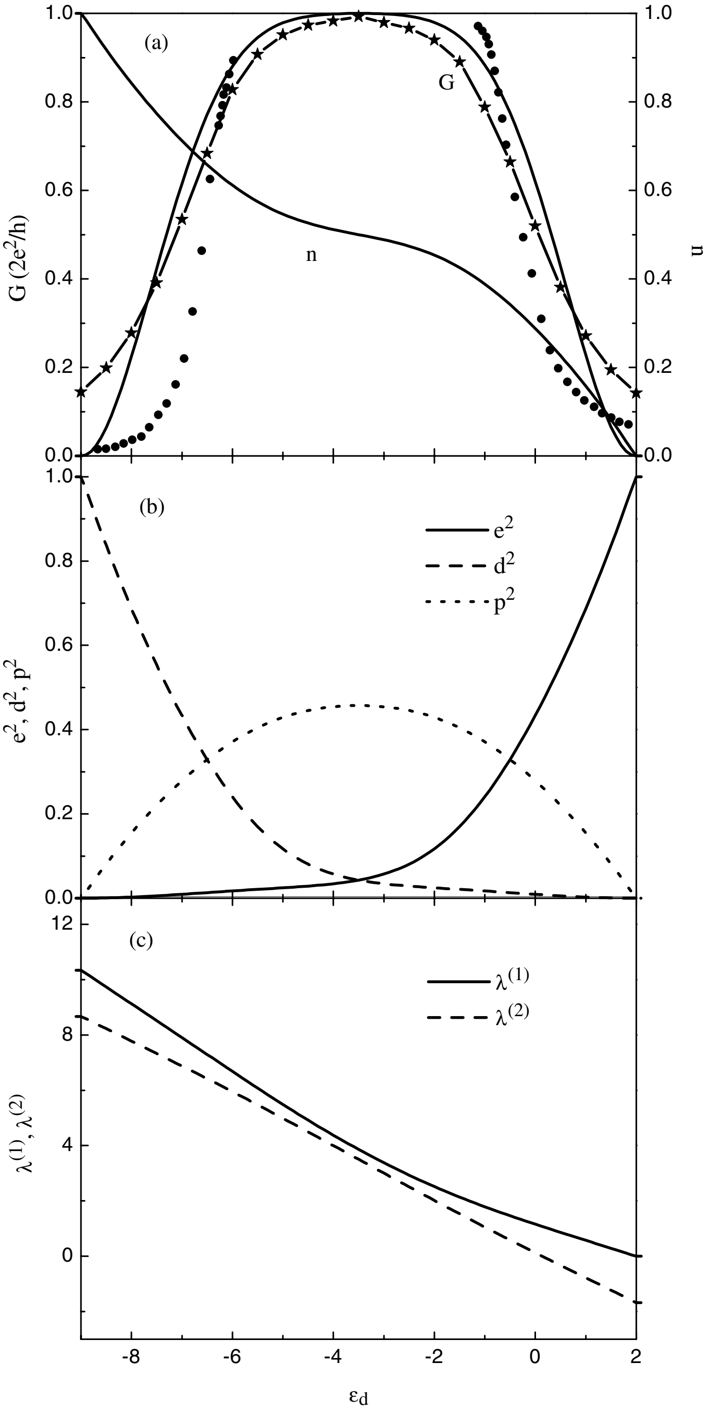

Figure 1. (a) The linear conductance at absolute zero temperature and the electron occupation number in the QD, (b) the slave-boson-operator occupied-state numbers e^2, p^2, and d^2, and (c) the Lagrange multipliers $\lambda^{(1)}$ and $\lambda^{(2)}$ versus the dot energy level for $U = 7$. Solid dots and stars in (a) denote the experimental [8] and NRG calculation results, respectively. Γ is chosen as the energy unit.

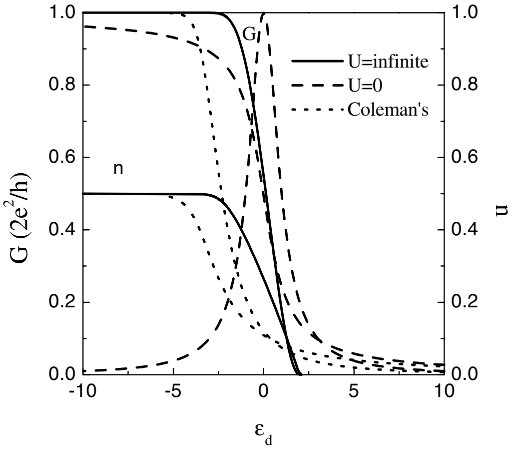

Figure 2. The linear conductance through the QD and the electron occupation number in the QD at zero temperature calculated by applying the present SBMFT with $U = \infty$ (solid lines) and $U = 0$ (dashed lines) as functions of the dot energy level. For comparison, the corresponding results obtained by means of the Coleman formulation are also plotted.

