Emergence of quantum hydrodynamic sound mode of a quantum Brownian particle in a one-dimensional molecular chain

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We have theoretically investigated a long-time transport process of a quantum Brownian particle interacting with a thermal phonon field in a one-dimensional molecular chain. A kinetic equation is derived from a quantum Liouville equation in a weak-coupling case by applying a complex spectral representation of Liouvillean. Due to a characteristic Poincaré resonance for a quantum one-dimensional system, there are an infinite number of degeneracy for collision invariants. In the hydrodynamic situation, the degeneracy is lifted by the first order of perturbation of the flow term, resulting in a new hydrodynamic mode, i.e., quantum hydrodynamic sound mode. It is found that the time evolution of the quantum hydrodynamic sound mode obeys a macroscopic linear wave equation for the probability distribution of the quantum particle. It is remarkable that the stability of the wave packet of the sound wave increases as temperature increases. As a demonstration, the sound wave of the minimum uncertainty wave packet is theoretically analyzed.

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I. INTRODUCTION

Recent developments of ultrafast spectroscopy have allowed to measure an early stage of the relaxation process of excitons in semiconductors[1–8] and molecules,[9–11] and stimulate the theoretical analysis of the non-Markovian effect of short-time relaxation process of open quantum systems[12–14] based on the kinetic equation for the nonequilibrium quantum Brownian motion.[15–20] However, there remain a lot of interesting phenomena for long-time Markovian relaxation process yet to be analyzed by quantum kinetic theory such as the spectrum of the collision operator for spatially homogeneous systems, quantum hydrodynamic modes for inhomogeneous systems, and so on.

In this paper we will show that the quantum hydrodynamic sound modes may exist in a one-dimensional molecular chain in which a quantum particle is interacting with a thermally equilibrated acoustic-phonon field. The present system may represent the transport of a vibrational excitation (a vibron) in a molecular chain.[21–28]

We will derive a quantum kinetic equation for these systems on the basis of complex spectral representation of the quantum Liouville operator that gives a microscopic foundation of the irreversible kinetic theory.[29,30] We will show that the one dimensionality of the system is essential to allow the quantum hydrodynamic sound mode. Indeed, only for the one-dimensional case, the collision invariants of the collision operator of the homogeneous kinetic equation have a degeneracy. As is well known, the degeneracy of the collision invariants is lifted by the flow term in the inhomogeneous kinetic equation resulting in the macroscopic transport mode such as sound wave and diffusion mode in hydrodynamic situation where the length scale of the spatial inhomogeneity is longer than the mean-free path of the particle.[31,32] In our system, we will see that the degeneracy of the collision invariants is also lifted by the first-order perturbation in terms of the flow term so that a quantum sound wave transport appears in addition to the diffusion mode. This is the main result of the present work. Our result is quite contrast to the result of the conventional kinetic theory of the quantum Brownian motion which is based on stochastic approximation: Only the diffusion mode is allowed to appear as a macroscopic transport mode in the conventional kinetic theory.[33–43]

The time evolution of this sound wave obeys a macroscopic linear wave equation for the probability itself and not for the probability amplitude. This sound wave is macroscopic because the wave equation represents a collective motion over macroscopic length much greater than a mean-free length. As in the usual case, the quantum hydrodynamic sound wave becomes more stable as temperature rises since this sound wave is caused by the interaction with thermal phonon field. But this remarkable fact is counterintuitive since the random collision with the thermal phonon might disturb the coherent motion.

In Sec. II we present a model Hamiltonian which describes a system where a quantum particle is weakly coupled with a thermally equilibrated acoustic-phonon field in one-dimensional molecular chain. In Sec. III, we derive a kinetic equation for a momentum distribution for the quantum particle by applying a complex spectral representation of the Liouvillean. We will see that the resonance condition for the one-dimensional system leads to an infinite number of collision invariants. In Sec. IV, a kinetic equation for the spatially inhomogeneous distribution is investigated. We reveal that the quantum sound wave arises as a macroscopic transport mode as a result that the degeneracy of the collision invariants is removed by the flow term. The time evolution of the sound wave following the macroscopic wave equation is demonstrated to show the stability of the sound wave compared to the free motion. Section V is devoted to some discussions, where a relaxation time and velocity of the kinetic sound wave are evaluated for concrete systems. Short summary of the complex spectral representation is presented in Appendix B following the brief summary of the Liouville-space representation in Appendix A. The classical limit of

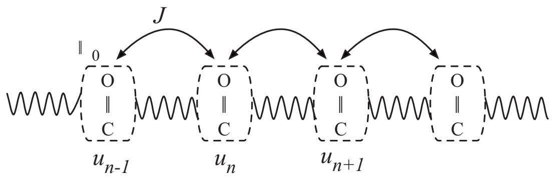

FIG. 1. One-dimensional molecular chain.

the kinetic equation is discussed in Appendix D. In the high-temperature case, the eigenvalue problem of the collision operator is solved analytically, which is shown in Appendix E.

II. MODEL

In this paper, we will discuss a characteristic feature of the kinetic equation for one-dimensional quantum system that leads to quantum hydrodynamic sound wave. As a working example of the one-dimensional quantum system, we will consider here the Davydov Hamiltonian that is a simple model for a molecular chain.[22] In this system, an intramolecular vibration, such as C=O vibration, transfers along the chain due to the dipole-dipole interactions, forming a vibrational exciton (a vibron), and a vibron is weakly interacting with a longitudinal-acoustic phonon of a backbone molecular chain. The physical situation is schematically shown in Fig. 1.[22–28] Then the Hamiltonian is given by[22]

$$H = \sum_n E_0 B_n^\dagger B_n - J\sum_n (B_{n+1}^\dagger B_n + B_n^\dagger B_{n+1}) + \sum_q \hbar\omega_q b_q^\dagger b_q + g\chi \sum_n B_n^\dagger B_n (u_{n+1} - u_{n-1}). \tag{1}$$

Here, B_n is annihilation operator for an intramolecular vibration with a high frequency $E_0/\hbar$ at site n and J denotes the dipole-dipole interaction between the intramolecular vibrations, and b_q is annihilation operator of the acoustic molecular lattice phonon with $\omega_q = c|q|$. The fourth term represents the vibron-phonon coupling due to the modulation of the on-site energy by the molecular displacements, where g is a dimensionless coupling constant. The molecular displacement u_n may be written in terms of the normal mode

$$u_n = \sum_q \sqrt{\frac{\hbar}{2L\rho_M \omega_q}} (b_q + b_{-q}^\dagger) e^{iqnd}, \tag{2}$$

where d is a lattice constant, L is the length of the chain, and ρ_M is the molecular mass density.

Since H conserves the number of a vibron quanta, we restrict ourselves to the single vibron subspace. By transformation to the momentum representation

$$|p\rangle \equiv \frac{1}{\sqrt{(L/d)}} \sum_p \exp\left(\frac{ipdn}{\hbar}\right) B_n^\dagger |vac\rangle, \tag{3}$$

where $|vac\rangle$ denotes the vacuum state for the vibron, the total Hamiltonian H in Eq. (1) is rewritten as

$$H = H_0 + gH_{\rm int}, \tag{4}$$

where

$$H_0 = \sum_p \varepsilon_p |p\rangle\langle p| + \sum_q \hbar\omega_q b_q^\dagger b_q, \tag{5}$$

$$H_{\rm int} = \frac{1}{\sqrt{\Omega}} \sum_{p,q} V_q |p + \hbar q\rangle\langle p| (b_q + b_{-q}^\dagger), \tag{6}$$

with $\Omega \equiv L/2\pi$. The vibron energy ε_p in Eq. (5) is given by

$$\varepsilon_p = E_0 - 2J\cos\left(\frac{pd}{\hbar}\right). \tag{7}$$

In this paper, we consider the long wavelength situation of $pd/\hbar \ll 1$, where ε_p is assumed to be

$$\varepsilon_p \simeq J\left(\frac{pd}{\hbar}\right)^2 \equiv \frac{p^2}{2m}, \tag{8}$$

aside from a constant $E_0 - 2J$. Therefore the vibron behaves as a free quantum particle with the effective mass

$$m = \frac{\hbar^2}{2Jd^2}. \tag{9}$$

In Eq. (6) the coupling constant V_q is given in the long-wavelength situation by

$$V_q = \Delta_0 |q| \sqrt{\frac{\hbar}{4\pi\rho_M\omega_q}}, \tag{10}$$

with $\Delta_0 \equiv 2i\chi d$. We impose a periodic boundary condition leading to the discrete momenta and wave numbers with $p/\hbar$, $q = 2\pi j/L$, respectively, where $j = 0, \pm 1, \pm 2, \ldots$. The model Hamiltonian (4) together with Eqs. (5) and (6) has also been used to describe a free electron coupling with acoustic-phonon field through the deformation-potential interaction in semiconductors.[44–46]

The time evolution of the density matrix $\rho(t)$ of the total system obeys the quantum Liouville equation

$$i\frac{\partial}{\partial t}\rho(t) = \mathcal{L}\rho(t), \tag{11}$$

where the Liouvillean $\mathcal{L}$ is defined by $\mathcal{L}\rho \equiv [H, \rho]/\hbar$.

We focus on the time evolution of the reduced density matrix of the particle defined by

$$f(t) \equiv {\rm Tr}_{\rm ph}[\rho(t)], \tag{12}$$

where ${\rm Tr}_{\rm ph}$ means the partial trace over the phonon states. We assume that in the initial state the phonon system is in thermal equilibrium represented by

$$\rho_{\rm ph}^{\rm eq} = \frac{1}{Z_{\rm ph}} \exp\left[-\sum_q \beta\hbar\omega_q b_q^\dagger b_q\right], \tag{13}$$

with a phonon partition function

$$Z_{\rm ph} \equiv \prod_q (1 - \exp[-\beta\hbar\omega_q])^{-1}, \tag{14}$$

where $\beta \equiv 1/k_B T$ with the Boltzmann constant k_B. Note that the time evolution of the phonon distribution $\rho_{\rm ph}$ deviated from the thermal equilibrium is proportional to $1/L$ so that the deviation from the phonon equilibrium is neglected in a large system $L \gg 1$.[40]

The reduced density operator of the particle may be represented by the eigenvectors of the unperturbed particle Hamiltonian, $f_{p,p'}(t) \equiv \sqrt{\Omega}\langle p|f(t)|p'\rangle$, where $\sqrt{\Omega}$ comes from the normalization in the representation of the Wigner basis. (see Appendix A) We shall instead express the reduced density operator in terms of "Wigner representation" in the momentum space of the particle[30,40,47],

$$f_k(P,t) \equiv \langle\langle k,P|f(t)\rangle\rangle = \sqrt{\Omega}\langle P+\hbar k/2|f(t)|P-\hbar k/2\rangle, \tag{15}$$

where $|f(t)\rangle\rangle$ stands for a vector in the Liouville space. The inner product in the Liouville space is defined by $\langle\langle A|B\rangle\rangle \equiv \mathrm{Tr}[A^\dagger B]$, where A and B are any Hilbert operators of the particle. The Wigner basis $|k,P\rangle\rangle$ is defined by $|k,P\rangle\rangle \equiv \sqrt{\Omega}|P+\hbar k/2\rangle\langle P-\hbar k/2|$. (see Appendix A) The representation of a density matrix in the Liouville space is summarized in Appendix A.

The Fourier transform of $f_k(P,t)$ for k gives the Wigner function in phase space

$$f^W(X,P,t) \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} f_k(P,t)\exp[ikX]dk. \tag{16}$$

The Fourier component of $f_0(P,t)$ represents a homogeneous component of the distribution while $k\neq 0$ component represents an inhomogeneous component in space.

We consider such a large system that the wave number can be regarded as a continuous variable. We will take a continuous limit $L\to\infty$ in appropriate places. However, as far as P variables are concerned, there is no confusion to take $L\to\infty$ limit at this stage. Hence, hereafter we will use a notation for P of

$$\frac{1}{\Omega}\sum_P \to \int dP, \quad \Omega\delta^{Kr}_{P,P'} \to \delta(P-P'). \tag{17}$$

III. KINETIC EQUATION OF MOMENTUM DISTRIBUTION

The equation of motion of the reduced distribution function $f_k(P,t)$ is obtained by using the complex spectral representation of the Liouvillean as shown in Appendices B and C.[30] The collision operator, which is the time-evolution generator of the equation of motion of $f_k(P,t)$, is evaluated up to the second order of the interaction in the weak-coupling case. The kinetic equation thus derived is the same as obtained by taking a so-called g^2t approximation.[47,48] In this section we consider the time evolution of the momentum distribution with $k=0$ component $f_0(P,t)$ in Eq. (15).

The kinetic equation of the reduced distribution $|f(t)\rangle\rangle$ is given in Eq. (C6). By taking $k=0$, we have

$$i\frac{\partial}{\partial t}\hat{P}^{(0)}|f(t)\rangle\rangle = \hat{\bar{\Psi}}_2^{(0)}(+i0)\hat{P}^{(0)}|f(t)\rangle\rangle, \tag{18}$$

where $P^{(k)}$ is the projection operator onto the k component of the particle defined by $P^{(k)} \equiv \int dP|k,P\rangle\rangle\langle\langle k,P|$. By multiplying $\langle\langle 0,P|$ from the left, we obtain

$$\frac{\partial}{\partial t}f_0(P,t) = \hat{\mathcal{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right)f_0(P,t), \tag{19}$$

where $\hat{\mathcal{K}}^{(0)}(P,\partial/\partial P)$ is expressed as a matrix element of the collision operator $\hat{\bar{\Psi}}_2^{(0)}$ given in Eq. (C5) (See Appendix C for a derivation),

$$\langle\langle 0,P|\hat{\bar{\Psi}}_2^{(0)}|0,P'\rangle\rangle = g^2\langle\langle 0,P|\mathrm{Tr}_{\mathrm{ph}}\left[\hat{P}^{(0,0)}\mathcal{L}_{\mathrm{int}}\hat{Q}^{(0,0)}\frac{1}{i0^+-\mathcal{L}_0}\hat{Q}^{(0,0)}\mathcal{L}_{\mathrm{int}}\hat{P}^{(0,0)}\rho^{\mathrm{eq}}_{\mathrm{ph}}\right]|0,P'\rangle\rangle \equiv i\langle\langle 0,P|\hat{\mathcal{K}}^{(0)}|0,P'\rangle\rangle$$
$$\equiv i\hat{\mathcal{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\delta(P-P'). \tag{20}$$

In Eq. (20) $\mathcal{L}_0$ is the unperturbed Liouvillean and $\mathcal{L}_{\mathrm{int}}$ is the interaction part of the Liouvillean, corresponding to H_0 in Eq. (5) and H_{int} in Eq. (6), respectively. The superoperator $\hat{P}^{(0,0)}$ denotes the projection operator for the density matrix onto the $k=0$ component of the particle and $\nu=0$ component of the phonon field, as defined in Eq. (B2). The superoperator $\hat{Q}^{(0,0)}=1-\hat{P}^{(0,0)}$ is the projection operator complement to $\hat{P}^{(0,0)}$. Since $\mathcal{L}_0$ has continuous spectrum for large $L\gg 1$, the Poincaré resonance occurs in Eq. (20), letting the system nonintegrable and irreversible.[30]

The explicit form of the collision operator $\hat{\mathcal{K}}^{(0)}$ is obtained by calculating Eq. (20) for the present case Eq. (4) and is given by

$$\hat{\mathcal{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right) = -\frac{2\pi g^2}{\hbar^2}\int dq|V_q|^2\left\{\delta\left(\frac{\varepsilon_P-\varepsilon_{P+\hbar q}}{\hbar}+\omega_q\right)n(q)\right.$$
$$\left.+\delta\left(\frac{\varepsilon_{P-\hbar q}-\varepsilon_P}{\hbar}+\omega_q\right)[n(q)+1]\right\}$$
$$+\frac{2\pi g^2}{\hbar^2}\int dq|V_q|^2\left\{\delta\left(\frac{\varepsilon_{P-\hbar q}-\varepsilon_P}{\hbar}+\omega_q\right)n(q)\right.$$
$$\times\exp\left[-\hbar q\frac{\partial}{\partial P}\right]$$
$$+\delta\left(\frac{\varepsilon_P-\varepsilon_{P+\hbar q}}{\hbar}+\omega_q\right)[n(q)+1]$$

$$\times \exp\left[\hbar q \frac{\partial}{\partial P}\right]\Bigg\}, \tag{21}$$

where $n(q)$ denotes the Planck's distribution

$$n(q) \equiv \frac{1}{\exp[\beta\hbar\omega_q]-1}, \tag{22}$$

and $\exp[\pm\hbar q\,\partial/\partial P]f(P)=f(P\pm\hbar q)$.

