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Effect of transport coefficients on the time dependence of a density matrix

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Abstract. For Lindblad's master equation of open quantum systems with the Hamiltonian in a general quadratic form, the propagator of the density matrix is calculated analytically by using path-integral techniques. The time-dependent density matrix is applied to nuclear barrier penetration in heavy ion collisions with inverted oscillator and double-well potentials. The quantum mechanical decoherence of pairs of phase space histories in the propagator is studied and it is shown that the decoherence depends crucially on the transport coefficients.

(Some figures in this article are in colour only in the electronic version; see `www.iop.org`)

1. Introduction

In many problems of nuclear physics and quantum optics, where one deals with open quantum systems, the memory time of the environment is very short and a Markovian approximation is suitable. Disregarding the averaging over the intrinsic degrees of freedom, one can consider an open system starting from the general Markovian master equation for the reduced density matrix of the collective degrees of freedom as given by Lindblad [1],

$$\frac{\mathrm{d}\hat{\rho}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}[\hat{H}_0, \hat{\rho}] + \frac{1}{2\hbar}\sum_j \left(\left[\hat{V}_j\hat{\rho}, \hat{V}_j^+\right] + \left[\hat{V}_j, \hat{\rho}\hat{V}_j^+\right]\right) \tag{1}$$

where $\hat{H}_0$ is the Hamiltonian of the collective subsystem and $\hat{V}_j$ are operators acting in the Hilbert space of the subsystem. The terms in the sum of equation (1) are responsible for the friction and diffusion and supply the irreversibility of the dynamics of the open quantum system. Omitting these terms we obtain a standard form for the evolution equation of the density matrix for closed systems. This equation and similar equations were used, for example, in [2–12].

Path-integral methods are a conventional tool to describe open quantum systems [10–18]. Here, we use the results of Strunz [10] elaborated with path-integral techniques and derive analytical expressions for the time-dependent density matrix for a general Hamiltonian of quadratic form with an inverse oscillator potential which can be applied to the description of fission and fusion through potential barriers in nuclear physics. The decoherence of pairs of phase space trajectories will be studied in the semiclassical limit for different choices of the effects of the environment on the system. As was shown in [11], the initial Gaussian distribution remains to Gaussian in an oscillator potential. We extend this statement for any quadratic form

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of the Hamiltonian of the subsystem. By a direct numerical solution of equation (1) we consider the evolution of the density matrix in time in a double-well potential under various sets of transport coefficients. Such potentials are more useful and realistic for investigating nuclear fission problems than inverse oscillator potentials.

2. Path-integral propagator and decoherence

With the propagator $G(q, q', t; q_0, q_0', 0)$ of the density matrix one can find the density matrix $\langle q|\hat{\rho}(t)|q'\rangle$ (in a coordinate representation) at any time from the initial one $\langle q|\hat{\rho}(t = 0)|q'\rangle$:

$$\langle q|\hat{\rho}(t)|q'\rangle = \int \mathrm{d}q_0 \int \mathrm{d}q_0' \, G(q, q', t; q_0, q_0', 0)\langle q_0|\hat{\rho}(t = 0)|q_0'\rangle. \tag{2}$$

In the one-dimensional case an expression for the phase space path integral of the propagator corresponding to (1) was derived in [10] as

$$\begin{aligned} G(q, q', t; q_0, q_0', 0) &= \int_{(q_0,0)}^{(q,t)} D[\alpha] \int_{(q_0',0)}^{(q',t)} D[\alpha'] \exp\left(\frac{\mathrm{i}}{\hbar} S[\alpha; \alpha']\right) \\ S[\alpha; \alpha'] = S[q, p; q', p'] &= \int_0^t \mathrm{d}\tau \, \{\dot{q}(\tau)p(\tau) - H_{\mathrm{eff}}(q(\tau), p(\tau))\} \\ &\quad - \int_0^t \mathrm{d}\tau \, \{\dot{q}'(\tau)p'(\tau) - H_{\mathrm{eff}}^*(q'(\tau), p'(\tau))\} \\ &\quad - \mathrm{i}\sum_j \int_0^t \mathrm{d}\tau \, \{V_j(q(\tau), p(\tau))V_j^*(q'(\tau), p'(\tau))\} \end{aligned} \tag{3}$$

