Effect of the Kondo correlation on thermopower in a Quantum Dot

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In this paper we study the thermopower of a quantum dot connected to two leads in the presence of Kondo correlation by employing a modified second-order perturbation scheme at nonequilibrium. A simple scheme, Ng’s ansatz [Phys. Rev. Lett. 76, 487 (1996)], is adopted to calculate nonequilibrium distribution Green’s function and its validity is further checked with regard to the Onsager relation. Numerical results demonstrate that the sign of the thermopower can be changed by tuning the energy level of the quantum dot, leading to a oscillatory behavior with a suppressed magnitude due to the Kondo effect. We also calculate the thermal conductance of the system, and find that the Wiedemann-Franz law is obeyed at low temperature but violated with increasing temperature, corresponding to emerging and quenching of the Kondo effect.

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I. INTRODUCTION

Observation of the Kondo effect in a semiconductor quantum dot (QD)\textsuperscript{1,2} which provided a testing ground of the quantum behavior of electron wave functions and many-body effects, has stimulated a great deal of experimental\textsuperscript{3-4} and theoretical\textsuperscript{5-7} investigation. So far, many interesting features in QD, such as Kondo-assisted enhancement of conductance, its specific temperature dependence, a peak splitting in a magnetic field, zero-bias maximum of differential conductance, its specific temperature dependence, a peak splitting in a magnetic field, zero-bias maximum of

energy level of the quantum dot, leading to a oscillatory behavior with a suppressed magnitude due to the Kondo effect. We also calculate the thermal conductance of the system, and find that the Wiedemann-Franz law is obeyed at low temperature but violated with increasing temperature, corresponding to emerging and quenching of the Kondo effect.

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In this paper we will provide another validity check of Ng’s ansatz by analyzing the particle current and thermal flux through QD connecting to two reservoirs on the basis of Anderson single-impurity model by means of nonequilibrium GF with the help of Langreth continuation rules and Ng’s ansatz. We find that the resulting particle current and heat flux driven by bias voltages and temperature gradients between two leads satisfy the Onsager relation in nearly equilibrium regime,\(^2^0\) thus provide a natural check on the validity of derivation of the lesser GF.

To date, most theoretical calculation and experimental measurement on the thermopower of QD have focused in the Coulomb blockade (CB) regime,\(^2^1\) which have revealed that when the gate voltage defining QD is swept, the thermopower oscillates about zero (sawtooth behavior) with a period equal to that of the CB oscillations in electric conductance. However, thermopower across QD in the Kondo regime is still much less studied.\(^2^2,^2^3\) The second purpose of this paper is to investigate the Kondo effect on the linear thermopower of QD basing on Ng’s ansatz.

We organize the rest parts of the paper as following. In the second section we derive particle current and thermal flux formulas through interacting QD within the framework of nonequilibrium GF. The electric and thermoelectric transport coefficients are derived in the presence of both chemical potential and temperature gradients between two leads and automatically satisfy Onsager relation in the linear transport regime. We note that within this approximation, the same current formula as that in Ref. 25 is derived without the presumption of proportional coupling \(\Gamma_L(\omega) = \lambda \Gamma_R(\omega)\). In section 3, numerical calculation of linear Kondo-type thermopower \(S\) in QD are reported as a function of gate voltage and temperature, which shows a gate-voltage-controlled change of sign and largely suppressed oscillatory magnitude due to the Kondo effect. We also discuss the thermal conduction coefficient \(\kappa\) and its violations of the well-known Wiedemann-Franz law. Finally, a conclusion is given in Section 4.

II. THERMAL CURRENT FORMULA AND ONSAGER RELATION

Transport through a QD coupled to two reservoirs in the presence of external voltages and temperature gradient between two reservoirs can be described by the Anderson single impurity model:

\[
H = \sum_{\eta,k,\sigma} \epsilon_{\eta k \sigma} c_{\eta k \sigma}^\dagger c_{\eta k \sigma} + \epsilon_d \sum_\sigma c_{d \sigma}^\dagger c_{d \sigma} + \sum_{\eta,k,\sigma} (V_{\eta} c_{\eta k \sigma}^\dagger c_{d \sigma} + \text{H.c.}),
\]