SBMFT, while there is only one parameter, b, in Coleman's formulation. In the following, we apply this new approach to investigate the effects of Coulomb correlation on the linear and non-linear transport through QD.

4. Calculations and discussion

In this section, we employ the newly developed SBMFT to numerically investigate the Kondo correlation effect on linear and non-linear transport through the QD for a special case: that with the finite on-site Coulomb interaction $U = 7$. The calculation is performed only at zero temperature in the present paper. For simplicity, we assume that the QD system is symmetric and choose the mixing constant Γ as the energy unit.

4.1. Linear transport

Using equation (19), we can calculate the linear conductance G of the QD at absolute zero temperature. Figure 1 depicts: the calculated conductance G and the electron occupation number n per spin (a); the expectation values of slave-boson operators e^2, p^2, and d^2 (b); and the Lagrange multipliers $\lambda^{(1)}$, $\lambda^{(2)}$ (c) as functions of the gate voltage, the discrete energy level of the QD with $U = 7$. For comparison, the experimental data (from figure 5(b) in reference [8]) and the results of the NRG calculation for zero temperature are also plotted, respectively, as solid circles and stars in figure 1(a). The numerical results give a good explanation for the measured and NRG conductances in the symmetric case $-1.2U \lesssim \epsilon_d \lesssim 0.2U$. However, there is a big discrepancy between them in the extremely asymmetric regimes, where the conductance computed from the present model shows a sudden drop to zero, which is at variance with the gradual decrease of the experimental and the NRG results. We think that this behaviour can be attributed to the limitation of zero temperature. Extension of the present approach from zero temperature to finite temperature will be our next project. In figure 2, we plot the conductance and occupation number per spin versus energy level for two special cases, $U = \infty$ and $U = 0$. The Coulomb correlation can significantly affect transport through the QD as demonstrated in this figure. It is easily observed from figure 2 that only when the chemical potentials of the two leads are in alignment with the energy level of the QD is the resonance condition satisfied and does the conductance reach unity at $\epsilon_d = 0$ (because of assumption of $\mu_L = \mu_R = 0$ in the calculation). Nevertheless, the Coulomb correlation can greatly enhance the conductance of the QD in the Kondo regime.

The Anderson model has three different regimes parametrized by the energy level ϵ_d: the Kondo regime with $\epsilon_d \lesssim -0.5$; the mixed-valence regime with $-0.5 \lesssim \epsilon_d \lesssim 0$; and the empty-orbital regime with $\epsilon_d \gtrsim 0$, each of which has different transport properties. In the empty-orbital regime, there are few electrons in the QD. The empty-state number e^2 is larger than p^2 and d^2 as observed from figure 1(b). As the energy level ϵ_d decreases, e^2 evidently reduces and the singly occupied-state number p^2 starts to increase and reaches a maximum at the symmetric point $\epsilon_d = -U/2$, which corresponds to an odd number of electrons residing in the QD with $n = 0.5$ and the most pronounced Kondo effect, $G = 2e^2/h$. Subsequently, with further decrease of the energy level, lots of electrons reside in the QD and e^2 tends to zero. Also p^2 begins to reduce. But the doubly occupied-state number d^2 has a remarkable value and finally an even number of electrons enter into the QD with $n = 1$, which weakens the Coulomb correlation effect. However, since the infinite Coulomb interaction can prevent there being a doubly occupied state in the QD, there is always a significant Kondo correlation effect throughout the whole Kondo regime as shown in figure 2. Moreover, we can clearly observe from figure 1(a) that the calculated conductance G agrees well with the experimental results for the non-Kondo regimes with $\epsilon_d \lesssim -0.5$. Meanwhile, figure 2 demonstrates that there are great differences between the conductances G derived from the present SBMFT and from the Coleman formulation in the non-Kondo regimes. In consequence, these results show that this especially designed SBMFT provides a good tool for investigating linear transport through QD over a very wide range of the energy level ϵ_d near symmetric point. We can qualitatively conclude, from numerical calculations for different strengths of the on-site Coulomb interaction U, that the validity limitation of the present approach is about $-1.2U \lesssim \epsilon_d \lesssim 0.2U$, even though only results for the particular system parameter $U = 7$ are presented in this paper. Note that the validity regime is rather wide, including both Kondo and non-Kondo regimes, in contrast to the usual finding that the slave-boson mean-field approximation completely fails in describing charge fluctuation.