In $\hat{\mathcal{K}}^{(0)}$, the delta function represents the quantum-mechanical resonance indicating both the energy and the momentum conservations in the elementary collision process between the quantum Brownian particle and a phonon.

Let us recall that the well-known fact that the collision operator of the kinetic equation for the classical one-dimensional gas vanishes in the weak-coupling case because the Fourier component of the interaction potential V_q vanishes at the resonance point given by the argument of the delta function, in spite of the fact that the corresponding collision operator for the quantum one-dimensional gas does not vanish.[47] It is interesting that a similar phenomena occurs in our system, i.e., $\hat{\mathcal{K}}^{(0)}$ vanishes in the classical limit of $\hbar \to 0$ in Eq. (21), as proven in Appendix D. This means that the dissipation in the present weakly coupled system is a pure quantum effect in the one-dimensional chain.

Now we introduce the following units: $l_u \equiv \hbar/mc$ (length unit), $\varepsilon_u \equiv mc^2$ (energy unit), $t_u \equiv \hbar/mc^2$ (time unit), $p_u \equiv mc$ (momentum unit), and $T_u \equiv mc^2/k_B$ (temperature unit).[45] With these units the energy dispersions of the particle and phonon read $\bar{\varepsilon}_{\bar{p}}=\bar{p}^2/2$ and $\bar{\omega}_{\bar{q}}=|\bar{q}|$, respectively. The interaction potential V_q is rewritten in the dimensionless form as

$$\bar{V}_{\bar{q}} = \bar{\Delta}_0|\bar{q}|\frac{1}{\sqrt{4\pi\bar{\rho}_M\bar{\omega}_{\bar{q}}}}; \quad \bar{\Delta}_0 \equiv \Delta_0/\varepsilon_u. \tag{23}$$

Hereafter we will use the dimensionless unit and omit the sign of the bar for the dimensionless quantities unless necessary.

In order to solve the kinetic Eq. (19) we consider the eigenvalue problem of the collision operator

$$\hat{\mathcal{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\phi_j^{(0)}(P) = \lambda_j^{(0)}\phi_j^{(0)}(P), \tag{24}$$

where (0) denotes $k=0$ component of the distribution; $\phi_j^{(0)}(P)$ is a momentum distribution function.

We shall now introduce a similitude transformation of the distribution function $\phi_j(P)$ with use of $\hat{T}$ as follows:

$$\bar{\bar{\phi}}_j(P) = \hat{T}\phi_j(P) = \varphi_{\rm eq}^{-1/2}(P)\phi_j(P), \tag{25}$$

where $\varphi_{\rm eq}(P)$ is the equilibrium distribution in the dimensionless form

$$\varphi_{\rm eq}(P) = \exp[-\beta\varepsilon_P]\sqrt{\beta/2\pi}. \tag{26}$$

We also introduce the vector notation corresponding to Eq. (25) as

$$|\bar{\bar{\phi}}_j\rangle\rangle = \hat{T}|\phi_j\rangle\rangle, \tag{27}$$

where

$$\langle\langle 0,P|\hat{T}|0,P'\rangle\rangle = \hat{T}\delta(P-P') = \varphi_{\rm eq}^{-1/2}(P)\delta(P-P'). \tag{28}$$

With use of Eqs. (25) and (27), the Hermite conjugate to $|\bar{\bar{\phi}}_j\rangle\rangle$ can be written by

$$\langle\langle\bar{\bar{\phi}}_j|0,P\rangle\rangle = \bar{\bar{\phi}}_j^*(P) = \phi_j^*(P)\varphi_{\rm eq}^{-1/2}(P) = \langle\langle\phi_j|\hat{T}|0,P\rangle\rangle. \tag{29}$$

The collision operator $\hat{K}^{(0)}$ in Eq. (20) is also transformed to $\bar{\bar{K}}^{(0)}$ by $\hat{T}$ as

$$\begin{aligned}\langle\langle 0,P|\bar{\bar{K}}^{(0)}|0,P'\rangle\rangle &\equiv \langle\langle 0,P|\hat{T}\hat{\mathcal{K}}^{(0)}\hat{T}^{-1}|0,P'\rangle\rangle \\ &= \bar{\bar{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\delta(P-P'),\end{aligned} \tag{30}$$

where

$$\bar{\bar{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right) = \varphi_{\rm eq}^{-1/2}(P)\hat{K}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\varphi_{\rm eq}^{1/2}(P). \tag{31}$$

It if found from Eqs. (21), (31), and (30) that $\bar{\bar{K}}^{(0)}$ satisfies Hermiticity,

$$[\langle\langle 0,P|\bar{\bar{K}}^{(0)}|0,P'\rangle\rangle]^* = \langle\langle 0,P'|\bar{\bar{K}}^{(0)}|0,P\rangle\rangle, \tag{32}$$

while $\hat{K}^{(0)}$ is non-Hermitian operator, i.e.,

$$[\langle\langle 0,P|\hat{K}^{(0)}|0,P'\rangle\rangle]^* \neq \langle\langle 0,P'|\hat{K}^{(0)}|0,P\rangle\rangle. \tag{33}$$

In the transformed vector space, the eigenvalue problem [Eq. (24)] reads

$$\bar{\bar{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\bar{\bar{\phi}}_j(P) = \lambda_j^{(0)}\bar{\bar{\phi}}_j(P), \tag{34}$$

where $\lambda_j^{(0)}$ takes a real number. The eigenvectors of the Hermite operator $\bar{\bar{K}}^{(0)}$ form the complete orthonormal basis in the transformed vector space as follows:

$$\begin{aligned}\langle\langle\bar{\bar{\phi}}_i^{(0)}|\bar{\bar{\phi}}_j^{(0)}\rangle\rangle &= \int dP\langle\langle\bar{\bar{\phi}}_i^{(0)}|0,P\rangle\rangle\langle\langle 0,P|\bar{\bar{\phi}}_j^{(0)}\rangle\rangle \\ &= \int \varphi_{\rm eq}^{-1}(P)\phi_i^{(0)*}(P)\phi_j^{(0)}(P)dP = \delta_{i,j}\end{aligned} \tag{35}$$

and

$$\sum_j |\bar{\bar{\phi}}_j\rangle\rangle\langle\langle\bar{\bar{\phi}}_j| = 1, \tag{36}$$

which is alternatively expressed as

$$\sum_j \bar{\bar{\phi}}_j^*(P)\bar{\bar{\phi}}_j(P) = \delta(P-P'). \tag{37}$$

In the original vector space spanned by $\{|\phi_j\rangle\rangle\}$, this closure relation is represented by

$$\sum_j \varphi_{\rm eq}^{-1}(P)\phi_j^*(P)\phi_j(P') = \delta(P-P'). \tag{38}$$

It is readily seen from Eq. (32) that $\bar{\bar{K}}^{(0)}$ satisfies the relation

$$[\langle\langle\bar{\bar{\phi}}_i|\bar{\bar{K}}^{(0)}|\bar{\bar{\phi}}_j\rangle\rangle]^* = \langle\langle\bar{\bar{\phi}}_j|\bar{\bar{K}}^{(0)}|\bar{\bar{\phi}}_i\rangle\rangle, \tag{39}$$

where

$$\langle\langle\bar{\bar{\phi}}_j|\bar{\bar{K}}^{(0)}|\bar{\bar{\phi}}_i\rangle\rangle = \int dP \bar{\bar{\phi}}_j^*(P)\bar{\bar{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\bar{\bar{\phi}}_i(P)$$
$$= \int dP \varphi_{\rm eq}^{-1}(P)\phi_j^*(P)\hat{K}^{(0)}\left(P,\frac{\partial}{\partial P}\right)\phi_i(P). \tag{40}$$

The time evolution of the momentum distribution function is then given by

$$f_0(P,t) = \langle\langle 0,P|f(t)\rangle\rangle = \langle\langle 0,P|\hat{T}^{-1}|\bar{\bar{f}}(t)\rangle\rangle$$
$$= \sum_j e^{\lambda_j^{(0)}t}\phi_j^{(0)}(P)\langle\langle\bar{\bar{\phi}}_j^{(0)}|\bar{\bar{f}}(0)\rangle\rangle, \tag{41}$$

where $|\bar{\bar{f}}(t)\rangle\rangle = \hat{T}|f(t)\rangle\rangle$ defined by Eq. (27).

Calculating $\langle\langle\bar{\bar{\phi}}_j^{(0)}|\bar{\bar{\mathcal{K}}}^{(0)}|\bar{\bar{\phi}}_j^{(0)}\rangle\rangle$ with Eqs. (21) and (40) for the eigenstates, we find

$$\lambda_j^{(0)} = -2\pi g^2\int\int dPdq|V_q|^2\varphi_{\rm eq}^{-1}(P)n(q)\times\delta(\varepsilon_P-\varepsilon_{P+q}+\omega_q)$$
$$\times|\phi_j^{(0)}(P)-e^{\beta\omega_q}\phi_j^{(0)}(P+q)|^2 \le 0, \tag{42}$$

which guarantees the monotonous approach to the steady state for Eq. (19), i.e., the H theorem: All the states but the collision invariant $\phi_0^{(0)}(P)$ with $\lambda_0^{(0)}=0$ exponentially decay. Equation (42) shows that the collision invariant $\phi_0^{(0)}(P)$ should satisfy the detailed balance condition,

$$\phi_0^{(0)}(P) = \exp[\beta\omega_q]\phi_0^{(0)}(P+q), \tag{43}$$

for the value of q determined by the resonance condition represented by the energy delta function.

The delta function for the energy in $\hat{\mathcal{K}}^{(0)}$ representing the resonance effect plays a key role to the emergence of the quantum hydrodynamic sound mode as will be shown below. The states satisfying the resonance condition, $\varepsilon_{P\pm q}-\varepsilon_P = \pm\omega_q$, are obtained by the intersections of the particle and the phonon energy-dispersion curves as shown in Fig. 2(a), where the particle and the phonon dispersions are drawn by the black and the gray lines, respectively. The resonance condition is satisfied for three consecutive states, $|0,P_{0;n-1}\rangle\rangle$, $|0,P_{0;n}\rangle\rangle$, and $|0,P_{0;n+1}\rangle\rangle$ through one phonon absorption or emission process, where

$$P_{0;n} \equiv (-1)^n(P_0-2n) \quad (n=0,\pm1,\pm2,\ldots) \tag{44}$$

with

$$|P_0| \le 1. \tag{45}$$

We can see a sequence of states including a particular state $|0,P_0\rangle\rangle$ with $|P_0|\le 1$ through transitions by the particle-phonon interaction, as shown in Fig. 2(a). An entire momentum space is therefore a summation of an infinite number of disjoint sets of states corresponding to each value of P_0 with $|P_0|\le 1$.

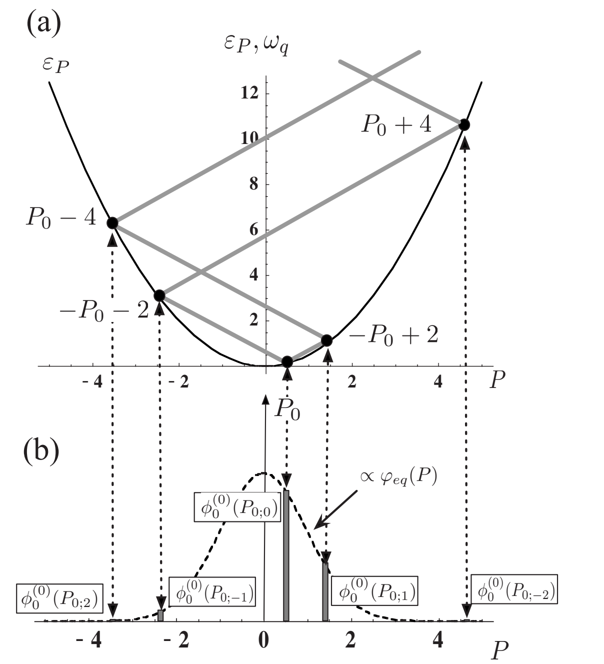

FIG. 2. (a) The states satisfying resonance conditions, where the particle and the phonon dispersions are shown by solid and gray lines, respectively. (b) A distribution of a collision invariant associated with the value of P_0.

As a consequence, there are an infinite number of collision invariants $\phi_0^{(0)}$ corresponding to the disjoint momentum subspaces specifying with a continuous value of P_0 with $|P_0|\le 1$. Considering Eq. (43) and due to the fact that successive states $|0,P_{0;n-1}\rangle\rangle$, $|0,P_{0;n}\rangle\rangle$, and $|0,P_{0;n+1}\rangle\rangle$ satisfy the resonance condition, $\phi_0^{(0)}(P)$ corresponding to a P_0 satisfies that

$$\exp[\beta\varepsilon_{P_{0;n}}]\phi_0^{(0)}(P_{0;n}) = \exp[\beta\varepsilon_{P_{0;n\pm1}}]\phi_0^{(0)}(P_{0;n\pm1}) \tag{46}$$

for any integer n as shown in Fig. 2(b). Taking into account the normalization condition, we can then obtain a collision invariant for a particular disjoint set of states accompanied with P_0 in the form of a probability density as

$$\phi_0^{(0)}(P) = \mathcal{N}_{P_0}^{-1}\sum_n\exp[-\beta\varepsilon_P]\delta(P-P_{0;n}) \equiv \psi_{P_0}(P), \tag{47}$$

where $\mathcal{N}_{P_0}$ is determined by the normalization condition (35) as

$$\mathcal{N}_{P_0} = \left[\sqrt{2\pi/\beta}\sum_n\exp(-\beta\varepsilon_{P_{0;n}})\right]^{1/2}. \tag{48}$$

Both the $\psi_{P_0}(P)$ and $\mathcal{N}_{P_0}$ defined by Eqs. (47) and (48), respectively, are the functions of P_0 through Eq. (44), where P_0 runs from −1 to 1. Replacing P_0 in $\psi_{P_0}(P)$ and $\mathcal{N}_{P_0}$ with $P_{0;n}$ defined by Eq. (44), we find the relation

$$\psi_{P_{0;n}}(P) = \psi_{P_0}(P) \quad \text{and} \quad \mathcal{N}_{P_{0;n}} = \mathcal{N}_{P_0}. \tag{49}$$

This indicates together with Eq. (44) that we can extend the range of P_0 in $\psi_{P_0}(P)$ and $\mathcal{N}_{P_0}$ to the entire range of $-\infty$ to ∞.