where \(\epsilon_{\eta k \sigma}\) represents the conduction electron energy of the lead \(\eta\), and \(\epsilon_d\) is the discrete energy level in the QD. \(c_{\eta k \sigma}^\dagger\) (\(c_{\eta k \sigma}\)) are the creation (annihilation) operators for electrons in the lead \(\eta\) (=L, R), while \(c_{d \sigma}^\dagger\) (\(c_{d \sigma}\)) for electrons in the QD. When a total external voltage \(V\) is applied between the two leads, their chemical potential difference is \(\mu_L - \mu_R = eV\). The two leads are assumed to be in local equilibrium with respective temperature \(T_\eta\) and their distribution functions are given by \(f_\eta(\omega) = [1 + \exp (\omega - \mu_\eta)/k_B T_\eta]^{-1}\) \((\eta = L, R)\). This assumption is practically correct because the two reservoirs respond to an external perturbation much faster than the center region, i.e., the QD. The other parameters \(U\) and \(V_\eta\), stand for the Coulomb interaction, and the coupling between the QD and the reservoir \(\eta\), respectively. For the transport problem concerned in this paper, electrons in the QD are in a nonequilibrium state, to be determined by their coupling to two leads and by the applied voltage. In order to describe the nonequilibrium state of electrons, we define the retarded (advanced) and lesser (greater) GFs for the QD as follows: \(G_{\eta d}^{(r)}(t, t') \equiv \pm \Theta(t \mp t') \langle c_{d \sigma}(t') c_{d \sigma}^\dagger(t) \rangle\), \(G_{\eta d}^{(a)}(t, t') \equiv i \langle c_{d \sigma}(t') c_{d \sigma}(t) \rangle\) and \(G_{\eta d}^{(c)}(t, t') \equiv i \langle c_{d \sigma}(t) c_{d \sigma}^\dagger(t') \rangle\).

The particle current \(J_\eta\) and energy flux \(J_{E\eta}\) flowing from the lead \(\eta\) to the QD can be evaluated, respectively, from the rate of change of the electron number operator \(N_\eta(t) = \sum_{k,\sigma} c_{\eta k \sigma}^\dagger c_{\eta k \sigma}(t)\) and the rate of change of energy operator \(H_\eta(t) = \sum_{k,\sigma} \epsilon_{\eta k \sigma} c_{\eta k \sigma}^\dagger c_{\eta k \sigma}(t)\) of the lead \(\eta\):\(^2^4\)

\[
J_\eta(t) = -\frac{1}{\hbar} \frac{dN_\eta}{dt} = -i\frac{1}{\hbar} \left\langle \left[H, \sum_{k,\sigma} c_{\eta k \sigma}^\dagger c_{\eta k \sigma}(t)\right] \right\rangle = i\frac{1}{\hbar} \left\langle \sum_{k,\sigma} [V_\eta c_{\eta k \sigma}^\dagger c_{d \sigma}(t) - V_{\eta}^* c_{d \sigma}^\dagger(t)c_{\eta k \sigma}(t)] \right\rangle,
\]

\[
J_{E\eta}(t) = -\frac{1}{\hbar} \frac{dH_\eta}{dt} = -i\frac{1}{\hbar} \left\langle \left[H, \sum_{k,\sigma} \epsilon_{\eta k \sigma} c_{\eta k \sigma}^\dagger(t)c_{\eta k \sigma}(t)\right] \right\rangle = i\frac{1}{\hbar} \left\langle \sum_{k,\sigma} \epsilon_{\eta k \sigma} [V_\eta c_{\eta k \sigma}^\dagger(t) c_{d \sigma}(t) - V_{\eta}^* c_{d \sigma}^\dagger(t)c_{\eta k \sigma}(t)] \right\rangle,
\]

which involve the time-diagonal parts of the correlation functions: \(G_{\eta d,\eta}^{(r)}(t, t') \equiv i \langle c_{\eta k \sigma}^\dagger(t') c_{d \sigma}(t) \rangle\) and \(G_{\eta d,\eta}^{(c)}(t, t') \equiv i \langle c_{d \sigma}(t') c_{\eta k \sigma}(t) \rangle\). According to Ref. 24, the thermal flux \(J_{Q\eta}\) flowing from the lead \(\eta\) to the QD is determined as

\[
J_{Q\eta} = J_{E\eta} - \mu_\eta J_\eta.
\]