with phase space paths $[\alpha] = [q, p]$, where q and p are the position and momentum, respectively. The effective Hamiltonian is given by

$$H_{\mathrm{eff}} = H_0 - \tfrac{1}{2}\mathrm{i}\sum_j |V_j|^2.$$

Here, the quantities H_0, $|V_j|^2$, V_j and V_j^* are the Wigner transforms of the operators $\hat{H}_0$, $\hat{V}_j^+\hat{V}_j$, $\hat{V}_j$ and $\hat{V}_j^+$ in (1), respectively.

Choosing an inverse oscillator potential, we write the Hamiltonian of the collective subsystem in a more general quadratic form

$$\hat{H}_0 = \frac{1}{2m}\hat{p}^2 - \tfrac{1}{2}m\omega^2\hat{q}^2 + \tfrac{1}{2}\mu(\hat{p}\hat{q} + \hat{q}\,\hat{p}). \tag{4}$$

The environment operators are assumed to be linear,

$$\hat{V}_j = A_j\hat{p} + B_j\hat{q} \qquad \hat{V}_j^+ = A_j^*\hat{p} + B_j^*\hat{q} \qquad j = 1, 2. \tag{5}$$

In this paper A_j and B_j are arbitrary complex numbers. A specific choice of time-dependent quantities A_j and B_j allows one to obtain the equations with friction and diffusion coefficients depending on time and thus to extend the Lindblad equations to the strong-coupling case and non-Markovian processes [19, 20]. However, a detailed analysis of this possibility is necessary.

As shown in [10] for the similar case of an harmonic oscillator, the integrals in (3) over the momentum yield Gaussian integrals and can be evaluated. Then the propagator is reduced to path integrals in coordinate space [10]:

$$G(q,q',t;q_0,q_0',0)=\int_{q_0}^{q(t)}D[q]\int_{q_0'}^{q'(t)}D[q']\exp\left(\frac{\mathrm{i}}{\hbar}S[q;q']\right)$$
$$S[q;q']=S_{\mathrm{cl}}[q]-S_{\mathrm{cl}}[q']-\mathrm{i}\hbar\lambda t+\Phi[q,q']+\tfrac{1}{2}\mathrm{i}D[q,q']^2. \tag{6}$$

In equation (6) the classical action of the isolated system S_{cl}, the phase function $\Phi[q,q']$ and the square of the decoherence amplitude $D[q,q']$ can be expressed as

$$S_{\mathrm{cl}}=\int_0^t \mathrm{d}\tau\ \left\{\tfrac{1}{2}m\dot{q}^2+\tfrac{1}{2}m\omega^2q^2\right\} \tag{7}$$

$$\Phi[q,q']=m\lambda\int_0^t \mathrm{d}\tau\ (\dot{q}q'-q\dot{q}')+m\tfrac{1}{2}(\lambda_p-\lambda_q)$$
$$\times\int_0^t \mathrm{d}\tau\ (q'\dot{q}'-q\dot{q})-m\tfrac{1}{2}(\lambda_p\lambda_q)\int_0^t \mathrm{d}\tau\ (q^2-q'^2) \tag{8}$$

$$D[q,q']^2=\frac{2}{\hbar}\left\{(D_{pp}+m^2\lambda_p^2D_{qq}+2m\lambda_pD_{pq})\int_0^t \mathrm{d}\tau\ (q-q')^2-2m(D_{pq}+m\lambda_pD_{qq})\right.$$
$$\left.\times\int_0^t \mathrm{d}\tau\ (q-q')(\dot{q}-\dot{q}')+m^2D_{qq}\int_0^t \mathrm{d}\tau\ (\dot{q}-\dot{q}')^2\right\}. \tag{9}$$

