Oscillator Bath
A Model for Dissipation

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1 Introduction to the problem

The central question of this paper is how I can model dissipation and how does dissipation affect a physical system? Since in a dissipative system the energy is not conserved, our system loses energy to it's environment. So our "universe" consists of the system plus the environment. How do we now describe the environment? The answer is that the environment is a set of harmonic oscillators coupled with the system: the oscillator bath! See also [1], page 392, for further details. This description is called the system-plus-bath model and is the most successful way to describe dissipation.

Additionally, we want that our system with the coordinate q obeys a phenomenological damped equation of motion of the following form

$$M\ddot{q} + \eta\dot{q} + \frac{\partial V(q)}{\partial q} = F_{ext}(t) \tag{1}$$

where η is the friction coefficient which in our case is frequency independent, M is the mass, $V(q)$ is the potential and F_{ext} might be an external force.

2 Hamiltonian of the system-plus-bath model

The Hamiltonian of the system-plus-bath model is composed of three components

$$H = H_S + H_B + H_I \tag{2}$$

where

$$H_S = \frac{M}{2}\dot{q}^2 + V(q) \tag{3}$$

is the Hamiltonian of the isolated system,

$$H_B = \sum_{\alpha=1}^{N} \left(\frac{m_\alpha}{2}\dot{x}_\alpha^2 + \frac{m_\alpha \omega_\alpha^2}{2} x_\alpha^2 \right) \tag{4}$$

describes the the bath of N harmonic oscillators and

$$H_I = -\sum_{\alpha=1}^{N} F_\alpha(q) x_\alpha + \phi(m_\alpha, \omega_\alpha, F_\alpha(q)) \tag{5}$$

is the interaction term.

The function ϕ serves to compensate renormalization effects. If we assume that ϕ is zero and ask what is the minimum value of the potential energy of the universe which can be attained for given q, then we will see that we need to set

$$x_\alpha = \frac{F_\alpha(q)}{m_\alpha \omega_\alpha^2} \tag{6}$$

for all α and the resulting effective potential $V_{eff}(q)$ is given by

$$V_{eff}(q) = V(q) - \sum_{\alpha=1}^{N} \frac{F_\alpha^2(q)}{2m_\alpha \omega_\alpha^2}. \tag{7}$$

Since we would like that the damped and undamped system "feel" the same observable potential, we don't want to have this renormalization effect of the potential and have to set therefore

$$\phi = \sum_{\alpha=1}^{N} \frac{F_\alpha^2(q)}{2m_\alpha \omega_\alpha^2}. \tag{8}$$

Additionally, we want that the coupling is strictly linear in q with

$$F_\alpha(q) = C_\alpha q \tag{9}$$

where C_α is a constant. The resulting Hamiltonian for the system-plus-bath model is now given by the following expression

$$H = \frac{M}{2}\dot{q}^2 + V(q) + \sum_{\alpha=1}^{N} \left(\frac{m_\alpha}{2}\dot{x}_\alpha^2 + \frac{m_\alpha \omega_\alpha^2}{2} x_\alpha^2 \right) - \sum_{\alpha=1}^{N} C_\alpha x_\alpha q + \sum_{\alpha=1}^{N} \frac{C_\alpha^2 q^2}{2m_\alpha \omega_\alpha^2}. \tag{10}$$

3 Integrating out the bath

We define the density matrix ρ of our universe as

$$\rho(q_i, [x_{\alpha_i}]; q_f, [x_{\alpha_f}]; \beta) \equiv \sum_n \psi_n^*(q_i, [x_{\alpha_i}])\psi_n(q_f, [x_{\alpha_f}]) \exp(-\beta E_n) \tag{11}$$

and the propagator (reduced density matrix) of the system by

$$K(q_i, q_f, \beta) \equiv \int \prod_\alpha dx_{\alpha_i} \rho(q_i, [x_{\alpha_i}]; q_f, [x_{\alpha_i}]; \beta) \tag{12}$$

with $\beta^{-1} = k_B \vartheta$ where ϑ is the temperature and where x_i and q_i are the initial and x_f and q_f the final coordinates of the bath respectively of the system. Writing $T = \beta\hbar$, we have

$$K(q_i, q_f, T) = \int \prod_\alpha dx_{\alpha_i} \sum_n \psi_n^*(q_i, [x_{\alpha_i}])\psi_n(q_f, [x_{\alpha_i}]) \exp\left(-\frac{E_n T}{\hbar}\right). \tag{13}$$