With the help of the Langreth analytic continuation rules,\(^2^6\) we obtain the following expressions:
\[ J_\eta = i \int \frac{d\omega}{2\pi\hbar} \Gamma_\eta(\omega) \sum_\sigma \left\{ G_{da}^<(\omega) + f_\eta(\omega) [G_{da}^r(\omega) - G_{da}^a(\omega)] \right\}, \tag{5} \]

\[ J_{Q\eta} = i \int \frac{d\omega}{2\pi\hbar} \Gamma_\eta(\omega) \sum_\sigma (\omega - \mu_\eta) \left\{ G_{da}^<(\omega) + f_\eta(\omega) [G_{da}^r(\omega) - G_{da}^a(\omega)] \right\}, \tag{6} \]

in terms of the QD’s GFs in the Fourier space. Here \( \Gamma_\eta(\omega) = 2\pi \sum_{k,\sigma} |V_\eta|^2 \delta(\omega - \epsilon_{k\sigma}) \) denotes the strength of coupling between the QD level and the lead \( \eta \).

In the presence of both a strong Coulomb interaction in QD and tunnelings between QD and leads, it is difficult to evaluate the retarded GF \( G_{da}^r \) of QD accurately. Several approximation schemes have been proposed in literature to derive \( G_{da}^r \), such as EOM with the decoupling approximation, SOPT, etc., where a retarded (advanced) self-energy for the interacting QD is written as \( \Sigma^{(r)}(\omega) = \Sigma_0^{(r)}(\omega) + \Sigma_i^{(r)}(\omega) \), with \( \Sigma_0^{(r)} = \mp i \sum_\eta \Gamma_\eta(\omega)/2 \) being the noninteracting part coming from the tunneling of electrons from the impurity state to outside leads, and \( \Sigma_i^{(r)} \) being the interacting part derived within these approximation approaches. The retarded (advanced) GF \( G_{da}^{r,a} \) thus has the form

\[ G_{da}^{r,a}(\omega) = \frac{1}{\omega - \epsilon_d - \Sigma^{(r,a)}(\omega)}. \tag{7} \]

Unfortunately, one can not straightforwardly get the lesser GF for the strongly correlated systems under out-of-equilibrium circumstance, as does for the retarded GF. Several years ago, Ng proposed a simple scheme to obtain the lesser GF \( G_{da}^< \) from the retarded and advanced terms in order to study ac Kondo resonances in nonlinear transport based on EOM approach. He assumed that \( \Sigma^<(\omega) = \Sigma_0^<(\omega) + \Sigma_i^<(\omega) \) with \( \Sigma_0^<(\omega) = -i \sum_\eta \Gamma_\eta(\omega)[1 - f_\eta(\omega)] \) are noninteracting lesser and greater self-energies. These lesser and greater self-energies are requested to satisfy the Keldysh relation \( \Sigma^< - \Sigma^> = \Sigma^r - \Sigma^a \), leading to

\[ A = \frac{\Sigma^r - \Sigma^a}{\Sigma_0^r - \Sigma_0^a}, \tag{8} \]

or in explicit form,

\[ \Sigma^<(\omega) = -2i \frac{\sum_\eta \Gamma_\eta(\omega) f_\eta(\omega)}{\sum_\eta \Gamma_\eta(\omega)} \text{Im}\Sigma^r. \tag{9} \]

The lesser GF \( G_{da}^< = \Sigma^<|G_{da}^r|^2 \) is thus obtained. This is the central result of Ng’s scheme. It has three advantages, initially addressed by Ng, that (i) it is exact in the equilibrium limit \( \mu_L = \mu_R \), (ii) it is exact in the noninteracting \( (U = 0) \) limit under general nonequilibrium situations, and (iii) the continuity equation \( J_L(t) = -J_R(t) \) is automatically satisfied in the steady state limit.\(^9\) With the help of this ansatz, as long as one obtains the retarded GF properly describing the strongly correlated system from certain approximative method, the lesser GF can be derived, and thus the transport problem can be investigated. By means of Eq. (9), we easily obtain

\[ J_\eta = -\frac{2}{\hbar} \int d\omega \Gamma(\omega) \frac{[f_\eta(\omega) - f_\eta(\omega)] \text{Im}G_{da}^r(\omega)}{\text{Im}\Sigma^r}, \tag{10} \]