The quantum mechanical diffusion coefficients are $D_{qq}=\frac{1}{2}\hbar\sum_j|A_j|^2$ for coordinate, $D_{pp}=\frac{1}{2}\hbar\sum_j|B_j|^2$ for momentum and $D_{qp}=-\frac{1}{2}\hbar\mathrm{Re}\sum_j A_j^*B_j$ for the mixed case. The frictional damping rate $\lambda=-\mathrm{Im}\sum_j A_j^*B_j$ and the diffusion coefficients must satisfy the constraint: $D_{pp}D_{qq}-D_{pq}^2\geqslant\lambda^2\hbar^2/4$ with $D_{qq}>0$, $D_{pp}>0$ which ensures the non-negativity of the density matrix at any time. The values $\lambda_p=\lambda+\mu$ and $\lambda_q=\lambda-\mu$ ($\lambda_p+\lambda_q=2\lambda$) are friction coefficients for coordinate and momentum, respectively. Both position and momentum undergo a direct damping and diffusion process in contrast to the classical case. If $D[q,q']$ increases with time for $q\neq q'$, then the propagator suppresses the non-diagonal components of the density matrix. Thus, the interference between different positions q and q' becomes weaker.

Since H_{eff} depends at most quadratically on p and q, the path integrals are Gaussian. In that case a semiclassical solution of the path integrals with the method of stationary phases leads to an exact analytical evaluation of the propagator. First, equations of motion along the path trajectories $q(\tau)$ and $q'(\tau)$ (complex trajectories) are calculated with the condition of stationary phase $\delta S[q,p;q',p']=0$ with S of equation (3). The following equations for $Q_1=q+q'$, $Q_2=q-q'$, $P_1=p+p'$ and $P_2=p-p'$ result, which are solved with the boundary conditions $\boldsymbol{q}=(q(0)=q_0,q(t),q'(0)=q_0',q'(t))$.

$$\begin{pmatrix}\dot{Q}_1\\ \dot{P}_1\\ \dot{Q}_2\\ \dot{P}_2\end{pmatrix}=\begin{pmatrix}-\lambda_q & m^{-1} & 4\mathrm{i}D_{pq}/\hbar & -4\mathrm{i}D_{qq}/\hbar\\ m\omega^2 & -\lambda_p & 4\mathrm{i}D_{pp}/\hbar & -4\mathrm{i}D_{pq}/\hbar\\ 0 & 0 & \lambda_p & m^{-1}\\ 0 & 0 & m\omega^2 & \lambda_q\end{pmatrix}\begin{pmatrix}Q_1\\ P_1\\ Q_2\\ P_2\end{pmatrix}. \tag{10}$$

Next, the solutions $q(\tau)$ and $q'(\tau)$ of equation (10) depending on the parameters q_0, $q(t)$, q_0' and $q'(t)$ are inserted into the action function $S[q;q']$ of equation (6) and integrated over τ.

The square of the decoherence amplitude is found as

$$D[q,q']^2 = \sinh^{-2}[\psi t](A_t(q_0-q_0')^2 - A_{-t}(q(t)-q'(t))^2 + B_t(q_0-q_0')(q(t)-q'(t))) \tag{11}$$

where $\psi = \sqrt{\omega^2 + (\lambda_q-\lambda_p)^2/4}$ and

$$\begin{aligned} A_t = {} & \frac{D_{pp} - m(m\omega^2 D_{qq} + (\lambda_q-\lambda_p)D_{pq})}{2\hbar\lambda} \\ & + \exp[2\lambda t]\psi^2 \frac{D_{pp} - m(-2D_{pq}\lambda_p + mD_{qq}(\omega^2 - 2\lambda\lambda_p))}{2\hbar\lambda(\lambda_p\lambda_q - \omega^2)} \\ & + \frac{\psi}{2\hbar(\omega^2-\lambda_p\lambda_q)} \sinh[2\psi t]\left\{D_{pp} + m(2D_{pq}\lambda_p + mD_{qq}(\omega^2 - \lambda_p(\lambda_q-\lambda_p))\right\} \\ & - \frac{1}{2\hbar(\omega^2-\lambda_p\lambda_q)} \cosh[2\psi t]\{-\lambda D_{pp} + m[(-2D_{pq} + m(\lambda_q-\lambda_p)D_{qq})\psi^2 \\ & -\lambda(-D_{pq}(\lambda_q-\lambda_p) + mD_{qq}(\omega^2 + 0.5(\lambda_q-\lambda_p)^2))]\} \end{aligned} \tag{12}$$

