We develop the strong coupling quantum thermodynamics based on the solution of the exact master equation. We find that both the Hamiltonian and the temperature must be renormalized due to the system-reservoir couplings. With the renormalized Hamiltonian and temperature, the exact steady state of open quantum systems can be expressed as a standard Gibbs state. The exact steady-state particle distributions obey the Bose-Einstein distribution or the Fermi-Dirac distribution only for the renormalized energy and temperature. In this formulation, heat and work are quantum mechanically defined, from which we compute the specific heat and examine the consistency of the theory. Consequently, thermodynamic laws and statistical mechanics emerge naturally and rigorously from quantum evolution of open systems.

Thermodynamics and statistical mechanics are built with the equilibrium hypothesis [1, 2]. That is, over a sufficiently long time, a macroscopic system which is very weakly coupled with a thermal reservoir can always reach thermal equilibrium, and the equilibrium statistical distribution does not depend on the initial state of the system. A question arises naturally is what happens for a microscopic system coupling strongly with a reservoir. Solving this problem from dynamical evolution of quantum systems has been a big challenge in physics [3–15].

In the past decades, experimental investigations on quantum heat engines have attracted a great interest on the realization of thermalization and the formulation of quantum thermodynamics [16–38]. Besides searching new thermal phenomena arising from quantum coherence and quantum entanglement, tremendous works have been focused on the questions: how thermodynamic laws naturally emerge from quantum dynamics and how these laws may be changed when the system-reservoir couplings become strong [39–43]. Due to various assumptions and approximations one inevitably takes in addressing these questions, no consensus has been reached in building quantum thermodynamics at strong coupling. In this Letter, we will attempt to answer these questions based on the exact solution of the exact master equation for a class of open quantum systems [54–63].

The difficulty of establishing quantum thermodynamics at strong coupling is twofold: (i) How to systematically determine the internal energy from the system Hamiltonian which may be modified by the strong coupling? (ii) How to correctly count the entropy production if the steady state of the system may deviate from a Gibbs state? To answer these questions, we begin with a single-mode bosonic open system (such as a photonic mode in a microwave cavity or a phononic mode in lattices) coupled to a thermal reservoir through particle exchange interactions. Later, we will generalize to more general systems. The total Hamiltonian of the system, the reservoir and coupling between them is a Fano-Anderson Hamiltonian [64, 65]:

\[ H = H_s + H_r + H_{sr} = \hbar \omega_s a^\dagger a + \sum_k \hbar \omega_k b^\dagger_k b_k + \sum_k \hbar (V_k a^\dagger b_k + V_k^* b_k^\dagger a), \]

where \( a^\dagger \) and \( b_k \) (and \( b_k^\dagger \)) are the creation (annihilation) operators of the bosonic modes in the system and the reservoir with frequency \( \omega_k \) and continuous spectrum \( \omega_k \), respectively, \( V_k \) is the coupling amplitude between them. The thermal reservoir is initially in Gibbs state \( \rho_{\theta_s}(t_0) = e^{-\beta_s H_E} / Z_{\theta_s} \), where \( \beta_s = 1 / k_B T_0 \), \( T_0 \) is the temperature of the reservoir at initial time \( t_0 \), and \( Z_{\theta_s} = \text{Tr}_E [e^{-\beta_s H_E}] \) is the partition function. The system can be initially in arbitrary state \( \rho_s(t_0) \).

The exact master equation of the reduced density matrix \( \rho_s(t) = \text{Tr}_r [e^{-\beta_s H_E(t-t_0)} \rho_s(t_0) e^{\beta_s H_E(t-t_0)}] \), which determines the time evolution of the system, can be rigorously derived by integrating out all the reservoir degrees of freedom [54].

