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The Harmonic Oscillator in a Heat Bath

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Abstract. We study the time evolution of a quantum-mechanical harmonic oscillator in interaction with an infinite heat bath, which is supposed to be initially in the canonical equilibrium at some temperature. We show that the oscillator relaxes from an arbitrary initial state to its canonical state at the same temperature, and that in the weak coupling limit the relaxation is Markovian, that is exponential. In contrast to earlier treatments of the problem [4, 5], the results are obtained without assuming any particular special form for the self-interaction of the heat bath. No use is made of coarse graining, finite memory assumptions or randomly varying Hamiltonians.

1. Introduction

It is well known that for a finite heat bath it is not possible to prove convergence to an equilibrium state in the limit $t \to \infty$ because of the existence of Poincaré recurrences [8, 11, 15]. However, for large systems these recurrences become extremely infrequent and we can eliminate them by passing to the limit of an infinite heat bath. Since the techniques for passing from a finite heat bath to an infinite one are by now well known [2, 5] we immediately consider the Hamiltonian given formally by

$$H_\lambda = H_0 + \lambda H_1 \tag{1.1}$$

where

$$H_0 = \tfrac{1}{2}(p^2 + \omega^2 q^2) + \tfrac{1}{2} : \sum_{n=-\infty}^{\infty} p_n^2 + \sum_{m,n=-\infty}^{\infty} \alpha_{m-n} q_m q_n : \tag{1.2}$$

and

$$H_1 = \sum_{n=-\infty}^{\infty} \gamma_n q_n q \, . \tag{1.3}$$

Here $\{p_m, q_m\}_{m=-\infty}^{\infty}$ are the canonical coordinates of the infinite heat bath and p, q are the canonical coordinates of the oscillator whose time evolution we shall study. We suppose that α is a real symmetric sequence such that for some $\delta > 0$

$$\sum_{n=-\infty}^{\infty} |\alpha_n| \, e^{\delta |n|} < \infty \, . \tag{1.4}$$

As in [5] we must also suppose that α is a positive definite sequence, but we actually suppose slightly more, that

$$\varrho(\theta) \equiv \sum_{n=-\infty}^{\infty} \alpha_n e^{in\theta} > 0 \tag{1.5}$$

for all $0 \leqq \theta \leqq 2\pi$. It is clear that ϱ is a real analytic periodic function on $[0, 2\pi]$ with strictly positive minimum and maximum values. The corresponding convolution operator on $l^2(\mathbb{Z})$, which we also denote by α, is therefore positive, bounded and invertible. We put on γ the initial hypotheses that γ is real and

$$\sum_{n=-\infty}^{\infty} |\gamma_n|^2 < \infty \tag{1.6}$$

so that γ defines an element of $l^2(\mathbb{Z})$. We shall subsequently put further regularity conditions on γ. Since we are interested in the time evolution of the system only for very small λ, we shall feel free to add terms of order λ^2 to the Hamiltonian H_λ if convenient.

We outline the well-known procedure for realising H_λ as a self-adjoint operator on Fock space [1, 14]. Let $\mathcal{H}$ be the real test function space

$$\mathcal{H} = \mathbb{R} \oplus l^2(\mathbb{Z}) \tag{1.7}$$

and let $\mathcal{F}$ be the boson Fock space over $\mathcal{H}_{\mathbb{C}}$. For $f \in \mathcal{H}$ let $a^*(f)$ and $a(f)$ be the usual creation and annihilation operators in $\mathcal{F}$ so that

$$a(g)\, a^*(f) - a^*(f)\, a(g) = \langle f, g \rangle\, 1\,. \tag{1.8}$$

Let A_λ be the bounded positive operator on $\mathcal{H}$ given by the matrix

$$A_\lambda = \left(\begin{array}{c|c} \omega^2 & \lambda\gamma \\ \hline \lambda\gamma & \alpha \end{array}\right) \tag{1.9}$$

and let H_λ be the free Hamiltonian on $\mathcal{F}$ constructed from $A_\lambda^{\frac{1}{2}}$ on $\mathcal{H}$. Dropping temporarily the subscript λ, let

$$\phi_t(f) = \frac{1}{\sqrt{2}}\, e^{iHt}\{a^*(A^{-\frac{1}{4}}f) + a(A^{-\frac{1}{4}}f)\} \tag{1.10}$$

and

$$\pi_t(g) = \frac{i}{\sqrt{2}}\, e^{iHt}\{a^*(A^{\frac{1}{4}}g) - a(A^{\frac{1}{4}}g)\} \tag{1.11}$$

so that

$$\phi_t(f)\, \pi_t(g) - \pi_t(g)\, \phi_t(f) = i\langle f, g \rangle\, 1\,. \tag{1.12}$$

Elementary calculations give

$$\begin{aligned} \phi_t(f) = {} & \frac{1}{\sqrt{2}}\{a^*[\cos(A^{\frac{1}{2}}t)\, A^{-\frac{1}{4}}f] + ia^*[\sin(A^{\frac{1}{2}}t)\, A^{-\frac{1}{4}}f]\} \\ & + \frac{1}{\sqrt{2}}\{a[\cos(A^{\frac{1}{2}}t) A^{-\frac{1}{4}}f] - ia[\sin(A^{\frac{1}{2}}t) A^{-\frac{1}{4}}f]\} \\ = {} & \phi_0\{\cos(A^{\frac{1}{2}}t)\, f\} + \pi_0\{A^{-\frac{1}{2}}\sin(A^{\frac{1}{2}}t)\, f\} \end{aligned} \tag{1.13}$$

and

$$\pi_t(g) = \frac{i}{\sqrt{2}} \{a^*[\cos(A^{\frac{1}{2}}t)\, A^{\frac{1}{4}}g] + ia^*[\sin(A^{\frac{1}{2}}t)\, A^{\frac{1}{4}}g]\}$$

$$- \frac{i}{\sqrt{2}} \{a[\cos(A^{\frac{1}{2}}t) A^{\frac{1}{4}}g] - ia[\sin(A^{\frac{1}{2}}t) A^{\frac{1}{4}}g]\} \tag{1.14}$$

$$= -\phi_0\{\sin(A^{\frac{1}{2}}t)\, A^{\frac{1}{2}}g\} + \pi_0\{\cos(A^{\frac{1}{2}}t)\, g\}\,.$$

From these equations it follows that

$$\frac{\partial}{\partial t}\phi_t(f) = \pi_t(f)\,, \tag{1.15}$$

$$\frac{\partial}{\partial t}\pi_t(g) = -\phi_t(Ag) \tag{1.16}$$

and these equations are the justification for regarding H_λ as the rigorously defined self-adjoint operator corresponding to Eqs. (1.1)–(1.3).