Then $\psi_{P_0}(P)$ and $\mathcal{N}_{P_0}$ become the periodic functions of P_0 with the periodicity of 4. [See also Eq. (64)]

The fact that there are an infinite number of collision invariants $\psi_{P_0}(P)$ is a consequence of a strong constraint on the momentum and energy exchange due to the conservation relation. This is quite contrary to the case of an ordinary Brownian particle with a unique collision invariant, where the momentum and energy are freely exchanged with the thermal bath without any constraint.

Now we solve the eigenvalue problem of $\hat{\mathcal{K}}^{(0)}$. Substituting Eq. (21) into Eq. (24), we have the explicit expression of the eigenvalue equation (24) for a given P_0 as a simultaneous equation of $\phi_j(P_{0;n})$ $(n=-\infty,\ldots,-1,0,1,\ldots,\infty)$

$$-[n(P_{0;n+1}-P_{0;n})+n(P_{0;n-1}-P_{0;n})+1]\phi_j(P_{0;n}) + n(P_{0;n}-P_{0;n-1})\phi_j(P_{0;n-1})+[n(P_{0;n}-P_{0;n+1})+1]\phi_j(P_{0;n+1}) = \frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\phi_j(P_{0;n}) \quad (n>0), \tag{50a}$$

$$-[n(P_{0;1}-P_{0;0})+n(P_{0;-1}-P_{0;0})]\phi_j(P_{0;0}) + [n(P_{0;0}-P_{0;-1})+1]\phi_j(P_{0;-1})+[n(P_{0;0}-P_{0;1})+1]\phi_j(P_{0;1}) = \frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\phi_j(P_{0;0}), \tag{50b}$$

$$-[n(P_{0;n-1}-P_{0;n})+n(P_{0;n+1}-P_{0;n})+1]\phi_j(P_{0;n}) + n(P_{0;n}-P_{0;n+1})\phi_j(P_{0;n+1})+[n(P_{0;n}-P_{0;n-1})+1]\phi_j(P_{0;n-1}) = \frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\phi_j(P_{0;n}) \quad (n<0), \tag{50c}$$

where $|\lambda_{j'}^{(0)}|>|\lambda_j^{(0)}|$ for $j'>j$. On the left-hand side of Eq. (50), the first term represents the loss term of $\phi_j(P_{0;n})$, and the second and third terms represent the gain terms of $\phi_j(P_{0;n})$. The Eq. (50) is expressed in the matrix form as

$$\sum_{n'=-\infty}^{\infty}\hat{\mathcal{K}}_{n,n'}^{(0)}\phi_j(P_{0;n'}) = \frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\phi_j(P_{0;n}), \tag{51}$$

where $\hat{\mathcal{K}}_{n,n'}^{(0)}=\langle\langle 0,P_{0;n}|\hat{\mathcal{K}}^{(0)}|0,P_{0;n'}\rangle\rangle$ which is a non-Hermitian tridiagonal matrix. The non-Hermitian tridiagonal matrix $\hat{\mathcal{K}}_{n,n'}^{(0)}$ is cast into a Hermitian tridiagonal matrix $\bar{\bar{\mathcal{K}}}_{n,n'}^{(0)}$ by the similitude transformation defined by Eq. (30) as

$$\bar{\bar{\mathcal{K}}}_{n,n'}^{(0)} \equiv \langle\langle 0,P_{0;n}|\bar{\bar{K}}^{(0)}|0,P_{0;n'}\rangle\rangle = \langle\langle 0,P_{0;n}|\hat{T}\hat{\mathcal{K}}^{(0)}\hat{T}^{-1}|0,P_{0;n'}\rangle\rangle = [\varphi_{\rm eq}(P_{0;n})]^{-1/2}\hat{\mathcal{K}}_{n,n'}^{(0)}[\varphi_{\rm eq}(P_{0;n'})]^{1/2}, \tag{52}$$

where the spectrum of $\bar{\bar{\mathcal{K}}}^{(0)}$ is identical with that of $\hat{\mathcal{K}}^{(0)}$. In order to diagonalize rigorously the Hermitian matrix $\bar{\bar{\mathcal{K}}}_{n,n'}^{(0)}$, we have to use an infinite set of basis states $\{|0;P_{0;n}\rangle\rangle\}$ $(n=-\infty,\ldots,\infty)$. However, we can approximately diagonalize in numerical calculation using enough number of the basis states $\{|0;P_{0;n}\rangle\rangle\}$. The Hermitian matrix of $\bar{\bar{\mathcal{K}}}^{(0)}$ is numerically diagonalized among enough number of basis states of $\{|0;P_{0;n}\rangle\rangle\}$ for the eigenvalues to converge.

The spectrum of $\hat{\mathcal{K}}^{(0)}$ is obtained by numerically solving the eigenvalue problem in terms of the continued fraction method.[49] In Fig. 3, we display the spectrum of $\hat{\mathcal{K}}^{(0)}$ for several temperatures, where $P_0=0.5$ is used. It is found that the spectrum of $\hat{\mathcal{K}}^{(0)}$ is discrete. The discreteness of the spectrum ensures the existence of the local equilibrium (hence the hydrodynamic modes) in the present one-dimensional system.[31] It is found that all the values of $\lambda_j^{(0)}$ depend on the value of P_0, except for the collision invariants $\psi_{P_0}(P)$ with $\lambda_0^{(0)}=0$. However, the dependence of $\lambda_j^{(0)}$ for $j\neq 0$ on P_0 is very weak for $\lambda_j^{(0)}<1$.

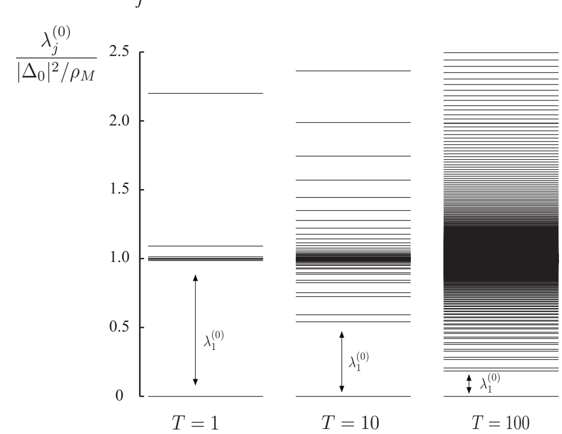

FIG. 3. The spectrum of $\hat{\mathcal{K}}^{(0)}$ for the effective temperatures, $T=1$, 10, and 100. $P_0=0.5$ is used.

The quantity $t_r \equiv 1/|\lambda_1^{(0)}|$ determines the relaxation time taken for the system to relax into the steady state by the random collision with the thermal phonon field, where $|\lambda_1^{(0)}|$ is the lowest nonvanishing eigenvalue of $\hat{\mathcal{K}}^{(0)}$. We have shown in Appendix E that $|\lambda_1^{(0)}|$ is proportional to the coupling potential $|\Delta_0|^2$, and $1/\sqrt{T}$ for $T \gg 1$.

IV. QUANTUM HYDRODYNAMIC SOUND WAVE

Now we turn our attention to the time evolution of spatially inhomogeneous distribution $f_k(P,t)$ with $k \neq 0$. The time evolution obeys the kinetic equation which is derived by the complex spectral representation method as shown in Appendix C. The kinetic equation for the reduced distribution $|f(t)\rangle\rangle$ is given in Eq. (C6),

$$i\frac{\partial}{\partial t}\hat{P}^{(k)}|f(t)\rangle\rangle = \hat{\bar{\bar{\Psi}}}_2^{(k)}(w_{kP}+i0)\hat{P}^{(k)}|f(t)\rangle\rangle. \tag{53}$$

By multiplying $\langle\langle k,P|$ from the left, we have

$$\frac{\partial}{\partial t}f_k(P,t) = \hat{\mathcal{K}}^{(k)}\left(P,\frac{\partial}{\partial P}\right)f_k(P,t), \tag{54}$$

where $\hat{\mathcal{K}}^{(k)}(P,\partial/\partial P)$ is expressed as a matrix element of the collision operator $\hat{\bar{\bar{\Psi}}}_2^{(k)}(w_{kP}+i0)$ as given in Eq. (C5),

$$\langle\langle k,P|\hat{\bar{\bar{\Psi}}}_2^{(k)}(w_{kP}+i0)|k,P'\rangle\rangle = w_{kP} + g^2\langle\langle k,P|\mathrm{Tr}_{\mathrm{ph}}\left[\hat{P}^{(k,0)}\mathcal{L}_{\mathrm{int}}\hat{Q}^{(k,0)}\frac{1}{w_{kP}+i0-\mathcal{L}_0}\hat{Q}^{(k,0)}\mathcal{L}_{\mathrm{int}}\hat{P}^{(k,0)}\rho_{\mathrm{ph}}^{\mathrm{eq}}\right]|k,P'\rangle\rangle = i\langle\langle k,P|\hat{\mathcal{K}}^{(k)}|k,P'\rangle\rangle$$
$$\equiv i\hat{\mathcal{K}}^{(k)}\left(P,\frac{\partial}{\partial P}\right)\delta(P-P'). \tag{55}$$

The explicit expression of $\hat{\mathcal{K}}^{(k)}(P,\partial/\partial P)$ for the present model is given by Eq. (C9).

In this section we consider the inhomogeneous distribution whose space variation is so slow that the range of inhomogeneity measured by $L_h = 1/|k|$ is far larger than the mean-free length inversely proportional to the relaxation time $L_r = 1/t_r$, i.e., we consider the time evolution of $f_k(P,t)$ for $|k| \ll |\lambda_1^{(0)}|$ which corresponds to $c|k| \ll |\lambda_1^{(0)}|$ with dimension unit. It is only in this case that the phenomenological concepts in hydrodynamics, such as sound modes, diffusion modes, etc., have a microscopic dynamical justification.[31,47] In this case, the denominator of the resolvent in Eq. (C9) can be approximated as follows:

$$w_{kP} + i0 - (w_{k-q,P-q/2} + \omega_q) = \frac{q}{2}(k-q) + qP - \omega_q + i0 \tag{56a}$$

$$\simeq -\frac{q^2}{2} + qP - \omega_q + i0 \tag{56b}$$

$$= i0 - (w_{-q,P-q/2} + \omega_q), \tag{56c}$$

where we have assumed $k \ll q$ in Eq. (56b). This assumption is justified in the hydrodynamic situation because the interaction potential V_q given by Eq. (10) is a short-range potential with an interaction range determined by $1/q$ which is much smaller than the macroscopic spatial range $1/k$ to be concerned. The neglect of the k dependence of the resolvent in Eq. (55) can approximate $\hat{\mathcal{K}}^{(k)}$ as

$$\hat{\mathcal{K}}^{(k)}\left(P,\frac{\partial}{\partial P}\right) \simeq -ikP + \hat{\mathcal{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right), \tag{57}$$

with the collision operator $\hat{\mathcal{K}}^{(0)}(P,\partial/\partial P)$ of the homogeneous distribution given in Eq. (21).

The eigenvalue problem corresponding to Eq. (54) is now written by

$$\left[\hat{\mathcal{K}}^{(0)}\left(P,\frac{\partial}{\partial P}\right) - ikP\right]\phi_j^{(k)}(P) = \lambda_j^{(k)}\phi_j^{(k)}(P). \tag{58}$$

We note that $\hat{\mathcal{K}}^{(0)}$ does not commute with ikP since $\hat{\mathcal{K}}^{(0)}$ involves $\partial/\partial P$ seen in Eq. (21). By using the same similitude transformation as in Eqs. (27) and (30), we rewrite the eigenvalue problem (58) as

$$\left[\bar{\bar{\mathcal{K}}}^{(0)}\left(P,\frac{\partial}{\partial P}\right) - ikP\right]\bar{\bar{\phi}}_j^{(k)}(P) = \lambda_j^{(k)}\bar{\bar{\phi}}_j^{(k)}(P). \tag{59}$$

The distribution function may be expanded in terms of the eigenfunctions $\phi_j^{(k)}(P)$ in the same manner of Eq. (41) by

$$f_k(P,t) = \langle\langle k,P|f(t)\rangle\rangle = \langle\langle k,P|\hat{T}^{-1}|\bar{\bar{f}}(t)\rangle\rangle$$
$$= \sum_j \exp[\lambda_j^{(k)}t]\phi_j^{(k)}(P)\langle\langle\bar{\bar{\tilde{\phi}}}_j^{(k)}|\bar{\bar{f}}(0)\rangle\rangle, \tag{60}$$

where the inner product $\langle\langle\bar{\bar{\tilde{\phi}}}_j^{(k)}|\bar{\bar{f}}(0)\rangle\rangle$ is defined by Eq. (35).

In the hydrodynamic situation, the flow term (that is a time-symmetric part) is treated as a small perturbation for the collision operator $\hat{\mathcal{K}}^{(0)}$ (that is a time asymmetric part) in Eq. (58).[31] The eigenvalues and eigenfunctions are then obtained in the expansion of k,

$$\lambda_j^{(k)} = \lambda_{j;0}^{(k)} + k\lambda_{j;1}^{(k)} + k^2\lambda_{j;2}^{(k)} + \cdots \tag{61a}$$

$$|\phi_j^{(k)}\rangle\rangle = \hat{P}^{(k)}|\phi_j^{(k)}\rangle\rangle = |\phi_{j;0}^{(k)}\rangle\rangle + k|\phi_{j;1}^{(k)}\rangle\rangle + k^2|\phi_{j;2}^{(k)}\rangle\rangle + \cdots, \tag{61b}$$

where $\lambda_{j;0}^{(k)}=\lambda_j^{(0)}$ and $\phi_{j;0}^{(k)}(P)\equiv\langle\langle k,P|\phi_{j;0}^{(k)}(P)\rangle\rangle=\phi_j^{(0)}(P)$ are the eigenvalues and the eigenfunctions, respectively, of $\hat{\mathcal{K}}^{(0)}$ given in Eq. (24).

