Numerical study of non-adiabatic quantum thermodynamics of the driven resonant level model: non-equilibrium entropy production and higher order corrections

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Abstract
We present our numerical study on quantum thermodynamics of the resonant level model subjected to non-equilibrium condition as well as external driving. Following our previous work on non-equilibrium quantum thermodynamics (Dou \textit{et al} 2020 \textit{Phys. Rev. B} 101 184304), we expand the density operator into a series of power in the driving speed, where we can determine the non-adiabatic thermodynamic quantities. Particularly, we calculate the non-equilibrium entropy production rate as well as higher order non-adiabatic corrections to the energy and/or population, which is not determined previously in Dou \textit{et al} (2020 \textit{Phys. Rev. B} 101 184304). In the limit of weak system-bath coupling, our results reduce to the one from the quantum master equation.

Keywords: quantum thermodynamics, entropy production, non-adiabatic, dissipation and fluctuation, quantum master equation

(Some figures may appear in colour only in the online journal)

1. Introduction

The study of dynamics and thermodynamics for a quantum system strongly coupled to a set of baths are of great interests recently [1–11], particularly due to its applications in nano technology, quantum information, and quantum measurement [12–16]. Quantum thermodynamics address the energy and information flow of a system consisting of a few atoms or qubits interacting strongly to non-equilibrium environments [1, 17–21]. Moreover, to make a useful quantum engine, external driving is usually applied. The finite speed driving can introduce non-adiabatic effects, including entropy production, friction (or dissipation), and fluctuation [22–27].

The driven resonant-level model has been studied extensively for thermodynamics in the strongly coupled regimes [3, 17, 28, 29]. At equilibrium (with one bath or no current), studies based on different methods (e.g. symmetric splitting [28, 30], scattering matrix [31], and non-equilibrium Green’s function [3]) arrive at a (somewhat) consistent quantum description of the thermodynamics. In particular, the first order non-adiabatic corrections to work, population, and entropy...
have been identified. Furthermore, the entropy production is proportional to the frictional work and remains positive at equilibrium, which is consistent with the second law of thermodynamics. That being said, the out of equilibrium cases (baths with different temperatures or chemical potentials) are far less understood, except for a few recent developments [31–34]. Furthermore, there are far less studies on the higher order non-adiabatic corrections to the thermodynamic quantities, which is a challenging task.

In the previous studies [35, 36], by expanding the density operator into a series of power in the driving speed, we formulate a general description of quantum thermodynamics for a generic model strongly coupled to one or more baths. We identify the non-adiabatic corrections to thermodynamic quantities, such as work, population, and entropy. In particular, the non-adiabatic entropy production rate is given by [36]

$$
\delta \dot{S} = -k_B \sum_{\alpha} \int_0^\infty \dot{\rho}_\alpha \dot{R}_\alpha tr(e^{-\frac{iHt}{\hbar}}/\hbar \partial \ln \rho_\alpha)dt.
$$

(1)

Here, $\dot{\rho}_\alpha$ is the steady state density of the total system. $H$ is the total Hamiltonian, which depends on a set of external parameters $[R_\alpha]$. Here $\alpha$ (and $\nu$) indicates the degrees of freedom (DoFs) of the driving parameters. $R_\alpha$ is the driving speed. $k_B$ is the Boltzmann constant. The above equation can be recasted into a Kubo transformed correlation function of the generalized random force using the Barker–Campell–Hassdrauff formula, where $\partial \ln \rho_\alpha$ is what we refer to as the generalized random force. Such that we have proven that the entropy production rate is always positive, which is consistent with the second law of thermodynamics. At equilibrium, the steady state density reduces to equilibrium density, such that we can show that the non-adiabatic entropy is proportional to the friction (or non-adiabatic correction to the work). Out of equilibrium, however, we have not been able to calculate $\delta \dot{S}$ explicitly due to the difficulty of determining $\dot{\rho}_\alpha$.

In the present manuscript, we calculate this entropy production rate explicitly for the driven resonant level model, which is not determined previously in [36]. We discretize the continuous bath DoFs and diagonalize the total Hamiltonian numerically. In doing so, we can identify the steady state density and calculate relevant thermodynamic quantities. We show that the numerical results recover analytical solutions when available. Also not determined previously, we identify the second order correction to the populations using analytical analysis as well as the solutions from hierarchical quantum master equation (HQME) [36–39].

We organize the manuscript as follows. In section 2, we present our analysis as well as our numerical methods to calculate thermodynamic quantities for the resonant level model. In section 3, we show our numerical results in non-adiabatic corrections to population, work as well entropy production. We conclude our work in section 4.
\[ W = \text{tr}(\dot{\rho} \hat{H}) \]  
\[ S = -k_B \text{tr}(\dot{\rho} \ln \dot{\rho}) \]  

Here \( \dot{\rho} \) is the total density operator (including the system and baths). Note that, the dot population and work are local quantities since the driving \( \partial_t \hat{H} \) and the dot number operator \( \dot{d} \) are local. The entropy defined above is an extensive quantity which includes the system and the bath. As being clear below, the total entropy is a sum of the nonadiabatic entropy production and heat. The nonadiabatic entropy production will be local. Such that the definitions of the entropy and the heat have to be consistent. See discussions in [35, 36]. Since the Hamiltonian is quadratic, we can rewrite the total Hamiltonian in equation (2) as

\[ \hat{H} = \sum_{ij} h_{ij} \hat{b}^\dagger_i \hat{b}_j \]  

