Dual Spaces Structure of Quantum Kinetic Equations

—— *Quantum Systems vs Classical Systems* ——

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The relation between the Hilbert space structure and the generalized spaces structure represented by dual states for dissipative kinetic equation is discussed for quantum systems. As working examples, we consider the systems of a harmonic oscillator or a particle interacting with a thermal reservoir and construct analytic solutions to the eigenvalue problem of the quantum collision operators of these systems. The generalized spaces structure of the eigenfunctions indicates that dissipation destroys the Hilbert space structure of the undamped system. In the Wigner representation where the quantum collision operators closely resemble the classical kinetic operators in phase space, the Hilbert space structure can be restored to certain extent by introducing a weighted norm or a similarity transformation on the operators. However, in the position space where the collision operators have no classical counterpart, generalized spaces description cannot be avoided.

§1. Introduction

The conventional quantum mechanics occurs in the Hilbert space and evolves in a time unitary way.[1)] To incorporate dissipative phenomena such as resonances and damping into the picture, we have to give up unitary time evolution. The spectrum of the Hamiltonian then turns complex and the Hilbert space structure cannot be maintained. Hence, generalized spaces structure of quantum mechanics represented by the dual states emerges.[2)]

In a parallel line of thought that occurred much earlier in classical kinetic theory, Boltzmann's pioneering work on dilute gas[3)] was intended to obtain an irreversible picture of classical system out of reversible Hamiltonian dynamics. As a result, the kinetic operators that govern the time evolution of damped or diffusive systems possess complex eigenvalues. The dynamics should also then occur in the generalized spaces. It may occur either on the level of the full Liouville dynamics,[4)] or on the level of the reduced dynamics, which is our focus here.

The reduced dynamics of the subsystem can be obtained through the Markovian approximation,[5)] in which the memory effect in the dynamics is effectively neglected. As a result, the reduced dynamics dictated by the collision (kinetic) operator lies in the generalized spaces. It obeys exact exponential decay law and possesses complex eigenvalues. This will be shown through examples involving a harmonic oscillator or a particle in a thermal reservoir by solving the eigenvalue problem of the collision operators analytically.

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An issue arises with regard to the necessity of such these generalized spaces description, in view of some procedures in classical kinetic theory that may bring back both the left and right eigenfunctions to the Hilbert space (square integrable). By applying the same procedures on the quantum collision operators in the Wigner representation that bears a much similar structure to the classical kinetic operators in phase space, we find that the Hilbert space structure can be restored to some extent, a statement that will be clarified later. However, if we want to describe the quantum dynamics in the more natural position space that does not have classical counterpart, the generalized spaces description cannot be avoided.

§2. Free harmonic oscillator

We begin with a simple harmonic oscillator. The time evolution of its density function $i\partial\phi/\partial t = C_0\phi$ is governed by the Liouville operator, $C_0\cdot = [H_0, \cdot]/\hbar$, where $H_0 = \hbar\omega_0 a^\dagger a$ is the free oscillator Hamiltonian with natural frequency ω_0 and annihilation operator a. In the position coordinate, we denote the density function by $\phi(x,\tilde{x}) \equiv \langle x|\phi|\tilde{x}\rangle$. Using the coordinate representation of $a^\dagger|x\rangle = \frac{1}{\sqrt{2}}(x+\partial/\partial x)|x\rangle$ and $a|x\rangle = \frac{1}{\sqrt{2}}(x-\partial/\partial x)|x\rangle$, the Liouville operator becomes

$$C_0(x,\tilde{x}) = \frac{\omega_0}{2}\left(-\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial\tilde{x}^2} + x^2 - \tilde{x}^2\right), \tag{2·1}$$

where $x \equiv \sqrt{m\omega_0/\hbar}\,q$ is the dimensionless position, m being the mass of the oscillator and q the usual position coordinate with the dimension of length.

The Liouville operator is the difference between two simple oscillators' Hamiltonian acting on different position coordinates. The solution to the eigenvalue problem $C_0\phi_\nu = \omega_\nu\phi_\nu$ is therefore the product of the wave functions of two oscillators,

$$\phi_{mn}(x,\tilde{x}) = \frac{1}{\sqrt{2^{m+n}m!n!\pi}}\,e^{-x^2/2-\tilde{x}^2/2}H_m(x)H_n(\tilde{x}), \quad m,\,n = 0,1,2,3,\ldots, \tag{2·2}$$

with eigenvalue $\omega_{mn} = \omega_0(m-n)/2$, where H_n is the Hermite polynomial. The quantum mechanical vacuum f_{00} is infinitely degenerate in the diagonal states $m = n$. The eigenfunctions are square integrable under the norm

$$\langle\langle\phi_{mn}|\phi_{m'n'}\rangle\rangle \equiv \int_{-\infty}^{\infty}dx\int_{-\infty}^{\infty}d\tilde{x}\,\phi^*_{mn}(x,\tilde{x})\phi_{m'n'}(x,\tilde{x}) = \delta_{m,m'}\delta_{n,n'}\,. \tag{2·3}$$

Since the collision operator is Hermitian $C_0^\dagger = C_0$, its left eigenfunctions are separately identical with its right eigenfunctions, and are also square integrable.