Here we focus on the realization of thermalization and the formulation of quantum thermodynamics at strong coupling. In this Letter, we will attempt to answer these questions based on the exact solution of the exact master equation for a class of open quantum systems [54–63].

\[ \frac{d}{dt} \rho_s(t) = \frac{1}{i\hbar} \left[ H_s^R(t), \rho_s(t) \right] + \gamma(t, t_0) \left\{ 2a \rho_s(t)a^\dagger - a^\dagger a \rho_s(t) - \rho_s(t) a^\dagger a \right\} + \gamma(t, t_0) \left\{ a a^\dagger \rho_s(t) - \rho_s(t) a a^\dagger \right\}. \]  

(1)

where

\[ H_s^R(t) = \hbar \omega_s(t, t_0) a^\dagger a \]  

(2)

is the renormalized Hamiltonian specified by superscript index \( r \). The real coefficients \( \omega_s(t, t_0), \gamma(t, t_0) \) and \( \tilde{\gamma}(t, t_0) \) describe the renormalized frequency, dissipation and fluctuations arising from the coupling. These coefficients are determined by the relations

\[ i\omega_s(t, t_0) + \gamma(t, t_0) = -\dot{u}(t, t_0) / u(t, t_0), \]  

(3a)

\[ \tilde{\gamma}(t, t_0) = \dot{v}(t, t) - 2v(t, t) \text{Re}[\ddot{u}(t, t_0) / u(t, t_0)], \]  

(3b)

where \( u(t, t_0) \) and \( v(t, t) \) are the non-equilibrium Green functions obeying the integro-differential equations.

\[ \frac{d}{dt} u(t, t_0) + i\omega_s u(t, t_0) + \int_{t_0}^t d\tau g(t, \tau) u(\tau, t_0) = 0, \]  

(4a)

\[ v(t, t_0) = \int_{t_0}^t d\tau_1 \int_{t_0}^{\tau_1} d\tau_2 \frac{\partial}{\partial \tau_2} \frac{1}{g(\tau_2, \tau_1)} u^{\dagger}(\tau_2, \tau_1). \]  

(4b)

The intergral kernels, \( g(t, \tau) = \int_0^\infty d\omega J(\omega)e^{-i\omega(t-\tau)} \) and \( \tilde{g}(t, \tau) = \int_0^\infty d\omega J(\omega)\tilde{\pi}(\omega, T_0)e^{-i\omega(t-\tau)} \), characterize the back-reactions between the system and the reservoir. Here \( J(\omega) \equiv \sum_k |V_k|_2^2 \delta(\omega - \omega_k) \) is the spectral density and \( \tilde{\pi}(\omega, T_0) = \frac{1}{e^{\beta_s \omega} - 1} \) is the initial particle distribution in the reservoir.
For any arbitrary initial state of the system \( \rho_{\omega_0}(t_0) = \sum_{m=0}^{\infty} \rho_{\omega_0} |m \rangle \langle m | \) (either a pure state \( \rho_{\omega_0} = c_0 |c_0 \rangle \langle c_0 | \), or a mixed state \( \rho_{\omega_0} \neq c_0 |c_0 \rangle \langle c_0 | \), where \( c_0 \) is a complex number), the exact solution of Eq. (1) can be found [27]

\[
\rho_{\omega}(t) = \sum_{i,m=0}^{\infty} \min_{(1,m)} \sum_{k=0}^{\infty} d_k A_{ik}^{\dagger}(t) \rho^{(i)}(t) A_{mk}(t)
\]

(5)

where \( \rho^{(i)}(t) = \sum_{n=0}^{\infty} |v(t,n)\rangle \langle n| \), \( A_k^{\dagger}(t) = \frac{\sqrt{\pi}}{(i-k) \sqrt{2 \rho^{(i)(t)}}} \left[ u(t,n) - k \right]^{\dagger} 
\]
and \( d_k = \left[ 1 - |v(t,n)|^2 \right] / \sqrt{v^{(i)(t)}} \). As a self-consistent check, we can calculate the average particle number from the above solution, \( \bar{n}(t) \equiv \sum_{n=0}^{\infty} n |v(t,n)|^2 \), where \( \bar{n}(t) \) is the solution of Eq. (4a)

\[
\rho_{\omega}(t) = \frac{1}{1 + v(t)} e^{\ln[v(t)]} u(t) + v(t).
\]

(6)

Here \( u(t_0) \) and \( v(t) \) are determined by Eq. (4).