\( \hat{b}_i \) is the annihilation operator of the Fermions in the system and baths, i.e. \( \{ \hat{b}_i \} = \{ \hat{c}_{\alpha d}, \hat{c}_{\alpha R} \} \). \( \hat{h} \) is the matrix representation of the one-body Hamiltonian. The thermodynamic quantities can be then rewritten using the one-body density operator \( \hat{\sigma} \):

\[ N = \langle \hat{d} | \hat{\sigma} | \hat{d} \rangle \]  
\[ W = \hat{\varepsilon}_d \langle \hat{d} | \hat{\sigma} | \hat{d} \rangle = \hat{\varepsilon}_d N \]  
\[ S = -k_B \text{Tr}(\hat{\sigma} \ln \hat{\sigma} + (1 - \hat{\sigma}) \ln (1 - \hat{\sigma})) \]  

Here \( \text{Tr} \) denotes the one-body trace (trace in orbital representation), and \( \hat{\sigma} \) is the one-body density operator for the total system (system + baths), which is defined as \( \sigma_{ij} = \text{tr}(\rho \hat{b}^\dagger_i \hat{b}_j) \). Note that for the resonant level model, work \( W \) is proportional to dot population by a factor of \( \hat{\varepsilon}_d \), where \( \hat{\varepsilon}_d \) is the speed of driving. Such that we will mainly focus on population and entropy below.

The task is then to calculate the density operator, which can be very difficult for the time-dependent Hamiltonian. The density operator follows the von Neumann equation,

\[ \frac{d}{dt} \hat{\sigma} = -i \frac{\hbar}{\varepsilon_d} [\hat{h}, \hat{\sigma}] \]  

Again, \( \hat{h} \) is the one-body Hamiltonian in equation (10). Here, \( \frac{d}{dt} \) is the total derivative with respect to time. With external driving, the total derivative can be separated into partial derivatives, i.e. \( \frac{d}{dt} = \frac{d}{dt} + \hat{\varepsilon}_d \partial_t \). \( \hat{\varepsilon}_d \) is the parameter (on-site energy of the dot level) that depends on time, \( \hat{\varepsilon}_d \) is the speed of the driving parameter. Such that the equation of motion for the density matrix can be rewritten as

\[ \partial_t \hat{\sigma} = -\hat{\varepsilon}_d \partial_t \hat{\sigma} - i \frac{\hbar}{\varepsilon_d} [\hat{h}, \hat{\sigma}] \]  

In the limit of slow driving, we can expand the density operator into a series of power in the driving speed,

\[ \hat{\sigma} = \hat{\sigma}^{(0)} + \hat{\sigma}^{(1)} + \hat{\sigma}^{(2)} + \cdots \]  

By matching the order in driving speed from both sides of the above equation, we arrive at a set of equations:

\[ \partial_t \hat{\sigma}^{(0)} = -\frac{i}{\hbar} \left[ \hat{h}, \hat{\sigma}^{(0)} \right] \]  
\[ \partial_t \hat{\sigma}^{(n)} = -\hat{\varepsilon}_d \partial_t \hat{\sigma}^{(n-1)} - \frac{i}{\hbar} \left[ \hat{h}, \hat{\sigma}^{(n)} \right], n \geq 1 \]  

The steady state solution of equation (17) gives us the 0th order density matrix, \( \hat{\sigma}^{(0)} = \hat{\sigma}_{ss} \). Note that we refer to the steady state in the strictly adiabatic limit, i.e. the zeroth order in driving speed. Note also that the dynamics in equation (17) unitary, where the Hamiltonian includes the system and baths. Still we can define the steady state of the full Hamiltonian in the same spirit of the scattering matrix techniques. See discussion in the next subsection and in [26, 36]. With the steady state zeroth order solution, we can proceed to calculate the higher order density matrix

\[ \hat{\sigma}^{(n)} = -\hat{\varepsilon}_d \int_0^\infty e^{-\hat{h}(t-t')/\hbar} \partial_t \hat{\sigma}^{(n-1)} e^{\hat{h}(t-t')/\hbar} dt' \]  
\[ \approx -\hat{\varepsilon}_d \int_0^\infty e^{-iht/\hbar} \partial_t \hat{\sigma}^{(n-1)} e^{ihtr/\hbar} dt. \]  

In the second line of the above equation, we have used the Markovian approximation, assuming the timescale of driving is much smaller as compared with the timescale for the relaxation. The Markovian approximation is consistent with the slow driving approximation.