For $j=0$ the degeneracy of the collision invariants may be removed by the perturbation of the flow term. According to the ordinary kinetic theory, the resultant perturbed states yield the hydrodynamic modes, such as sound modes, diffusion modes, corresponding to the first- and second-order perturbations, respectively.[31] Note that the degeneracy of $j=0$ is classified by P_0 as shown in Eq. (45). Since the collision invariants $\psi_{P_0}(P)$ given by Eq. (47) consists both of even and odd functions of P, the degeneracy of the collision invariants $\psi_{P_0}(P)$ are removed by the first-order perturbation of the flow term which is an odd function of P. We denote $\lambda_{P_0}^{(k)}\equiv\lambda_{0;1}^{(k)}$ which is associated with the collision invariant $\psi_{P_0}(P)$ and $|\phi_{P_0}^{(k)}\rangle\rangle\equiv|\phi_{0;0}^{(k)}\rangle\rangle$ for a particular value of P_0. We then have for the first-order approximation in k

$$k\lambda_{P_0}^{(k)} = \langle\langle\bar{\bar{\phi}}_{P_0;0}^{(k)}|(-ikP)|\bar{\bar{\phi}}_{P_0;0}^{(k)}\rangle\rangle, \tag{62a}$$

$$=(-ik)\frac{\Sigma_{n=-\infty}^{\infty}P_{0;n}\exp[-\beta\varepsilon_{P_{0;n}}]}{\Sigma_{n=-\infty}^{\infty}\exp[-\beta\varepsilon_{P_{0;n}}]}, \tag{62b}$$

$$=(-ik)\frac{\int P\psi_{P_0}(P)dP}{\int\psi_{P_0}(P)dP}, \tag{62c}$$

$$\equiv -ik\sigma(P_0,\beta), \tag{62d}$$

which gives

$$\lim_{T\to 0}\sigma(P_0,\beta)=P_0. \tag{63}$$

Note that the flow term $(-ikP)$ is diagonalized among the collision invariant $\langle\langle\bar{\bar{\phi}}_{P_0'}|(-ikP)|\bar{\bar{\phi}}_{P_0}\rangle\rangle\propto\delta(P_0'-P_0)$ so that each $\phi_{P_0}^{(k)}(P)=\psi_{P_0}(P)$ becomes a hydrodynamic mode in the first-order approximation in k.[31]

As will be shown in Eq. (69), $\sigma(P_0,\beta)$ is a sound velocity, corresponding to a hydrodynamic mode $\psi_{P_0}(P)$ associated with a P_0. With use of Eq. (44), we find the periodicity of $\sigma(P_0,\beta)$,

$$\sigma(P_{0;n},\beta)=\sigma(P_0,\beta)\quad(n=\pm1,\pm2,\pm3,\ldots). \tag{64}$$

Since $P_{0;n}$ in Eq. (44) runs from $-\infty$ to ∞, $\sigma(P,\beta)$ defined by Eqs. (62d) and (64) is a continuous periodic function of P with the periodicity of 4. In Fig. 4(a), we show the sound velocity as a function of P for several temperatures: $T(=1/\beta)=0.1$, 1.0, and 3.0. The temperature dependence of $\sigma(P,\beta)$ are also shown in Fig. 4(b) for several values of P. Starting from $\sigma(P,\beta)=P$ at $T=0$, as temperature increases, $\sigma(P,\beta)$ increases to a maximum value and then asymptotically decreases to 0.

Now we consider the time evolution of the distribution according to Eq. (54). For $t=t_0\gtrsim t_r$, the system reaches to the steady state of the momentum distribution, i.e., the local equilibrium has been attained. In this situation, the momentum distribution is expressed as a linear combination of the collision invariants $\psi_{P_0}(P)$ given by Eq. (47),

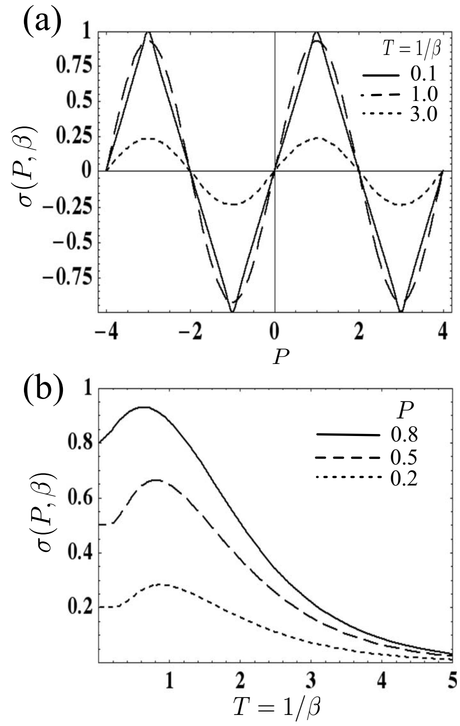

FIG. 4. Sound velocity as a function (a) of P and (b) of T.

$$f_k^{\rm LE}(P)\equiv\int_{-1}^{1}\psi_{P_0}(P)\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle dP_0, \tag{65}$$

where the superscript LE stands for the local equilibrium that still evolves in time by the generator of motion $\hat{\mathcal{K}}^{(k)}$ in Eq. (57). Equation (65) indicates that in the local equilibrium the weight of each collision invariants $\psi_{P_0}(P)$ is uniquely determined by a given initial distribution. That is how the initial momentum distribution keeps its memory for long time at any temperatures in the present one-dimensional chain system. Substituting $\psi_{P_0}(P)$ given by Eq. (47) into Eq. (65) and taking into account the relation of Eq. (49), we have

$$\begin{aligned}f_k^{\rm LE}(P)&=\int_{-1}^{1}dP_0\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle\sum_n\frac{\exp[-\beta\varepsilon_{P_{0;n}}]}{\mathcal{N}_{P_0}}\delta(P-P_{0,n})\\&=\int_{-1}^{1}dP_0\sum_n\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle\frac{\exp[-\beta\varepsilon_{P_{0;n}}]}{\mathcal{N}_{P_{0;n}}}\delta(P-P_{0,n})\\&=\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle\frac{\exp[-\beta\varepsilon_P]}{\mathcal{N}_P}\int_{-1}^{1}dP_0\sum_n\delta(P-P_{0,n})\\&=\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle\frac{\exp[-\beta\varepsilon_P]}{\mathcal{N}_P}.\end{aligned} \tag{66}$$

Time evolution of the distribution is given by substituting Eq. (62d) into Eq. (60) as

$$f_k(P,t) = \int_{-1}^{1} dP_0 \exp[\lambda_{P_0}^{(k)}(t-t_0)]\psi_{P_0}(P)\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle$$
$$= \int_{-1}^{1} dP_0 \sum_n \exp[-ik\sigma(P_{0;n},\beta)(t-t_0)]$$
$$\times \langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle \frac{\exp[-\beta\varepsilon_{P_{0;n}}]}{\mathcal{N}_{P_{0;n}}}\delta(P-P_{0;n})$$
$$= \exp[-ik\sigma(P,\beta)(t-t_0)]\langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle \frac{\exp[-\beta\varepsilon_P]}{\mathcal{N}_P}. \quad (67)$$

Fourier transform of Eq. (67) gives a Wigner function [Eq. (16)] in phase space as

$$f^W(X,P,t) = \frac{1}{2\pi}\int dk \exp[ik\{X-\sigma(P,\beta)(t-t_0)\}]$$
$$\times \langle\langle\bar{\bar{\phi}}_{P_0}^{(k)}|\bar{\bar{f}}(0)\rangle\rangle \frac{\exp[-\beta\varepsilon_P]}{\mathcal{N}_P}. \quad (68)$$

Differentiating Eq. (68) twice with respect to X and t, we then obtain a macroscopic wave equation for $t \gtrsim t_r$ with a sound velocity $\sigma(P,\beta)$ as

$$\frac{\partial^2}{\partial t^2} f^W(X,P,t) = \sigma^2(P,\beta)\frac{\partial^2}{\partial X^2} f^W(X,P,t). \quad (69)$$

This clearly reveals that there appears the quantum hydrodynamic sound mode in macroscopic sense in the exactly same manner as in the classical gas system.[31]

Let us illustrate a time evolution of a Wigner distribution in the case where the initial distribution is given by the minimum uncertainty wave packet with a mean at $X=0$ in space and at $P=P_{\rm intl}$ in momentum spaces,

$$f^W(X,P,0) = \frac{1}{\pi}\exp\left[-\frac{X^2}{(\Delta x)^2} - (P-P_{\rm intl})^2(\Delta x)^2\right]. \quad (70)$$

The standard deviation $\delta X(0)$ in space is given by

$$\delta X(0) \equiv \sqrt{\langle X\rangle_0^2 - \langle X\rangle_0^2} = (\Delta x)/\sqrt{2}, \quad (71)$$

where the subscript of 0 stands for $t=0$ and that in momentum is given by $\delta P(0)=1/2[\delta X(0)]$.

In Fig. 5(a) we show a minimum uncertainty wave packet with $\Delta x=3.0$ and $P_{\rm intl}=0.5$, giving a peak at $X=0$ and $P=P_{\rm intl}=0.5$ with $\delta X(0)=3/\sqrt{2}\simeq 2.1$ and $\delta P(0)=(3\sqrt{2})^{-1}\simeq 0.23$. Since $\delta X(0) \gg \delta P(0)$, this wave packet becomes macroscopic in space. A bird's-eye view and the contour plot of the wave packet are shown in the left and the right columns, respectively.

After the relaxation time at $t=t_0 \gtrsim t_r$, the system has reached to the local equilibrium where the momentum distribution relaxes into the equilibrium,

$$\int f^W(X,P,t_0)dX = f_0^{\rm LE}(P) \quad (t_0 \gtrsim t_r) \quad (72)$$

while the spatial distribution is unchanged

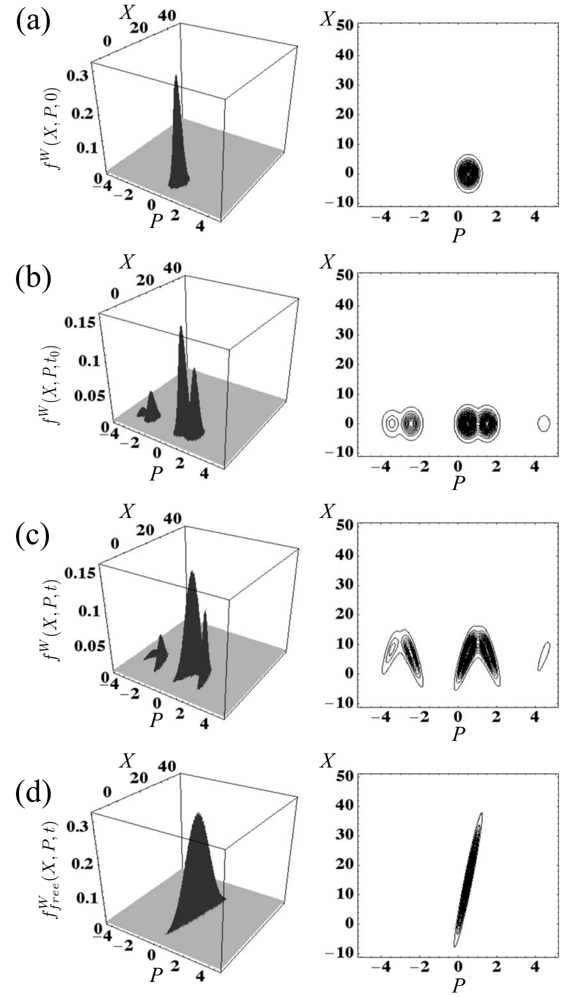

FIG. 5. Propagation of the wave packet for the particle distribution as a quantum hydrodynamic sound wave at $T=2.5$. A bird's-eye view and a contour plot are shown in right and left columns, respectively, for initial (a) distribution at $t=0$, (b) distribution at local equilibrium at $t=t_0 \gtrsim t_r$, and (c) $t-t_0=30\hbar/mc^2$. The wave packet for the free particle with the same initial condition at $t=30\hbar/mc^2$ is shown in (d).

$$\int f^W(X,P,t_0)dP = \int f^W(X,P,0)dP. \quad (73)$$

We show the Wigner distribution at $t_0(\gtrsim t_r)$ for a temperature $T=2.5$ in Fig. 5(b). The distribution has side peaks at $P_{0;1}=1.5$, $P_{0;-1}=-2.5$, and $P_{0;2}=3.5$ besides the main peak at $P_{0;0}=P_{\rm intl}=0.5$, corresponding to the distribution of $\psi_{P_0}(P)$ shown in Fig. 2(b). Each peak has a same width in P direction of $\delta P(0)\simeq 0.23$. As the temperature increases, the satellite peak intensities increase as seen from Eq. (47).

Then the wave packet propagates in space following the macroscopic wave Eq. (69) as shown in Fig. 5(c). During the propagation in space while the distribution does not change along P direction, it is dispersed along X direction since the wave packet [Eq. (68)] is composed of various plane waves with different sound velocities shown in Fig. 4(a). Reflecting the periodicity of $\sigma(P,\beta)$ as a function of P, the dispersed

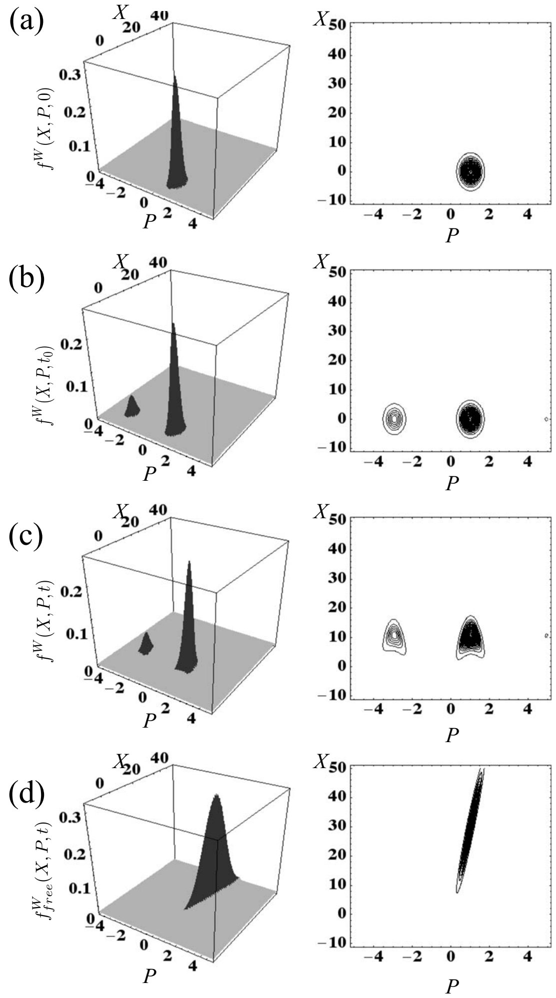

FIG. 6. Propagation of the wave packet of the particle distribution for the same parameters as in Fig. 5 except for $P_{\rm intl}=1.0$. A bird's-eye view and a contour plot are shown in right and left columns, respectively, for initial (a) distribution at $t=0$, (b) distribution at local equilibrium at $t=t_0 \gtrsim t_r$, and (c) $t-t_0=30\hbar/mc^2$. The wave packet for the free particle with the same initial condition at $t=30\hbar/mc^2$ is shown in (d).

distribution function demonstrates the same periodicity as in Fig. 4(a) besides the Boltzmann factor.

For comparison we display in Fig. 5(d) the time evolution of the Wigner distribution of a free particle without the interaction with the phonons for the same initial condition given by Eq. (70). The distribution of the free particle is immediately spread out in space because of the phase mixing effect as a consequence of the nonlinearity in energy with respect to a momentum p, $\varepsilon_p \propto p^2$. It is, therefore, quite intriguing and counterintuitive that the random collision of the quantum particle with thermal phonon field makes the macroscopic coherent motion of the particle far more stable than the free particle motion.

In Fig. 6, we also show the propagation of the wave packet of the particle distribution for the same parameters as in the case of Fig. 5 except for $P_{\rm intl}=1.0$. In this case, the main peak at $P_{0;0}=P_{\rm intl}$ and the first satellite peak at $P_{0;1}$ is merged at $P=1.0$, and the small satellite at $P=-3.0$ corresponds to $P_{0;-1}$ and $P_{0;2}$, as shown in Fig. 6(b). The propagation of the wave packet following the macroscopic wave Eq. (69) is shown in Fig. 6(c). Compared to Fig. 5(c), the distribution along X direction is greatly suppressed as a result that $\sigma(P,\beta)$ is slightly changed around $P=1.0$ and $P=-3.0$ as a function of P as shown in Fig. 4(a). It is, therefore, intriguing that the minimum uncertainty wave packet propagates without being spread even under the random collision with the phonon field.