For a given spectral density \( J(\omega) \), if no localized mode exists [51, 09], the solution of Eq. (4a) \( u(t \to \infty, t_0) \to 0 \) when the system reaches the steady state. As a result,

\[
\rho_{\omega}(t \to \infty) = \lim_{t \to \infty} \sum_{n=0}^{\infty} \frac{|v(t,n)|^2}{1 + v(t)} |n\rangle \langle n|
\]

\[
\pi(t \to \infty) = \lim_{t \to \infty} v(t) = \int d\omega D(\omega) \pi(\omega, T_0)
\]

(7a)

where \( D(\omega) = \frac{J(\omega)}{\omega - \omega - \Delta(\omega)} \) is the frequency shift. Equation (7a) is the exact steady-state solution of the system for arbitrary system-reservoir coupling strengths.

Now we can build quantum thermodynamics from the above solution. First, we plot in Fig. 1(a) (the red-dashed line) the exact solution \( \pi(t \to \infty) \) of Eq. (7b) as a function of the coupling strength \( \eta \) for the Ohmic spectral density \( J(\omega) = \eta \omega \) [14, 5]. As one can see, \( \pi(t \to \infty) \) diverges significantly from \( \pi(\omega, T_0) \) (the green-dot line) as \( \eta \) increases. This derivation shows how the system-reservoir coupling changes the intrinsic thermal property of the system. The master equation Eq. (1) shows that the Hamiltonian of the system must be renormalized from \( H_{\omega_0} \) to \( H_{\omega} \) with the energy \( \omega \), being shifted to \( \omega \) due to the system-reservoir coupling, where the renormalized frequency \( \omega \ = \omega \ (t \to \infty) \) can be exactly calculated from Eq. (3a) (see Fig. 1(b)). We also plot in Fig. 1(a) (the blue-dashed-dot line) the particle distribution with the renormalized energy: \( \pi(\omega, T_0) \to \frac{1}{Z} \). It shows that \( \pi(\omega_0, T_0) \) changes with increasing \( \eta \), similar to the exact solution \( \pi(t \to \infty) \) but there is still obvious difference between them.

Note that the exact solution \( \rho_{\omega}(t \to \infty) \) of Eq. (7a) is a Gibbs state. This indicates that the exact particle distribution \( \pi(t \to \infty) \) should obey the Bose-Einstein distribution for arbitrary coupling. To find such a distribution that agrees with the solution Eq. (7a), one possibility is to renormalize the temperature because no other thermal quantity can be modified in the Gibbs state for photon and phonon systems. Physically, both system and reservoir evolve into the nonequilibrium state \( \rho(t) \) after the initial time \( t_0 \). A new equilibrium temperature must be generated when the system and reservoir reach the steady state. According to the axiomatic description of thermodynamics [70, 71], the temperature is defined as the change of internal energy with respect to the thermal entropy of the system. The internal energy can be determined by the renormalized Hamiltonian in Eq. (1): \( E(t) = Tr_\pi[H_{\omega}(t) \rho_\omega(t)] \). Because the steady state Eq. (7a) is still a Gibbs state, the nonequilibrium entropy should be the von Neumann entropy [53, 70, 72]: \( S(t) = -k_B Tr_\pi[\rho_\omega(t) \ln \rho_\omega(t)] \). The time-dependence of \( E(t) \) and \( S(t) \) are plotted in Fig. 1(c)-(d). Thus, the renormalized dynamical temperature can be defined [71],

\[
T'(t) = \frac{dT(t) - dS(t)}{dE(t)} - Tr_\pi[H_{\omega}(t) \frac{d\rho_\omega(t)}{dS(t)}]
\]

(8)