### 2.2.1. Zeroth order quantities

Since the zeroth order entropy is an extensive quantity, we mainly calculate the zeroth order dot population here. To do so, we need to diagonalize the one-body Hamiltonian:

\[ \hat{h} = \sum_{k\alpha} \epsilon_{k\alpha} |\psi_{k\alpha}\rangle \langle \psi_{k\alpha}|. \]  

The diagonalization can be done analytically through the following transformation [40, 41]:

\[ |\psi_{k\alpha}\rangle = |\epsilon_{k\alpha} \rangle + \frac{V_{k\alpha}}{\epsilon_{k\alpha} - \epsilon_d + i\Gamma/2} \times \left( |\hat{d}\rangle + \sum_{k'\alpha'} \epsilon_{k'\alpha'} |\epsilon_{k'\alpha'} \rangle \langle \epsilon_{k'\alpha'}| \right). \]  

Here, \( \Gamma \) is the hybridization function defined in equation (6), and \( \eta \) is an positive infinitesimal. The diagonalization can be achieved through the scattering matrix approach (See e.g. [42–44]). With the diagonalized Hamiltonian, we can determine the steady-state single particle density matrix

\[ \hat{\sigma}^{(0)} = \sum_{k\alpha} f(\epsilon_{k\alpha} - \mu) |\psi_{k\alpha}\rangle \langle \psi_{k\alpha}|. \]
Here, \( f \) is the Fermi function \( f(\epsilon_{\alpha} - \mu_{\alpha}) = [1 + e^{\beta(\epsilon_{\alpha} - \mu_{\alpha})}]^{-1} \), and \( \mu_{\alpha} \) is the chemical potential for the \( \alpha \) lead.

Correspondingly, the zeroth order entropy is

\[
S^{(0)} = -k_{B} \text{Tr}(\hat{\sigma}^{(0)} \ln \hat{\sigma}^{(0)} + (1 - \hat{\sigma}^{(0)}) \ln(1 - \hat{\sigma}^{(0)})).
\]

(23)

Note that the zeroth order entropy is the total adiabatic entropy, which includes the entropy in the system and the baths. The derivative with respect to the driving parameters give rise to adiabatic heat:

\[
\hat{Q}^{(1)} = \hat{T} \partial_{\epsilon} S^{(0)}
\]

\[
= -k_{B} \text{Tr}_{d} \text{Tr} \left[ \partial_{\epsilon_{d}} \sigma^{(0)} \ln \sigma^{(0)} - \partial_{\epsilon_{d}} \sigma^{(0)} \ln \left( 1 - \sigma^{(0)} \right) \right].
\]

(24)

The and the zeroth order population is

\[
N^{(0)} = \left\langle d \right| \hat{\sigma}^{(0)} \left| d \right\rangle = \frac{1}{2\pi} \int d\epsilon \Lambda(\epsilon) f(\epsilon).
\]

(25)

Here, \( \Lambda(\epsilon) \) is the spectral function

\[
\Lambda(\epsilon) = \frac{\Gamma}{(\epsilon - \epsilon_{d})^{2} + (\Gamma/2)^{2}},
\]

(26)

and \( f(\epsilon) \) is the weighted Fermi function \( f(\epsilon) = \sum_{\alpha} \frac{1}{\beta} \ln \left[ 1 + e^{\beta(\epsilon - \mu_{\alpha})} \right]^{-1} \). Details of the deviation are shown in appendix A.

2.2.2. First order quantities. Now we turn to the first order correction. With 0th order \( \hat{\sigma}^{(1)} \), we can proceed to calculate the first order density:

\[
\hat{\sigma}^{(1)} = -\dot{\epsilon}_{d} \int_{0}^{\infty} e^{-i\dot{\epsilon}_{d}/\hbar} \partial_{\epsilon_{d}} \hat{\sigma}^{(0)} e^{i\dot{\epsilon}_{d}/\hbar} dt.
\]

(27)

The first order correction to the population is then given by

\[
N^{(1)} = \left\langle d \right| \hat{\sigma}^{(1)} \left| d \right\rangle = -\frac{\hbar \dot{\epsilon}_{d}}{4\pi} \int d\epsilon \Lambda^{2} \partial_{\epsilon} f(\epsilon).
\]

(28)

Detailed derivation can be found in the appendix of [35, 45]. Note that the population is linearly proportional to driving speed \( \dot{\epsilon}_{d} \). Such that the first order work depends on \( \dot{\epsilon}_{d} \) quadratically, \( W^{(1)} = \gamma^{(1)} \dot{\epsilon}_{d}^{2} \). Here \( \gamma^{(1)} \) is the frictional coefficient:

\[
\gamma^{(1)} = \frac{N^{(1)}}{\dot{\epsilon}_{d}} = -\frac{\hbar}{4\pi} \int d\epsilon \Lambda^{2} \partial_{\epsilon} f(\epsilon),
\]

(29)

which accounts for the dissipative effects.

We could also define a correlation function of the random force to qualify the fluctuation

\[
D_{\mu \nu} = \int_{0}^{\infty} \langle e^{i\dot{H}/\hbar} \delta F_{\mu} e^{-i\dot{H}/\hbar} \delta F_{\nu}(0) \rangle_{S}
\]

\[
= \delta F_{\nu} = \partial_{\epsilon} \hat{H} - tr(\partial_{\epsilon} \hat{H} \hat{\rho}_{\alpha})
\]

(30)

\[
(31)
\]

\( (\cdots)_{S} \) denote the symmetric average of the correlation functions. Here \( \nu \) and \( \mu \) are DoF for the motion. In the driven resonant level model, where the driving parameter is on-site energy, we have \( \nu = \mu = \epsilon_{d} \), such that we can calculate the fluctuation analytically

\[
\hat{D} = \frac{\hbar}{4\pi} \int d\epsilon \Lambda^{2} \partial_{\epsilon} f(\epsilon) \hat{f}(\epsilon).
\]

(32)