$$\begin{aligned} B_t = {} & \frac{\psi \sinh[(\psi-\lambda)t]}{\hbar\lambda(\omega^2-\lambda_p\lambda_q)}\left\{\psi[-D_{pp} + m(-2D_{pq}\lambda_p + mD_{qq}(\omega^2 - 2\lambda\lambda_p))]\right. \\ & \left. -\lambda[D_{pp} + m(2D_{pq}\lambda_p + mD_{qq}(\omega^2 - \lambda_p(\lambda_q-\lambda_p)))]\right\} \\ & - \frac{\psi \sinh[(\psi+\lambda)t]}{\hbar\lambda(\omega^2-\lambda_p\lambda_q)}\left\{\psi[-D_{pp} + m(-2D_{pq}\lambda_p + mD_{qq}(\omega^2 - 2\lambda\lambda_p))]\right. \\ & \left. +\lambda[D_{pp} + m(2D_{pq}\lambda_p + mD_{qq}(\omega^2 - \lambda_p(\lambda_q-\lambda_p)))]\right\}. \end{aligned}$$

Similar analytical expressions are obtained for the action $S_{\rm cl}$ and phase $\Phi[q,q']$. Then, the propagator (6) is finally evaluated as

$$G(q,q',t;q_0,q_0',0) = \frac{m\psi}{2\pi\hbar\sinh(\psi t)} \exp(\lambda t)\exp(\mathrm{i}S_R/\hbar)\exp(-D[q,q']^2/(2\hbar))$$

$$\begin{aligned} S_R &= S_{\rm cl}[q] - S_{\rm cl}[q'] + \Phi[q,q'] \\ &= \frac{m\omega}{2\sinh(\psi t)}\left\{\cosh(\psi t-\phi)[q_0^2 - q_0'^2] + \cosh(\psi t+\phi)[q^2 - q'^2]\right. \\ &\quad \left. -2\cosh(\phi)\cosh(\lambda t)[q_0 q - q_0' q'] - 2\cosh(\phi)\sinh(\lambda t)[q_0 q' - q_0' q]\right\} \end{aligned} \tag{13}$$

where $\sinh\phi = (\lambda_q-\lambda_p)/(2\omega)$. This propagator is correct for any quadratic Hamiltonian and is a generalization of the results of [10–12], where propagators were obtained for harmonic and inverted oscillators only. For the initial density matrix ($\bar q(0)$ and $\bar p(0)$ are mean values)

$$\begin{aligned} \langle q|\hat\rho(0)|q'\rangle &= (2\pi\sigma_{qq}(0))^{-1/2} \\ &\quad \times \exp\left[-\frac{1}{4\sigma_{qq}(0)}\{(q-\bar q(0))^2 + (q'-\bar q(0))^2\} - \frac{\mathrm{i}}{\hbar}\bar p(0)(q'-q)\right] \end{aligned} \tag{14}$$

the density matrix at time t is calculated with (2) and (13) as follows:

$$\begin{aligned} \langle q|\hat\rho(t)|q'\rangle = {} & \frac{1}{\sqrt{2\pi\sigma_{qq}(t)}} \exp\left[-\frac{1}{2\sigma_{qq}(t)}\left(\tfrac{1}{2}(q+q') - \bar q(t)\right)^2\right. \\ & -\frac{1}{2\hbar^2}\left(\sigma_{pp}(t) - \frac{\sigma_{pq}^2(t)}{\sigma_{qq}(t)}\right)(q-q')^2 \\ & \left. +\frac{\mathrm{i}\sigma_{pq}(t)}{\hbar\sigma_{qq}(t)}\left(\tfrac{1}{2}(q+q') - \bar q(t)\right)(q-q') + \frac{\mathrm{i}}{\hbar}\bar p(t)(q-q')\right] \end{aligned} \tag{15}$$