Now, the change of the internal energy in time contains two parts. One is the change of the system Hamiltonian \( H_\omega(t) \) (through the change of the energy level \( \hbar \omega(t) \)) which corresponds to quantum work done on the system [72]. The other is the change of the density state \( \rho_\omega(t) \) which corresponds to quantum heat associated with the entropy production. Thus,

\[
dE(t) = Tr_\pi[\rho_\omega(t) dH_{\omega}(t)] + Tr_\pi[H_{\omega}(t) d\rho_\omega(t)]
\]

\[
dW(t) + dQ(t) = dE(t) + T'(t) dS(t).
\]

(9)

Because the steady state Eq. (7a) is a Gibbs state, it can be also expressed as

\[
\rho_{\omega}(t) = \sum_{n=0}^{\infty} \frac{|n\rangle \langle n|}{Z} e^{-\beta' H_{\omega}(t)}
\]

(10)

where \( H_{\omega}(t) = \frac{1}{e^{\beta' H_{\omega}(t) - \beta' H_{\omega}(t)} - 1} \) is the Bose-Einstein distribution and \( Z' = Tr_\pi[e^{-\beta' H_{\omega}(t)}] \) with \( \beta' = 1/k_B T' \).
and $T^r = T^r(t \to \infty)$ is the renormalized equilibrium temperature at steady state (see Fig. 1b). We plot $\pi(\omega^r_s, T^r)$ with the renormalized energy and temperature (the black-dot line) in Fig. 1a. Remarkably, it precisely reproduces the exact solution Eq. (7b), i.e., $\pi(t \to \infty) = \pi(\omega^r_s, T^r)$. This is a substantial test of the temperature renormalization in strong coupling quantum thermodynamics.

Furthermore, in the very weak coupling regime $\eta \ll \eta_c$, we have $\Delta(\omega) \to 0$ and $D(\omega) \to \delta(\omega - \omega_o)$ so that in the steady state, Eq. (7b) is directly reduced to $\pi \to \pi(\omega_o, T_0)$ [27] [38], and

$$\rho_s = \sum_{n=0}^{\infty} \frac{|\pi(\omega_o, T_0)|^n}{1 + \pi(\omega_o, T_0)} |n\rangle\langle n| = \frac{1}{Z} e^{-\beta_0 H_S}, \quad (11)$$

which recovers the expected solution in the weak coupling regime. Figure 1 also shows that $\hbar \omega_o^r \to \hbar \omega_o$ and $T^r \to T_0$ at very weak coupling. Thus, the equilibrium hypothesis of thermodynamics and statistical mechanics is proven rigorously from quantum dynamics.

Because Eqs. (7a) and (10) are identical and Eq. (10) is the standard Gibbs state, all the thermodynamic laws are naturally preserved with the renormalized Hamiltonian and temperature, including the second thermodynamic law which is a consequence of the Gibbs state obtained by maximizing the von Neumann entropy. The quantum work and heat in Eq. (9) are well defined and $T^r(t)$, $dW(t) = T_r \rho_s(t) dH^r_S(t)$, $dQ(t) = T_r [H^r_S(t)\rho_s(t)] = T^r(t)dS(t)$. The quantum Helmholtz free energy defined by a Legendre transformation from $E(t)$ is [53] [70]:

$$F(t) = E(t) - T^r(t)S(t) \quad t \to S - (1/\beta^r) \ln Z^r, \quad (12)$$

and $dF(t) = dW(t) - S(t)dT^r(t)$ which leads to the consistency that the quantum thermodynamic work done on the system can be identified with the change of the Helmholtz free energy of the system in isothermal processes [70]. Moreover, the specific heat calculated from the internal energy and from the Gibbs state with the renormalized Hamiltonian and temperature are also identical, as shown in Fig. 2

$$C = \frac{dQ}{dT^r} = T^r \frac{dS}{dT^r} = \frac{\partial E}{\partial T^r}, \quad (13)$$

where the third thermodynamic law is justified from the specific heat at arbitrary coupling: $C \sim T^r$ as $T^r \to 0$.