We then turn to the first order correction to entropy, which can be calculated through Taylor expansion of equation (13):

\[
S^{(1)} = -k_{B} \text{Tr} \left[ \hat{\sigma}^{(1)} \ln \hat{\sigma}^{(0)} - \hat{\sigma}^{(1)} \ln \left( 1 - \hat{\sigma}^{(0)} \right) \right].
\]

(33)

The non-adiabatic entropy rate is the derivative of the above equation.

\[
\dot{S}^{(2)} = \partial_{\epsilon} S^{(1)} = \frac{\hat{Q}^{(2)}}{\hat{T}} + \delta \hat{S}.
\]

(34)

The first term in equation (34) is the first order correction to the heat [36]

\[
\hat{Q}^{(2)} = -k_{B} \text{Tr}_{d} \text{Tr} \left[ \partial_{\epsilon_{d}} \sigma^{(1)} \ln \sigma^{(0)} - \partial_{\epsilon_{d}} \sigma^{(1)} \ln \left( 1 - \sigma^{(0)} \right) \right].
\]

(35)

The second term \( \delta \hat{S} \) in equation (34) is the additional entropy production rate due to the external driving

\[
\delta \hat{S} = -k_{B} \dot{\epsilon}_{d} \left[ \hat{\sigma}^{(1)} \partial_{\epsilon} \ln \hat{\sigma}^{(0)} - \hat{\sigma}^{(1)} \partial_{\epsilon} \ln \left( 1 - \hat{\sigma}^{(0)} \right) \right].
\]

(36)

At equilibrium, we can calculate the entropy production rate explicitly and show that

\[
\gamma^{(1)} = \beta D = \frac{\hbar T \delta \hat{S}}{\dot{\epsilon}_{d}}.
\]

(37)

The first equality in the above equation is the fluctuation-dissipation theorem. Under non-equilibrium condition, the fluctuation-dissipation theorem is no longer obeyed and we have not been able to determine the entropy production rate. In section 2.3, we will show how to evaluate entropy production rate numerically.

2.2.3. Second order quantities. Evaluation of the second order corrections to thermodynamic quantities is very tricky, which will require

\[
\hat{\sigma}^{(2)} = \int_{0}^{\infty} e^{-i\dot{H}/\hbar} \partial_{\epsilon_{d}} \sigma^{(1)} e^{i\dot{H}/\hbar} dt.
\]

(38)

Nevertheless, as shown in appendix B, we manage to evaluate the second order correction to the population analytically for the equilibrium case,

\[
N^{(2)} = \left\langle d \right| \hat{\sigma}^{(2)} \left| d \right\rangle = \frac{\hbar \dot{\epsilon}_{d}^{2}}{12\pi} \int d\epsilon \Lambda^{3} \partial_{\epsilon}^{2} f(\epsilon).
\]

(39)
Similarly to the first order case, we can define the friction term \( \gamma^{(2)} \) as

\[
\gamma^{(2)} = \frac{N^{(2)}}{\epsilon_d^2} = \frac{\hbar^2}{12\pi} \int d\epsilon A^3 \partial_\epsilon^2 f(\epsilon).
\]  

(40)

Out of equilibrium, we do not have analytical results for the second order corrections. Similar to the zeroth and first order case, we could simply replace \( f \) by \( \tilde{f} \) in the above equation as our trial results. Note that, this out-of-equilibrium solution is ad hoc. In general, however, the higher order correction can be evaluated numerically using HQME.

2.3. Numerical methods

The derivations in evaluating the non-adiabatic corrections can be very lengthy and a compact form of solutions may not available for certain quantities. In this subsection, we consider a finite number of DoFs for the baths in a similar fashion to the [46], such that we can evaluate non-adiabatic corrections numerically. Note that we do not solve the full dynamics using the numerical method blow. Rather, we compute the steady state solution by diagonalizing the discrete Hamiltonian. The non-adiabatic density (and other quantities) are then computed from the steady state density using equation (27).

To do so, we discrete the baths DoFs, and we build the one-body Hamiltonian \( \hat{h} \) with finite number of levels from the baths. \( \hat{h} \) can be written in the matrix form:

\[
\hat{h} = \begin{pmatrix}
\epsilon_d & V_L^\dagger & V_R^\dagger \\
V_L & \hat{\epsilon}_L & 0 \\
V_R & 0 & \hat{\epsilon}_R
\end{pmatrix}
\]  

(41)

Here, \( V_{\alpha} = \{ V_{i\alpha} \} \) is a vector representation of the system-bath coupling, and \( \epsilon_{\alpha} = \{ \epsilon_{i\alpha} \} \) is a matrix representation of the energies in the baths.

We then proceed to build the steady state density matrix \( \hat{\sigma}_{ss} \). We first define non-interacting density operator

\[
\hat{\sigma}_0 = \begin{pmatrix}
f(\epsilon_d - \frac{1}{2} \mu_L - \frac{1}{2} \mu_R) & 0 & 0 \\
0 & f(\hat{\epsilon}_L - \mu_L) & 0 \\
0 & 0 & f(\hat{\epsilon}_R - \mu_R)
\end{pmatrix}.
\]  

(42)

The interacting steady-state density operator is obtained by transforming \( \hat{h} \) in the basis where \( \hat{h} \) is diagonal and zero out all non-diagonal terms of \( U^\dagger \hat{h}_0 U \). Here \( U^\dagger \) diagonalizes the \( \hat{h} \). Such that \( \hat{\sigma}_{ss} \) and \( \hat{h} \) are both diagonal in such a basis.

\[
\hat{h} = \sum_m \epsilon_d |m\rangle \langle m| \]

(43)

\[
\hat{\sigma}_{ss} = \sum_m \sigma_m |m\rangle \langle m|
\]  

(44)

Such a scheme is similar to the scattering formulation of the density operator [26].