We know from the path integral formalism that we can write the propagator as a path integral

$$K(q_i, q_f, T) = \int_{q(0)=q_i}^{q(T)=q_f} Dq(\tau) \int \prod_\alpha dx_{\alpha_i} \int_{x_\alpha(0)=x_{\alpha_i}}^{x_\alpha(T)=x_{\alpha_i}} Dx_\alpha(\tau) \exp\left(-\frac{1}{\hbar}\int_0^T L_E d\tau\right) \tag{14}$$

where L_E is the Euclidean Lagrangian given by the expression

$$L_E = \frac{M}{2}\dot{q}^2 + V(q) + \sum_{\alpha=1}^{N} \left(\frac{m_\alpha}{2}\dot{x}_\alpha^2 + \frac{m_\alpha \omega_\alpha^2}{2} x_\alpha^2 \right) + \sum_{\alpha=1}^{N} C_\alpha x_\alpha q + \sum_{\alpha=1}^{N} \frac{C_\alpha^2 q^2}{2m_\alpha \omega_\alpha^2}. \tag{15}$$

Let's have now a closer look at the following part of the integral over L_E appearing in the exponent. We define

$$Q(T) = \int_0^T \left(\frac{m}{2}\dot{x}^2 + \frac{m\omega^2}{2}x^2 + Cxq \right) d\tau. \tag{16}$$

For convenience I left the index α away. By parametrizing $x(\tau) = z(\tau) + y(\tau)$ where $z(\tau)$ is a path that makes the largest contribution to $K(q_i, q_f, T)$ and the boundary conditions $y(0) = y(T) = 0$ for y we can write $Q(T)$ as

$$\begin{aligned} Q(T) &= \underbrace{\int_0^T \left(\frac{m}{2}\dot{z}^2 + \frac{m\omega^2}{2}z^2 + Czq \right) d\tau}_{I} + \underbrace{\int_0^T \left(m\dot{z}\dot{y} + m\omega^2 zy + Cyq \right) d\tau}_{II} \\ &\quad + \underbrace{\int_0^T \left(\frac{m}{2}\dot{y}^2 + \frac{m\omega^2}{2}y^2 \right) d\tau}_{III} \end{aligned} \tag{17}$$

Because $z(\tau)$ makes the largest contribution to $K(q_i, q_f, T)$ (in other words it minimizes the action in the exponent!) it must satisfy the Euler-Lagrange equations and we get from there the following equation of motion

$$m\ddot{z} - m\omega^2 z - Cq = 0. \tag{18}$$

After partial integration of the first term in integral II we can write

$$II = \int_0^T \left(-m\ddot{z}y + m\omega^2 zy + Cyq \right) d\tau = \int_0^T -y \underbrace{\left[m\ddot{z} - m\omega^2 z - Cq \right]}_{=0} d\tau = 0. \tag{19}$$

Writing $z(\tau) = \frac{1}{T}\sum_n \tilde{z}(\nu_n)\exp(i\nu_n\tau)$ (Fourier transformation) with $\nu_n = \frac{2\pi n}{T}$ and analogue for $q(\tau)$, we can write the equation of motion (18) as

$$\frac{1}{T}\sum_n \exp(i\nu_n\tau)\left[-m\nu_n^2\tilde{z}(\nu_n) - m\omega^2\tilde{z}(\nu_n) - C\tilde{q}(\nu_n) \right] = 0. \tag{20}$$

The expression in the brackets must therefore be zero for each n and we get

$$\tilde{z}(\nu_n) = -\frac{C\tilde{q}(\nu_n)}{m(\nu_n^2 + \omega^2)} \tag{21}$$

from where we get the term for

$$z(\tau) = \frac{1}{T}\sum_n \left(-\frac{C\tilde{q}(\nu_n)}{m(\nu_n^2 + \omega^2)} \right) \exp(i\nu_n\tau). \tag{22}$$