Now we extend the above formulation to multi-level systems coupled with multi-reservoirs (including both bosonic and fermionic systems) [74]. Using the second quantization, the Hamiltonian of a microscopic system can be written as $H_S = \sum_{\alpha} \varepsilon_{\alpha} a_{\alpha}^\dagger a_{\alpha}$ in the energy eigenbasis. Similarly, the Hamiltonian of multiple reservoirs can also be written as $H_R = \sum_{\alpha} H_{R,\alpha} = \sum_{\alpha k} \varepsilon_{\alpha k} b_{\alpha k}^\dagger b_{\alpha k}$, where the index $\alpha$ denotes different reservoirs with spectrum $\varepsilon_{\alpha k}$ which must be continuous. The basic process characterizing exchanges of energies, particles and informations between the system and reservoirs is $H_{gs} = \sum_{\alpha k} \left( V_{\alpha k} a_{\alpha k}^\dagger b_{\alpha k} + V_{\alpha k}^\ast b_{\alpha k}^\dagger a_{\alpha k} \right)$. Thus, the total Hamiltonian $H = H_s + H_R + H_{gs}$ is a generalized Fano-Anderson Hamiltonian [61] [64] [65] which has been widely used in nuclear, atomic and optical systems as well as in condensed matter physics [75] [76].

We have derived the exact master equation of the above open systems [54] [57]. The result is indeed a generalization of Eq. (1)

$$\frac{d}{dt}\rho_s(t) = -i[H_s(t), \rho_s(t)] + \sum_{ij} \left( \gamma_{ij}(t, t_0) [2a_{i}^\dagger \rho_s(t) a_{i}^\dagger - a_{i}^\dagger a_{i} \rho_s(t) - \rho_s(t) a_{i}^\dagger a_{i} + \gamma_{ij}(t, t_0) [a_{i}^\dagger \rho_s(t) a_{j} + a_{i} a_{j}^\dagger \rho_s(t) - \rho_s(t) a_{j} a_{i}^\dagger] \right) \quad (14)$$

where the upper and lower signs correspond respectively to the bosonic and fermionic cases, $H_s(t) = \sum_{ij} \varepsilon_{ij}(t, t_0) a_{i}^\dagger a_{j}$ is the renormalized system Hamiltonian; $\gamma_{ij}(t, t_0)$ and $\tilde{\gamma}_{ij}(t, t_0)$ characterize the dissipation and fluctuations induced by reservoirs: $i\varepsilon_{ij}(t, t_0) + \gamma_{ij}(t, t_0) = -[\mathbf{u}(t, t_0) \mathbf{u}^{-1}(t, t_0)]_{1j}$, $\tilde{\gamma}_{ij}(t, t_0) = \delta_{ij}(t) - [\mathbf{u}(t, t_0) \mathbf{u}^{-1}(t, t_0) \mathbf{v}(t, t) + \mathbf{h}(t)]_{ij}$. They are all determined by Green function $\mathbf{u}_{ij}(t, t_0) \equiv \langle [a_{i}(t), a_{j}^\dagger(t_0)] \rangle$ obeying the time-convolution Dyson equation:

$$\frac{d}{dt}\mathbf{u}(t, t) = i\mathbf{\epsilon}(t, t_0) + \int_{t_0}^{t} dt' \mathbf{g}(t, t') \mathbf{u}(t', t_0), \quad t > t_0 \to 0, \quad (15)$$

and $\mathbf{u}(t, t)$ obeying the fluctuation-dissipation relation [54]: $\mathbf{v}(t, t) = \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \mathbf{u}(t, t_1) \mathbf{g}(t_1, t_2) \mathbf{u}(t_2, t)$. The integral kernels $\mathbf{g}(t, t') = \sum_{\alpha} \mathbf{d}(\mathbf{J}_{\alpha}(t) e^{-i\epsilon(t-t')}), \tilde{\mathbf{g}}(t, t') = \sum_{\alpha} \mathbf{d}(\mathbf{J}_{\alpha}(t) e^{-i\epsilon(t-t')}), \mathbf{J}_{\alpha}(t) = \sum_{\alpha k} V_{\alpha k} V_{\alpha k}^\ast \delta(\epsilon - \epsilon_{\alpha k})$ is the spectral density associated with reservoir $\alpha$, and $\mathbf{f}(\epsilon, t_0, \mu_\alpha) = 1/\epsilon^{-\mu_\alpha}/k_B T_0 + 1$ is the bosonic or fermionic distribution with chemical potential $\mu_\alpha$ and temperature $T_0$ at initial time $t = t_0$.