With the eigenvalues and eigenbasis of \( \hat{h} \) and \( \hat{\sigma}_{ss} \), the zeroth order population is easily obtained:

\[
N^{(0)} = \sum_m |\langle d|m \rangle|^2 \sigma_m.
\]  

(45)

The first order correction requires \( \hat{\sigma}^{(1)} \) (equation (27)), which can be evaluated in the eigenbasis of \( \hat{h} \):

\[
\hat{\sigma}^{(1)} = \pi \hbar \hat{h} \sum_m |m\rangle \langle m| \partial_\epsilon \sigma_{ss} \langle n| \delta(\epsilon_m - \epsilon_n) |n\rangle.
\]  

(46)

Using Hellman–Feynman theorem, we can rewrite the above as (see the appendix in [35])

\[
\hat{\sigma}^{(1)} = \pi \hbar \hat{h} \sum_m |m\rangle \langle m| \frac{\sigma_m - \sigma_n}{\epsilon_m - \epsilon_n} \delta(\epsilon_m - \epsilon_n) |\langle d|n \rangle|^2.
\]  

(47)

Such that the first order population is

\[
N^{(1)} = \pi \hbar \hat{h} \sum_m |m\rangle \langle m| \left( \frac{\sigma_m - \sigma_n}{\epsilon_m - \epsilon_n} \delta(\epsilon_m - \epsilon_n) |\langle d|n \rangle|^2 \right)
\]  

(48)

In numerical simulations, we replace the delta function by a Gaussian with a broadening parameter \( \eta \):

\[
\pi \delta(\epsilon_m - \epsilon_n) \rightarrow \sqrt{\frac{\pi}{2\eta^2}} \exp \left( -\frac{(\epsilon_m - \epsilon_n)^2}{2\eta^2} \right).
\]  

(49)

We also take care of the denominator \( \epsilon_m - \epsilon_n \) in equation (48) as

\[
\frac{\sigma_m - \sigma_n}{\epsilon_m - \epsilon_n} \rightarrow \text{Re} \frac{\sigma_m - \sigma_n}{\epsilon_m - \epsilon_n + i\eta}.
\]  

(50)

In practice, the broadening parameter \( \eta \) is set to be in the order of the energy spacing to better converge the results.

The correlation function in equation (30) can be recast in the eigenbasis (see the supplementary material in [45]):

\[
D = \pi \hbar \hat{h} \sum_m |\langle m|d \rangle|^2 \sigma_m (1 - \sigma_n) \delta(\epsilon_m - \epsilon_n) |\langle d|n \rangle|^2
\]  

(51)

which is readily to be calculated. Finally, \( \delta \hat{S} \) can be written in the eigenbasis as

\[
\delta \hat{S} = \pi \hbar \hat{h} \sum_m |\langle m|\hat{\sigma}^{(1)}|n\rangle |\partial_\epsilon \ln \sigma_{ss} - \ln(1 - \sigma_{ss})| |m\rangle.
\]  

(52)

Here, \( |\langle m|\partial_\epsilon \ln \sigma_{ss}|n\rangle \) is done numerically with finite difference. Note that \( |m\rangle \) is the adiabatic basis. To calculate the matrix element properly, we rotate the matrix in \( \ln \sigma_{ss} \) back to the diabatic basis. After done derivative, we rotate the matrix back to the adiabatic basis.
3. Results and discussion

3.1. Weak coupling limit: master equations

In this subsection, we consider the weak coupling limit. In such a limit, we can trace out the bath DoFs and derive an equation of motion for the dot density $\sigma_d$ only \cite{47, 48}:

$$\partial_t \sigma_d = -\epsilon_d \partial_\epsilon \sigma_d - \frac{\Gamma}{\hbar} \left[ \sigma_d - \overline{f}(\epsilon_d) \right].$$  \hspace{1cm}  \text{(53)}

Again, we can expand the dot density into a series of powers in terms of the driving speeds, $\sigma_d = \sigma_d^{(0)} + \sigma_d^{(1)} + \sigma_d^{(2)} + \cdots$. Similar to the procedures in section 2.2, we obtain the nth order population as

$$N^{(n)} = \overline{f}(\epsilon_d), \hspace{2cm} \text{for } n = 0, 1, 2, \cdots$$  \hspace{1cm}  \text{(54)}$$

$$N^{(1)} = -\frac{\hbar \epsilon_d}{\Gamma} \partial_\epsilon \overline{f}(\epsilon_d), \hspace{2cm} \text{for } n = 1$$  \hspace{1cm}  \text{(55)}$$

$$N^{(2)} = \frac{\hbar^2 \epsilon_d^2}{\Gamma^2} \partial_\epsilon^2 \overline{f}(\epsilon_d). \hspace{2cm} \text{for } n = 2$$  \hspace{1cm}  \text{(56)}$$