or in explicit form

$$\langle q|\hat{\rho}(t)|q'\rangle = \frac{m\psi}{2\sinh(\psi t)}\exp(\lambda t)\frac{1}{\sqrt{2\pi\sigma_{qq}(0)}}\frac{1}{\sqrt{4f_3f_6 - f_5^2}} \times \exp\left[-\frac{-f_2f_4f_5 + f_1f_5^2 + f_2^2f_6 + f_3(f_4^2 - 4f_1f_6)}{4f_3f_6 - f_5^2}\right] \tag{16}$$

where

$$\begin{aligned}
f_1 &= \sinh^{-2}[\psi t]\left(-\frac{\hbar\bar{q}^2(0)}{2\sigma_{qq}(0)}\sinh^2[\psi t] + \tfrac{1}{2}A_{-t}(q-q')^2 + \tfrac{1}{2}\mathrm{i}m\omega\cosh[\psi t+\phi]\sinh[\psi t](q^2 - q'^2)\right)\\
f_2 &= \sinh^{-2}[\psi t]\left(\frac{2\mathrm{i}\sigma_{qq}(0)\bar{p}(0) + \hbar\bar{q}(0)}{2\sigma_{qq}(0)}\sinh^2[\psi t] - \tfrac{1}{2}B_t(q-q') - \mathrm{i}m\omega\cosh[\phi]\sinh[\psi t](q\cosh[\lambda t] + q'\sinh[\lambda t])\right)\\
f_3 &= \sinh^{-2}[\psi t]\tfrac{1}{2}\left(\mathrm{i}m\omega\cosh[\psi t-\phi]\sinh[\psi t] - \frac{\hbar}{2\sigma_{qq}(0)}\sinh^2[\psi t] - A_t\right)\\
f_4 &= \sinh^{-2}[\psi t]\left(\frac{-2\mathrm{i}\sigma_{qq}(0)\bar{p}(0) + \hbar\bar{q}(0)}{2\sigma_{qq}(0)}\sinh^2[\psi t] + \tfrac{1}{2}B_t(q-q') + \mathrm{i}m\omega\cosh[\phi]\sinh[\psi t](q\sinh[\lambda t] + q'\cosh[\lambda t])\right)\\
f_5 &= \sinh^{-2}[\psi t]A_t\\
f_6 &= -\sinh^{-2}[\psi t]\tfrac{1}{2}\left(\mathrm{i}m\omega\cosh[\psi t-\phi]\sinh[\psi t] + \frac{\hbar}{2\sigma_{qq}(0)}\sinh^2[\psi t] + A_t\right).
\end{aligned} \tag{17}$$

Here, $\bar{q}(t)$ and $\bar{p}(t)$ are the mean values of $\hat{q}$ and $\hat{p}$, respectively, and $\sigma_{qq}(t)$, $\sigma_{pp}(t)$ and $\sigma_{pq}(t)$ the corresponding variances [8, 12]. Explicit expressions for these mean values and variances are given in [12]. The diagonal part of the density matrix (15) yields a Gaussian distribution at time t

$$\rho(q,t) = \langle q|\hat{\rho}(t)|q\rangle = (2\pi\sigma_{qq}(t))^{-1/2}\exp\left[-\frac{1}{2\sigma_{qq}(t)}(q-\bar{q}(t))^2\right] \tag{18}$$

where

$$\begin{aligned}
\bar{q}(t) &= \mathrm{e}^{-\lambda t}\left(\bar{q}(0)\left[\cosh(\psi t) + \frac{\lambda_p - \lambda_q}{\psi}\sinh(\psi t)\right] + \frac{1}{m\psi}\bar{p}(0)\sinh(\psi t)\right)\\
\sigma_{qq}(t) &= \frac{1}{2m^2\lambda(\omega^2 - \lambda_p\lambda_q)}\left[m^2(\omega^2 - 2\lambda_p\lambda)D_{qq} - D_{pp} - 2m\lambda_pD_{pq}\right]\\
&\quad + \mathrm{e}^{-2\lambda t}\left[\frac{2C_1}{m(\lambda_q - \lambda_p)} - \frac{1}{2m\omega^2}[(\lambda_q - \lambda_p)C_2 + 2C_3\psi]\cosh(2\psi t)\right.\\
&\quad \left. + \frac{1}{2m\omega^2}[(\lambda_q - \lambda_p)C_3 + 2C_2\psi]\sinh(2\psi t)\right]
\end{aligned} \tag{19}$$