If we define an operator B_λ on $\mathscr{H}$ by the matrix

$$B_\lambda = \left(\begin{array}{c|c} \omega & \lambda v \\ \hline \lambda v & \alpha^{\frac{1}{2}} \end{array}\right) \tag{1.17}$$

where

$$v = (\omega + \alpha^{\frac{1}{2}})^{-1}\gamma \in l^2(\mathbb{Z}) \tag{1.18}$$

then

$$B_\lambda^2 = \left(\begin{array}{c|c} \omega & \lambda v \\ \hline \lambda v & \alpha^{\frac{1}{2}} \end{array}\right)\left(\begin{array}{c|c} \omega & \lambda v \\ \hline \lambda v & \alpha^{\frac{1}{2}} \end{array}\right)$$

$$= \left(\begin{array}{c|c} \omega^2 + \lambda^2\|v\|^2 & \lambda\omega v + \lambda\alpha^{\frac{1}{2}}(v) \\ \hline \lambda\omega v + \lambda\alpha^{\frac{1}{2}}(v) & \alpha + \lambda^2 v \otimes \bar{v} \end{array}\right) \tag{1.19}$$

$$= A_\lambda + \lambda^2 \left(\begin{array}{c|c} \|v\|^2 & 0 \\ \hline 0 & v \otimes \bar{v} \end{array}\right)$$

$$= A_\lambda + O(\lambda^2)\,.$$

Since we shall have mainly to use $A_\lambda^{\frac{1}{2}}$ rather than A_λ, instead of calculating the complicated exact expression for $A_\lambda^{\frac{1}{2}}$ we now *redefine*

$$A_\lambda = B_\lambda^2 \tag{1.20}$$

where B_λ is given by Eq. (1.17). This amounts to changing A_λ, and hence H_λ, by a term of order λ^2, which we earlier stated we would regard as permissible.

We come now to the thermodynamic aspects of the model. Again dropping explicit reference to λ, we let the Weyl operators be

$$U(f, g) = \exp[i\phi_0(f) + i\pi_0(g)] \tag{1.21}$$

so that for all $f, g \in \mathscr{H}$, $U(f,g)$ is a well-defined unitary operator [1, 2, 14]. The canonical equilibrium state of the system at the inverse temperature β is given by specifying its expectation values for the Weyl operators. If H had discrete spectrum we could write

$$E_\beta(f,g) = \mathrm{tr}[U(f,g)\, e^{-\beta H}]/\mathrm{tr}[e^{-\beta H}] \tag{1.22}$$

from which can be deduced [2]

$$E_\beta(f,g) = \exp\left[-\frac{1}{4}\left\langle A^{-\frac{1}{2}}\coth\frac{\beta A^{\frac{1}{2}}}{2} f, f\right\rangle - \frac{1}{4}\left\langle A^{\frac{1}{2}}\coth\frac{\beta A^{\frac{1}{2}}}{2} g, g\right\rangle\right]. \tag{1.23}$$

In our case H does not have discrete spectrum but we can define E_β directly by Eq. (1.23). This amounts to changing from the Fock space representation of the CCR's to another representation [2], but we shall not need to consider this new representation explicitly.

Identifying any $x \in \mathbb{R}$ with the element $x \oplus 0$ of $\mathscr{H}$, the dynamics of the oscillator is given in the Heisenberg picture by

$$\alpha_t\{U(x,y)\} = M\{e^{iHt}\, U(x,y)\, e^{-iHt}\} \tag{1.24}$$

where, as in [4], M is the operation of taking the expectation with respect to the canonical equilibrium state at the inverse temperature β, of all expressions involving the field operators of the heat bath. This corresponds to the assumption that the oscillator is initially in an arbitrary state while the heat bath is initially in its thermal equilibrium state. Letting $P : \mathscr{H} \to \mathscr{H}$ be the projection

$$P(x \oplus \psi) = x \oplus 0 \tag{1.25}$$

we obtain from [4] the explicit formulae

Lemma 1.1. *For all $x, y \in \mathbb{R}$ and all $t \geqq 0$*

$$\alpha_t\{U(x,y)\} = U(x_t, y_t)\exp[-r_t/4] \tag{1.26}$$

where

$$x_t = P\{\cos(A^{\frac{1}{2}}t)\, x - A^{\frac{1}{2}}\sin(A^{\frac{1}{2}}t)\, y\}, \tag{1.27}$$

$$y_t = P\{A^{-\frac{1}{2}}\sin(A^{\frac{1}{2}}t)\, x + \cos(A^{\frac{1}{2}}t)\, y\}, \tag{1.28}$$

$$r_t = \langle A^{-\frac{1}{2}}\coth(\beta A^{\frac{1}{2}}/2)\, \xi_t, \xi_t\rangle + \langle A^{\frac{1}{2}}\coth(\beta A^{\frac{1}{2}}/2)\, \eta_t, \eta_t\rangle, \tag{1.29}$$

$$\xi_t = (1-P)\{\cos(A^{\frac{1}{2}}t)\, x - A^{\frac{1}{2}}\sin(A^{\frac{1}{2}}t)\, y\}, \tag{1.30}$$

$$\eta_t = (1-P)\{A^{-\frac{1}{2}}\sin(A^{\frac{1}{2}}t)\, x + \cos(A^{\frac{1}{2}}t)\, y\}. \tag{1.31}$$

We are interested in studying the approach to equilibrium of the oscillator for a small coupling constant. This means that we must find asymptotic forms for $x_{\lambda,t}$, $y_{\lambda,t}$ and $r_{\lambda,t}$ in the limit as $t \to \infty$ and $\lambda \to 0$.

The order in which these two limits must be taken is critical and the correct sense in determined by the subsequent analysis.