Figure 3 clearly reveals the dependence on the Coulomb interaction U of the conductance G in these different regimes. It is evident from figure 3 that the Coulomb interaction substantially enhances the conductance through the QD in the Kondo regime $\epsilon_d = -2$ and a saturation value is reached after about $U = 8$. In contrast, the Coulomb correlation slightly suppresses the conductance in the other two regimes. Furthermore, the inset in figure 3 shows that the conductance declines more rapidly in the mixed-valence regime than in the empty regime. In the mixed-valence regime, and very close to the Kondo regime, the conductance G has a maximum value at about $U = 1$, then it decreases with the increase of the Coulomb interaction.

4.2. Nonlinear transport

In this subsection, we concentrate on the non-equilibrium transport through QD. For the sake of simplicity, the assumption that there is a symmetric voltage drop, $\mu_L = -\mu_R = eV/2$, through the whole system is made in our calculation. Then, considering symmetric coupling for two tunnel barriers, the differential conductance is symmetric under bias reversal. Since it is known that SBMFT has some problems in describing dynamical properties, non-linear results far from equilibrium have to be treated with more caution.

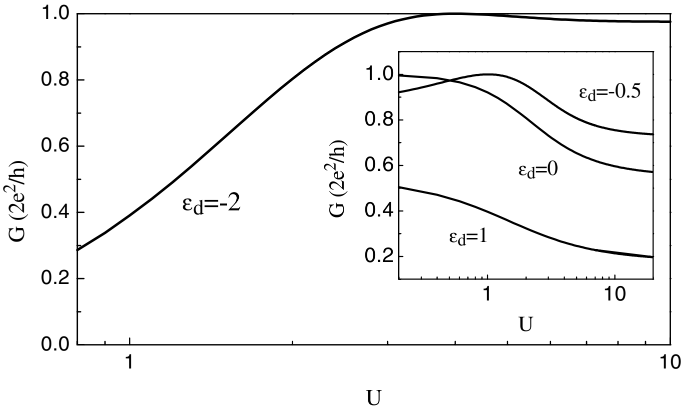

Figure 3. The Coulomb interaction dependence of the linear conductance at zero temperature through the QD. Inset: linear conductances for $\epsilon_d = -0.5$, $\epsilon_d = 0$ (the mixed-valence regime), and $\epsilon_d = 1$ (the empty-orbital regime).

Figure 4 illustrates the bias-voltage-dependent differential conductance $\mathrm{d}I/\mathrm{d}V$ for the QD with $U = 7$ in the Kondo regimes with $\epsilon_d = -2, -1$, and -0.5. For these specially chosen parameters, the Kondo temperatures T_K are about 0.14, 0.44, and 1.12, respectively (the exact Bethe *ansatz* gives the following dynamic energy scale: $T_K = U\sqrt{\beta}\exp(-\pi/\beta)/2\pi$, $\beta = -2U\Gamma/\epsilon_d(U + \epsilon_d)$). The inset in figure 4 depicts the calculated differential conductance versus external bias voltage in the non-Kondo regimes with $\epsilon_d = 1$, 1.5, and 1.8. The differential conductance has a sharp peak at zero bias voltage $V = 0$ in the Kondo regime. For these energy levels close to the Kondo regime, the differential conductance demonstrates a broadened zero-bias peak (note the big difference of the scales, i.e., the Kondo temperatures,

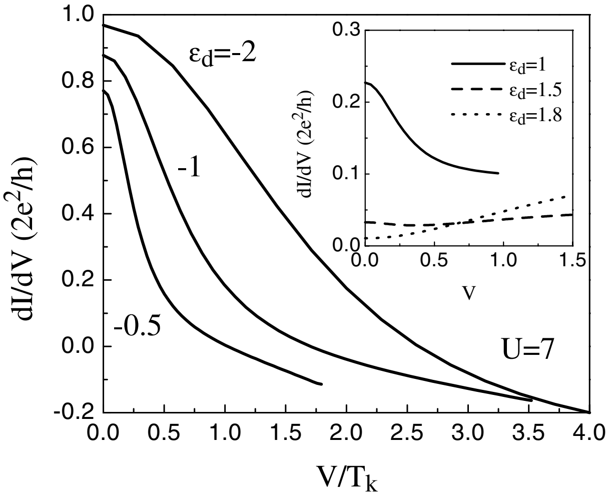

Figure 4. The zero-temperature differential conductance $\mathrm{d}I/\mathrm{d}V$ of the QD with $U = 7$ as a function of the external voltage at several different discrete energy levels, $\epsilon_d = -2, -1$, and -0.5. The inset shows these results at $\epsilon_d = 1$, 1.5, and 1.8. A pronounced zero-bias maximum is observed in the Kondo regime with $\epsilon_d = -2$, while a flat minimum appears in the empty-orbital regimes with $\epsilon_d = 1.5$ and 1.8.