§3. Damped oscillator – effect of dissipation

We now consider the effect of dissipation on the square integrability of the eigenfunctions. We consider an oscillator coupled linearly to a field[6)]

$$H = \hbar\omega_0 a^\dagger a + \textstyle\sum_k \hbar\omega_k a_k^\dagger a_k + \frac{\lambda}{\sqrt{L}}\sum_k v_k(a^\dagger a_k + a a_k^\dagger), \tag{3·1}$$

where λ is a dimensionless coupling constant and L is the space dimension of the box the system resides, before we take the thermodynamic limit.[7] On the level of Liouville dynamics, we assume the Van Hove limit[8] (weak coupling), average out the contribution of the field and eventually take the thermodynamic limit. As a result, we obtain the reduced dynamics of the oscillator governed by the collision operator, $C = C_0 + C_{\rm d}$, which is a completely positive Kassakowski-Lindblad's operator.[9] The contribution to the unitary component of the time evolution C_0 is the same as in §2, whereas the dissipative component is given by

$$C_{\rm d} f \equiv i\gamma(b+\tfrac{1}{2})(2afa^\dagger - a^\dagger af - fa^\dagger a) + i\gamma(b-\tfrac{1}{2})(2a^\dagger fa - aa^\dagger f - faa^\dagger)\,, \quad (3\cdot2)$$

where $\gamma = \lambda^2/(2L)\sum_k |v_k|^2\delta(\omega_k - \omega_0)$ is the damping constant and

$$b = \tfrac{1}{2}\coth(\hbar\omega_0/2k_BT) \xrightarrow{T\to\infty} \frac{k_BT}{\hbar\omega_0} \quad (3\cdot3)$$

is a thermal parameter related to the temperature of the field in thermal equilibrium.

Using the center $Q \equiv (x+\tilde{x})/2$ and relative $r \equiv x - \tilde{x}$ coordinates, the collision operator takes a compact form,

$$C(Q,r) = -\omega_0\left(\frac{\partial^2}{\partial Q\partial r} - Qr\right) + i\gamma\left(\frac{\partial}{\partial Q}Q - r\frac{\partial}{\partial r}\right) + i\gamma b\left(\frac{\partial^2}{\partial Q^2} - r^2\right)\,, \quad (3\cdot4)$$

where we have ignored the renormalization of the frequency that is not essential to our discussion.

The eigenvalue problem $Cf_\nu = z_\nu f_\nu$ can be solved analytically in the Wigner representation,[10] obtained through a Fourier transform on the r coordinate

$$\mathcal{F}[f] = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dr\, e^{-iPr} f(Q,r) \equiv f^{\rm w}(Q,P)\,. \quad (3\cdot5)$$

The collision operator in the Wigner representation is

$$C^{\rm w}(Q,P) = -i\omega_0\left(P\frac{\partial}{\partial Q} - Q\frac{\partial}{\partial P}\right) + i\gamma\left(\frac{\partial}{\partial Q}Q + \frac{\partial}{\partial P}P\right) + i\gamma b\left(\frac{\partial^2}{\partial Q^2} + \frac{\partial^2}{\partial P^2}\right)\,. \quad (3\cdot6)$$

We can learn about the classical behaviour of the oscillator by taking the ensemble average of the kinetic equation $i\partial f/\partial t = Cf$ over Q and P. We obtain the following set of coupled equations,

$$\langle\dot{Q}\rangle = \omega_0\langle P\rangle - \gamma\langle Q\rangle\,, \qquad \langle\dot{P}\rangle = -\omega_0\langle Q\rangle - \gamma\langle P\rangle\,, \quad (3\cdot7)$$

where dot represents time derivative. The motion of a damped oscillator is then

$$\langle Q\rangle_t = e^{-\gamma t}\left[\langle Q\rangle_0\cos\omega_0 t + \langle P\rangle_0\sin\omega_0 t\right]\,, \quad (3\cdot8)$$

$$\langle P\rangle_t = e^{-\gamma t}\left[\langle P\rangle_0\cos\omega_0 t - \langle Q\rangle_0\sin\omega_0 t\right]\,. \quad (3\cdot9)$$

Introducing the quantum analog of the classical action-angle variables,[11] $P \equiv \sqrt{2J}\cos\alpha$ and $Q \equiv \sqrt{2J}\sin\alpha$, the collision operator becomes separable,

$$C^{\mathrm{w}}(J,\alpha) = -i\omega_0\frac{\partial}{\partial\alpha} + i\gamma\left(b\frac{\partial}{\partial J}J\frac{\partial}{\partial J} + \frac{\partial}{\partial J}J + \frac{b}{4J}\frac{\partial^2}{\partial\alpha^2}\right). \tag{3·10}$$

The eigenvalue problem of C^{w} can now be solved[7] by separating the angle variable through the Fourier series $\exp(\pm in\alpha)$. We are then left with a second order differential equation in J, with the collision invariant (i.e., the eigenfunction with $z_\nu = 0$ that corresponds to the equilibrium solution of the kinetic equation $i\partial f^{\mathrm{w}}/\partial t = C^{\mathrm{w}} f^{\mathrm{w}}$)

$$f^{\mathrm{w}}_{\mathrm{eq}} = \frac{1}{\sqrt{2\pi b}}\exp(-J/b), \tag{3·11}$$

normalized according to Eq. (3·17) below.

To obtain the complete solutions to the kinetic equation, we go on to extract the factor $(J/b)^{n/2}f^{\mathrm{w}}_{\mathrm{eq}}$ from f^{w}_ν. We are then left with the differential equation

$$\left[bJ\frac{\partial^2}{\partial J^2} + b(1+n-J/b)\frac{\partial}{\partial J} + (m-n)\right]L^n_m(J/b) = 0, \tag{3·12}$$

satisfied by the associated Laguerre polynomials,[7] $L^n_m(J/b)$. The eigenvalues and eigenfunctions are

$$z^{\pm}_{mn} = \pm n\omega_0 - i\left(m - \tfrac{n}{2}\right)\gamma, \qquad m \geq n, \tag{3·13}$$

$$f^{\mathrm{w}\pm}_{mn}(J,\alpha) = \sqrt{\frac{(m-n)!}{m!^3}}\,e^{\pm in\alpha}(J/b)^{n/2}L^n_m(J/b)f^{\mathrm{w}}_{\mathrm{eq}}. \tag{3·14}$$

Thanks to the factor $\exp(-J/b)$ in $f^{\mathrm{w}}_{\mathrm{eq}}$ (3·11), the right eigenfunctions are square integrable with respect to the norm (3·17) defined below.