\[ J_{Q\eta} = -\frac{2}{\hbar} \int d\omega \Gamma(\omega)(\omega - \mu_\eta) \frac{[f_\eta(\omega) - f_\eta(\omega)] \text{Im}G_{da}^r(\omega)}{\text{Im}\Sigma^r}, \tag{11} \]

where \( \Gamma(\omega) = \Gamma_L(\omega)\Gamma_R(\omega)/[\Gamma_L(\omega) + \Gamma_R(\omega)] \) and \( \bar{\eta} \neq \eta \). Note that here we arrive at exactly the same current formula (10) as that in Ref. 25 without introducing the assumption of a proportional coupling \( \Gamma_L(\omega) = \lambda \Gamma_R(\omega) \) \( (\lambda = 1 \) constant). Since the pioneer work of Ng,\(^9\) several attempts have been made to generalize this ansatz to study Kondo-type transport in more complicated devices containing interacting QD, such as normal metal-QD-superconductor\(^{18}\) and superconductor-QD-superconductor\(^{19}\). Nevertheless, the validity of this ansatz is worth being further examined. As mentioned in the introduction, verification of the Onsager relation is a natural choice for this purpose.

The Onsager relation is concerned with the linear response of the particle current \( J_\eta \) [Eq. (10)] and the heat flux \( J_{Q\eta} \) [Eq. (11)] driven by small bias voltages \( \mu_\eta - \mu_{\bar{\eta}} = \delta \mu \) and small temperature gradients \( T_\eta - T_{\bar{\eta}} = \delta T \):

\[ J_\eta = -L_{11} \frac{\delta \mu}{T} - L_{12} \frac{\delta T}{T^2} = -\frac{2}{\hbar} \int d\omega \bar{T}(\omega) \left[ \left( \frac{\partial f_\eta(\omega)}{\partial \mu} \right)_{\bar{T}} \delta \mu + \left( \frac{\partial f_\eta(\omega)}{\partial T} \right)_{\bar{T}} \delta T \right], \tag{12} \]

\[ J_{Q\eta} = -L_{21} \frac{\delta \mu}{T} - L_{22} \frac{\delta T}{T^2} = -\frac{2}{\hbar} \int d\omega \bar{T}(\omega)(\omega - \mu_\eta) \left[ \left( \frac{\partial f_\eta(\omega)}{\partial \mu} \right)_{\bar{T}} \delta \mu + \left( \frac{\partial f_\eta(\omega)}{\partial T} \right)_{\bar{T}} \delta T \right], \tag{13} \]
with $T(\omega) = \Gamma(\omega) \text{Im} G_{\alpha\alpha}^{\text{r}}(\omega)_{\delta\mu=0,\delta T=0}$ and

$$
\mathcal{L}_{11} = \frac{2T}{\hbar} \int d\omega T(\omega) \left( \frac{\partial f_{\alpha}(\omega)}{\partial \mu} \right)_T, \quad \mathcal{L}_{12} = \frac{2T^2}{\hbar} \int d\omega T(\omega) \left( \frac{\partial f_{\alpha}(\omega)}{\partial T} \right)_\mu,
$$

$$
\mathcal{L}_{21} = \frac{2T}{\hbar} \int d\omega T(\omega)(\omega - \mu_\eta) \left( \frac{\partial f_{\alpha}(\omega)}{\partial \mu} \right)_T, \quad \mathcal{L}_{22} = \frac{2T^2}{\hbar} \int d\omega T(\omega)(\omega - \mu_\eta) \left( \frac{\partial f_{\alpha}(\omega)}{\partial T} \right)_\mu.
$$

We can easily see that Ng’s ansatz Eq. (9) preserves Onsager relation $\mathcal{L}_{12} = \mathcal{L}_{21}$ automatically. Furthermore, the result is independent of the approximation adopted in deriving the retarded GF.