Similarly, we can also obtain the friction and fluctuation,

$$\gamma^{(1)} = -\frac{\hbar}{\Gamma} \partial_\epsilon \overline{f}(\epsilon_d), \hspace{2cm} \text{for } n = 1$$  \hspace{1cm}  \text{(57)}$$

$$D = \frac{\hbar kT}{\Gamma} \overline{f}(\epsilon_d) [1 - \overline{f}(\epsilon_d)]. \hspace{2cm} \text{for } n = 1$$  \hspace{1cm}  \text{(58)}$$

To get the entropy production rate, we define the entropy for the dot as $S = -\sigma_d \ln \sigma_d - (1 - \sigma_d) \ln(1 - \sigma_d)$. Similar to the procedures in section 2.2, we arrive at the entropy production rate as

$$\frac{\hbar T \delta \dot{S}}{\epsilon_d} = [\gamma^{(1)}]^2 / (\beta D). \hspace{2cm} \text{(59)}$$

Note that the above equation is only true for the driven resonant level model in the weak coupling limit. We expect that our numerical results can reduce to the master equation results in the limit of $\Gamma < kT$. What is missing in the master equation is mainly the level broadening effects. Hence, we refer to the master equation results as unbroadened results.

3.2. Results

We now present our results in this subsection. In our numerical calculations, the number of the levels is set to be 1000 for both leads, and level spacing is set to be uniform. The bandwidth is 100$\Gamma$. Broadening term $\eta$ is equal to the energy spacing. This choice of the parameters allow us to converge our results sufficiently. We have also set the driving speed as $\hbar \epsilon_d = 0.1 \Gamma^2$.

3.2.1. Zeroth and first order results. We first look at the zeroth and first order corrections to the thermodynamic quantities. In figure 2, we plot the dot population $N^{(0)}$ and $N^{(1)}$ as a function of $\epsilon_d$ at equilibrium where $\mu_L = \mu_R = -2\Gamma$. In such a case, analytical results are available. Notice the good agreement between the numerical results and the analytical results for both the zeroth order and first order populations. In the numerical calculations, the main source of the error is the discretization of finite bandwidth. This agreement verify the reliability of the numerical method. The results from master equation having a sharper feature as compared to the other results, suggesting the missing of the level broadening effects. Note also that the first order correction to the population $N^{(1)}$ shows a peak at $\epsilon_d = \mu_L = \mu_R$.

In figure 3, we plot friction, fluctuation, and entropy production rate as a function of $\epsilon_d$ at equilibrium. In equation (37), we have shown that friction, fluctuation, and entropy production rate are proportional to each other analytically without non-equilibrium condition. Indeed, our numerical calculations further verify this statement. Such an agreement will no longer exist under non-equilibrium condition (as shown below).

Now, let us look at the non-equilibrium case. In figure 4, we plot $N^{(0)}$ and $N^{(1)}$ as a function of $\epsilon_d$ under non-equilibrium condition, where $\mu_L = -\mu_R = -2\Gamma$. Again, we see good agreement between the analytical solution and the
Figure 3. Friction, fluctuation, and entropy production rate as a function of \(\epsilon_d\) at equilibrium. \(\mu_L = \mu_R = -2\Gamma, \Gamma = k_B T\).

Figure 4. \(N^{(0)}\) and \(N^{(1)}\) as a function of \(\epsilon_d\) under nonequilibrium condition. \(\mu_L = -\mu_R = -2\Gamma, \Gamma = k_B T\).

Numerical calculation. The first order population \(N^{(1)}\) shows two peaks at \(\epsilon_d = \mu_L\) and \(\epsilon_d = \mu_R\) respectively, resulting a dip at \(\epsilon_d = \frac{1}{2}(\mu_L + \mu_R)\). Hence, the peaks are Fermi resonance in nature. Again, results from quantum master equation show sharper dips and peaks due to lack of broadening effects.

In figure 5, we plot friction, fluctuation, and entropy production rate as a function of \(\epsilon_d\) under non-equilibrium condition. Now we see that, unlike the equilibrium case, friction, fluctuation, and entropy production rate do not agree with each other. In fact, in general all three quantities can be recast into correlation functions [36]:

\[
\delta S = k_B\beta^2 \sum_{\alpha\nu} \langle \dot{R}_\alpha \dot{R}_\nu \int_0^\infty \langle \delta \dot{F}_\alpha(t)\delta \dot{F}_\nu \rangle \rangle dt \quad (60)
\]

\[
\gamma_{\alpha\nu} = \beta \int_0^\infty \langle \delta F_\alpha(t)\delta \dot{F}_\nu \rangle dt \quad (61)
\]

\[
D_{\alpha\nu} = \int_0^\infty \langle \delta \dot{F}_\alpha(t)\delta \dot{F}_\nu \rangle dt. \quad (62)
\]

Here \(\langle \cdots \rangle_K\) denotes Kubo transformed average of the correlation functions. \(\beta\) is the reduced temperature [26]. \(\delta \dot{F}_\alpha\) can be seen as the generalized random force:
Figure 5. Friction, fluctuation, and entropy production rate as a function of $\epsilon_d$ under nonequilibrium condition. $\mu_L = -\mu_R = -2\Gamma$, $\Gamma = k_B T$.

Figure 6. $\gamma^{(2)}$ as a function of $\epsilon_d$ under equilibrium ($\mu_L = \mu_R = 0$) and nonequilibrium condition ($\mu_L = -\mu_R = -2\Gamma$). $\Gamma = k_B T$.