The exact solution of Eq. (14) has recently been solved [27] [38] and its steady state (see Supplemental Materials [74])

$$\rho_s(t \to \infty) = \frac{1}{\det(I + \frac{\mathbf{n}}{I + \mathbf{a}})} \exp \left( \mathbf{a} \ln \frac{\mathbf{n}}{I + \mathbf{a}} \right) \quad (16)$$

which is again a Gibbs state. Here the one-column matrix $\mathbf{a} \equiv (a_{1}^\dagger, a_{2}^\dagger, a_{3}^\dagger, \cdots)$, $\mathbf{n}_{ij} = \lim_{t \to \infty} \mathbf{T}_{ij}(\rho_s(t) a_{i}^\dagger a_{j})$. This solution remains the same for initial system-reservoir correlated states [58] [63]. Thus, the nonequilibrium internal
energy, entropy and particle number can be determined

\[ E(t) = \text{Tr}_s[H_s^r(t)\rho_s(t)], \]
\[ S(t) = -k_B \text{Tr}_s[\rho_s(t) \ln \rho_s(t)], \]
\[ N(t) = \text{Tr}_s[\mathbf{a}^\dagger \mathbf{a} \rho_s(t)]. \]

(17)

and they are related to each other and form the fundamental

equation of quantum thermodynamics [53 70]:

\[ E(t) = E(\varepsilon_i^r(t), S(t), N(t)). \]

Here energy levels play a similar role as the volume [73]. Thus,

\[ dE(t) = dW + T'(t) dS(t) + \mu'(t) dN(t). \]

(18)

Quantum work \(dW(t)\) done on the system is the changes of energy levels without the changes of both particle distributions in levels and the average particle number,

\[ dW(t) = \text{Tr}_s[\rho_s(t) dH_s^r(t)] = \sum_{ij} n_{ij}(t) d\varepsilon_{s,ij}(t), \]

(19)

where \(n_{ij}(t) = \text{Tr}_s[a_i^\dagger a_j \rho_s(t)]\). Quantum heat \(dQ(t)\) (chemical work \(dW_c(t)\)) are the changes of particle distributions without the changes of energy levels and average particle number (entropy),

\[ dQ(t) + dW_c(t) = \text{Tr}_s[H_s^r(t) d\rho_s(t)] = \sum_{ij} \varepsilon_{s,ij}(t) d\mathbf{n}_{ij}(t) = T'(t) dS(t) + \mu'(t) dN(t). \]

(20)

Thus, the renormalized temperature and chemical potential are given by

\[ T'(t) = \frac{\partial E(t)}{\partial S(t)} \varepsilon_{s}(t, N(t)), \quad \mu'(t) = \frac{\partial E(t)}{\partial N(t)} \varepsilon_{s}(t, S(t)). \]

(21)

In shows that \(d\mathbf{n}_{ij}(t)\) characterizes both the state information exchanges (entropy production) and the matter exchanges (chemical process for massive particles) between the systems and the reservoir. For photon or phonon systems, particle number is the number of quantum energy \(\hbar \omega\) so that \(\mu'(t) = 0\). Now, Eq. (16) can be also expressed as

\[ \rho_s(t \rightarrow \infty) = \frac{1}{Z} \exp \left\{ -\beta'(H_s^r - \mu'a^\dagger a) \right\} \]

(22)

with the renormalized Hamiltonian \(H_s^r(t)\), temperature \(T'(t)\) and chemical potential \(\mu'(t)\) at steady-state limit \(t \rightarrow \infty\). Because the exact solution of the steady state is a Gibbs state, thermodynamic laws are all retained. This completes our formulation of quantum thermodynamics for arbitrary coupling.