### III. THERMOELECTRIC EFFECTS IN THE PRESENCE OF KONDO CORRELATION

As shown in Eq. (12), both the bias voltage and the temperature gradient between two reservoirs can give rise to particle current. The current induced purely by a small bias voltage reflects the electric conductance $G = -\frac{e^2}{h} \mathcal{L}_{11}$, while the thermopower $S$ measures the voltage difference needed to eliminate the current due to the temperature gradient between the leads, given in linear regime by

$$
S = -\frac{1}{eT} \frac{\mathcal{L}_{12}}{\mathcal{L}_{11}}.
$$

In this situation, we can simplify the thermal flux Eq. (13) as $J_{Q_\eta} = -\kappa \delta T$, in which

$$
\kappa = \frac{1}{T^2} \left( \mathcal{L}_{22} - \frac{\mathcal{L}_{21}^2}{\mathcal{L}_{11}} \right)
$$

is the thermal conductance.

Comparing the explicit expressions of $\mathcal{L}_{11}$ and $\mathcal{L}_{12}$ [Eq. (14)], we can roughly address that in low temperatures, the electric conductance $G$ is determined by the transmission probability, or the density-of-state (DOS) of QD, at the Fermi energy of the leads, while the linear thermopower $S$ depends sensitively on the energy dependence of DOS, implying that it contains information different from the electric conductance. So far, the thermopower of QD in the kondo regime is still much less studied in literature. In this section, we attempt to numerically calculate the linear Kondo-type thermoelectric effects in QD. The remaining task is to choose a suitable approximative scheme, which can provide the retarded self-energy (or DOS $\rho(\omega)$) capable of properly describing the Kondo physics in a wide range of parameters of interacting QD. In the present paper, a modified SOPT developed in Ref. 8 is adopted, in which

$$
\Sigma^r(\omega) = Un + \frac{a \Sigma^{(2)}(\omega)}{1 - b \Sigma^{(2)}(\omega)},
$$

with $a = n(1 - n)/n_0(1 - n_0)$ and $b = (1 - 2n)/n_0(1 - n_0)U$. $n$ is the occupation number of the QD level which should be determined self-consistently. $\Sigma^{(2)}$ and $n_0$ are, respectively, the second order self-energy in $U$ and a fictitious particle number, both of which are obtained from the bare GF $G_0^r = 1/(\omega - \epsilon_d - Un - \Sigma_0^r)$.

In actual calculation, an assumption that the tunneling strength is independent of incident energy is taken in the wide-band limit and a symmetric system $\Gamma_d(\omega) = \Gamma_R(\omega) = \Gamma$ is focused. In the following we take the coupling strength $\Gamma$ as the energy unit and the Fermi level of the lead to be zero.

In Figs. 1(a)-(d) we plot the equilibrium DOS $\rho(\omega)$ for the QD with $U = 7$ and several different energy levels $\epsilon_d = -2, -3.5, -5$ and 2 at different temperatures. We can observe that the Kondo resonance peak in DOS is clearly resolved for the Kondo systems $\epsilon_d = -2, -3.5$ and $-5$ at low temperature $T = 0.01$, but nearly disperses at high temperature $T = 1$. Of course there is no Kondo peak in DOS for the non-Kondo system $\epsilon_d = 2$. In Fig. 2, the calculated electric conductance $G(a)$, thermopower $S(b)$ and thermal conductance $\kappa(c)$ are displayed as functions of the gate voltage, i.e., the energy level in QD. As expected, the conductance demonstrates a single peak structure and nearly unitary limit near symmetric point $\epsilon_d = -U/2$ at very low temperature, splitting peaks with increasing temperature and a minimum at $\epsilon_d = -U/2$ for very high temperature. It manifests the equilibrium DOS of QD at the Fermi energy of the lead, $\rho(0)$, at low temperature, but not its concrete shape of the Kondo peak: symmetric or nonsymmetric (right or left of center) around the Fermi energy of the lead. In order to detect DOS in the whole range of energy, one has made an attempt to measure the differential conductance of QD. However, the finite bias voltages between two leads result in a large change of DOS, giving rise to a splitting of the Kondo peak. As mentioned above, an alternative way of addressing this problem is to explore the thermopower, because it is relevant with the product
of the incident electron energy $\omega$ and the DOS of QD $\rho(\omega)$. For example, the perfectly symmetric shape of DOS around $\omega = 0$ at the symmetric case $\epsilon_d = -3.5$, as shown in Fig. 1(b), results in exactly zero of the thermopower; while the positive (negative) thermopower is attributed to slightly slanting of DOS towards the left (right) for $\epsilon_d = -2 (-5)$ [Figs. 1(a) and (c)], implying an oscillatory behavior around zero which can be controlled by the gate voltage. We also observe from Fig. 2(b) that the magnitude of oscillating in thermopower is largely decreased with lowering temperature due to the Kondo-suppressed deviation of DOS from the symmetric shape. Fig. 2(c) reveals that the thermal conductance $\kappa$ has similar behavior as the electric conductance $G$ at low temperature, but quite different at high temperature $T = 1$.