Since C is a non-Hermitian operator, we need to also consider the left eigenvalue problem of its adjoint, $C^\dagger g_\nu = z^*_\nu g_\nu$, defined through $\langle\langle f_\mu|C^\dagger|g_\nu\rangle\rangle = \langle\langle g_\nu|C|f_\mu\rangle\rangle^*$,

$$C^{\mathrm{w}\dagger}(J,\alpha) = -i\omega_0\frac{\partial}{\partial\alpha} - i\gamma\left(b\frac{\partial}{\partial J}J\frac{\partial}{\partial J} - J\frac{\partial}{\partial J} + \frac{b}{4J}\frac{\partial^2}{\partial\alpha^2}\right). \tag{3·15}$$

Its solution can be obtained readily from its right counterpart by extracting the equilibrium solution from f^{w}_ν. We first write $f^{\mathrm{w}}_\nu = f^{\mathrm{w}}_{\mathrm{eq}}\bar{f}^{\mathrm{w}}_\nu$, and then take the complex conjugate over the resulting equation on $\bar{f}^{\mathrm{w}}_\nu$. If we now relabel the angle variable as $-\alpha$, we obtain $C^{\mathrm{w}\dagger}(J,\alpha)\bar{f}^{\mathrm{w}\pm *}_{mn}(J,-\alpha) = z^{\pm *}_{mn}\bar{f}^{\mathrm{w}\pm *}_{mn}(J,-\alpha)$. Using the fact that $\bar{f}^{\mathrm{w}\pm *}_{mn}(J,-\alpha) = \bar{f}^{\mathrm{w}\pm}_{mn}(J,\alpha)$, we can set

$$g^{\mathrm{w}\pm}_{mn}(J,\alpha) = e^{J/b}f^{\mathrm{w}\pm}_{mn}(J,\alpha). \tag{3·16}$$

Since the exponential decaying factor of $f^{\mathrm{w}}_{\mathrm{eq}} \sim \exp(-J/b)$ in $f^{\mathrm{w}\pm}_{mn}$ is canceled by the prefactor on the right-hand side of Eq. (3·16), the left eigenfunctions are no longer square integrable. As a result of dissipation, the biorthogonal pair of eigenfunctions

become objects in the generalized spaces. The normalized eigenfunctions satisfy the orthogonality and completeness relations ($\sigma = \pm$)

$$\langle\langle g_\nu | f_{\nu'} \rangle\rangle = \delta_{\nu,\nu'} \quad \leftrightarrow \quad \int_{-\infty}^{\infty} dJ \int_0^{2\pi} d\alpha \, (g_{mn}^{\mathrm{w}\sigma})^* f_{m'n'}^{\mathrm{w}\sigma'} = \delta_{m,m'}\delta_{n,n'}\delta_{\sigma,\sigma'}, \tag{3·17}$$

$$\sum_\nu |f_\nu\rangle\rangle\langle\langle g_\nu| = I \quad \leftrightarrow \quad \sum_\nu g_\nu(J,\alpha) f_\nu(J',\alpha') = \delta(\alpha-\alpha')\delta(J-J'). \tag{3·18}$$

They can be proved by using the orthogonality of the Fourier series and the associated Laguerre polynomials.[7)]

When we go back to the original position coordinates, the eigenfunctions become

$$f_{mn}^{\pm}(Q,r) = f_{\mathrm{eq}}(Q,r) \sum_{\mu=0}^{m-n} \sum_{\nu=0}^{\mu} \sum_{\sigma=0}^{n} c_{mn}^{\pm\mu\nu\sigma} \left(\frac{Q}{\sqrt{2b}}\right)^{2(\mu-\nu)+n-\sigma} H_{2\nu+\sigma}\left(\sqrt{b/2}\, r\right), \tag{3·19}$$

$$g_{mn}^{\pm}(Q,r) = \sqrt{\frac{b}{2}} \sum_{\mu=0}^{m-n} \sum_{\nu=0}^{\mu} \sum_{\sigma=0}^{n} c_{mn}^{\pm\mu\nu\sigma} \left(\frac{Q}{\sqrt{2b}}\right)^{2(\mu-\nu)+n-\sigma} \delta^{(2\nu+\sigma)}\left(\sqrt{b/2}\, r\right), \tag{3·20}$$

where the equilibrium state and the coefficient are respectively given by

$$f_{\mathrm{eq}}(Q,r) \equiv f_{00}(Q,r) = \frac{1}{\sqrt{2\pi b}} e^{-Q^2/2b - br^2/2}, \tag{3·21}$$

$$c_{mn}^{\pm\mu\nu\sigma} = (\pm 1)^{n+\sigma} \frac{(-1)^{\mu+\nu}}{i^n 2^{2\nu+\sigma}\mu!} \sqrt{\frac{(m-n)!}{m!}} \binom{m}{n+\mu} \binom{\mu}{\nu} \binom{n}{\sigma}. \tag{3·22}$$

The generalized spaces structure stands out clearly with the existence of the n-th derivative of the delta function with respect to x, $\delta^{(n)}(x)$, in the left eigenfunctions.

The $f_{mn}^{\pm}$ represent different correlation components of a density function ψ that belongs to the space of square integrable functions, whereas the $g_{mn}^{\pm}$ serve as projections onto these components. This can be seen by expanding ψ as

$$\psi(x,\tilde{x}) = \sum_\nu c_\nu f_\nu(x,\tilde{x}), \qquad c_\nu = \langle\langle g_\nu | \psi \rangle\rangle. \tag{3·23}$$

For instance, $g_{00} = \delta(r)$ projects out the probability components $\tilde{x} = x$ of the density functions.

§4. Can generalized spaces structure be avoided?

The structure of the quantum kinetic equations in the Wigner representation is very much similar to the classical kinetic equations in phase space, such as the Fokker-Planck equation.[12)] In classical kinetic theory, one can introduce a weighted norm or perform a similarity transformation on the kinetic equation to obtain a symmetrical left and right eigenfunctions. The left and right eigenfunctions then become square integrable. This seems to suggest a way to avoid the generalized spaces structure in the quantum case. One can then ask to what extent the generalized spaces structure can be avoided, to which we now turn our attention.