2. Estimates of Some Decay Functions

It is clear from Lemma 1.1 that the main problem consists of giving a detailed analysis of the spectral properties of the self-adjoint operator B_λ on $\mathscr{H}_{\mathbb{C}}$. This section is devoted to examining $\langle e^{iB_\lambda t} v, v \rangle$ in the limit $t \to \infty$ and $\lambda \to 0$, where v is the element $1 \oplus 0$ of $\mathscr{H}_{\mathbb{C}}$. The operator B_λ is identifiable with the Hamiltonian of a (somewhat generalised) Wigner-Weiskopf atom and the form of the limit has been found in several particular cases in the literature [3, 15]. We, however, need to repeat the calculations with more care since we are concerned to obtain estimates of the rate of convergence to the limit which are *uniform* with respect to time. The reader interested only in the results may proceed immediately from here to the statement of Theorem 2.5.

By taking Fourier transforms we may represent B_λ by the matrix

$$B_\lambda = \left(\begin{array}{c|c} \omega & \lambda h \\ \hline \lambda h & \varrho^{\frac{1}{2}} \end{array} \right) \tag{2.1}$$

acting on

$$\mathscr{H}_{\mathbb{C}} = \mathbb{C} \oplus L^2(-\pi, \pi) \tag{2.2}$$

where $h \in L^2(-\pi, \pi)$ is the Fourier transform of $v \in l^2(\mathbb{Z})$ and ϱ is the operator of multiplication by the function defined in Eq. (1.5). Now if ϱ were merely continuous then as an operator it could have pure point spectrum (if ϱ had an interval of constancy) or even singular continuous spectrum. The purpose of the rather strong condition (1.4) is to ensure that ϱ has only absolutely continuous spectrum, as will be seen below.

Since ϱ is real analytic there exists a partition

$$-\pi = a_0 < a_1 < \cdots < a_n = \pi$$

such that ϱ is strictly monotone in each interval $[a_{r-1}, a_r]$ with non-zero derivative in the interior of each interval. If $b_r = \varrho(a_r)^{\frac{1}{2}}$ we define a unitary equivalence

$$V: L^2(-\pi, \pi) \to \sum_{r=1}^{n} \oplus L^2(b_{r-1}, b_r)$$

by

$$V(\varphi) = \{\psi_r\}_{r=1}^n \tag{2.3}$$

where

$$\psi_r(y) = \varphi(x)\, |y'(x)|^{-\frac{1}{2}} \tag{2.4}$$

for $a_{r-1} < x < a_r$ and $y = \varrho(x)^{\frac{1}{2}}$. It is clear that if

$$V(\varrho^{\frac{1}{2}} \varphi) = \{\eta_r\}_{r=1}^n \tag{2.5}$$

then

$$\eta_r(y) = y\, \psi_r(y) \tag{2.6}$$

for all y and all r. Using V to identify

$$\mathscr{H}_{\mathbb{C}} = \mathbb{C} \oplus \sum_{r=1}^{n} \oplus L^2(b_{r-1}, b_r) \tag{2.7}$$

we obtain

$$B_r = \left(\begin{array}{c|c} \omega & \lambda k \\ \hline \lambda k & Q \end{array} \right) \tag{2.8}$$

where Q acts on $\sum_{r=1}^{n} \oplus L^2(b_{r-1}, b_r)$ as the usual multiplication operator

$$(Q\psi_r)(x) = x\psi_r(x) \tag{2.9}$$

and

$$k = V(\omega + \varrho^{\frac{1}{2}})^{-1}\gamma \in \sum_{r=1}^{n} \oplus L^2(b_{r-1}, b_r). \tag{2.10}$$

We now impose our final hypotheses on the model. The first is a regularity condition, that $\{k_r\}_{r=1}^{n}$ be C^∞ functions of compact support (this is actually unnecessarily strong). The more physically significant hypothesis is that ω should be one of the range of frequencies of the heat bath and that the interaction should couple the oscillator to that frequency. Specifically we assume that for some r

$$b_{r-1} < \omega < b_r \quad \text{and} \quad k_r(\omega) \neq 0. \tag{2.11}$$

This assumption is in contrast to that of Friedrichs in his treatment of the otherwise similar Lee model [6], where he supposes ω lies outside the spectrum of Q.

Lemma 2.1. *If λ is sufficiently small then B_λ has no pure point spectrum.*

Proof. Suppose $B_\lambda(x \oplus \psi) = \alpha(x \oplus \psi)$ for some $\alpha \in \mathbb{R}$. Then

$$\omega x + \lambda \sum_{r=1}^{n} \langle \psi_r, k_r \rangle = \alpha x, \tag{2.12}$$

$$\lambda x k_r + Q\psi_r = \alpha \psi_r. \tag{2.13}$$

If $x = 0$ then $\psi = 0$, and otherwise we may normalise by taking $x = 1$. Then

$$(Q - \alpha)\psi_r = -\lambda k_r \tag{2.14}$$

and the solubility conditions are that

$$(Q - \alpha)^{-1} k_r \in L^2(b_{r-1}, b_r) \tag{2.15}$$

and

$$\eta(\alpha) = 0 \tag{2.16}$$

where

$$\begin{aligned} \eta(z) &= \omega - z - \lambda^2 \sum_{r=1}^{n} \langle (Q - z)^{-1} k_r, k_r \rangle \\ &= \omega - z - \lambda^2 \int_{-\infty}^{\infty} \frac{\sum_{r=1}^{n} |k_r(s)|^2}{s - z} ds. \end{aligned} \tag{2.17}$$

Since the k_r are all continuous the first condition is equivalent to $\alpha \notin S$ where

$$S = \bigcup_{r=1}^{n} \operatorname{supp}(k_r)$$

is the support of k. Now $\eta(z)$ is the sum of $\omega - z$ and the Hilbert transform of $\sum_{r=1}^{n} |k_r|^2$. Since this second function is C^∞ of compact support its Hilbert transform is uniformly bounded on the entire complex plane and analytic with a cut along S. Let

$$A = \sup_{z \in \mathbb{C}} \left| \int_{-\infty}^{\infty} \frac{\sum_{r=1}^{n} |k_r(s)|^2}{s - z} ds \right| . \tag{2.18}$$

Since $\omega \in \operatorname{int}(S)$ there is a constant $B > 0$ such that

$$(\omega - B, \omega + B) \subseteqq S . \tag{2.19}$$

Then if $\alpha \notin S$ and $|\lambda| < (B/A)^{\frac{1}{2}}$

$$|\eta(z)| \geqq B - \lambda^2 A > 0 \tag{2.20}$$

so if $|\lambda| < (B/A)^{\frac{1}{2}}$, B_λ has no eigenvalue.