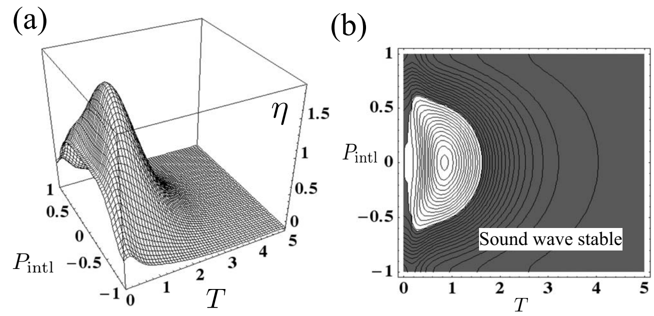

FIG. 7. Stability of the sound wave: (a) the ratio of the speed of broadening of (a) the wave packet, $\eta=G_{\rm sw}/G_{\rm free}$, and (b) a contour plot of η. The stable region of the sound wave against the free particle is shaded in (b).

We show in Fig. 7 the stability of the wave packet of the quantum hydrodynamic sound wave compared with the free particle. The standard deviation of the wave packet in space is given by

$$\delta X_{\rm sw}(t) \equiv \sqrt{\langle X^2\rangle_t - \langle X\rangle_t^2} = \left[\int\int X^2 f^W(X,P,t)dXdP - \left(\int\int X f^W(X,P,t)dXdP\right)^2\right]^{1/2}, \qquad (74)$$

which becomes broadened in time. For the sound wave, we obtain

$$\delta X_{\rm sw}(t) = \left[\frac{(\Delta x)^2}{2} + t^2 G_{\rm sw}(P_{\rm intl},\beta)\right]^{1/2}, \qquad (75)$$

where the broadening ratio $G_{\rm sw}$ is given by

$$G_{\rm sw}(P_{\rm intl},\beta) = \frac{(\Delta x)}{\sqrt{\pi}}\int dP\sigma^2(P,\beta)\exp[-(\Delta x)^2(P-P_{\rm intl})^2] - \left\{\frac{(\Delta x)}{\sqrt{\pi}}\int dP\sigma(P,\beta)\exp[-(\Delta x)^2(P-P_{\rm intl})^2]\right\}^2. \qquad (76)$$

The standard deviation of the free particle wave packet with the initial condition Eq. (70) is given by

$$\delta X_{\rm free}(t) = \left[\frac{(\Delta x)^2}{2} + t^2 G_{\rm free}\right]^{1/2}, \qquad (77)$$

with

$$G_{\text{free}} = \frac{1}{2(\Delta x)^2}. \tag{78}$$

In Fig. 7(a) we show the ratio of $\eta \equiv G_{\text{sw}}(P_{\text{intl}},\beta)/G_{\text{free}}$ as a function of P_{intl} and $T=1/\beta$, where the initial wave packet is assumed to be a minimum uncertainty wave packet with $\Delta x=3.0$. The contour plot of η is drawn in Fig. 7(b). Because of the periodicity of $\sigma(P,\beta)$ with respect to P as shown in Fig. 4(a) and Eq. (64), $G_{\text{sw}}(P_{\text{intl}},\beta)$ is periodic with respect to P_{intl}; $G_{\text{sw}}(P_{\text{intl}},\beta)=G_{\text{sw}}(P_{\text{intl}}\pm 2,\beta)$. For $\eta<1$, the broadening of the wave packet of the sound wave is slower than that of the free particle, indicating that the propagation of the sound wave is more stable than the free particle. The shaded region in Fig. 7(b) denotes the stable region of the sound wave. It is clearly seen from Fig. 7 that the stability of the sound mode increases as temperature increases.

As t increases to the order of $t\sim 1/k^2$, the second-order perturbation in Eq. (61) becomes nonnegligible. So the quantum hydrodynamic sound mode eventually disappears due to the diffusion process, similar to the case of the classical sound mode in gas.[31]

V. DISCUSSIONS AND CONCLUDING REMARKS

We have derived a kinetic equation for a quantum particle which is coupled with an acoustic phonon in one-dimensional system based on the formulation of complex spectral representation of the Liouvillean. As usual, the collision operator for the weakly coupled system has a contribution only from the resonance energy that is represented by the delta function for the unperturbed energy of the Brownian particle and the phonon. Because of this resonance condition, the momentum states are separated into an infinite number of independent disjoint sets for the one-dimensional system. As a result, there appears an infinite degeneracy in the collision invariants.

We have presented an analytic solution of the eigenvalue problem of the collision operator for the high-temperature case, as well as a numerical solution for more general case. These solutions show that the eigenvalues of the collision operator are discrete. Hence, there is a finite gap between the collision invariant and the first eigenstate. We also found that the relaxation time determined by the inverse of this gap is proportional to $|\Delta_0|^2$ and $1/\sqrt{T}$ for a high-temperature case.

Thanks to the discreteness of the spectrum of the collision operator, one can consider the so-called hydrodynamic situation where the flow term in the inhomogeneous situation may be considered as a small perturbation on the collision term. We then showed that the degeneracy of the collision invariants are lifted by the flow term in the first-order perturbation of the wave number, which yields the quantum hydrodynamic sound mode. Note that the flow term is time symmetric while the collision term breaks time symmetry. Hence, our quantum sound mode is a result of the dissipation. Indeed, we have seen that the stability of our quantum sound mode increases with temperature, which is counterintuitive, as the random collision of our Brownian particle with the thermal acoustic phonon stabilizes the propagation of the sound mode.

We note that there is no quantum sound mode in two- or three-dimensional systems. This is because there is no degeneracy in more than one-dimensional system. Indeed, in these systems the momentum states coupled to a particular $|\mathbf{P}_0\rangle$ state with $|\mathbf{P}_0|\leq mc$ due to the resonance condition of $\varepsilon_{\mathbf{P}\pm\hbar\mathbf{q}}-\varepsilon_{\mathbf{P}}=\pm\hbar\omega_{\mathbf{q}}$ are determined by a common line or surface, respectively, of the intersections of the particle and phonon dispersions. This is in contrast to the case of one-dimensional system where the coupled momentum states are determined in pointwise as shown in Fig. 2(a). Since these continuous common lines or surfaces corresponding to different $|\mathbf{P}_0\rangle$ states are intersected with each other, all the momentum states are connected. As a result there is no degeneracy of the collision invariants. In the two or three-dimensional systems, therefore, we have only a diffusion mode as for the hydrodynamic transport mode that comes from the second-order perturbation of the flow term.

Let us also remark the case where the particle is interacting with optical-phonon field instead of the acoustic-phonon field considered in this paper. For the optical phonon, the energy dispersion is described by $\omega_q=\omega_0$ (constant). For this case one can show that Poincaré resonance gives also rise to an infinite number of disjoint sets of momentum space, which then yields an infinite degeneracy of collision invariants, as in the case of the interaction with an acoustic-phonon filed. However, it is found that in this case the collision invariants are given by an even function of P. Since the flow term is an odd function of P, the degeneracy of the collision invariants are not removed by the first-order perturbation of the flow term, unlike the case of the acoustic phonon. Therefore, there does not appear the quantum hydrodynamic sound wave in the case of the interaction with an optical-phonon field.

In the weak-coupling case, the renormalization effect on the sound velocity appears from the second-order correction in terms of the interaction of $g\mathcal{L}_{\text{int}}$, just as the renormalization effect of the eigenenergies of a Hamiltonian appears from the second-order correction of an interaction. On the other hand, the decay of the sound mode also appears from the second-order correction of $g\mathcal{L}_{\text{int}}$. Therefore as long as we are concerned with a time region in which we can ignore the decay of the sound mode, we can consistently ignore the renormalization effect of the sound velocity.

Let us present an evaluation of the relaxation time and the sound velocity for a vibrational excitation (a vibron) in molecular chain which is a transfer mechanism of an bioenergy in α-helix protein.[22,23,25,26] The vibrational exciton (vibron) propagates under the thermal collision with a backbone delocalized molecular vibration. The effective mass of the vibron has been evaluated by the dipole-dipole interactions between the peptide units,[22] $m=\hbar^2/2d^2J\simeq 2\times 10^{-28}$ kg, where d is a periodicity of the unit peptide and J is a dipole-dipole interaction constant. The interaction potential and the acoustic-phonon velocity have been estimated in literatures[22]: $|\Delta_0|\simeq 0.5$ eV and $c\simeq 4000$ m/s. With these values, $l_u=\hbar/mc=1.3$ Å, the energy unit $\varepsilon_u=mc^2$ $=20$ meV$=230$ K, yielding the relaxation time $t_r\simeq 17$ fs at $T=310$ K. It should be noted that due to the large effective mass the energy unit ε_u is large. Therefore, the quantum resonance is prominent even at the physiological temperature, i.e., the effective temperature $\bar{T}_{\text{eff}} \equiv T/(\varepsilon_u/k_B) = 1.33$. As a result, the quantum hydrodynamic sound wave can be observed to propagate with the sound velocity of the same order of the acoustic-phonon velocity $c=4000$ m/s. Note that in this case we need to take into account the correct energy dispersion of the vibron which is different from that of the free particle. It is found that the relaxation dynamics of the vibron in α-helix protein shows a very interesting feature. This will be discussed in a forthcoming paper.[50]

The model Hamiltonian (4) has been used to account for the relaxation process of an electron (or an exciton) motion interacting with the acoustic-phonon mode in semiconductor crystals,[46] and semiconductor quantum wires where an electron is restricted in one-dimensional motion while the phonon is three dimensional.[51–53] In this respect, the present model may be oversimplified for an electron in semiconductor wire because the phonon is restricted in one-dimensional motion. But we think that the present analysis may shed new light on the transport processes of semiconductor wires so it is worth while to investigate its potential applicability to various solid-state nanomaterials, including semiconductor wires.

In this study we have considered the macroscopic transport process of the simplified one-dimensional molecular chain system. In reality, there are a lot of extrinsic factors which may hinder the appearance of the quantum sound wave, for example, imperfections of the chain, perturbations due to the side chains, quasi-one-dimensionality of the chain. In addition to the intrinsic diffusion process, the quantum sound mode decays due to these extrinsic disturbances. Even so, as long as the strength of the disturbances are small compared to the inverse of the relaxation time t_r, there is a time window in which the transport of the hydrodynamic sound wave is stable to be observed. We shall reveal the time region for the stable transport of the quantum sound wave in the forthcoming paper.[50]

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APPENDIX A: REPRESENTATION OF WIGNER BASIS IN LIOUVILLE SPACE AND THE EXPRESSION OF $\mathcal{L}_{\text{int}}$

In this section, we shall briefly review the Liouville-space representation of a Hilbert-space operator. In Appendix A–C, we present the results in the form with dimensions. The Liouville space is spanned by linear operators in $A, B, \ldots$ in the ordinary wave-function space.[30] As usual, the inner product of the Liouville space is defined by

$$\langle\langle A|B\rangle\rangle = \text{Tr}(A^\dagger B), \tag{A1}$$

where A and B are linear operators acting on wave functions, and $A^\dagger$ is a Hermite conjugate of A. For the case where the wave-function space is spanned by a complete orthonormal basis,

$$\sum_\alpha |\alpha\rangle\langle\alpha| = 1, \;\; \langle\alpha|\beta\rangle = \delta_{\alpha,\beta}, \tag{A2}$$

the Liouville space is spanned by a complete orthonormal basis of the dyads $|\alpha;\beta\rangle\rangle \equiv |\alpha\rangle\langle\beta|$, i.e.,

$$\sum_{\alpha,\beta} |\alpha;\beta\rangle\rangle\langle\langle\alpha;\beta| = 1, \quad \langle\langle\alpha;\beta|\alpha';\beta'\rangle\rangle = \delta_{\alpha,\alpha'}\delta_{\beta,\beta'}. \tag{A3}$$

The matrix element of the usual operator A in the wave-function space is given by

$$\langle\langle\alpha;\beta|A\rangle\rangle = \langle\alpha|A|\beta\rangle. \tag{A4}$$

For the present case, with use of the orthonormal eigenstates of the unperturbed Hamiltonian (5), we can take the orthonormal basis in the Liouville space as $|p;p'\rangle\rangle$ and $|n_q;n_q'\rangle\rangle$ for the particle and phonon systems for a q mode, respectively. In terms of these orthonormal basis, the Wigner basis are defined by

$$|k,P)) \equiv |p;p'\rangle\rangle = \left|P+\frac{\hbar k}{2};P-\frac{\hbar k}{2}\right\rangle\rangle \tag{A5}$$

for the particle state and

$$|\{\nu\},\{N\}\rangle\rangle \equiv |\{n\};\{n'\}\rangle\rangle = \left|\left\{N+\frac{\nu}{2}\right\};\left\{N-\frac{\nu}{2}\right\}\right\rangle\rangle \tag{A6}$$

for the phonon state, where $\{\cdots\}$ in Eq. (A6) denotes a direct product of all q modes of the phonon states. We note the difference of the notation between "semicolon" and "comma" in Eqs. (A5) and (A6). These Wigner basis form the orthonormal complete basis set

$$((k,P|k',P')) = \delta^{Kr}_{k,k'}\delta^{Kr}_{P,P'}, \quad \sum_k\sum_P |k,P))((k,P| = 1 \tag{A7}$$

for the particle states and

$$\langle\langle\{\nu\},\{N\}|\{\nu'\},\{N'\}\rangle\rangle = \delta^{Kr}_{\nu,\nu'}\delta^{Kr}_{N,N'},$$

$$\sum_{\nu,N} |\{\nu\},\{N\}\rangle\rangle\langle\langle\{\nu\},\{N\}| = 1, \tag{A8}$$

for the phonon states.

Here we introduce a new Wigner basis for the particle states as

$$|k,P\rangle\rangle \equiv \sqrt{\Omega}\,|k,P)), \tag{A9}$$

where $\Omega \equiv L/2\pi$. These new Wigner basis for the particle satisfy the orthonormal complete relation

$$\langle\langle k,P|k',P'\rangle\rangle = \Omega\,\delta^{Kr}_{P,P'}\delta^{Kr}_{k,k'}, \tag{A10}$$

$$\sum_k \frac{1}{\Omega} \sum_P |k,P\rangle\rangle\langle\langle k,P| = 1. \tag{A11}$$

We may take here $L \to \infty$ limit for the P variables, which leads to Eq. (17).