4.1. *Weighted norm*

A weight may be incorporated into the definition of a norm. It is customary to choose the weight to be the inverse of the equilibrium solution $1/f_{\rm eq}^{\rm w}$ of the kinetic equation.[12),13)] In order to preserve the expectation value of observables, the new left eigenfunctions acquire a factor of $f_{\rm eq}^{\rm w}$ [cf. square bracket in Eq. (4·1)], making it square integrable,

$$\langle\!\langle g_\mu | f_\nu \rangle\!\rangle_w = \int dQdP (f_{\rm eq}^{\rm w})^{-1}(Q,P) \Big[f_{\rm eq}^{\rm w}(Q,P) g_\mu^{\rm w*}(Q,P) \Big] f_\nu^{\rm w}(Q,P) \,. \tag{4·1}$$

The weighted norm has the disadvantage that the integration measure $dQdP/f_{\rm eq}^{\rm w}$ is divergent if we want to go back to the original position space, while maintaining the weighted structure. Another subtlety arises in view of the fact that the weight $f_{\rm eq}^{\rm w}$ is a function of the thermal parameter b. The eigenfunction expansion of ψ is absolutely convergent only for some range of b. In a simple example using the weight $1/f_{\rm eq}^{\rm w}(b') = \exp[(P^2+Q^2)/2b']$, the norm of the equilibrium function $\langle\!\langle f_{\rm eq}^{\rm w}(b) | f_{\rm eq}^{\rm w}(b) \rangle\!\rangle_w$ diverges whenever $1/2b' \geq 1/b$. However, the eigenfunction expansion of ψ still holds in the weak sense under the ensemble average of an observable F, which is assumed to be a polynomial in P and Q,[14)]

$$\langle F \rangle \equiv \int dQdP F(Q,P)\psi(Q,P) = \lim_{N\to\infty} \int dQdP F(Q,P) \sum_\nu^N c_\nu f_\nu(Q,P) \,. \tag{4·2}$$

Hence, even though the eigenfunctions become square integrable through a weighted norm, but the generalized spaces description reemerges in the eigenfunction expansion of the density functions.

4.2. *Similarity transformation*

The similarity transformation is defined on C as

$$\tilde{C}(\eta) \equiv \mathcal{S}[C](\eta) \equiv f_{\rm eq}^{-1/2}(\eta) C(\eta) f_{\rm eq}^{1/2}(\eta) \,, \tag{4·3}$$

where η may be either (Q,r) or (Q,P), and $f_{\rm eq}$ is the equilibrium solution of the collision operator, i.e., $Cf_{\rm eq}(\eta) = 0$. In order to preserve the scalar product in Eq. (3·17) in the Wigner representation, the left and right eigenfunctions transform accordingly as $\tilde{f}^{\rm w} = f^{\rm w}/\sqrt{f_{\rm eq}^{\rm w}}$ and $\tilde{g}^{\rm w} = \sqrt{f_{\rm eq}^{\rm w}} g^{\rm w}$. Consequently, the transformed eigenfunctions are brought back to the Hilbert space.

An interesting issue arises when we want to transform to the position space, in that the Fourier transform treats the Q and P coordinates dissymmetrically. Hence, the similarly transform collision operator in the position space

$$\tilde{C}'(Q,r) \equiv \mathcal{F}^{-1}\mathcal{S}\mathcal{F}[C] = C_0(Q,r) + i\gamma + i\gamma b \left(\frac{\partial^2}{\partial Q^2} - \frac{Q^2}{4b^2} - r^2 + \frac{1}{4b^2}\frac{\partial^2}{\partial r^2} \right) \,, \tag{4·4}$$

is no longer similarly related to the original one ($\tilde{C}' \neq \tilde{C}$)

$$\tilde{C}(Q,r) \equiv \mathcal{S}[C] = C_0(Q,r) - \omega_0 \left(\frac{Qr}{4} - \frac{br}{2}\frac{\partial}{\partial Q} - \frac{Q}{2b}\frac{\partial}{\partial r} \right)$$

$$+ i\gamma\left(\frac{1}{2} - r\frac{\partial}{\partial r}\right) + i\gamma b\left(\frac{\partial^2}{\partial Q^2} - \frac{Q^2}{4b^2} - \frac{r^2}{2}\right). \tag{4·5}$$

They have different equilibrium functions,

$$\tilde{f}'_{\rm eq} = \exp(-Q^2/4b - br^2), \qquad \tilde{f}_{\rm eq} = \exp(-Q^2/4b - br^2/4). \tag{4·6}$$

In other words, the Fourier transform and the similarity transform operations do not commute $[\mathcal{S}, \mathcal{F}] \neq 0$. Consequently, $\tilde{C}'(Q, r)$ effectively describes a different system not similarly related to the original one. We conclude that the generalized spaces structure in the position space cannot be transformed away through a similarity transformation.

§5. The Caldeira-Leggett equation

For the collision operator discussed in §3, the damping effect acts symmetrically on the Q and P space. We now consider damping effect that affects only the P space, with the collision operator

$$C^{\rm w}_{\rm CL} = -i\omega_0\left(P\frac{\partial}{\partial Q} - Q\frac{\partial}{\partial P}\right) + i\gamma\left(\frac{\partial}{\partial P}P + b\frac{\partial^2}{\partial P^2}\right). \tag{5·1}$$

It goes into the collision operator of the Caldeira-Leggett equation[15] in the high temperature limit (3·3). The Caldeira-Leggett equation was derived from the Hamiltonian

$$H_{\rm CL} = \hbar\omega_0 a^\dagger a + \textstyle\sum_k \hbar\omega_k a_k^\dagger a_k + \frac{\lambda}{\sqrt{L}}\sum_k v_k(a^\dagger + a)(a_k^\dagger + a_k), \tag{5·2}$$

in the high temperature limit through the path integral method.[15] Here we generalize this equation to arbitrary temperature and obtain Eq. (5·1). Compared to the Hamiltonian in previous example (3·1), $H_{\rm CL}$ includes the virtual transition interactions between the oscillator and field.