It can be proved under similar hypotheses that B_λ has no singular continuous spectrum. We need however a sharper result.

Lemma 2.2. *There are constants $K, \lambda_0 > 0$ such that if $|\lambda| \leqq \lambda_0$ then*

$$|\langle e^{-iB_\lambda t} v, v\rangle| \leqq \min(1, K/\lambda^2 t) . \tag{2.21}$$

Proof. We note that for $\operatorname{Im} z > 0$

$$\begin{aligned} \int_0^\infty \langle e^{-iB_\lambda t} v, v\rangle e^{izt} dt & \\ &= -i\langle (B_\lambda - z)^{-1} v, v\rangle \\ &= -i\eta(z)^{-1} \end{aligned} \tag{2.22}$$

because of the formula [7]

$$\begin{aligned} &(B_\lambda - z)^{-1} \\ &= \eta(z)^{-1} \left(\begin{array}{c|c} 1 & -\lambda (Q - \bar{z})^{-1} k \\ \hline -\lambda (Q - z)^{-1} k & \eta(z)(Q - z)^{-1} + \lambda^2 (Q - z)^{-1} k \otimes (Q - \bar{z})^{-1} k \end{array} \right) \end{aligned} \tag{2.23}$$

which is certainly valid for all $\operatorname{Im} z \neq 0$. Taking the limit as $y \downarrow 0$ we get

$$\int_0^\infty \langle e^{-iB_\lambda t} v, v\rangle e^{ixt} dt = -i\eta(x + i0)^{-1} \tag{2.24}$$

so that decay properties of $\langle e^{-iB_\lambda t}v, v\rangle$ can be deduced by Fourier analysis from smoothness properties of η. For $y>0$ and $t>0$

$$\langle e^{-iB_\lambda t}v, v\rangle\, e^{-yt} = \frac{-i}{2\pi}\int_{-\infty}^{\infty} \eta(x+iy)^{-1}\, e^{-ixt}\, dx \tag{2.25}$$

so

$$\langle e^{-iB_\lambda t}v, v\rangle = \frac{e^{yt}}{2\pi t}\int_{-\infty}^{\infty} \frac{\eta'(x+iy)}{\eta(x+iy)^2}\, e^{-ixt}\, dx\,. \tag{2.26}$$

Therefore

$$|\langle e^{-iB_\lambda t}v, v\rangle| \leqq \frac{e^{yt}}{2\pi t}\int_{-\infty}^{\infty} \left|\frac{\eta'(x+iy)}{\eta(x+iy)^2}\right| dx\,. \tag{2.27}$$

We make estimates of the integrand which are uniform with respect to $y>0$. We rewrite

$$\begin{aligned}\eta(z) &= \omega - z - \lambda^2 \int_{s=-\infty}^{\infty}\int_{u=0}^{\infty} i\sum_{r=1}^{n} |k_r(s)|^2\, e^{-isu+izu}\, du\, ds\\ &= \omega - z - i\lambda^2 \int_{-\infty}^{\infty} h(u)\, e^{izu}\, du\end{aligned} \tag{2.28}$$

where

$$h(u) = \int_{-\infty}^{\infty} \sum_{r=1}^{n} |k_r(s)|^2\, e^{-isu}\, ds\,. \tag{2.29}$$

Since k_r are C^∞ functions of compact support, h lies in the Schwartz space $\mathcal{S}$. Therefore

$$\begin{aligned}|\eta'(z)| &\leqq 1 + \lambda^2 \int_0^{\infty} u\,|h(u)|\, du\\ &\leqq 2\end{aligned} \tag{2.30}$$

provided λ is small enough, say $|\lambda| \leqq \lambda_1$.

We estimate $\eta(x+iy)$ differently depending on whether $(x-\omega)$ is small or not. If $|x-\omega| \geqq 2A\lambda^2$ then by Eqs. (2.17) and (2.18)

$$\begin{aligned}|\eta(z)| &\geqq |\omega - x| - \lambda^2 A\\ &\geqq \tfrac{1}{2}|\omega - x|\,.\end{aligned} \tag{2.31}$$

On the other hand for all $\operatorname{Im} z > 0$

$$\begin{aligned}|\eta(z)| &\geqq \operatorname{Im}\eta(z)\\ &= y + \lambda^2 \int_{-\infty}^{\infty} \frac{y\sum_{r=1}^{n}|k_r(s)|^2}{(s-x)^2+y^2}\, ds\\ &\geqq \lambda^2 \int_{-\infty}^{\infty} \frac{\sum_{r=1}^{n}|k_r(ys+x)|^2}{s^2+1}\, ds\\ &\geqq \lambda^2 \min_{|s|\leqq 1} \sum_{r=1}^{n} |k_r(ys+x)|^2\,.\end{aligned} \tag{2.32}$$

Now $\sum_{r=1}^{n} |k_r(\omega)|^2 > 0$ by (2.11), so there exist $C, \delta > 0$ such that if $|x-\omega| < 2\delta$ then

$$\sum_{r=1}^{n} |k_r(x)|^2 > C. \tag{2.33}$$

If now we define $\lambda_0 > 0$ so that $\lambda_0 \leqq \lambda_1$ and $2A\lambda_0^2 \leqq \delta$ then for all λ, z such that $|\lambda| \leqq \lambda_0$, $0 < y < \delta$ and $|x-\omega| < \delta$

$$|\eta(z)| \geqq \lambda^2 C. \tag{2.34}$$

Therefore if $|\lambda| \leqq \lambda_0$, $0 < y < \delta$ and $t \geqq 0$

$$|\langle e^{-iB_\lambda t} v, v\rangle| \leqq \frac{e^{yt}}{\pi t} \int_{-\infty}^{\infty} |\eta(x+iy)|^{-2}\, dx \tag{2.35}$$

by Eqs. (2.27) and (2.30),

$$= \frac{e^{yt}}{\pi t} \int_{|x-\omega| \geqq 2A\lambda^2} |\eta(x+iy)|^{-2} dx + \frac{e^{yt}}{\pi t} \int_{|x-\omega| \leqq 2A\lambda^2} |\eta(x+iy)|^{-2}\, dx$$

$$\leqq \frac{2e^{yt}}{\pi t} \int_{2A\lambda^2}^{\infty} 4x^{-2}\, dx + \frac{e^{yt}}{\pi t} 4A\lambda^2 (\lambda^2 C)^{-2}$$

by Eqs. (2.31) and (2.34),

$$\begin{aligned} &= \frac{e^{yt}}{\pi t} \{8/2A\lambda^2 + 4A\lambda^2/C^2\lambda^4\} \\ &= K e^{yt}/\lambda^2 t. \end{aligned} \tag{2.36}$$