in figure 4). This zero-bias maximum in the differential conductance has been derived from previous theoretical calculations and observed in experiments [3,4]. In contrast, the differential conductance predicts a weak zero-bias minimum in the non-Kondo regime with $\epsilon_d = 1.5$ and a slightly more obvious non-zero-bias maximum for $\epsilon_d = 1.8$. This prediction is in qualitative agreement with the modified SOPT investigation [16]. Note that the slave-boson mean-field approximation used in the present method is believed to be reliable for describing spin fluctuations (Kondo regime) but completely fails in describing charge fluctuations because quantum and thermal fluctuations are not included at the mean-field level. In fact, the high-frequency features in the DOS, i.e., charge-fluctuation peaks, play especially important roles in defining non-linear transport. Consequently, the validity of the application of the SBMFT in studying non-linear transport is not clear. Of course the KR slave-boson formulation provides a scheme for including fluctuations upon the mean-field solution [35], but this is beyond the scope of the present paper and will be included in a future project. In the present investigation, we perform our calculation of the differential conductance with bias voltages up to several multiples of the Kondo temperature T_K for the Kondo system, in which regime spin fluctuations make a primary contribution to transport. Therefore, we can comment that the results in figure 4 for the Kondo system properly describe the I–V characteristic of the QD. Meanwhile, for the non-Kondo systems, we limit our non-equilibrium calculation to low voltages $V < \mathrm{Min}(|\epsilon_d|, |U + \epsilon_d|)$, in which range the SBMFT is believed to approximately recover the main features of the DOS. Thus some qualitative features of the non-linear transport through QD in non-Kondo systems can be deduced from the present investigation, which can serve to furnish a deeper understanding of the properties of transport through QD. For example, both the present SBMFT and the modified SOPT calculations [16] for $\epsilon_d = 1.5$ and 1.8 show a non-zero-bias maximum in the differential conductance, although there is an obvious difference as regards magnitude. In fact, there have been many experiment-based arguments regarding the zero-bias minimum in the differential conductance in non-Kondo regimes [2–4]. Our results suggest that only when the energy levels are far enough away from the Kondo regime does the zero-bias minimum appear, and that further away from the Kondo regime there emerges a more obvious peak, but a weak zero-bias maximum still remains for $\epsilon_d = 1$. This seems to provide a basis for discussion of the zero-bias minimum in the differential conductance.

5. Conclusions

In this paper, we have studied the properties of linear and non-linear transport through QD by means of an alternative SBMFT on the basis of the saddle-point approximation of the slave-boson functional integral method, which is correct for arbitrary Coulomb correlation and naturally fulfils the Friedel–Langreth sum rule. The great advantage of the present method is that the correlation Hamiltonian for QD can be transformed to one without Coulomb correlation by introducing several auxiliary Bose field operators and the well-developed tunnelling formula for the non-interacting mesoscopic systems can be applied to investigate the transport through QD, which can avoid the difficulty as regards how to treat both the Coulomb interaction and the tunnelling between the QD and the two leads simultaneously. On the other hand, the NCA limits one to the case of the infinite Coulomb interaction. The EOM method underestimates the Kondo correlation effect at low temperature due to the decoupling approximation. The modified SOPT uses an equilibrium DOS to explore the non-equilibrium transport through QD.

We also provide a comparison between the KR formulation used in the present paper and the usual slave-boson formulation at the same slave-boson mean-field level. The theoretical derivation in section 3 reveals that the usual finite-U slave-boson formulation does not allow one to apply the slave-boson mean-field approximation. Moreover, a further comparison between the results obtained from our SBMFT and those derived from Coleman's formulation is performed, which suggests that the present SBMFT is a more precise theoretical tool for studying Kondo-type transport through QD.

In our numerical investigation, the zero-temperature linear conductance G versus the energy level is in good agreement with the experiment data. In the different regimes, the conductance G has different dependences on the Coulomb interaction. Our evaluation also displays a pronounced zero-bias enhancement of the differential conductance in the Kondo regime in comparison with the results obtained without the Coulomb correlation. In addition, a flat zero-bias minimum is predicted in our calculation for a non-Kondo system far enough away from the Kondo regime, which qualitatively agrees with previous studies and provides a basis for discussion of experiments.

Furthermore, the other great advantage of the new SBMFT is that it is very easy to extend to more complicated systems with strong Coulomb correlation effects. For example, it is straightforward to apply this tool to study Kondo-type transport through QD in the presence of an external magnetic field [28] or for multi-levels—and even the Kondo correlation coherent transport in hybrid mesoscopic systems (N–QD–S and S–QD–S) and the QD-modified AB ring systems. Studies of these systems are in progress.

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