Now we can write the integral I as following

$$\begin{aligned} I &= \frac{C^2}{2mT^2}\sum_n (i\nu_n)\frac{\tilde{q}(\nu_n)}{\nu_n^2 + \omega^2}\sum_l (i\nu_l)\frac{\tilde{q}(\nu_l)}{\nu_l^2 + \omega^2}\underbrace{\int_0^T \exp(i(\nu_n + \nu_l)\tau)d\tau}_{T\delta_{l,-n}} \\ &\quad + \frac{C^2\omega^2}{2mT^2}\sum_n \frac{\tilde{q}(\nu_n)}{\nu_n^2 + \omega^2}\sum_l \frac{\tilde{q}(\nu_l)}{\nu_l^2 + \omega^2}\underbrace{\int_0^T \exp(i(\nu_n + \nu_l)\tau)d\tau}_{T\delta_{l,-n}} \\ &\quad - \frac{C^2}{Tm}\int_0^T \sum_n \frac{\tilde{q}(\nu_n)}{\nu_n^2 + \omega^2}e^{i\nu_n\tau}q(\tau)d\tau \end{aligned} \tag{23}$$

$$= \frac{C^2}{2mT}\sum_n \left[(i\nu_n)(i\underbrace{\nu_{-n}}_{-\nu_n}) + \omega^2\right] \frac{\tilde{q}(\nu_n)\tilde{q}(\nu_{-n})}{(\nu_n^2+\omega^2)(\nu_{-n}^2+\omega^2)} \tag{24}$$

$$-2\int_0^T \frac{\tilde{q}(\nu_n)}{\nu_n^2+\omega^2}\exp(i\nu_n\tau)q(\tau)d\tau$$

$$= -\frac{C^2}{2mT}\int_0^T\int_0^T\sum_n \frac{\exp(-i\nu_n(\tau-\tau'))}{\nu_n^2+\omega^2}q(\tau)q(\tau')d\tau d\tau' \tag{25}$$

Integral III leads to a prefactor K_0 we are not very much interested in and I will only quote the result from the paper of Caldeira and Leggett (See also [1], page 402).

This leads directly to this expression for the propagator

$$K(q_i, q_f, T) = K_0 \int_{q(0)=q_i}^{q(T)=q_f} Dq(\tau)\exp\left(-\frac{S_0 + S_{bath}}{\hbar}\right) \tag{26}$$

with

$$K_0 = \prod_\alpha \frac{1}{2}\text{cosech}\left(\frac{\omega_\alpha T}{2}\right), \tag{27}$$

$$S_0 = \int_0^T \frac{M}{2}\dot{q}^2 + V(q)d\tau \tag{28}$$

and

$$S_{bath} = \underbrace{\int_0^T \sum_\alpha \frac{C_\alpha^2 q^2}{2m_\alpha\omega_\alpha^2}d\tau}_{IV} - \underbrace{\int_0^T\int_0^T \sum_\alpha \frac{C_\alpha^2}{2m_\alpha T}\sum_n \frac{\exp(-i\nu_n(\tau-\tau'))}{\nu_n^2+\omega^2}q(\tau)q(\tau')d\tau d\tau'}_{V}. \tag{29}$$

Writing IV and V with the Fourier coefficients

$$IV = \sum_\alpha \frac{C_\alpha^2}{2m_\alpha\omega_\alpha^2}\frac{1}{T}\sum_n \tilde{q}(\nu_n)\tilde{q}(-\nu_n), \tag{30}$$

$$V = \sum_\alpha \frac{C_\alpha^2}{2m_\alpha}\frac{1}{T}\sum_n \frac{1}{\nu_n^2+\omega_\alpha^2}\tilde{q}(\nu_n)\tilde{q}(-\nu_n) \tag{31}$$

we get for

$$S_{bath} = \frac{1}{T}\sum_n \tilde{q}(\nu_n)\tilde{q}(-\nu_n)\left[\sum_\alpha \frac{C_\alpha^2}{2m_\alpha}\left[\frac{\nu_n^2}{\omega_\alpha^2(\nu_n^2+\omega_\alpha^2)}\right]\right]. \tag{32}$$

We define now the spectral density $J(\omega)$ as

$$J(\omega) \equiv \frac{\pi}{2}\sum_\alpha \frac{C_\alpha^2}{m_\alpha\omega_\alpha}\delta(\omega-\omega_\alpha). \tag{33}$$

From a comparison of the equation of motion we get from L_E (15) and our phenomenological equation of motion (1) we get for $J(\omega) = \eta\omega$ where η is the friction coefficient which in our case is frequency independent (See also [1], page 446).