Here $\hat{Y}$ is an operator that accounts for particle transport [41]. $\delta F_\alpha$ is the random force defined in equation (31).

\[
\delta F_\alpha = -\frac{1}{\beta} \partial_\alpha \ln \rho_{ss} = \partial_\alpha \hat{Y} - \partial_\alpha Tr(\rho_{ss}(\partial_\alpha \hat{H} - \partial_\alpha \hat{Y})).
\]

(63)

Hence, friction, fluctuation, and entropy production rate are just correction functions of the two random force operators. Since $\delta \hat{S}$ and $D_{\alpha\nu}$ are the correlation functions of the same random force, such that $\delta \hat{S}$ and $D_{\alpha\nu}$ are positive definite, whereas in general $\gamma_{\alpha\nu}$ is not positive definite under non-equilibrium condition. Here, for the resonant level model, we see that $\gamma_{\alpha\nu}$ remains positive even out of equilibrium. However, for more complicated model, this is not true [49].

3.2.2. Second order results. We now look at the second order correction to the population (or second order friction). Here, HQME is used to simulate the exact dynamics for the driven resonant level model, where we can calculate the exact population as a function of time. We then estimate the
second order friction by subtracting the zeroth and first order correction:

\[ \gamma^{(2)} = \frac{(N - N(0) - \epsilon_d \gamma^{(1)})}{\epsilon_d^2}. \] (64)

In the above equation, we have ignored the third order and higher correction. In figure 6, we plot \( \gamma^{(2)} \) as a function of \( \epsilon_d \) from HQME with different driving speeds. At equilibrium, HQME results reproduce analytical results in equation (40). Out of equilibrium, we do not have analytical results for \( \gamma^{(2)} \). However, we simply replace \( f \) by \( \hat{f} \) in equation (40) as our trial solution. Such a solution agrees with the HQME results as well as results from master equations. Indeed, future work must verify this trial solution for the second order correction out of equilibrium.

4. Conclusion

Using the expansion of the density operator in the power of driving speed, we have identified the non-adiabatic correction to the quantum thermodynamic quantities in the strongly coupled regimes. With numerical tools, we have calculated non-adiabatic corrections for the resonant level model. We have verified our numerical results against analytical results for the zeroth and first order correction to the population in and out of equilibrium. We then have calculated the non-adiabatic entropy production out of equilibrium. We show that, at equilibrium, the friction, random force, and entropy production agree with each other. Out of equilibrium, friction, random force and entropy production are all correlation functions between different (generalized) random forces. Our results agree with the one from the master equation in the limit of weak couplings. Future work must study the non-adiabatic entropy production and higher order corrections go beyond simple resonant level model.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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Appendix A. Evaluation of \( \langle d | \delta(\epsilon - \hat{h}) | d \rangle \)

In this appendix, we draw certain identities and then evaluate \( \langle d | \delta(\epsilon - \hat{h}) | d \rangle \). To start with, we have the following identity:

\[ \delta(\epsilon - \hat{h})(\epsilon - \hat{h}) = (\epsilon - \hat{h})\delta(\epsilon - \hat{h}) = 0. \] (A1)

Taking \( \partial_{\epsilon_d} \) on both sides, we arrive at

\[ -\partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) + (\epsilon - \hat{h})\partial_{\epsilon_d} \delta(\epsilon - \hat{h}) = -\delta(\epsilon - \hat{h})\partial_{\epsilon_d} \hat{h} + \partial_{\epsilon_d} \delta(\epsilon - \hat{h})(\epsilon - \hat{h}) = 0. \] (A2)

Hence,

\[ \partial_{\epsilon_d} \hat{h} = (\epsilon - \hat{h})^{-1} \partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) = \delta(\epsilon - \hat{h})\partial_{\epsilon_d} \hat{h}(\epsilon - \hat{h})^{-1}. \] (A3)

Similarly, we can show that

\[ \partial_{\epsilon} \delta(\epsilon - \hat{h}) = - (\epsilon - \hat{h})^{-1} \delta(\epsilon - \hat{h}) = - \delta(\epsilon - \hat{h})(\epsilon - \hat{h})^{-1}. \] (A4)

The above equations will be useful for higher order corrections.

In the diagonal basis, we have

\[ \delta(\epsilon - \hat{h}) = \sum_{\kappa\alpha} |\psi_{\kappa\alpha}\rangle \delta(\epsilon - \epsilon_{\kappa\alpha}) \langle \psi_{\kappa\alpha}|, \] (A5)

such that

\[ \langle d | \delta(\epsilon - \hat{h}) | d \rangle = \sum_{\kappa\alpha} |\psi_{\kappa\alpha}\rangle^2 \delta(\epsilon - \epsilon_{\kappa\alpha}) \]

\[ = \sum_{\kappa\alpha} |V_{\kappa\alpha}|^2 \delta(\epsilon - \epsilon_{\kappa\alpha}) \]

\[ = \frac{1}{2\pi} \sum_{\alpha} |\Gamma_{\alpha}| \frac{\Gamma_{\alpha}}{(\epsilon - \epsilon_d)^2 + (\Gamma/2)^2} = A(\epsilon) \frac{1}{2\pi}. \] (A6)

Appendix B. Deviation of equation (39)

At equilibrium, the one-body steady state density is

\[ \tilde{\sigma}_{ss} = \langle \hat{h} \rangle = \int f(\epsilon) \delta(\epsilon - \hat{h}) \delta(\epsilon) \, d\epsilon, \] (B1)