These basis states are eigenvectors of the unperturbed Liouvillean $\mathcal{L}_0$ in the Liouville space

$$\mathcal{L}_0|k,P\rangle\rangle \otimes |\{\nu\},\{N\}\rangle\rangle = (w_{k,P} + \nu\omega)|k,P\rangle\rangle \otimes |\{\nu\},\{N\}\rangle\rangle, \tag{A12}$$

where

$$w_{k,P} \equiv \frac{1}{\hbar}(\varepsilon_{P+\hbar k/2} - \varepsilon_{P-\hbar k/2}), \tag{A13}$$

$$\nu\omega \equiv \sum_q \nu_q \omega_q. \tag{A14}$$

The Wigner basis forms a complete orthonormal basis set

$$\langle\langle k,P|k',P'\rangle\rangle \cdot \langle\langle\{\nu\},\{N\}|\{\nu'\},\{N'\}\rangle\rangle = \delta(P-P')\,\delta^{Kr}_{k,k'}\,\delta^{Kr}_{\{\nu\},\{\nu'\}}\,\delta^{Kr}_{\{N\},\{N'\}}, \tag{A15}$$

$$\sum_k \int dP|k,P\rangle\rangle\langle\langle k,P| \otimes \sum_{\nu,N} |\{\nu\},\{N\}\rangle\rangle\langle\langle\{\nu\},\{N\}| = 1. \tag{A16}$$

The matrix element of the usual operator A of a particle in the wave-function space is represented by Wigner basis as

$$A_k(P) \equiv \langle\langle k,P|A\rangle\rangle = \sqrt{\Omega}\langle P+\hbar k/2|A|P-\hbar k/2\rangle. \tag{A17}$$

The Liouvillean for the interaction parts $\mathcal{L}_{\rm int}$ is then represented in terms of these basis

$$\begin{aligned}\langle\langle k,P| \otimes \langle\langle\{\nu\},\{N\}|g\mathcal{L}_{\rm int}|\{\nu'\},\{N\}\rangle\rangle \otimes |k',P'\rangle\rangle &= \frac{g}{\sqrt{\Omega}}\sum_q V_q \delta^{kr}_{q,k-k'}\delta(P-P') \\ &\times \frac{1}{\hbar}\Bigg[\Bigg\{\sqrt{N_q+\frac{\nu'_q}{2}+\frac{1}{2}}\exp\left[-\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[\frac{1}{2}\frac{\partial}{\partial N_q}\right] - \sqrt{N_q-\frac{\nu'_q}{2}+\frac{1}{2}}\exp\left[\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[-\frac{1}{2}\frac{\partial}{\partial N_q}\right]\Bigg\}\delta^{Kr}_{\nu'_q,\nu_q+1}\bar{\delta}^{Kr}_{\{\nu\},\{\nu'\}} \\ &+ \Bigg\{\sqrt{N_{-q}+\frac{\nu'_{-q}}{2}+\frac{1}{2}}\exp\left[-\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[-\frac{1}{2}\frac{\partial}{\partial N_{-q}}\right] - \sqrt{N_{-q}-\frac{\nu'_{-q}}{2}+\frac{1}{2}}\exp\left[\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[\frac{1}{2}\frac{\partial}{\partial N_{-q}}\right]\Bigg\} \\ &\times \delta^{Kr}_{\nu'_{-q},\nu_{-q}-1}\bar{\delta}^{Kr}_{\{\nu\},\{\nu'\}}\Bigg],\end{aligned} \tag{A18}$$

where $\bar{\delta}^{Kr}_{\{\nu\},\{\nu'\}}$ denotes the Kronecker delta relation other than the q (or $-q$) mode. This represents the transition by $\mathcal{L}_{\rm int}$ from the state with a (k',ν') particle-phonon correlation to the states with a (k,ν) particle-phonon correlation.[47]

The interaction Liouvillean can be represented by a diagram in correlation dynamics as shown in Fig. 8,[47,54] where the diagrams corresponding to the first and second lines in Eq. (A18) are shown in Figs. 8(a) and 8(b), respectively. In Fig. 8, the solid and dashed lines represent correlations of a particle and phonon states, respectively.

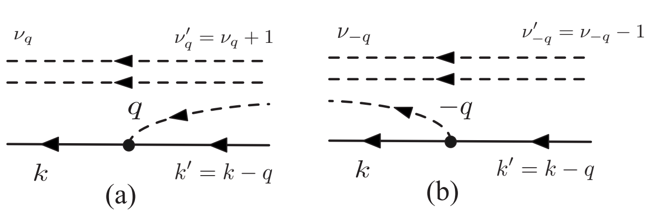

FIG. 8. Diagram of correlation dynamics for the interaction Liouvillean.

APPENDIX B: THE COMPLEX SPECTRAL REPRESENTATION OF LIOUVILLEAN AND SUBDYNAMICS

In this section, we shall briefly summarize the complex spectral representation of Liouvillean.[30] Useful formula for this paper are listed without proof. The reader may refer to some references for detail.[30,40]

In the complex spectral representation of Liouvillean, we consider the eigenvalue problem for each correlation subspace $(\mu)=(k,\nu)$ given by

$$\mathcal{L}|F_j^{(\mu)}\rangle\rangle = Z_j^{(\mu)}|F_j^{(\mu)}\rangle\rangle, \quad \langle\langle\tilde{F}_j^{(\mu)}|\mathcal{L} = \langle\langle\tilde{F}_j^{(\mu)}|Z_j^{(\mu)}, \tag{B1}$$

where the Liouvillean, $\mathcal{L}=\mathcal{L}_0+g\mathcal{L}_{\rm int}$, can have complex eigenvalues ${\rm Im}\, Z_j^{(\mu)} \neq 0$. It has been shown that the time evolution splits into two semigroups; one is oriented toward our future $t>0$ with ${\rm Im}\, Z_j^{(\mu)}<0$ (equilibrium is approached for $t\to\infty$) while the other is oriented toward our past $t<0$ with ${\rm Im}\, Z_j^{(\mu)}>0$. All irreversible processes have the same time orientation. To be self-consistent we choose the semigroup oriented toward our future, which determines the direction of the analytic continuation of the eigenfunction of $\mathcal{L}$.[29,30]

In terms of the eigenstates of $\mathcal{L}_0$ as defined in Eq. (A12), we introduce the projection operator as

$$\hat{P}^{(k,\nu)} = \sum_N \int dP|k,P\rangle\rangle\langle\langle k,P| \otimes |\{\nu\},\{N\}\rangle\rangle\langle\langle\{\nu\},\{N\}|, \tag{B2}$$

resulting in

$$\mathcal{L}_0\hat{P}^{(k,\nu)} = \hat{P}^{(k,\nu)}\mathcal{L}_0, \tag{B3a}$$

$$\hat{P}^{(k,\nu)}\hat{P}^{(k',\nu')} = \hat{P}^{(k,\nu)}\delta_{k,k'}\delta_{\nu,\nu'}, \tag{B3b}$$

$$\sum_{k,\nu}\hat{P}^{(k,\nu)} = 1. \tag{B3c}$$

We also introduce the projection operators

$$\hat{Q}^{(k,\nu)} = 1 - \hat{P}^{(k,\nu)} \tag{B4}$$

which are orthogonal to $\hat{P}^{(k,\nu)}$.

We solve the eigenvalue problem (B1) for the perturbed system with $g\neq 0$ under the boundary conditions for the unperturbed case

$$|F_j^{(\mu)}\rangle\rangle = \hat{P}^{(\mu)}|F_j^{(\mu)}\rangle\rangle,$$

$$\langle\langle\tilde{F}_j^{(\mu)}| = \langle\langle\tilde{F}_j^{(\mu)}|\hat{P}^{(\mu)} \quad \text{for} \quad g=0. \tag{B5}$$

Hence, $\hat{Q}^{(\mu)}|F_j^{(\mu)}\rangle\rangle=0$ for $g=0$. The $\hat{Q}^{(\mu)}$ components are created through the interaction for $g\neq 0$. The right and left eigenstates, $|F_j^{(\mu)}\rangle\rangle$ and $\langle\langle\tilde{F}_j^{(\mu)}|$, are biorthonormal sets satisfying

$$\langle\langle\tilde{F}_j^{(\mu)}|F_{j'}^{(\mu')}\rangle\rangle = \delta_{j,j'}\delta_{\mu,\mu'}, \quad \sum_{\mu,j}|F_j^{(\mu)}\rangle\rangle\langle\langle\tilde{F}_j^{(\mu)}| = 1. \tag{B6}$$

Applying the projection operators $\hat{P}^{(\mu)}$ and $\hat{Q}^{(\mu)}$ in Eqs. (B2) and (B4) to the Eq. (B1), we derive the set of equations

$$\hat{P}^{(\mu)}\mathcal{L}(\hat{P}^{(\mu)}|F_j^{(\mu)}\rangle\rangle + \hat{Q}^{(\mu)}|F_j^{(\mu)}\rangle\rangle) = Z_j^{(\mu)}\hat{P}^{(\mu)}|F_j^{(\mu)}\rangle\rangle, \tag{B7a}$$

$$\hat{Q}^{(\mu)}\mathcal{L}(\hat{P}^{(\mu)}|F_j^{(\mu)}\rangle\rangle + \hat{Q}^{(\mu)}|F_j^{(\mu)}\rangle\rangle) = Z_j^{(\mu)}\hat{Q}^{(\mu)}|F_j^{(\mu)}\rangle\rangle. \tag{B7b}$$

Equation (B7b) leads to

$$\hat{Q}^{(\mu)}|F_j^{(\mu)}\rangle\rangle = \hat{\mathcal{C}}^{(\mu)}(Z_j^{(\mu)})\hat{P}^{(\mu)}|F_j^{(\mu)}\rangle\rangle, \tag{B8}$$

where

$$\hat{\mathcal{C}}^{(\mu)}(z) = \frac{1}{z-\hat{Q}^{(\mu)}\mathcal{L}\hat{Q}^{(\mu)}}\hat{Q}^{(\mu)}g\mathcal{L}_{\rm int}\hat{P}^{(\mu)} \tag{B9}$$

is called the creation-of-correlation operator or simply the *creation operator*.[30] Substituting Eq. (B8) into Eq. (B7a), we obtain

$$\hat{\Psi}^{(\mu)}(Z_j^{(\mu)})|u_j^{(\mu)}\rangle\rangle = Z_j^{(\mu)}|u_j^{(\mu)}\rangle\rangle, \tag{B10}$$

where

$$|u_j^{(\mu)}\rangle\rangle = (N_j^{(\mu)})^{-1/2}\hat{P}^{(\mu)}|F_j^{(\mu)}\rangle\rangle \tag{B11}$$

and $N_j^{(\mu)}$ is a normalization constant which will be determined later. Here, $\hat{\Psi}^{(\mu)}$ is the *collision operator* familiar to nonequilibrium statistical mechanics.[31,32,47,48] This operator is associated to *diagonal transitions* between two states corresponding to the same projection operator $\hat{P}^{(\mu)}$,

$$\hat{\Psi}^{(\mu)}(z) = \hat{P}^{(\mu)}\mathcal{L}_0\hat{P}^{(\mu)} + \hat{P}^{(\mu)}g\mathcal{L}_{\rm int}\hat{P}^{(\mu)} + \hat{P}^{(\mu)}g\mathcal{L}_{\rm int}\hat{Q}^{(\mu)}\hat{\mathcal{C}}^{(\mu)}(z)\hat{P}^{(\mu)}. \tag{B12}$$

Note that Eq. (B10) is a nonlinear equation in the same sense of the Brillouin-Wigner perturbation method, i.e., the eigenvalue $Z_j^{(\mu)}$ appears in the collision operator.

Assuming completeness in the space $\hat{P}^{(\mu)}$, we may always construct a set of states $\{\langle\langle\tilde{u}_j^{(\mu)}|\}$ biorthogonal to $\{|u_j^{(\mu)}\rangle\rangle\}$, i.e.,

$$\langle\langle\tilde{u}_j^{(\mu)}|u_{j'}^{(\mu')}\rangle\rangle = \delta_{j,j'}\delta_{\mu,\mu'}, \quad \sum_{\mu,j}|u_j^{(\mu)}\rangle\rangle\langle\langle\tilde{u}_j^{(\mu)}| = 1. \tag{B13}$$

Formula (B10) shows that the $\hat{P}^{(\mu)}$ component of $|F_j^{(\mu)}\rangle\rangle$ (which is called "*privileged component*" of $|F_j^{(\mu)}\rangle\rangle$) is an eigenstates of the collision operator, which has the same eigenvalue $Z_j^{(\mu)}$ as the Liouvillean. The solution of the eigenvalue problem of the Liouvillean for our class of singular functions has unique features. The privileged components satisfy closed equations and the $\hat{Q}^{(\mu)}$ components are "driven" by the privileged components [See Eq. (B8)].

Combining Eq. (B8) with Eq. (B11), we obtain the right eigenstates of the Liouvillean given by

$$|F_j^{(\mu)}\rangle\rangle = \sqrt{N_j^{(\mu)}}[\hat{P}^{(\mu)} + \hat{\mathcal{C}}^{(\mu)}(Z_j^{(\mu)})]|u_j^{(\mu)}\rangle\rangle. \tag{B14}$$

Similarly, we obtain for the left eigenstates given by

$$\langle\langle\tilde{F}_j^{(\mu)}| = \langle\langle\tilde{v}_j^{(\mu)}|[\hat{P}^{(\mu)} + \hat{\mathcal{D}}^{(\mu)}(Z_j^{(\mu)})]\sqrt{N_j^{(\mu)}}, \tag{B15}$$

where the operator $\hat{\mathcal{D}}^{(\mu)}(Z_j^{(\mu)})$ is called the destruction-of-correlation operator, or the *destruction operator* for short, and is defined by [cf. Eq. (B9)]

$$\hat{\mathcal{D}}^{(\mu)}(z) = \hat{P}^{(\mu)}g\mathcal{L}_{\rm int}\hat{Q}^{(\mu)}\frac{1}{z-\hat{Q}^{(\mu)}\mathcal{L}\hat{Q}^{(\mu)}}\hat{Q}^{(\mu)}. \tag{B16}$$

Again $\hat{\mathcal{D}}^{(\mu)}(z)$ corresponds to the off-diagonal transitions; $\hat{\mathcal{D}}^{(\mu)}(z)=\hat{P}^{(\mu)}\hat{\mathcal{D}}^{(\mu)}(z)\hat{Q}^{(\mu)}$. Using $\hat{\mathcal{D}}^{(\mu)}(z)$, the collision operator $\hat{\Psi}^{(\mu)}(z)$ is also written as

$$\hat{\Psi}^{(\mu)}(z) = \hat{P}^{(\mu)}\mathcal{L}_0\hat{P}^{(\mu)} + \hat{P}^{(\mu)}g\mathcal{L}_{\rm int}\hat{P}^{(\mu)} + \hat{P}^{(\mu)}\hat{\mathcal{D}}^{(\mu)}(z)\hat{Q}^{(\mu)}g\mathcal{L}_{\rm int}\hat{P}^{(\mu)}. \tag{B17}$$

The states $\langle\langle\tilde{v}_j^{(\mu)}|$ are the left eigenstates of the collision operator $\hat{\Psi}^{(\mu)}$,

$$\langle\langle \tilde{v}_j^{(\mu)} | \hat{\Psi}^{(\mu)}(Z_j^{(\mu)}) = \langle\langle \tilde{v}_j^{(\mu)} | Z_j^{(\mu)}. \tag{B18}$$

We have revealed so far the correspondence between the eigenvalue problems of the Liouvillean $\mathcal{L}$ and the collision operator $\hat{\Psi}^{(\mu)}$. Now we shall derive the kinetic equation from the solution of the eigenvalue problem of $\mathcal{L}$. In order to connect the kinetic theory to the eigenvalue problem of $\mathcal{L}$, we first introduce the *global* creation and destruction operators as

$$\mathbf{C}^{(\mu)} \equiv \sum_j \hat{\mathcal{C}}^{(\mu)}(Z_j^{(\mu)}) |u_j^{(\mu)}\rangle\rangle\langle\langle \tilde{u}_j^{(\mu)}|, \tag{B19a}$$

$$\mathbf{D}^{(\mu)} \equiv \sum_j |v_j^{(\mu)}\rangle\rangle\langle\langle \tilde{v}_j^{(\mu)}| \hat{\mathcal{D}}^{(\mu)}(Z_j^{(\mu)}). \tag{B19b}$$