So we can write S_{bath} as

$$S_{bath} = \frac{1}{T}\sum_n \tilde{q}(\nu_n)\tilde{q}(-\nu_n)\frac{1}{\pi}\int_o^\infty \frac{J(\omega)}{\omega}\frac{\nu_n^2}{\nu_n^2+\omega^2}d\omega \tag{34}$$

$$= \frac{1}{T}\sum_n \tilde{q}(\nu_n)\tilde{q}(-\nu_n)\frac{\eta|\nu_n|}{\pi}\underbrace{\int_0^\infty \frac{1}{1+y^2}dy}_{=\frac{\pi}{2}} \tag{35}$$

$$= \frac{\eta}{2T}\sum_n |\nu_n|\tilde{q}(\nu_n)\tilde{q}(-\nu_n) \tag{36}$$

With $\nu_n = \frac{2\pi n}{T} = \Delta\nu n \Rightarrow \frac{1}{T} = \frac{\Delta\nu}{2\pi}$ and $T = \frac{\hbar}{k_B\vartheta}$ in the limit of temperature $\vartheta \to 0 \Rightarrow T \to \infty$ we can write $\frac{1}{T} = \frac{d\nu}{2\pi}$ and the sum becomes an integral. So we get the final form of S_{bath}

$$S_{bath} = \frac{\eta}{4\pi}\int_{-\infty}^\infty |\nu|\tilde{q}(\nu)\tilde{q}(-\nu)d\nu = \frac{\eta}{4\pi}\int_{-\infty}^\infty\int_{-\infty}^\infty \left(\frac{q(\tau)-q(\tau')}{\tau-\tau'}\right)^2 \mathrm{d}\tau\mathrm{d}\tau'. \tag{37}$$

I quote here the second expression just for completeness because Caldeira and Leggett work with this form. But I found the first form where only the Fourier coefficients of the system coordinate q appear more convenient to work with.

4 Dissipative tunneling

4.1 Potential

As an example of the effect of dissipation on quantum mechanics we discuss now the tunneling out of a quadratic-plus-cubic potential of the form

$$V(q) = \frac{M\omega_0^2}{2}q^2 + \frac{M\omega_0^2}{2}\frac{q^3}{q_0} = \frac{27}{4}V_0\left[\left(\frac{q}{q_0}\right)^2 - \left(\frac{q}{q_0}\right)^3\right] \tag{38}$$

where V_0 is the height of the barrier and q_0 is the distance under the barrier. See also Figure 1.

4.2 Tunneling rate

The tunneling rate Γ out of the metastable minimum of the potential is given by

$$\Gamma = \sqrt{\Delta\frac{S_{eff}}{2\pi\hbar}}\exp\left(\frac{-S_{eff}}{\hbar}\right) \tag{39}$$

with

$$S_{eff} = \underbrace{\int_{-\infty}^\infty \frac{M}{2}\dot{q}^2 + V(q)d\tau}_{S_0} + \underbrace{\frac{\eta}{4\pi}\int_{-\infty}^\infty |\nu|\tilde{q}(\nu)\tilde{q}(-\nu)d\nu}_{S_{bath}} \tag{40}$$

where Δ is a ratio of determinants with the dimensions of $(frequency)^2$. See also [1], page 406, for further details.