But the left-hand side of the inequality is independent of y so letting $y \downarrow 0$ we get

$$|\langle e^{-iB_\lambda t} v, v\rangle| \leqq K/\lambda^2 t. \tag{2.37}$$

The other part of (2.21) is trivial.

For completeness we use the result to prove

Lemma 2.3. *If $|\lambda| < \lambda_0$ then B_λ has no singular continuous spectrum.*

Proof. Let L be the closed subspace of $\mathscr{H}$ generated by

$$\{e^{iB_\lambda t} v : t \in \mathbb{R}\}.$$

Then L is invariant under B_λ and $v, k \in L$. If g is the positive definite function

$$g(t) = \langle e^{-iB_\lambda t} v, v\rangle \tag{2.38}$$

then by Eq. (2.21), $g \in L^2(\mathbb{R})$, so by Bochner's theorem and Plancherel's theorem, g is the Fourier transform of an absolutely continuous measure. Therefore B_λ has absolutely continuous measure. Therefore B has absolutely continuous spectrum within L. In $L^\perp$, $B_\lambda = B_0$, which within $L^\perp$ has only absolutely continuous spectrum since $v \in L$.

The importance of Lemma 2.2 is that it shows that the relevant quantity in determining the rate of convergence to zero of $\langle e^{iB_\lambda t}v, v\rangle$ as $t\to\infty$ for small λ is the combination

$$\tau=\lambda^2 t\,. \tag{2.39}$$

This re-scaled time has already appeared in many contexts in non-equilibrium statistical mechanics [3, 8, 12]. If we now define

$$\Phi(\lambda,\tau)=e^{-i\omega t}\langle e^{iB_\lambda t}v, v\rangle \tag{2.40}$$

where t and τ are related as above then Lemma 2.2 gives the estimate

$$|\Phi(\lambda,\tau)|\leqq \min\{1, K/\tau\} \tag{2.41}$$

for all $r\geqq 0$ and $|\lambda|\leqq\lambda_0$.

Lemma 2.4. *There exists a constant* $c=a+ib$ *with* $a>0$ *such that*

$$\lim_{\lambda\to 0}\Phi(\lambda,\tau)=e^{-c\tau} \tag{2.42}$$

uniformly for τ *in any interval* $[0,\tau_0]$.

Proof. The method is to expand $\Phi(\lambda, t)$ as a perturbation series in λ. Let

$$B_\lambda=\left(\begin{array}{c|c}\omega & \lambda k\\ \hline \lambda k & Q\end{array}\right),\qquad A=\left(\begin{array}{c|c}0 & k\\ \hline k & 0\end{array}\right) \tag{2.43}$$

so that

$$B_\lambda=B_0+\lambda A\,. \tag{2.44}$$

By [10]

$$\begin{aligned} e^{iB_\lambda t}&=e^{iB_0 t}+i\lambda\int_{s=0}^{t} e^{iB_0(t-s)}A\,e^{iB_0 s}\,ds\\ &\quad+(i\lambda)^2\int_{s=0}^{t}\int_{u=0}^{s} e^{iB_0(t-s)}A\,e^{iB_0(s-u)}A\,e^{iB_0 u}\,du\,ds+\cdots \end{aligned} \tag{2.45}$$

the series converging in norm for all finite t. Therefore

$$\begin{aligned} \Phi(\lambda,\tau)&=1+i\lambda\int_{s=0}^{t} e^{-i\omega t}\langle e^{iB_0(t-s)}A\,e^{iB_0 s}v,v\rangle\,ds\\ &\quad+(i\lambda)^2\int_{s=0}^{t}\int_{u=0}^{s} e^{-i\omega t}\langle e^{iB_0(t-s)}A\,e^{iB_0(s-u)}A\,e^{iB_0 u}v,v\rangle\,du\,ds+\cdots. \end{aligned} \tag{2.46}$$

One easily sees that the odd terms contribute nothing to the series and that

$$\Phi(\lambda,\tau)=\sum_{n=0}^{\infty}(i\lambda)^{2n}I_n(t) \tag{2.47}$$

where

$$\begin{aligned} I_n(t)&=\int_{t_1=0}^{t}\int_{t_2=0}^{t_1}\int_{t_{2n}=0}^{t_{2n-1}} e^{-i\omega t}e^{i\omega(t-t_1)}\langle e^{iQ(t_1-t_2)}k,k\rangle\cdots\\ &\quad\cdots e^{i\omega(t_{2n-2}-t_{2n-1})}\langle e^{iQ(t_{2n-1}-t_{2n})}k,k\rangle\, e^{i\omega t_{2n}}\,dt_1\ldots dt_{2n}\\ &=\int_{t_1=0}^{t}\int_{t_2=0}^{t_1}\int_{t_{2n}=0}^{t_{2n-1}} h(t_1-t_2)\,h(t_3-t_4)\ldots h(t_{2n-1}-t_{2n})\,dt_1\ldots dt_{2n} \end{aligned} \tag{2.48}$$

where

$$h(s)=e^{-i\omega s}\langle e^{iQs}k,k\rangle \tag{2.49}$$

so that by our regularity assumptions on k, h lies in Schwarz space $\mathscr{S}$. Now $I_n(0)=0$ and

$$\begin{aligned}\frac{dI_n(t)}{dt} &= \int_{t_2=0}^{t}\int_{t_{2n}=0}^{t_{2n-1}} h(t-t_2)\,h(t_3-t_4)\dots h(t_{2n-1}-t_{2n})\,dt_2\dots dt_{2n} \\ &= \int_{s=0}^{t} h(t-s)\,I_{n-1}(s)\,ds\,.\end{aligned} \tag{2.50}$$