The time evolution of the position and momentum of the oscillator is

$$\langle\dot{Q}\rangle = \omega_0\langle P\rangle, \qquad \langle\dot{P}\rangle = -\omega_0\langle Q\rangle - \gamma\langle P\rangle, \tag{5·3}$$

respectively. It oscillates with the frequency $\omega' \equiv \sqrt{\omega_0^2 - \gamma^2/4}$ as

$$\langle Q\rangle_t = e^{-\gamma t/2}\left[\langle Q\rangle_0\cos\omega' t + \left(\tfrac{\omega_0}{\omega'}\langle P\rangle_0 + \tfrac{\gamma}{2\omega'}\langle Q\rangle_0\right)\sin\omega' t\right], \tag{5·4}$$

$$\langle P\rangle_t = e^{-\gamma t/2}\left[\langle P\rangle_0\cos\omega' t - \left(\tfrac{\omega_0}{\omega'}\langle Q\rangle_0 + \tfrac{\gamma}{2\omega'}\langle P\rangle_0\right)\sin\omega' t\right]. \tag{5·5}$$

The equilibrium solution of $C^{\rm w}_{\rm CL}$ is

$$F^{\rm w}_{\rm eq} \equiv F^{\rm w}_{00} = \frac{1}{\sqrt{2\pi b}}\, e^{-(P^2+Q^2)/2b}, \tag{5·6}$$

which is identical to Eq. (3·21). The nonequilibrium modes can be worked out by assuming series solution in powers of $F^{\rm w}_{\rm eq}P^aQ^b$, up to order $N \equiv a + b$. Due to

the bilinear structure of the collision operator, the N odd and the N even order polynomials are disconnected. In this way, we find that the eigenvalues of $C^{\rm w}_{\rm CL}F^{\rm w}_{\nu} = \lambda_{\nu}F^{\rm w}_{\nu}$ are

$$\lambda_{n,m} = -in\gamma - 2m\omega', \qquad \begin{aligned} n &= 0, \tfrac{1}{2}, 1, \tfrac{3}{2}, 2, ..., \\ m &= \pm n, \pm(n-1), ..., \pm\tfrac{1}{2} \text{ or } 0, \end{aligned} \tag{5·7}$$

where integer and half integer n correspond to the solutions in even and odd N, respectively. We list a few eigenfunctions in Appendix A. Due to the factor $F^{\rm w}_{\rm eq}$ in $F^{\rm w}_{m,n}$, the right eigenfunctions are square integrable.

The left eigenvalue problem can be similarly solved as in §3. We extract the equilibrium solution through $F^{\rm w}_{n,m} = N_{n,m}F^{\rm w}_{\rm eq}\bar{F}^{\rm w}_{n,m}$, and then take the complex conjugate. After relabeling Q as $-Q$, we obtain $C^{\rm w\dagger}_{\rm CL}\bar{F}^{\rm w*}_{n,m}(-Q,P) = \lambda^{*}_{n,m}\bar{F}^{\rm w*}_{n,m}(-Q,P)$, where the adjoint operator is

$$C^{\rm w\dagger}_{\rm CL} = -i\omega_0\left(P\frac{\partial}{\partial Q} - Q\frac{\partial}{\partial P}\right) + i\gamma\left(-P\frac{\partial}{\partial P} + b\frac{\partial^2}{\partial P^2}\right). \tag{5·8}$$

From the left eigenvalue problem $C^{\rm w\dagger}_{\rm CL}G^{\rm w}_{n,m} = \lambda^{*}_{n,m}G^{\rm w}_{n,m}$ and the relation $\bar{F}^{\rm w*}_{n,m} = \bar{F}^{\rm w}_{n,-m}$ (cf. Appendix A), we have

$$G^{\rm w}_{n,m}(Q,P) = \bar{N}_{n,m}\bar{F}^{\rm w}_{n,-m}(-Q,P) = \frac{\bar{N}_{n,m}}{N_{n,-m}}(F^{\rm w}_{\rm eq})^{-1}F^{\rm w}_{n,-m}(-Q,P). \tag{5·9}$$

The left eigenfunctions are not square integrable, since the regulating factor $F^{\rm w}_{\rm eq}$ in $F^{\rm w}_{n,-m}(-Q,P)$ is canceled by the corresponding prefactor $(F^{\rm w}_{\rm eq})^{-1}$, as is seen from the right-hand side of (5·9). The $F^{\rm w}_{n,m}$ and $G^{\rm w}_{n,m}$ form a complete set of biorthonormal basis as in Eqs. (3·17) and (3·18).

Once again we find that the right eigenfunctions belong to the space of square integrable functions, whereas the left eigenfunctions are not square integrable and they are represented as distributions in the position space. Due to the similar structure of the collision operators, the discussion in §4 can be applied to the present case directly. We conclude that a dissymmetrical damping that acts only on the P space also destroys the Hilbert space structure of the simple harmonic oscillator.

§6. Damped particle in thermal reservoir

It is interesting to compare the results obtained in the previous collision operators to ones in the following phenomenological collision operator for the Wigner representation,

$$K^{\rm w}(Q,P) = -i\omega_0 P\frac{\partial}{\partial Q} + i\gamma\left(\frac{\partial}{\partial P}P + b\frac{\partial^2}{\partial P^2}\right). \tag{6·1}$$

In the high temperature limit this reduces to the well known classical Kramers equation for a free particle that is subject to the thermal fluctuation (3·3). The quantum

effect is in b defined at (3·3). We phenomenologically obtained this form of the collision operator by comparing this to the quantum collision operators (3·6) and (5·1), and did not microscopically obtain this form by starting with a given Hamiltonian as done in the previous sections. Comparing (6·1) especially with (5·1), this collision operator (6·1) seems us to be a reasonable quantum collision operator that describes the situation for a particle moving in a thermal bath without any external potential. The first term on the right-hand side of (6·1) is a flow term that initiates the free motion of the particle, the second term induces friction and the third term causes diffusion.