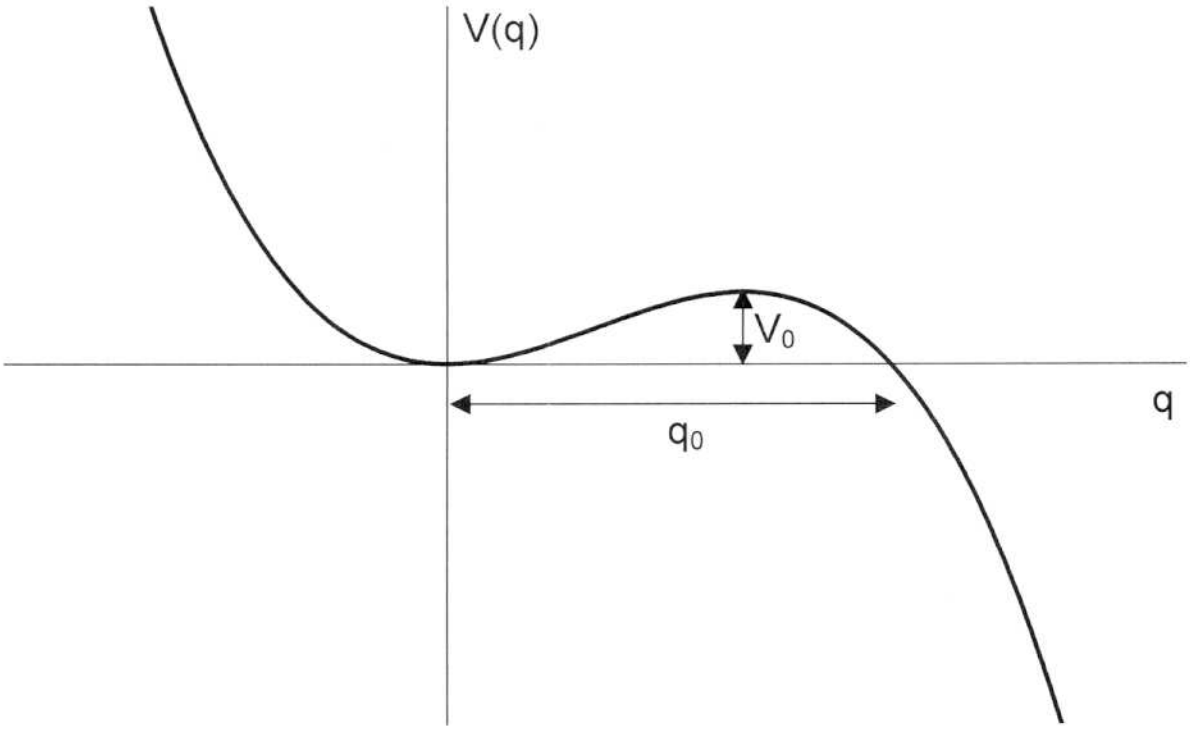

Figure 1: Potential of the form (38)

4.3 Limit of weak damping

For weak damping, we take the solution of the equation of motion for the problem without dissipation. As we already know (see also talk four about imaginary time) this is the bounce (instanton) solution in the inverted potential. The equation of motion for the bounce in the inverted potential is

$$M\ddot{q} - \frac{\partial V(q)}{\partial q} = 0 = M\ddot{q} - M\omega_0^2 q + \frac{3M\omega_0^2}{2q_0} q^2. \tag{41}$$

This differential equation has the solution

$$q_w(\tau) = \frac{q_0}{\cosh^2\left(\frac{\omega_0 \tau}{2}\right)}. \tag{42}$$

Because we are only interested in the effect of the dissipation that is caused by the bath, the tunneling rate is given by

$$\Gamma = \Gamma_w \exp\left(-\frac{S_{bath}}{\hbar}\right). \tag{43}$$

We need now the Fourier coefficients of $q_w(\tau)$ which are given by

$$\tilde{q}_w(\nu) = q_0 \frac{4\pi|\nu|}{\omega_0^2 \sinh\left(\frac{|\nu|\pi}{\omega_0}\right)}. \tag{44}$$

The resulting action for S_{bath} is now

$$S_{bath} = \frac{12\zeta(3)}{\pi^3}\eta q_0^2. \tag{45}$$

We get therefore the final result for the tunneling rate in the limit of weak damping

$$\Gamma = \Gamma_w \exp\left(-\frac{12\zeta(3)}{\pi^3\hbar}\eta q_0^2\right). \tag{46}$$

4.4 Limit of strong damping

In the limit of strong damping we neglect the kinetic term $\frac{M}{2}\dot{q}^2$ in the effective action S_{eff}. Therefore S_{eff} is given by

$$S_{eff} = \int_{-\infty}^{\infty} V(q)d\tau + \frac{\eta}{4\pi}\int_{-\infty}^{\infty} |\nu|\tilde{q}(\nu)\tilde{q}(-\nu)d\nu. \tag{47}$$

We request now that the Variation of S_{eff} must vanish an we get a new equation of motion in the limit of strong damping

$$M\omega_0^2\tilde{q}(\nu) - \frac{3M\omega_0^2}{2q_0 2\pi}\int_{-\infty}^{\infty} \tilde{q}(\nu-\gamma)\tilde{q}(\gamma)d\gamma + \eta|\nu|\tilde{q}(\nu) = 0. \tag{48}$$

With the ansatz $\tilde{q}(\nu) = Q\exp(\frac{\nu}{\nu_0})$ we get the following equation

$$M\omega_0^2 - \frac{3M\omega_0^2}{2q_0 2\pi}(\nu_0 + |\nu|)Q + \eta|\nu| = 0. \tag{49}$$

This must be valid for all frequencies ν! Especially for $\nu = 0$. We get now

$$Q = \frac{4\pi\eta q_0}{3M\omega_0^2} \tag{50}$$

and

$$\nu_0 = \frac{M\omega_0^2}{\eta}. \tag{51}$$

This results in the following expression for $\tilde{q}_s(\nu)$

$$\tilde{q}_s(\nu) = \frac{4\pi\eta q_0}{3M\omega_0^2}\exp\left(-\frac{|\nu|\eta}{M\omega_0^2}\right). \tag{52}$$