From this it follows that

$$I_n(t)=\int_{t_1=0}^{t}\int_{t_2=0}^{t-t_1}\int_{t_n=0}^{t-t_1-\dots-t_{n-1}}(n!)^{-1}(t-t_1-\dots-t_n)^n\,h(t_1)\cdots h(t_n)\,dt_1\dots dt_n \tag{2.51}$$

since the latter expression satisfies the same relations. This may be rewritten as

$$I_n(t)=\frac{t^n}{n!}\int_{t_1=0}^{\infty}\cdots\int_{t_n=0}^{\infty}K_t(t_1\dots t_n)\,h(t_1)\dots h(t_n)\,dt_1\dots dt_n \tag{2.52}$$

where

$$K_t(t_1\dots t_n)=\begin{cases}[1-(t_1+\dots+t_n)/t]^n & \text{if } 0\leqq t+\dots+t_n\leqq t\\ 0 & \text{otherwise}.\end{cases} \tag{2.53}$$

Substituting back into Eq. (2.47) gives

$$\Phi(\lambda,\tau)=\sum_{n=0}^{\infty}\frac{(-\tau)^n}{n!}\int_0^{\infty}\cdots\int_0^{\infty}K_t(t_1\dots t_n)\,h(t_1)\dots h(t_n)\,dt_1\dots dt_n\,. \tag{2.54}$$

Since $0\leqq K_t\leqq 1$, if $0\leqq\tau\leqq\tau_0$ the series is uniformly dominated by

$$\sum_{n=0}^{\infty}\frac{\tau_0^n}{n!}\left(\int_0^{\infty}|h(s)|\,ds\right)^n<\infty\,. \tag{2.55}$$

Moreover since

$$\lim_{t\to\infty}K_t(t_1\dots t_n)=1 \tag{2.56}$$

the individual terms of Eq. (2.54) converge as $\lambda\to 0$ for fixed τ. Therefore the series of Eq. (2.54) converges uniformly for $0\leqq\tau\leqq\tau_0$ with sum

$$\sum_{n=0}^{\infty}\frac{(-\tau)^n}{n!}\left(\int_0^{\infty}h(s)\,ds\right)^n=e^{-c\tau} \tag{2.57}$$

where

$$c=\int_0^{\infty}h(s)\,ds\,. \tag{2.58}$$

From its definition

$$\begin{aligned} h(s) &= e^{-i\omega s} \sum_{r=1}^{n} \int_{-\infty}^{\infty} e^{ixs} |k_r(x)|^2 \, dx \\ &= \int_{-\infty}^{\infty} e^{ixs} \sum_{r=1}^{n} |k_r(x+\omega)|^2 \, dx . \end{aligned} \tag{2.59}$$

Therefore $h \in \mathscr{S}$ and $h(-s) = \overline{h(s)}$ for all s. Hence, writing $c = a + ib$,

$$\begin{aligned} a &= \tfrac{1}{2} \int_{-\infty}^{\infty} h(s) \, ds \\ &= \frac{1}{4\pi} \sum_{r=1}^{n} |k_r(\omega)|^2 \end{aligned} \tag{2.60}$$

which is strictly positive by Eq. (2.11).

It is very significant that the convergence in the above lemma is not just uniform on each finite interval $[0, \tau_0]$, but uniform on the entire interval $[0, \infty)$. We choose to state the result without explicit reference to the re-scaled time.

Theorem 2.5. *Given* $\varepsilon > 0$ *there exists* $\lambda_\varepsilon > 0$ *such that if* $|\lambda| < \lambda_\varepsilon$ *then for all* $0 \leqq t < \infty$

$$|\langle e^{iA_\lambda^{\frac{1}{2}} t} v, v\rangle - e^{i\omega t - c\lambda^2 t}| < \varepsilon . \tag{2.61}$$

Proof. We have to prove that

$$\lim_{\lambda \to 0} \Phi(\lambda, \tau) = e^{-c\tau} \tag{2.62}$$

uniformly for $0 \leqq \tau < \infty$. Given $\varepsilon > 0$, there exists $\lambda_0, \tau_0 > 0$ such that if $|\lambda| < \lambda_0$ and $\tau \geqq \tau_0$ then

$$|\Phi(\lambda, \tau)| < \varepsilon/2 \tag{2.63}$$

and

$$|e^{-c\tau}| < \varepsilon/2 \tag{2.64}$$

by Eq. (2.41). By Lemma 2.4 there exists $\lambda_\varepsilon \leqq \lambda_0$ such that if $0 \leqq \tau \leqq \tau_0$ and $|\lambda| < \lambda_\varepsilon$ then

$$|\Phi(\lambda, \tau) - e^{-c\tau}| < \varepsilon . \tag{2.65}$$

Putting these together gives the result that if $|\lambda| < \lambda_\varepsilon$ then

$$|\Phi(\lambda, \tau) - e^{-c\tau}| < \varepsilon$$

for all $0 \leqq \tau < \infty$.

3. Approach to Equilibrium

We use the estimates of Section 2 to study the time evolution of the harmonic oscillator in interaction with the heat bath. The first theorem we obtain was proved for a particular special heat bath in [5].

Theorem 3.1. *The harmonic oscillator converges from an arbitrary initial state to an equilibrium state which, in the weak coupling limit, is its canonical state at the inverse temperature* β.