The physical meaning of the equation can be obtained by considering the average motion of the particle

$$\langle \dot{Q} \rangle = \omega_0 \langle P \rangle \,, \qquad \langle \dot{P} \rangle = -\gamma \langle P \rangle \,, \tag{6·2}$$

$$\langle \dot{Q^2} \rangle = \langle QP \rangle \,, \qquad \langle \dot{P^2} \rangle = -\langle P^2 \rangle + 2\gamma b \,, \qquad \langle \dot{QP} \rangle = -\gamma \langle QP \rangle + \omega_0 \langle P^2 \rangle \,, \tag{6·3}$$

which has the solution

$$\langle Q \rangle_t = \langle Q \rangle_0 + \tfrac{\omega_0}{2\gamma}(1 - e^{-\gamma t}) \langle P \rangle_0 \,, \qquad \langle P \rangle_t = e^{-\gamma t} \langle P \rangle_0 \,, \tag{6·4}$$

$$\langle Q^2 \rangle_t = \langle Q^2 \rangle_0 + \tfrac{\omega_0^2 b}{\gamma} t + \left[\tfrac{1}{\gamma} \langle \dot{Q^2} \rangle_0 - \tfrac{\omega_0^2 b}{\gamma^2} \right] \left(1 - e^{-\gamma t} \right) + \tfrac{\omega_0^2}{2\gamma^2} \left[\langle P^2 \rangle_0 - b \right] \left(1 - e^{-\gamma t} \right)^2 \,, \tag{6·5}$$

$$\langle P^2 \rangle_t = b(1 - e^{-2\gamma t}) + \langle P^2 \rangle_0 e^{-2\gamma t} \,. \tag{6·6}$$

The behaviors of the average position and momentum (6·4) indicate that the collision operator is describing a damped particle in a thermal bath, in contrast to the previous examples of damped harmonic oscillators, see Eqs. (3·8)–(3·9) and (5·4)–(5·5). The linear term of t in $\langle Q^2 \rangle_t$ gives rise to a non-vanishing diffusion coefficient

$$D \equiv \frac{\hbar}{m\omega_0} \lim_{t \to \infty} \frac{\langle Q^2 \rangle_t - \langle Q \rangle_t^2}{t} = \frac{\hbar \omega_0}{m\gamma} b \xrightarrow{T \to \infty} \frac{k_B T}{m\gamma} \,. \tag{6·7}$$

The solutions to the right eigenvalue problem $K^{\mathrm{w}} u_\nu^{\mathrm{w}} = \mu_\nu u_\nu^{\mathrm{w}}$ and its left counterpart can be obtained as follows.[13] We notice that the final equilibrium function is proportional to $\exp(-P^2/2b)$ and we can separate the Q coordinate from the first term of K^{w} with $\exp(ikQ)$. So we write $u_\nu^{\mathrm{w}} = \exp(-P^2/2b) \exp(ikQ) u'_\nu$ and the eigenvalue problem turns into a standard second order differential equation,[16]

$$b \frac{d^2 u'_\nu}{dP^2} - P \frac{du'_\nu}{dP} + \frac{i}{\gamma}(\mu_\nu - \omega_0 k P) u'_\nu = 0 \,. \tag{6·8}$$

Writing $u'_\nu \equiv \exp(-i\omega_0 k P/\gamma) \tilde{u}_\nu$ and introducing the variable $\xi \equiv P/\sqrt{2b} + i\sqrt{2b}\omega_0 k/\gamma$, it reduces to an equation satisfied by the Hermite polynomials,

$$\frac{d^2 \tilde{u}_\nu}{d\xi^2} - 2\xi \frac{d\tilde{u}_\nu}{d\xi} + 2 \left(\frac{i}{\gamma} \mu_\nu - \frac{b\omega_0^2}{\gamma^2} k^2 \right) \tilde{u}_\nu = 0 \,. \tag{6·9}$$

The solution is

$$\mu_{nk} = -i\gamma \left(n + \tfrac{b\omega_0^2}{\gamma^2} k^2 \right) \,, \qquad n = 0, 1, 2, \ldots \,, \quad k = \text{real}, \tag{6·10}$$

$$u^{\rm w}_{nk}(Q,P) = \frac{e^{b\omega_0^2 k^2/\gamma^2}}{\sqrt{2^n n!}}\, u^{\rm w}_{\rm eq}(P) e^{ikQ - i\omega_0 kP/\gamma}\, H_n\left(\frac{P}{\sqrt{2b}} + i\sqrt{2b}\frac{\omega_0}{\gamma}k\right), \tag{6·11}$$

with the equilibrium solution

$$u^{\rm w}_{\rm eq}(P) \equiv u^{\rm w}_{00}(P) = \frac{1}{2\pi\sqrt{2\pi b}} \exp(-P^2/2b)\,. \tag{6·12}$$

The normalization is determined by the orthonormality relation (6·15) below. Due to the flow term, the component in the Q space is a plane wave and does not belong to the Hilbert space in the first place. However, the eigenfunctions as a function of P are still square integrable as far as the P space are concerned. We will therefore focus our attention on the P space component in our discussion below.