In the last, we consider a fermionic system, a single electron transistor made of a quantum dot coupled to a source and a drain, the two leads which are treated as two reservoirs [53 66] 77], also see the Supplemental Materials [73]. The total Hamiltonian is

\[ H = \sum_{\sigma,\sigma',k} \varepsilon_{\sigma} a_{\sigma \sigma'}^\dagger a_{\sigma \sigma'} + \sum_{\sigma,\sigma',k} \varepsilon_{\sigma} b_{\sigma \sigma'}^\dagger b_{\sigma \sigma'} + \sum_{\sigma,\sigma',k} (V_{\sigma \omega} b_{\sigma \omega}^\dagger b_{\sigma' \omega} + V_{\sigma' \omega} b_{\sigma' \omega}^\dagger b_{\sigma \omega}). \]

Here \(\sigma = \uparrow, \downarrow\) label electron spin states, \(\alpha = L, R\) label the left and right leads. The two leads are setup initially in thermal states with different initial temperatures and chemical potentials \(T_{L,R}\) and \(\mu_{L,R}\). Let \(|0\rangle, |1\rangle, |2\rangle, |3\rangle\) (the empty state, the spin up and down states and the double occupied state, respectively) be the basis of the 4-dim dot Hilbert space. If the dot is initially empty, the 4 × 4 reduced density matrix solved from the exact master equation is [73 79]:

\[ \rho_{\alpha}(t) = \det[I - \mathbf{v}(t, t)], \]
\[ \rho_{ii}(t) = \nu_i(t) - \rho_{33}(t) (i = 1, 2), \]
\[ \rho_{12}(t) = \nu_{12}(t) = \rho_{21}(t), \]
\[ \rho_{33} = \det[\mathbf{u}], \]
and other matrix elements are zero, where \(\mathbf{u} = \mathbf{v}(t, t)\), see after Eq. (15).

The spectral densities \(J_{\sigma}(t)\) which characterize system-reservoir couplings and reservoir spectra take a Lorentzian form [55 80–83]:

\[ J_{\sigma,ij}(t) = \Gamma_{t} 2 |\varepsilon_{\sigma} - \varepsilon_{\sigma'}|/k_B T_{\sigma}^* + 1 \]

with the exact solution of the occupation numbers \(\pi_{\sigma,ij}(t \rightarrow \infty)\), they are completely the same. This provides again a consistent test of the formulation for fermionic systems.

\[ \text{FIG. 3: (a) The renormalized energy levels } \varepsilon_{s,ij}^c,\text{ temperature } T^* \text{ and chemical potential } \mu^* \text{ and (b) the comparison of Fermi-Dirac distribution } f(\varepsilon_{s,ij}^c, T^*, \mu^*) \text{ with the exact solution of the } \pi_{s,ij}^c(t \rightarrow \infty) \text{ as a function of the coupling strength } \Gamma. \text{ Other parameters: } \varepsilon_{\uparrow} = 3 \varepsilon_{\downarrow}, k_B T_{L,R} = (3, 0.1) \varepsilon_{\downarrow}, \mu_{L,R} = (5, 2) \varepsilon_{\downarrow}, \text{ and } d = 10 \varepsilon_{\downarrow}.\]

In conclusion, we build the strong coupling quantum thermodynamics based on the exact solution for a class of open quantum systems. The Hamiltonian of systems and the temperature (also the chemical potentials for massive particles) must be renormalized at strong coupling. The Hamiltonian renormalization can be systematically determined from the Dyson equation Eq. (15). The temperature (or chemical potential) renormalization is axiomatically determined form the changes of the renormalized internal energy with respect to the von Neumann entropy (or average particle number) of the systems. They can be generalized to other open systems. We also show that the steady state of systems is given by the standard Gibbs state in terms of the renormalized Hamiltonian, temperature and chemical potentials. The results are justified with a criterion that the exact steady-state solution of particle distributions obey the Bose-Einstein distribution and the Fermi-Dirac distribution only for the renormalized energy, temperature and chemical potential.

This work is supported by Ministry of Science and Technology of Taiwan, Republic of China under Contract No. MOST-108-2112-M-006-009-MY3.
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