Proof. The canonical state φ_β of the oscillator at the inverse temperature β is given in terms of the expectations of the Weyl operators by

$$\begin{aligned}&\langle \varphi_\beta, U(x,y)\rangle \\ &\quad = \mathrm{tr}[U(x,y)\exp\{-\beta(p^2+\omega^2 q^2)/z\}]/\mathrm{tr}[\exp\{-\beta(p^2+\omega^2 q^2)/2\}] \\ &\quad = \exp[-s_\beta(x,y)/4] \end{aligned} \tag{3.1}$$

where

$$s_\beta(x,y) = \omega^{-1} x^2 \coth(\beta\omega/2) + \omega y^2 \coth(\beta\omega/2)\,. \tag{3.2}$$

Calculating first in the Heisenberg picture, it is sufficient by Lemma 1.1 to show that if $\varepsilon > 0$ there are constants $\lambda_\varepsilon, \tau_\varepsilon > 0$ such that if $|\lambda| < \lambda_\varepsilon$ and $\tau \geqq \tau_\varepsilon$ then

$$|x_{\lambda,t}| < \varepsilon\,; \qquad |y_{\lambda,t}| < \varepsilon\,; \qquad |r_{\lambda,t} - s_\beta| < \varepsilon\,. \tag{3.3}$$

By Lemma 1.1 and Lemma 2.2 if $|\lambda| < \lambda_0$

$$\begin{aligned}|x_{\lambda,t}| &= |\langle \cos(A_\lambda^{\frac{1}{2}} t)\, v, v\rangle - \langle A_\lambda^{\frac{1}{2}} \sin(A_\lambda^{\frac{1}{2}} t)\, v, v\rangle| \\ &= |\langle \cos(A_\lambda^{\frac{1}{2}} t)\, v, v\rangle - \omega\langle \sin(A_\lambda^{\frac{1}{2}} t)\, v, v\rangle + \langle \sin(A_\lambda^{\frac{1}{2}} t)(\omega - A_\lambda^{\frac{1}{2}})\, v, v\rangle| \\ &\leqq (1+\omega)\,|\langle e^{iA_\lambda^{\frac{1}{2}} t} v, v\rangle| + \|(\omega - A_\lambda^{\frac{1}{2}})\, v\| \\ &\leqq (1+\omega)\, K/\tau + |\lambda|\, \|k\| \\ &< \varepsilon \end{aligned} \tag{3.4}$$

provided λ is small enough and τ is large enough. $y_{\lambda,t}$ is dealt with similarly.

Since $A_\lambda \to A_0$ in norm as $\lambda \to 0$, and A_0 is invertible, $A_0^{\pm\frac{1}{2}} \coth(\beta A_\lambda^{\frac{1}{2}}/2)$ converges in norm to $A_0^{\pm\frac{1}{2}} \coth(\beta A_0^{\frac{1}{2}}/2)$ as $\lambda \to 0$ by [13]. Moreover P commutes with A_0 and

$$\langle A_0^{\pm\frac{1}{2}} \coth(\beta A_0^{\frac{1}{2}}/2)\, v, v\rangle = \omega^{\pm 1} \coth(\beta\omega/2)\,. \tag{3.5}$$

Using these facts and writing

$$u = \cos(A_\lambda^{\frac{1}{2}} t)\, x - A_\lambda^{\frac{1}{2}} \sin(A_\lambda^{\frac{1}{2}} t)\, y \tag{3.6}$$

$$v = A_\lambda^{-\frac{1}{2}} \sin(A_\lambda^{\frac{1}{2}} t)\, x + \cos(A_\lambda^{\frac{1}{2}} t)\, y \tag{3.7}$$

we find that

$$\begin{aligned}
r_{\lambda,t} &= \langle A_\lambda^{-\frac{1}{2}} \coth(\beta A_\lambda^{\frac{1}{2}}/2)(1-P)u, (1-P)u\rangle \\
&\quad + \langle A_\lambda^{\frac{1}{2}} \coth(\beta A_\lambda^{\frac{1}{2}}/2)(1-P)v, (1-P)v\rangle \\
&= \langle A_\lambda^{-\frac{1}{2}} \coth(\beta A^{\frac{1}{2}}/2)u, u\rangle + \langle A_\lambda^{\frac{1}{2}} \coth(\beta A_\lambda^{\frac{1}{2}}/2)v, v\rangle \qquad (3.8)\\
&\quad - \langle A_0^{-\frac{1}{2}} \coth(\beta A_0^{\frac{1}{2}}/2)u, Pu\rangle \\
&\quad - \langle A_0^{\frac{1}{2}} \coth(\beta A_0^{\frac{1}{2}}/2)v, Pv\rangle + o(1) \\
&= \langle A_\lambda^{-\frac{1}{2}} \coth(\beta A^{\frac{1}{2}}/2)x, x\rangle + \langle A_\lambda^{\frac{1}{2}} \coth(\beta A_\lambda^{\frac{1}{2}}/2)y, y\rangle \\
&\quad - \omega^{-1} \coth(\beta\omega/2)\langle Pu, u\rangle \\
&\quad - \omega \coth(\beta\omega/2)\langle Pv, v\rangle + o(1) \\
&= \omega^{-1} x^2 \coth(\beta\omega/2) + \omega y^2 \coth(\beta\omega/2) \\
&\quad - \omega^{-1} \coth(\beta\omega/2)\{x^2 \langle\cos(A_\lambda^{\frac{1}{2}}t)v, v\rangle^2 \qquad (3.9)\\
&\quad - 2xy\omega\langle\cos(A_\lambda^{\frac{1}{2}}t)v, v\rangle\langle\sin(A_\lambda^{\frac{1}{2}}t)v, v\rangle + y^2\omega^2\langle\sin(A_\lambda^{\frac{1}{2}}t)v, v\rangle^2\} \\
&\quad - \omega \coth(\beta\omega/2)\{\omega^{-2} x^2 \langle\sin(A_\lambda^{\frac{1}{2}}t)v, v\rangle^2 \\
&\quad + 2xy\omega^{-1}\langle\cos(A_\lambda^{\frac{1}{2}}t)v, v\rangle\langle\sin(A_\lambda^{\frac{1}{2}}t)v, v\rangle + y^2\langle\cos(A_\lambda^{\frac{1}{2}}t)v, v\rangle^2\} + o(1) \\
&= s_\beta(1 - |\Phi(\lambda, \tau)|^2) + o(1),
\end{aligned}$$

this estimate being uniform with respect to τ. The required limiting property of $r_{\lambda,t}$ follows.