The solution to the left eigenvalue problem can be obtained by first extracting the equilibrium solution from the eigenvalue problem of Eq. (6·1) through $u^{\rm w}_\nu = \exp(-P^2/2b)\bar{u}_\nu$. We then take an overall complex conjugate on the resulting equation. After relabeling Q as $-Q$, we obtain

$$\left[-i\omega_0 P\frac{\partial}{\partial Q} - i\gamma\left(-P\frac{\partial}{\partial P} + b\frac{\partial^2}{\partial P^2}\right)\right]\bar{u}^*_\nu(-Q,P) = \mu^*_\nu \bar{u}^*_\nu(-Q,P)\,. \tag{6·13}$$

The operator on the left-hand side of the equation is the adjoint operator $K^{\rm w\dagger}$. A comparison with the left eigenvalue problem $K^{\rm w\dagger}v^{\rm w}_\nu = \mu^*_\nu v^{\rm w}_\nu$ enables us to set

$$v^{\rm w}_{nk}(Q,P) = \bar{u}^{\rm w*}_\nu(-Q,P) = e^{P^2/2b}\, u^{\rm w*}_{nk}(-Q,P)\,, \tag{6·14}$$

which is not square integrable in the P space, since the prefactor $\exp(P^2/2b)$ on the right-hand side of (6·14) cancels the regulating factor $u^{\rm w}_{\rm eq}$ in $u^{\rm w*}_{nk}(-Q,P)$. These eigenfunctions form a complete set of biorthonormal basis,

$$\int_{-\infty}^{\infty} dP \int_{-\infty}^{\infty} dQ\, v^{\rm w*}_{nk}(Q,P) u^{\rm w}_{n'k'}(Q,P) = \delta_{n,n'}\delta(k-k')\,, \tag{6·15}$$

$$\sum_{n=0}^{\infty}\int_{-\infty}^{\infty} dk\, u^{\rm w}_{nk}(Q,P) v^{\rm w*}_{nk}(Q',P') = \delta(Q-Q')\delta(P-P')\,, \tag{6·16}$$

which can be proved by means of the orthogonality of the Hermite functions.[13)]

The eigenfunctions in the position space are

$$u_{nk}(Q,r) = \frac{(i\sqrt{b})^n}{\sqrt{n!}}\frac{e^{\omega_0^2 bk^2/\gamma^2}}{\sqrt{2\pi b}} e^{ikQ}\, e^{-\frac{b}{2}(r-\omega_0 k/\gamma)^2}\left(r + \frac{\omega_0}{\gamma}k\right)^n, \tag{6·17}$$

$$v_{nk}(Q,r) = \frac{(-i)^n}{\sqrt{2^n n!}}\frac{e^{\omega_0^2 bk^2/\gamma^2}}{\sqrt{2\pi b}} e^{ikQ}\, H_n\left(\frac{1}{\sqrt{2b}}\frac{\partial}{\partial r} + \frac{\omega_0}{\gamma}\sqrt{2b}k\right)\delta\left(r + \frac{\omega_0}{\gamma}k\right). \tag{6·18}$$

The occurrence of the Dirac delta function clearly shows that the biorthogonal basis belongs to the generalized spaces, besides the factor $\exp(ikQ)$ that is also an object in the generalized spaces.

§7. Conclusion

On the level of Liouville space, the reduced dynamics of a quantum oscillator or a particle interacting with a thermal reservoir acquires generalized spaces structure due to the existence of damping on the subsystem. This is explicitly indicated by the generalized spaces structure of the complete set of biorthogonal basis of the eigenvalue problem of the collision operators. The density functions of the reduced system thus belong to the space of well-behaved functions, which permit eigenfunction expansion in the space of the right eigenfunctions. While the right eigenfunctions represent different correlation components of the reduced dynamics, its dual, the left eigenfunctions, serve as projections onto these correlation components. The left eigenfunctions are represented by distributions in the position space. Because of the duality between the position and momentum space representations in quantum mechanics, the same conclusion holds in the momentum space representation of the quantum kinetic equations.

In the Wigner representation, the quantum kinetic equation of the reduced systems closely resemble the classical kinetic equation in phase space. Usual procedures employed in classical kinetic theory, such as introducing a weighted norm or carrying out a similarity transformation on the collision operator, can be used to restore the Hilbert space structure of the quantum kinetic equations to certain extent. However, on the level of the position or momentum spaces where the quantum dynamics can find no classical counterpart, the generalized spaces structure of the dissipative systems cannot be avoided. This may be considered as a manifestation of the distinction between classical systems that naturally occur in the phase space and quantum systems that naturally occur in the position or momentum space.

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Appendix A

—— *List of Eigenfunctions of* $C^{\mathrm{w}}_{\mathrm{CL}}$ ——

Using the variables $\bar{P} \equiv P/\sqrt{2b}$, $\bar{Q} \equiv Q/\sqrt{2b}$, and $\bar{\lambda}_{n,m} \equiv -n + im\bar{\omega}'$, where $\bar{\omega}' \equiv 2\omega'/\gamma$ and $\lambda_{n,m} = i\gamma\bar{\lambda}_{n,m}$, the first few eigenfunctions can be obtained from the list by $F^{\mathrm{w}}_{n,m} = N_{n,m}F^{\mathrm{w}}_{\mathrm{eq}}\bar{F}^{\mathrm{w}}_{n,m}$ and $G^{\mathrm{w}}_{n,m}(Q,P) = \bar{N}_{n,m}\bar{F}^{\mathrm{w}}_{n,-m}(-Q,P)$. In the equations, $\tilde{\lambda}_\nu \equiv \sqrt{\bar{\lambda}_\nu}$. Note that since $\bar{\lambda}^*_{n,m} = \bar{\lambda}_{n,-m}$, we have $\bar{F}^{\mathrm{w}*}_{n,m} = \bar{F}^{\mathrm{w}}_{n,-m}$.