A Fourier-Back-Transformation gives us $q_s(\tau)$

$$q_s(\tau) = \frac{4}{3}q_0\frac{1}{1+(\nu_0\tau)^2}. \tag{53}$$

For the effective action S_{eff} results now

$$S_{eff} = \frac{2\pi}{9}\eta q_0^2. \tag{54}$$

The final result for the tunneling rate in the limit of strong damping is therefore

$$\Gamma = \Gamma_s \exp\left(-\frac{2\pi}{9\hbar}\eta q_0^2.\right) \tag{55}$$

4.5 Summary

It is somehow astonishing that in both cases, weak and strong damping, linear friction suppresses the tunneling rate Γ by a factor $\exp(-\alpha\frac{\eta q_0^2}{\hbar})$ where the prefactor α is in both cases of order unity. In the case of weak damping, I evaluated for $\alpha_w = \frac{12\zeta(3)}{\pi^3} = 0.46522$ and in the case of strong damping I got for $\alpha_s = \frac{2\pi}{9} = 0.69813$.

Figure 2 shows a plot of the coordinates $q_w(\tau)$ (42) and $q_s(\tau)$ (53) respectively for the following values: $\omega_0 = 1$, $q_0 = 1$, $M = 1$ and $\eta = 10$.

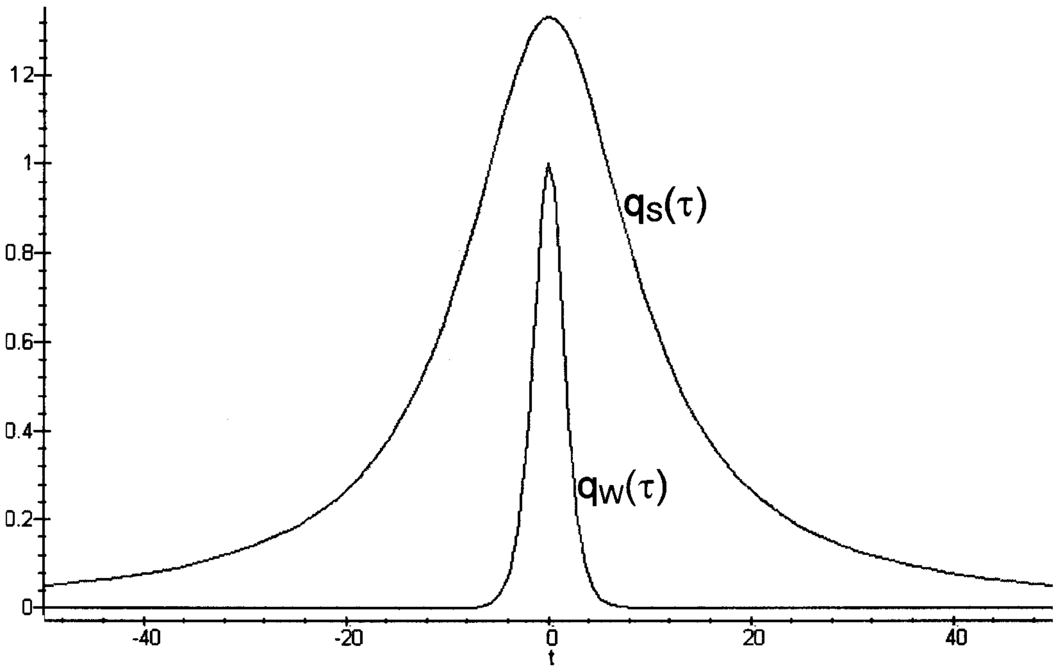

Figure 2: Plot of $q_w(\tau)$ and $q_s(\tau)$ with $\omega_0 = 1$, $q_0 = 1$, $M = 1$ and $\eta = 10$

References

[1] Caldeira A. O. and Leggett A. J., Quantum Tunelling in a Dissipative System, Annals of Physics 149, 374 - 456 (1983)

[2] Caldeira A. O. and Leggett A. J., Influence of Dissipation on Quantum Tunelling in Macroscopic Systems, Physical Review Letters Vol. 46, 211 - 214 (1981)

[3] Weiss U., Quantum Dissipative Systems, World Scientific (1993)

[4] Feynman R. P. and Hibbs A. R., Path integrals and Quantum Mechanics, McGraw-Hill (1965)

[5] Feynman R. P., Statistical Mechanics, Addison-Wesley (1972)