We finally transform to the Schrödinger picture in the same manner as in [4]. Let ψ be an arbitrary initial state of the harmonic oscillator and let the corresponding state at time $t \geqq 0$ be ψ_t, so that

$$\langle\psi_t, U(x,y)\rangle = \langle\psi, \alpha_{\lambda,t}\{U(x,y)\}\rangle. \qquad (3.10)$$

Then

$$\begin{aligned}
&\lim_{\lambda\to 0,\, \lambda^2 t\to\infty} \langle\psi_t, U(x,y)\rangle \\
&\quad = \lim_{\lambda\to 0,\, \lambda^2 t\to\infty} \langle\psi, U(x_{\lambda,t}, y_{\lambda,t})\rangle \exp[-r_{\lambda,t}/4] \\
&\quad = \langle\psi, U(0,0)\rangle \exp[-s_\beta/4] \qquad (3.11)\\
&\quad = \exp[-s_\beta/4] \\
&\quad = \langle\varphi_\beta, U(x,y)\rangle.
\end{aligned}$$

We can similarly follow the approach to equilibrium in the weak coupling limit. Since the diffusion becomes slower as $\lambda \to 0$ this must be done using the re-scaled time τ. Also because of the "fast" oscillation term in Eq. (2.61) we must compare the time evolution with the free evolution by changing to the interaction representation – as in scattering theory [10]. The following theorem is an exact analogue of Lemma 2.3 of [4]. However it is a result of much greater scope since only regularity conditions are imposed on the heat bath interactions whereas in [4] we were confined to a particular special heat bath.

Theorem 3.2. *If $\tau = \lambda^2 t$ then for each $\tau \geqq 0$*

$$\lim_{\lambda \to 0} e^{-iH_0 t} \alpha_{\lambda,t}\{U(x,y)\} e^{iH_0 t} = U(x^{(\tau)}, y^{(\tau)}) \exp[-r^{(\tau)}/4] \tag{3.12}$$

where

$$x^{(\tau)} = e^{-a\tau} \cos(b\tau)\, x + e^{-a\tau} \omega \sin(b\tau)\, y\,, \tag{3.13}$$

$$y^{(\tau)} = -e^{-a\tau} \omega^{-1} \sin(b\tau)\, x + e^{-a\tau} \cos(b\tau)\, y\,, \tag{3.14}$$

$$r^{(\tau)} = \{\omega^{-1} x^2 \coth(\beta\omega/2) + \omega y^2 \coth(\beta\omega/2)\}\, \{1 - e^{-2a\tau}\}\,. \tag{3.15}$$

Proof. As in [4]

$$e^{-iH_0 t} \alpha_{\lambda,t}\{U(x,y)\} e^{iH_0 t} = U(u_{\lambda,t}, v_{\lambda,t}) \exp[-r_{\lambda,t}/4] \tag{3.16}$$

where

$$u_{\lambda,t} = x_{\lambda,t} \cos(\omega t) + y_{\lambda,t} \omega \sin(\omega t)\,, \tag{3.17}$$

$$v_{\lambda,t} = -x_{\lambda,t} \omega^{-1} \sin(\omega t) + y_{\lambda,t} \cos(\omega t)\,. \tag{3.18}$$

Therefore

$$\begin{aligned} \omega^{-\frac{1}{2}} x^{(\tau)} + i\omega^{\frac{1}{2}} y^{(\tau)} &= \lim_{\lambda \to 0} \{\omega^{-\frac{1}{2}} u_{\lambda,t} + i\omega^{\frac{1}{2}} v_{\lambda,t}\} \\ &= \lim_{\lambda \to 0} \{\omega^{-\frac{1}{2}} x_{\lambda,t} + i\omega^{\frac{1}{2}} y_{\lambda,t}\} e^{-i\omega t} \\ &= \lim_{\lambda \to 0} \{\omega^{-\frac{1}{2}} x \langle \cos(A_\lambda^{\frac{1}{2}} t) v, v\rangle - \omega^{\frac{1}{2}} y \langle \sin(A_\lambda^{\frac{1}{2}} t) v, v\rangle \\ &\quad + i\omega^{-\frac{1}{2}} x \langle \sin(A_\lambda^{\frac{1}{2}} t) v, v\rangle + i\omega^{\frac{1}{2}} y \langle \cos(A_\lambda^{\frac{1}{2}} t) v, v\rangle\} e^{-i\omega t} \\ &= \lim_{\lambda \to 0} (\omega^{-\frac{1}{2}} x + i\omega^{\frac{1}{2}} y) \langle e^{iA_\lambda^{\frac{1}{2}} t} v, v\rangle e^{-i\omega t} \\ &= (\omega^{-\frac{1}{2}} x + i\omega^{\frac{1}{2}} y) e^{-c\tau} \end{aligned} \tag{3.19}$$

by Eqs. (1.27), (1.28) and (2.42). Separating real and imaginary parts gives the expressions for $x^{(\tau)}$ and $y^{(\tau)}$. That for $r^{(\tau)}$ can be obtained immediately from Eq. (3.9).

The above result can be interpreted in terms of the theory of Markov semigroups.

Theorem 3.3. *If we define*

$$\gamma_\tau\{U(x,y)\} = U(x^{(\tau)}, y^{(\tau)}) \exp[-r^{(\tau)}/4] \tag{3.20}$$

then for all $\sigma, \tau \geqq 0$

$$\gamma_\sigma \gamma_\tau \{U(x,y)\} = \gamma_{\sigma+\tau}\{U(x,y)\}\,. \tag{3.21}$$

Proof. Writing $z = \omega^{-\frac{1}{2}} x + i\omega^{\frac{1}{2}} y$ we have shown that

$$z^{(\tau)} = z e^{-c\tau} \tag{3.22}$$

and

$$\begin{aligned} r^{(\tau)} &= \coth(\beta\omega/2) |z|^2 (1 - e^{-2a\tau}) \\ &= \coth(\beta\omega/2) \{|z|^2 - |z^{(\tau)}|^2\}\,. \end{aligned} \tag{3.23}$$

The semigroup property follows immediately from these two equations.

We make some comments on this last theorem. It was shown in [5] that for a finite coupling constant λ, and for the corresponding classical problem, there is an essentially unique heat bath for which the induced diffusion of the oscillator is Markovian. The quantum mechanical analogue of this particular heat bath does not induce Markovian diffusion on the oscillator, and indeed there is no sensible quantum mechanical heat bath (of this type) which, for finite λ, induces Markovian diffusion on the oscillator. What we have shown is that nevertheless in the weak coupling limit one does obtain Markovian diffusion for every heat bath of this type.

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