Then, we can write the eigenstates as

$$|F_j^{(\mu)}\rangle\rangle = [N_j^{(\mu)}]^{1/2} (\hat{P}^{(\mu)} + \mathbf{C}^{(\mu)}) |u_j^{(\mu)}\rangle\rangle, \tag{B20a}$$

$$\langle\langle \tilde{F}_j^{(\mu)}| = \langle\langle \tilde{v}_j^{(\mu)}| (\hat{P}^{(\mu)} + \mathbf{D}^{(\mu)}) [N_j^{(\mu)}]^{1/2}. \tag{B20b}$$

The normalization constant may be found from the biorthonormality condition of the eigenstates Eq. (B6) as

$$[N_j^{(\mu)}]^{-1} = \langle\langle \tilde{v}_j^{(\mu)} | [\hat{A}_j^{(\mu)}]^{-1} | u_j^{(\mu)}\rangle\rangle, \tag{B21}$$

where

$$\hat{A}_j^{(\mu)} = [(\hat{P}^{(\mu)} + \mathbf{D}^{(\mu)})(\hat{P}^{(\mu)} + \mathbf{C}^{(\mu)})]^{-1} = [\hat{P}^{(\mu)} + \mathbf{D}^{(\mu)}\mathbf{C}^{(\mu)}]^{-1}. \tag{B22}$$

The global collision operators associated with the creation operator $\mathbf{C}^{(\mu)}$ are given by

$$\Theta_C^{(\mu)} \equiv \sum_j \hat{\Psi}^{(\mu)}(Z_j^{(\mu)}) |u_j^{(\mu)}\rangle\rangle\langle\langle \tilde{u}_j^{(\mu)}| = \sum_j Z_j^{(\mu)} |u_j^{(\mu)}\rangle\rangle\langle\langle \tilde{u}_j^{(\mu)}| \tag{B23}$$

and with the destruction operator $\mathbf{D}^{(\mu)}$ they are given by

$$\Theta_D^{(\mu)} \equiv \sum_j |v_j^{(\mu)}\rangle\rangle\langle\langle \tilde{v}_j^{(\mu)}| \hat{\Psi}^{(\mu)}(Z_j^{(\mu)}) = \sum_j |v_j^{(\mu)}\rangle\rangle\langle\langle \tilde{v}_j^{(\mu)}| Z_j^{(\mu)}. \tag{B24}$$

This is the direct way to see that the Liouvillean shares the same eigenvalues with the collision operator. Substituting Eq. (B12) into Eqs. (B23) and (B24), respectively, we have

$$\Theta_C^{(\mu)} = \hat{P}^{(\mu)}\mathcal{L}_0\hat{P}^{(\mu)} + \hat{P}^{(\mu)} g\mathcal{L}_{\rm int}\mathbf{C}^{(\mu)}\hat{P}^{(\mu)} \tag{B25}$$

and

$$\Theta_D^{(\mu)} = \hat{P}^{(\mu)}\mathcal{L}_0\hat{P}^{(\mu)} + \hat{P}^{(\mu)}\mathbf{D}^{(\mu)} g\mathcal{L}_{\rm int}\hat{P}^{(\mu)}. \tag{B26}$$

In general, we have $\Theta_C^{(\mu)} \neq \Theta_D^{(\mu)}$ [cf. Eqs. (B12) and (B17)].

The concept of *subdynamics* has been introduced in the works by Prigogine *et al.*[29,30,32,40,55] The relation of subdynamics to the complex spectral representation can be obtained through the projection operators $\Pi^{(\mu)}$ defined by

$$\Pi^{(\mu)} \equiv \sum_j |F_j^{(\mu)}\rangle\rangle\langle\langle \tilde{F}_j^{(\mu)}|. \tag{B27}$$

They satisfy the orthogonality and completeness relations,

$$\mathcal{L}\Pi^{(\mu)} = \Pi^{(\mu)}\mathcal{L}, \tag{B28a}$$

$$\Pi^{(\mu)}\Pi^{(\mu')} = \Pi^{(\mu)}\delta_{\mu\mu'}, \tag{B28b}$$

$$\sum_\mu \Pi^{(\mu)} = 1. \tag{B28c}$$

Therefore, $\Pi^{(\mu)}$ is an extension of $\hat{P}^{(\mu)}$ to the total Liouvillean $\mathcal{L}$.

The *dressed* distribution function for the collective modes associated with each subspace is given by

$$|\rho^{(\mu)}\rangle\rangle \equiv \Pi^{(\mu)}|\rho\rangle\rangle. \tag{B29}$$

The privileged component defined by $\hat{P}^{(\mu)}\rho^{(\mu)}(t)$ obeys the Markovian equation which reads

$$i\frac{\partial}{\partial t}\hat{P}^{(\mu)}|\rho^{(\mu)}(t)\rangle\rangle = \Theta_C^{(\mu)}\hat{P}^{(\mu)}|\rho^{(\mu)}(t)\rangle\rangle. \tag{B30}$$

In the weak-coupling case, we expand $\hat{\Psi}^{(\mu)}(z)$ in Eq. (B12) up to the second order of $\mathcal{L}_{\rm int}$,

$$\hat{\Psi}^{(\mu)}(z) \simeq \hat{\Psi}_2^{(\mu)}(w_\mu + i0)$$

$$= \hat{P}^{(\mu)}\mathcal{L}_0\hat{P}^{(\mu)} + g^2\hat{P}^{(\mu)}\mathcal{L}_{\rm int}\hat{\mathcal{C}}_1^{(\mu)}(w_\mu + i0)\hat{P}^{(\mu)}, \tag{B31a}$$

$$= \hat{P}^{(\mu)}\mathcal{L}_0\hat{P}^{(\mu)} + g^2\hat{P}^{(\mu)}\hat{\mathcal{D}}_1^{(\mu)}(w_\mu + i0)\mathcal{L}_{\rm int}\hat{P}^{(\mu)}, \tag{B31b}$$

where we have assumed $\hat{P}^{(\mu)}\mathcal{L}_{\rm int}\hat{P}^{(\mu)}=0$ which is the case we consider in this paper. In Eq. (B31a) $\hat{\mathcal{C}}_1^{(\mu)}(z)$ is given by

$$g\mathcal{C}_1^{(\mu)}(z) = \frac{1}{z - \mathcal{L}_0}\hat{Q}^{(\mu)} g\mathcal{L}_{\rm int}\hat{P}^{(\mu)}, \tag{B32}$$

and in Eq. (B31b) $\hat{\mathcal{D}}_1^{(\mu)}(z)$ is given by

$$g\mathcal{D}_1^{(\mu)}(z) = \hat{Q}^{(\mu)} g\mathcal{L}_{\rm int}\hat{P}^{(\mu)}\frac{1}{z - \mathcal{L}_0}. \tag{B33}$$

Substituting Eq. (B25) with Eq. (B31) and Eq. (B32) into Eq. (B30), we then have in the weak-coupling case the Markovian dissipative equation

$$i\frac{\partial}{\partial t}\hat{P}^{(\mu)}|\rho(t)\rangle\rangle = \hat{\Psi}_2^{(\mu)}(w^{(\mu)} + i0)\hat{P}^{(\mu)}|\rho(t)\rangle\rangle. \tag{B34}$$

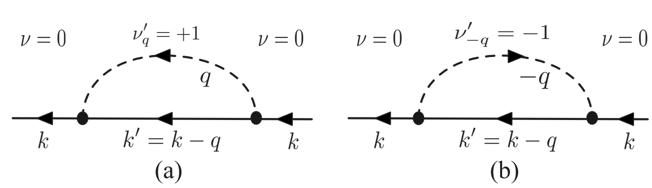

FIG. 9. Diagram of the collision operator $\bar{\Psi}_2^{(k)}(w_{kP}+i0)$.

APPENDIX C: DERIVATION OF THE KINETIC EQUATIONS

In this section, we shall derive the kinetic equations of the reduced distribution by applying Eq. (B34) into our model. Keeping in mind that $(\mu)=(k,0)$ in Eq. (B34) and taking a trace over the phonon field, we have

$$i\frac{\partial}{\partial t}\sum_N \langle\langle\{0\},\{N\}|\hat{P}^{(k,0)}|\rho(t)\rangle\rangle = \sum_N \langle\langle\{0\},\{N\}|\hat{\Psi}_2^{(k,0)}(w_{kP}+i0)\hat{P}^{(k,0)}|\rho(t)\rangle\rangle, \tag{C1a}$$

$$\Leftrightarrow i\frac{\partial}{\partial t}\langle\langle k,P|f(t)\rangle\rangle = \sum_{N,N'}\int dP'\langle\langle k,P|\langle\langle\{0\},\{N\}|\hat{\Psi}_2^{(k,0)}(w_{kP}+i0)|\{0\},\{N'\}\rangle\rangle|k,P'\rangle\rangle\langle\langle k,P'|\langle\langle\{0\},\{N'\}|\rho(t)\rangle\rangle, \tag{C1b}$$

where

$$\langle\langle k,P|\langle\langle\{0\},\{N\}|\hat{\Psi}_2^{(k,0)}(w_{kP}+i0)|\{0\},\{N'\}\rangle\rangle|k,P'\rangle\rangle$$

$$= w_{kP}\delta(P-P')\delta^{Kr}_{\{N\},\{N'\}} + g^2\langle\langle k,P|\langle\langle\{0\},\{N\}|\hat{P}^{(k,0)}\mathcal{L}_{\rm int}\hat{Q}^{(k,0)}\frac{1}{z-\mathcal{L}_0}\hat{Q}^{(k,0)}\mathcal{L}_{\rm int}\hat{P}^{(k,0)}|\{0\},\{N'\}\rangle\rangle|k,P'\rangle\rangle \tag{C2a}$$

$$\equiv \hat{\Psi}_2^{(k,0)}\left(P,\frac{\partial}{\partial P},\{N\},\frac{\partial}{\partial\{N\}}\right)\delta(P-P')\,\delta^{Kr}_{\{N\},\{N'\}}. \tag{C2b}$$

Substituting Eq. (C2b) into Eq. (C1b) leads to

$$i\frac{\partial}{\partial t}\langle\langle k,P|f(t)\rangle\rangle = \sum_N \hat{\Psi}_2^{(k,0)}\left(P,\frac{\partial}{\partial P},\{N\},\frac{\partial}{\partial\{N\}}\right)\langle\langle k,P|\langle\langle\{0\},\{N\}|\rho(t)\rangle\rangle. \tag{C3}$$

By using the fact that the phonon distribution does not deviate from the thermal equilibrium in a large volume system, we can cast Eq. (C3) into the form of

$$i\frac{\partial}{\partial t}\langle\langle k,P|f(t)\rangle\rangle = \sum_N \hat{\Psi}_2^{(k,0)}\left(P,\frac{\partial}{\partial P},\{N\},\frac{\partial}{\partial\{N\}}\right)\rho_{\rm ph}^{\rm eq}(N)\langle\langle k,P|f(t)\rangle\rangle, \tag{C4}$$

where $\rho_{\rm ph}^{\rm eq}(N)=\exp[-\Sigma_q\beta\hbar\omega_q N_q]/Z_{\rm ph}$. We define a collision operator $\hat{\bar{\Psi}}_2^{(k)}(w_{kP}+i0)$ acting on the particle distribution whose matrix elements are determined by

$$\langle\langle k,P|\hat{\bar{\Psi}}_2^{(k)}(w_{kP}+i0)|k,P'\rangle\rangle \equiv \left\{\sum_N \hat{\Psi}_2^{(k,0)}\left(P,\frac{\partial}{\partial P},\{N\},\frac{\partial}{\partial\{N\}}\right)\rho_{\rm ph}^{\rm eq}(N)\right\}\delta(P-P') \tag{C5a}$$

$$= w_{kP}\delta(P-P') + g^2\langle\langle k,P|\mathrm{Tr}_{\rm ph}\left[\hat{P}^{(k,0)}\mathcal{L}_{\rm int}\hat{Q}^{(k,0)}\frac{1}{w_{kP}+i0-\mathcal{L}_0}\hat{Q}^{(k,0)}\mathcal{L}_{\rm int}\hat{P}^{(k,0)}\rho_{\rm ph}^{\rm eq}\right]|k,P'\rangle\rangle. \tag{C5b}$$

Substituting Eq. (C5) into Eq. (C4), we obtain the kinetic equation of the reduced distribution as

$$i\frac{\partial}{\partial t}\hat{P}^{(k)}|f(t)\rangle\rangle = \hat{\bar{\Psi}}_2^{(k)}(w_{kP}+i0)\hat{P}^{(k)}|f(t)\rangle\rangle, \tag{C6}$$

where $\hat{P}^{(k)} \equiv \int dP|k,P\rangle\rangle\langle\langle k,P|$.

The second term of Eq. (C5b) consists of the two terms which are represented by the diagrams in Fig. 9. The explicit expressions of these terms are given by

$$\frac{g^2}{\hbar^2\Omega}\sum_q\sum_N V_q\left\{\sqrt{N_q+1}\,\exp\left[-\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[\frac{1}{2}\frac{\partial}{\partial N_q}\right] - \sqrt{N_q}\,\exp\left[\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[-\frac{1}{2}\frac{\partial}{\partial N_q}\right]\right\}\frac{1}{z-(w_{k-q,P}+\omega_q)}$$
$$\times V_{-q}\left\{\sqrt{N_q+\frac{1}{2}}\exp\left[\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[-\frac{1}{2}\frac{\partial}{\partial N_q}\right] - \sqrt{N_q+\frac{1}{2}}\exp\left[-\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[\frac{1}{2}\frac{\partial}{\partial N_q}\right]\right\}\rho_{\rm ph}^{\rm eq}(N)\delta(P-P') \tag{C7}$$

for Fig. 9(a) and

$$\frac{g^2}{\hbar^2\Omega}\sum_q\sum_N V_q\left\{\sqrt{N_{-q}}\exp\left[-\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[-\frac{1}{2}\frac{\partial}{\partial N_{-q}}\right]-\sqrt{N_{-q}+1}\exp\left[\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[\frac{1}{2}\frac{\partial}{\partial N_{-q}}\right]\right\}\frac{1}{z-(w_{k-q,P}-\omega_{-q})}$$
$$\times V_{-q}\left\{\sqrt{N_{-q}+\frac{1}{2}}\exp\left[\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[\frac{1}{2}\frac{\partial}{\partial N_{-q}}\right]-\sqrt{N_{-q}+\frac{1}{2}}\exp\left[-\frac{\hbar q}{2}\frac{\partial}{\partial P}\right]\exp\left[-\frac{1}{2}\frac{\partial}{\partial N_{-q}}\right]\right\}\rho_{\rm ph}^{\rm eq}(N)\,\delta(P-P') \quad \text{(C8)}$$

for Fig. 9(b), where $\rho_{\rm ph}^{\rm eq}(N)\equiv\exp[-\Sigma_q\beta\hbar\omega_qN_q]/Z_{\rm ph}$. By taking the thermodynamic limit in Eqs. (C7) and (C8) and combining them with the first term of Eq. (C5b), we obtain the explicit expression of $\hat{\hat{\Psi}}_2^{(k)}(z)$ as

$$\langle\langle k,P|\hat{\hat{\Psi}}_2^{(k)}(z)|k,P'\rangle\rangle$$
$$=\left\{w_{kP}+\frac{g^2}{\hbar^2}\int dq|V_q|^2\left[\left\{\frac{1}{z-(w_{k-q,P-\hbar q/2}+\omega_q)}+\frac{1}{z+(w_{k-q,P-\hbar q/2}+\omega_q)}\right\}(n(q)+1)(1-\exp[-\beta\omega_q]\exp[-\hbar q\,\partial/\partial P])\right.\right.$$
$$\left.\left.+\left\{\frac{1}{z-(w_{k-q,P+\hbar q/2}+\omega_q)}+\frac{1}{z+(w_{k-q,P+\hbar q/2}+\omega_q)}\right\}n(q)(1-\exp[\beta\omega_q]\exp[\hbar q\,\partial/\partial P])\right]\right\}\delta(P-P'). \quad \text{(C9)}$$