Use the identity in appendix A, we can show that

\[ \hat{\sigma}^{(1)} = -\pi \hbar \epsilon_d \int d\epsilon \delta(\epsilon - \hat{h}) \partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) \partial_{\epsilon} f(\epsilon), \] (B2)

Taking the derivative of \( \hat{\sigma}^{(1)} \) with respect to \( \epsilon_d \), we have

\[ \partial_{\epsilon_d} \hat{\sigma}^{(1)} = -\pi \hbar \epsilon_d \int d\epsilon \partial_{\epsilon_d} \delta(\epsilon - \hat{h}) \partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) \partial_{\epsilon} f(\epsilon) \]

\[ -\pi \hbar \epsilon_d \int d\epsilon \delta(\epsilon - \hat{h}) \partial_{\epsilon_d} \hat{h} \partial_{\epsilon_d} \delta(\epsilon - \hat{h}) \partial_{\epsilon} f(\epsilon) \]

\[ = -\pi \hbar \epsilon_d \int d\epsilon \delta(\epsilon - \hat{h})^{-1} \partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) \partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) \]

\[ \times \partial_{\epsilon} f(\epsilon) - \pi \hbar \epsilon_d \int d\epsilon \delta(\epsilon - \hat{h}) \partial_{\epsilon_d} \hat{h} \delta(\epsilon - \hat{h}) \]

\[ \times \partial_{\epsilon_d} \hat{h} (\epsilon - \hat{h})^{-1} \partial_{\epsilon} f(\epsilon). \] (B3)

We have used the identities shown in appendix A. To evaluate \( \hat{\sigma}^{(2)} \), we first calculate the following term,
\[
\int_0^\infty e^{i\hat{h}t/\hbar} \int d\epsilon (\epsilon - \hat{h})^{-1}\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial} \hat{h} \\
\times \delta(\epsilon - \hat{h})\partial_{\epsilon\partial} f(\epsilon) e^{-i\phi t/\hbar} \\
= \sum_{\text{map}} \int_0^\infty d\epsilon (\epsilon - \epsilon_p)\langle n| \partial_{\epsilon\partial}\hat{h}|n\rangle \delta(\epsilon - \epsilon_p)\partial_{\epsilon\partial} f(\epsilon) \langle n| \\
= \pi \hbar \sum_{\text{map}} \delta(\epsilon_0 - \epsilon_m)\langle n| \langle m| \partial_{\epsilon\partial}\hat{h}\rangle |p\rangle \\
\times \delta(\epsilon - \epsilon_m)\langle p| \partial_{\epsilon\partial}\hat{h}|n\rangle \delta(\epsilon - \epsilon_m)\partial_{\epsilon\partial} f(\epsilon) \langle n| \\
= \pi \hbar \sum_{\text{map}} \int d\epsilon (\epsilon - \epsilon_m)^{-1} \langle m| \partial_{\epsilon\partial}\hat{h}\rangle |p\rangle \\
\times \delta(\epsilon - \epsilon_m)\langle p| \partial_{\epsilon\partial}\hat{h}|n\rangle \delta(\epsilon - \epsilon_m)\partial_{\epsilon\partial} f(\epsilon) \langle n| \\
= -\pi \hbar \int d\epsilon \delta(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial} f(\epsilon). 
\]

Similarly,

\[
\int_0^\infty e^{i\hat{h}t/\hbar} \int d\epsilon (\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})^{-1} \\
\times \partial_{\epsilon\partial} f(\epsilon) e^{-i\phi t/\hbar} \\
= -\pi \hbar \int d\epsilon \delta(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial} f(\epsilon). 
\]

Therefore,

\[
\hat{\sigma}^{(2)} = -i\hat{\epsilon} \int_0^\infty e^{i\phi t/\hbar} \int d\epsilon \delta(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial} \hat{h} \\
\times \delta(\epsilon - \hat{h})\partial_{\epsilon\partial} f(\epsilon) \\
- \pi \hbar \int d\epsilon \delta(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial}\hat{h}(\epsilon - \hat{h})\partial_{\epsilon\partial} f(\epsilon). 
\]

We then proceed to evaluate \( N^{(2)} \):

\[
N^{(2)} = \langle d| \sigma^{(2)}| d \rangle = -\frac{\hbar^2}{4\pi} \int d\epsilon \partial_{\epsilon\partial}(A(\epsilon)A^\dagger(\epsilon))\partial_{\epsilon\partial} f(\epsilon) \\
= -\frac{\hbar^2}{12\pi} \int d\epsilon \partial_{\epsilon\partial} A(\epsilon)\partial_{\epsilon\partial} f(\epsilon) \\
= -\frac{\hbar^2}{12\pi} \left[ A(\epsilon)\partial_{\epsilon\partial} f(\epsilon) \right]^{\infty}_0 + \frac{\hbar^2}{12\pi} \int d\epsilon A(\epsilon)\partial_{\epsilon\partial} f(\epsilon) \\
= \frac{\hbar^2}{12\pi} \int d\epsilon A(\epsilon)\partial_{\epsilon\partial} f(\epsilon), 
\]

which gives us the results shown in equation (39). We have used the fact that \( \partial_{\epsilon\partial} \hat{h} = |d| |d\rangle \).

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