Fig. 3 displays the temperature dependence of these three quantities. We observe from Fig. 3(b) that the thermopower shows a logarithmic rise-up with increasing temperature, leading to a broad maximum, and subsequently decreases in the high temperature regime. But temperature increasing can not cause a change of the sign of the thermopower, except for very high temperature where the Kondo effect is quenched. Fig. 3(c) shows that the thermal conductance has similar temperature dependence for these different systems. As a result, the thermal conductance is not a suitable tool to explore the Kondo effect. The interesting physical quantity is the ratio between the thermal and electric conductance. The classical theory yields that thermal and electric transport in bulk metals satisfy the Wiedemann-Franz law $\kappa/TG = \pi^2/3e^2$. In mesoscopic system transport occurs through a small confined region, and consequently does not satisfy the Wiedemann-Franz law in general. We depict this ratio in Fig. 4. Surprising recovery of the Wiedemann-Franz law is observed at very low temperature, where transport through QD is dominated by Kondo correlation, implying that the Landau Fermi liquid state is rebuilt in this situation. But substantial deviation from the classical value emerges with increasing temperature due to disappearance of the Kondo effect. This temperature behavior provides a good trademark for exploring the onset of Kondo correlation.

IV. CONCLUSION

We have studied the particle current and thermal flux through interacting QD on the basis of the nonequilibrium Green’s function approach and Ng’s ansatz. The advantage of the ansatz is its capability of evaluating the lesser (greater) GF from the retarded and advanced GFs derived in certain rational approximation scheme. The validity about the ansatz and the resulting linear transport coefficients have been examined in term of Onsager relation. We have also emphasized that the same electric current formula as in Ref. 25 can be obtained without the assumption of proportional coupling $\Gamma_L(\omega) = \lambda \Gamma_R(\omega)$.

In the wide band limit, a modified SOPT has been employed to calculate the retarded GF for interacting QD and with this retarded GF the thermoelectric effect in the Kondo regime has been investigated. We have found that the thermopower exhibits a oscillatory behavior around zero due to nonsymmetric shape of the Kondo peak in the DOS, giving rise to a change of sign of the thermopower which is controllable by tuning the gate voltage. These results demonstrate that measuring thermopower can provide useful information of the DOS in QD. Furthermore, our calculation reveals that the magnitude of oscillation is largely suppressed by the Kondo effect. Finally, we have explored the temperature characteristic of the thermoelectric effect and predicted that at low temperature regime thermal transport satisfies the classical Wiedemann-Franz law, which can be taken as a trace of the Kondo correlation.

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Fig. 1 The DOS of the interacting QD $U = 7$ calculated from the modified SOPT with several energy levels $\epsilon_d = -2$ (a), $-3.5$ (b), $-5$ (c), 2 (d) and different temperatures $T = 0.01$, 0.5, and 1. In this and following figures, $\Gamma$ is chosen as energy unit.

Fig. 2 (a) The electric conductance $G$, (b) the thermopower $S$, and (c) the thermal conductance $\kappa$, as functions of the energy level for several different temperatures $T = 0.01$, 0.5, and 1. The on-site Coulomb interaction in the QD is $U = 7$.

Fig. 3 (a) The electric conductance, (b) the thermopower, and (c) the thermal conductance vs temperature for the QD with $U = 7$ and $\epsilon_d = -1$, 0, and $-5$.

Fig. 4 The ratio factor between the electric conductance and thermal conductance vs temperature for the QD with the same parameters as in Fig. 3.
(b) \( U=7 \), \( \epsilon_d=-2 \)

(c) \( \epsilon_d=-5 \)

(d) \( \epsilon_d=-3.5 \)

- \( T=0.01 \)
- \( 0.5 \)
- \( 1 \)
\( U = 7 \)

\[ 3\kappa /\pi^2 TG (1/e^2) \]

- \( \varepsilon_d = -1 \)
- \( 0 \)
- \( -5 \)