APPENDIX D: CLASSICAL LIMIT

In this section, we prove that the collision operator given by Eq. (21) vanishes in the classical limit ($\hbar\to 0$), which suggests that no dissipation takes place in the present one-dimensional chain under the g^2t approximation. For this purpose, we start with Eqs. (C7) and (C8) and expand them in terms of $\hbar$, rather than to directly expand Eq. (21). Instead of $\{N\}$ and $\{\nu\}$, we use the action $\{J\}$ and angle $\{\alpha\}$ variables defined by[47,54]

$$x_q=\sqrt{\frac{2J_q}{m\omega_q}}\sin\alpha_q,\quad p_q=\sqrt{2J_qm\omega_q}\cos\alpha_q, \quad \text{(D1)}$$

where $x_q=\sqrt{\hbar/2m\omega_q}(b_q+b_q^\dagger)$ and $p_q=-i\sqrt{m\hbar\omega_q/2}(b_q-b_q^\dagger)$. We then have the following relations,

$$N_q\to\frac{J_q}{\hbar},\quad \sum_N\to\frac{1}{\hbar}\int dJ,\quad \rho_{\rm ph}^{\rm eq}(N)\to\hbar\rho_{\rm ph}^{\rm eq}(J), \quad \text{(D2)}$$

where the equilibrium distribution for the phonon system is represented by

$$\rho_{\rm ph}^{\rm eq}(J)=\prod_q\beta\omega_q\exp\left[-\sum_q\beta\omega_qJ_q\right]. \quad \text{(D3)}$$

The expressions of Eqs. (C7) and (C8) are cast into the form of

$$\frac{g^2}{\hbar^2\Omega}\sum_q\int dJV_q\frac{1}{\hbar}\left\{\sqrt{J_q+\hbar}\exp\left[\frac{\hbar}{2}\left(-q\frac{\partial}{\partial P}+\frac{\partial}{\partial J_q}\right)\right]\right.$$
$$\left.-\sqrt{J_q}\exp\left[\frac{\hbar}{2}\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\right]\right\}\frac{1}{z-(w_{-q,P}+\omega_q)}$$
$$\times V_{-q}\left\{\sqrt{J_q+\frac{\hbar}{2}}\exp\left[\frac{\hbar}{2}\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\right]\right.$$
$$\left.-\sqrt{J_q+\frac{\hbar}{2}}\exp\left[\frac{\hbar}{2}\left(-q\frac{\partial}{\partial P}+\frac{\partial}{\partial J_q}\right)\right]\right\}\rho_{\rm ph}^{\rm eq}(J)\,\delta(P-P') \quad \text{(D4)}$$

and

$$\frac{g^2}{\hbar^2\Omega}\sum_q\int dJV_{-q}\frac{1}{\hbar}\left\{\sqrt{J_q}\exp\left[\frac{\hbar}{2}\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\right]\right.$$
$$\left.-\sqrt{J_q+\hbar}\exp\left[\frac{\hbar}{2}\left(-q\frac{\partial}{\partial P}+\frac{\partial}{\partial J_q}\right)\right]\right\}\frac{1}{z-(w_{q,P}-\omega_q)}$$
$$\times V_q\left\{\sqrt{J_q+\frac{\hbar}{2}}\exp\left[\frac{\hbar}{2}\left(-q\frac{\partial}{\partial P}+\frac{\partial}{\partial J_q}\right)\right]\right.$$
$$\left.-\sqrt{J_q+\frac{\hbar}{2}}\exp\left[\frac{\hbar}{2}\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\right]\right\}\rho_{\rm ph}^{\rm eq}(J)\,\delta(P-P'), \quad \text{(D5)}$$

respectively, where we have replaced q with $-q$ in Eq. (D5). In the classical limit, we may neglect the action $\hbar$ compared to J_q. By expanding the exponentials in terms of $\hbar$, the above expressions reduce to

$$g^2\int dq\int dJ\frac{|V_q|^2}{\hbar}\left(-q\frac{\partial}{\partial P}+\frac{\partial}{\partial J_q}\right)\frac{J_q}{z-(w_{-q,P}+\omega_q)}$$
$$\times\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\rho_{\rm ph}^{\rm eq}(J)\,\delta(P-P') \quad \text{(D6)}$$

and

$$g^2\int dq\int dJ\frac{|V_q|^2}{\hbar}\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\frac{J_q}{z-(w_{q,P}-\omega_q)}$$
$$\times\left(-q\frac{\partial}{\partial P}+\frac{\partial}{\partial J_q}\right)\rho_{\rm ph}^{\rm eq}(J)\,\delta(P-P'), \quad \text{(D7)}$$

respectively, where we have replaced $\Omega^{-1}\Sigma_q$ with $\int dq$. By summing up Eqs. (D6) and (D7), and taking $z=+i0$, we obtain

$$\langle\langle 0,P|\hat{\hat{\Psi}}_2^{(0)}(+i0)|0,P'\rangle\rangle = 2i\pi g^2\int dq\int dJ\frac{|V_q|^2}{\hbar} \times\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)J_q\delta(qP/m-c|q|) \times\left(q\frac{\partial}{\partial P}-\frac{\partial}{\partial J_q}\right)\rho_{\rm ph}^{\rm eq}(J)\delta(P-P') \tag{D8a}$$

$$=2i\pi g^2 k_BT\int dq\frac{|V_q|^2}{\hbar\omega_q}\frac{\partial}{\partial P}q\delta(qP/m-c|q|) \times\left(q\frac{\partial}{\partial P}+\frac{\omega_q}{k_BT}\right)\delta(P-P') \tag{D8b}$$

$$=\frac{ig^2|\Delta_0|^2k_BT}{2c^2\rho_M}\int dq\frac{\partial}{\partial P}q\delta[q(P/m-cq/|q|)] \times\left(q\frac{\partial}{\partial P}+\frac{\omega_q}{k_BT}\right)\delta(P-P'), \tag{D8c}$$

where we have integrated for J with use of Eq. (D3) in Eq. (D8b), and have used Eq. (10) in Eq. (D8c). The expression (D8c) is identical with the one Bak *et al.* have derived in three-dimensional case. [See Eq. (19) in Ref. 54].

Since the integrand includes the factor of $q\delta[q(P/m\pm c)]$, the one-dimensional integration for q vanishes, resulting in $\langle\langle 0,P|\hat{\hat{\Psi}}_2^{(0)}(+i0)|0,P'\rangle\rangle=0$. This proves that no dissipation occurs in the present one-dimensional chain when the interaction of the quantum particle and the phonon field is considered up to the second order in the collision operator. The situation is similar to the one-dimensional gas system where the collision operator vanishes in the second-order approximation for the collision operator.[47] On the other hand, in two- and three-dimensional cases the integration for q turns out to be

$$\int d\mathbf{q}\mathbf{q}\delta\left(\mathbf{q}\cdot\frac{\mathbf{P}}{m}\pm c\right)\left(\mathbf{q}\cdot\frac{\partial}{\partial\mathbf{P}}+\frac{\omega_q}{k_BT}\right). \tag{D9}$$

The two- or three-dimensional integration for $\mathbf{q}$ gives a finite value for the collision operator as long as the particle velocity $|\mathbf{P}|/m$ exceeds over c; the dissipation occurs for this case, which is nothing but the Cherenkov radiation.[47]

It is worth while to emphasize the two aspects of the $\hbar\to 0$ limit. First the $h\to 0$ is equivalent to the limit of $T\to\infty$ in terms of the average phonon number $\langle N\rangle=\langle J\rangle/\hbar \simeq k_BT/\hbar\omega$. In this limit, we may neglect the elementary action $\hbar$ compared to J in Eqs. (D4) and (D5). The other aspect of the $\hbar\to 0$ limit is seen in the resonance condition represented by the delta function in the collision operator. For a finite $\hbar$, the resonance condition in Eq. (21), $\varepsilon_{P\pm\hbar q}-\varepsilon_P=\pm\hbar\omega_q$, reads

$$\frac{(P\pm\hbar q)^2}{2m}-\frac{P^2}{2m}=\pm c\hbar|q| \Leftrightarrow \pm\frac{qP}{m}+\frac{\hbar q^2}{2m}=\pm c|q|. \tag{D10}$$

This represents both the energy and the momentum conservations in the elementary collision process between the quantum Brownian particle and a phonon. A nonzero value of $|q|=|2P\pm mc|/\hbar$ satisfies Eq. (D10), resulting in the finite value of the collision operator in quantum mechanics as shown in Eq. (44) or Fig. 2(a). Note that, since the quantum resonance condition is irrespective of temperature, the collision operator exists for any temperatures as long as we keep $\hbar$ finite. On the other hand, when $\hbar\to 0$ is taken in Eq. (D10), the classical resonance condition is satisfied only for $q=0$, as shown in Eq. (D8c), resulting in the vanishing collision operator.

APPENDIX E: THE ANALYTIC SOLUTION FOR A HIGH TEMPERATURE CASE

In this section, we show the approximate solution of the eigenvalue problem of $\hat{\mathcal{K}}^{(0)}$ and the temperature dependence of the relaxation time. First we note that the collision operator $\hat{\mathcal{K}}^{(0)}$ has a property for symmetry of

$$\hat{\mathcal{K}}^{(0)}\left(P,\frac{P}{\partial P}\right)=\hat{\mathcal{K}}^{(0)}\left(-P,-\frac{\partial}{\partial P}\right) \tag{E1}$$

which enables us to divide the whole momentum space into two independent subspaces as

$$|0,P^S\rangle\rangle \equiv \frac{1}{\sqrt{2}}(|0,P\rangle\rangle+|0,-P\rangle\rangle)(P^S\geq 0), \tag{E2a}$$

$$|0,P^S\rangle\rangle \equiv \frac{1}{\sqrt{2}}(|0,P\rangle\rangle-|0,-P\rangle\rangle)(P^A> 0), \tag{E2b}$$

where $|0,P^S\rangle\rangle$ and $|0,P^A\rangle\rangle$ denote the symmetric and antisymmetric basis in the momentum distribution space, respectively. In this section, we consider the distribution $\chi_j(P)$ deviated from the equilibrium, instead of $\phi_j(P)$,

$$\phi_j(P)\equiv\varphi_{\rm eq}(P)\chi_j(P), \tag{E3}$$

where $\varphi_{\rm eq}(P)$ is given by Eq. (26). Corresponding to the symmetrized basis of $|0,P^S\rangle\rangle$ and $|0,P^A\rangle\rangle$, the momentum distribution function is classified into two subspaces as

$$\chi_j^S(P)\equiv\langle\langle 0,P^S|\chi_j\rangle\rangle=\frac{1}{\sqrt{2}}[\chi_j(P)+\chi_j(-P)], \tag{E4a}$$

$$\chi_j^A(P)\equiv\langle\langle 0,P^A|\chi_j\rangle\rangle=\frac{1}{\sqrt{2}}[\chi_j(P)-\chi_j(-P)]. \tag{E4b}$$

With use of Eqs. (21), Eq. (24) is classified into two kinetic equations for each subspace,

$$\hat{\mathcal{K}}^S\left(P^S,\frac{P^S}{\partial P^S}\right)\chi_j^S(P^S)=\lambda_j^{(0)}\chi_j^S(P^S), \tag{E5a}$$

$$\hat{\mathcal{K}}^A\left(P^A,\frac{P^A}{\partial P^A}\right)\chi_j^A(P^A)=\lambda_j^{(0)}\chi_j^A(P^A). \tag{E5b}$$

With use of Eqs. (E1) and (21), explicit expression of these eigenvalue problems are written as

$$\frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\chi_j^S(P^S)=\{n[2(P^S+1)]+n[2(P^S-1)]+1\}\chi_j^S(P^S)-n[2(P^S+1)]\chi_j^S(P^S+2)-\{n[2(P^S-1)]+1\}\chi_j^S(P^S-2)\quad (P^S>1), \tag{E6a}$$

$$\frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\chi_j^S(P^S)=\{n[2(P^S+1)]+n[2(P^S-1)]\}\chi_j^S(P^S)-n[2(P^S+1)]\chi_j^S(P^S+2)-n[2(P^S-1)]\chi_j^S(P^S-2)\quad (1>P^S\geq 0), \tag{E6b}$$

and

$$\frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\chi_j^A(P^A)=\{n[2(P^A+1)]+n[2(P^A-1)]+1\}\chi_j^A(P^A)+n[2(P^A+1)]\chi_j^A(P^A+2)+\{n[2(P^A-1)]+1\}\chi_j^A(P^A-2)\quad (P^A>1), \tag{E7a}$$

$$\frac{\lambda_j^{(0)}}{|\Delta_0|^2/\rho_M}\chi_j^A(P^A)=\{n[2(P^A+1)]+n[2(P^A-1)]\}\chi_j^A(P^A)+n[2(P^A+1)]\chi_j^A(P^A+2)+n[2(P^A-1)]\chi_j^A(P^A-2)\quad (1>P^A>0). \tag{E7b}$$

For a high-temperature and high-momentum case,

$$T\gg 1,\quad P^S,P^A\gg 1, \tag{E8}$$

we can approximate in Eqs. (E6) and (E7) that

$$n_{2(P+1)}-n_{2(P-1)}+1\simeq 1, \tag{E9a}$$

$$n_{2(P+1)}+n_{2(P-1)}+1\simeq 2n_{2P}, \tag{E9b}$$

and

$$\chi_j(P\pm 2)\simeq\chi_j(P)\pm 2\frac{d}{dP}\chi_j(P)+2\frac{d^2}{dP^2}\chi_j(P). \tag{E10}$$

Substituting Eqs. (E10) into Eq. (E6a) or (E7a), we have a eigenvalue problem presented as a differential equation,

$$-\frac{T}{P}\frac{d^2}{dP^2}\chi_j(P)+\frac{d}{dP}\chi_j(P)=\frac{\lambda_j^{(0)}}{2|\Delta_0|^2/\rho_M}\chi_j(P), \tag{E11}$$

where we assume $n_P\simeq T/P$. By taking a new variable ξ and corresponding distribution $g_j(\xi)$ as

$$\xi\equiv\frac{P}{\sqrt{2T}},\quad g_j(\xi)\equiv\exp[-\lambda_j\xi\sqrt{T/2}]\chi_j(\xi), \tag{E12}$$

the eigenvalue Eq. (E11) is reduced to the following Hermite-type differential equation:

$$\frac{d^2}{d\xi^2}g_j(\xi)-2\left(\xi-\sqrt{\frac{T}{2}}\lambda_j\right)\frac{d}{d\xi}g_j(\xi)+2\left(\frac{T}{4}\lambda_j^2\right)g_j(\xi)=0. \tag{E13}$$

The solutions are obtained as

$$g_j(\xi)=H_j(\xi-\lambda_j\sqrt{T/2}) \tag{E14}$$

where $H_j(x)$ is a jth degree Hermite polynomial. The eigenvalue is given by

$$\lambda_j=2\sqrt{\frac{j}{T}}\quad (j=0,1,2,\ldots). \tag{E15}$$

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