$$\bar{F}^{\mathrm{w}}_{0,0} = 1, \tag{A·1}$$

$$\bar{F}^{\mathrm{w}}_{\frac{1}{2},\pm\frac{1}{2}} = \tilde{\lambda}_{\frac{1}{2},\pm\frac{1}{2}}\bar{P} + \tilde{\lambda}_{\frac{1}{2},\mp\frac{1}{2}}\bar{Q}, \tag{A·2}$$

$$\bar{F}^{\mathrm{w}}_{1,\pm1} = 1 + \left(\tilde{\lambda}_{1,\pm1}\bar{P} + \tilde{\lambda}_{1,\mp1}\bar{Q}\right)^2, \tag{A·3}$$

$$\bar{F}^{\mathrm{w}}_{1,0} = -\tilde{\lambda}_{1,\pm1}\tilde{\lambda}_{1,\mp1} + \left|\tilde{\lambda}_{1,\pm1}\bar{P} + \tilde{\lambda}_{1,\mp1}\bar{Q}\right|^2, \tag{A·4}$$

$$\bar{F}^{\mathrm{w}}_{\frac{3}{2},\pm\frac{3}{2}} = \frac{9}{2}\left(\tilde{\lambda}_{\frac{3}{2},\pm\frac{3}{2}}\bar{P} + \tilde{\lambda}_{\frac{3}{2},\mp\frac{3}{2}}\bar{Q}\right) + \left(\tilde{\lambda}_{\frac{3}{2},\pm\frac{3}{2}}\bar{P} + \tilde{\lambda}_{\frac{3}{2},\mp\frac{3}{2}}\bar{Q}\right)^3, \tag{A·5}$$

$$\begin{aligned}\bar{F}^{\mathrm{w}}_{\frac{3}{2},\pm\frac{1}{2}} = {} & -3\left(\tilde{\lambda}^2_{\frac{3}{2},\pm1}\tilde{\lambda}_{\frac{3}{2},\mp\frac{3}{2}}\bar{P} + \tilde{\lambda}^2_{\frac{3}{2},\mp1}\tilde{\lambda}_{\frac{3}{2},\pm\frac{3}{2}}\bar{Q}\right) + \tilde{\lambda}^2_{\frac{3}{2},\pm\frac{3}{2}}\tilde{\lambda}_{\frac{3}{2},\mp\frac{3}{2}}\bar{P}^3 \\ & + 3\tilde{\lambda}_{\frac{3}{2},\pm\frac{3}{2}}\tilde{\lambda}^2_{\frac{3}{2},\mp\frac{1}{2}}\bar{P}^2\bar{Q} + 3\tilde{\lambda}_{\frac{3}{2},\mp\frac{3}{2}}\tilde{\lambda}^2_{\frac{3}{2},\pm\frac{1}{2}}\bar{P}\bar{Q}^2 + \tilde{\lambda}^2_{\frac{3}{2},\mp\frac{3}{2}}\tilde{\lambda}_{\frac{3}{2},\pm\frac{3}{2}}\bar{Q}^3.\end{aligned} \tag{A·6}$$

The normalization constants are chosen so that the orthonormality and completeness relations (6·15)–(6·16) between the eigenfunctions hold.

$$N_{0,0} = \bar{N}_{0,0} = 1, \qquad N_{\frac{1}{2},\pm\frac{1}{2}} = \mp i\bar{N}_{\frac{1}{2},\pm\frac{1}{2}} = \sqrt{2/\bar{\omega}'}, \tag{A·7}$$

$$N_{1,0} = \bar{N}_{1,0} = 1/\bar{\omega}', \qquad N_{1,\pm1} = -\bar{N}_{1,\pm1} = 1/\sqrt{2\bar{\omega}'^2}, \tag{A·8}$$

$$N_{\frac{3}{2},\pm\frac{3}{2}} = \pm i\bar{N}_{\frac{3}{2},\pm\frac{3}{2}} = 2/9\sqrt{\bar{\omega}'^3}, \qquad N_{\frac{3}{2},\pm\frac{1}{2}} = \mp i\bar{N}_{\frac{3}{2},\pm\frac{1}{2}} = 2/\sqrt{3\bar{\omega}'}^3. \tag{A·9}$$

References

1) P. A. M. Dirac, *The Principle of Quantum Mechanics,* 4th ed. (Clarendon Press, Oxford, 1958).
2) E. C. G. Sudarshan, C. B. Chiu and Vitorio Gorini, Phys. Rev. D **18** (1978), 2914.
   A. Bohm, *Rigged Hilbert Space and Quantum Mechanics*, Lecture Notes in Phys. Vol. 78 (Springer-Verlag, Berlin, 1978).
3) L. Boltzmann, *Lectures on Gas Theory*, translated by S. Brush (University of California Press, Berkeley and Los Angeles, 1964).
4) T. Petrosky and I. Prigogine, Adv. Chem. Phys. **99** (1997), 1.
5) V. Gorini, A. Frigerio, M. Verri, A. Kossakowski and E. C. G. Sudarshan, Rep. Math. Phys. **13** (1978), 149.
6) K. O. Friedrichs, Commun. Pure Appl. Math. **1** (1948), 361.
7) I. Prigogine, *Non-Equilibrium Statistical Mechanics* (Wiley Interscience, 1962).
8) L. Van Hove, Physica **21** (1955), 517.
9) V. Gorini, A. Kossakowski and E. C. G. Sudarshan, J. Math. Phys. **17** (1976), 821.
   G. Lindblad, Commun. Math. Phys. **48** (1976), 119.
10) E. P. Wigner, Phys. Rev. **40** (1932), 749.
    M. Hillery, R. F. O'Connell, M. O. Scully and E. P. Wigner, Phys. Rep. **106** (1984), 121.
11) See, for example, T. Petrosky and V. Barsegov, Phys. Rev. E **65** (2002), 046102.
12) H. Risken, *The Fokker-Planck Equation: Methods of Solution and Applications*, 2nd ed. (Springer-Verlag, Berlin, 1989).
13) P. Résibois and M. de Leener, *Classical Kinetic Theory of Fluids* (John Wiley & Sons, 1977).
14) K. Kanki, S. Tanaka and T. Petrosky, to be published.
15) A. O. Caldeira and A. J. Leggett, Physica A **121** (1983), 587.
16) H. Bateman et al., *Higher Transcendental Functions*, Vol. I (McGraw-Hill Book Company Inc., 1953), p. 249.