with the following notation:

$$C_1 = \frac{m\omega^2(\lambda_q - \lambda_p)}{4\psi^2}\left[\sigma_{qq}(0) - \frac{1}{m^2\omega^2}\sigma_{pp}(0) + \frac{\lambda_q - \lambda_p}{m\omega^2}\sigma_{pq}(0) - \frac{1}{\lambda}D_{qq} + \frac{1}{m^2\omega^2\lambda}D_{pp} - \frac{(\lambda_q - \lambda_p)}{m\omega^2\lambda}D_{pq}\right]$$

$$C_2 = \frac{1}{4\psi^2}\left[\frac{\lambda_q - \lambda_p}{m}(\sigma_{pp}(0) - m^2\omega^2\sigma_{qq}(0)) + 4\omega^2\sigma_{pq}(0) + \frac{1}{\omega^2 - \lambda_p\lambda_q} \times\left(\frac{2\omega^2 - \lambda_p\lambda_q}{m}[D_{pp} + m^2\omega^2 D_{qq}] + \frac{\lambda_q^2}{m}D_{pp} + \lambda_p^2 m\omega^2 D_{qq} + 4\lambda\omega^2 D_{pq}\right)\right]$$

$$C_3 = -\frac{1}{2m\psi}\left[m^2\omega^2\sigma_{qq}(0) + \sigma_{pp}(0) + \frac{1}{\omega^2 - \lambda_p\lambda_q}(\lambda_q D_{pp} + 2m\omega^2 D_{pq} + m^2\omega^2\lambda_p D_{qq})\right].$$

For the values $\lambda_p = \lambda_q = 0$, $D_{pp} = D_{qq} = D_{pq} = 0$, $\sigma_{pp}(0) = \hbar^2/(4\sigma_{qq}(0))$ and $\sigma_{qp}(0) = 0$, we obtain the same result with these expressions as in [21, 22]. For $\lambda_q = 0$, $D_{pp} = D_{qq} = D_{pq} = 0$ and $\sigma_{pp}(0) = \hbar^2/(4\sigma_{qq}(0))$ and $\sigma_{qp}(0) = 0$, our results coincide in the underdamped limit with the results of [23], where tunnelling was studied with the inverted Caldirola–Kanai Hamiltonian. For $\lambda_q = 0$ and $D_{qq} = 0$, our result can be transformed to that of [24].

3. Calculated results

The influence of the friction and diffusion coefficients on the tunnelling was considered in [11, 12, 25]. Here, we study the time dependence of the decohering amplitude and the non-diagonal part of the density matrix for different sets of the transport coefficients. In order to demonstrate the effect of the diffusion and friction coefficients of the coordinate, D_{qq} and λ_q, on the change of the distance between phase space trajectories, we take a simple expression for the diffusion coefficients:

$$\begin{aligned} D_{pp} &= (1+\kappa)\lambda m\hbar\omega_{\text{eff}}\coth(\hbar\omega_{\text{eff}}/(2kT))/2 \\ D_{qq} &= (1-\kappa)\hbar\lambda\coth(\hbar\omega_{\text{eff}}/(2kT))/(2m\omega_{\text{eff}}) \qquad D_{pq} = 0 \end{aligned} \tag{20}$$

where κ is an adjustable parameter. The parameter ω_{eff} could be found from a microscopic consideration of the open system. In order to ensure the non-negativity of the density matrix at any time, the inequality $(1-\kappa^2)\coth^2(\hbar\omega_{\text{eff}}/(2kT)) \geqslant 1$ must be true. With $\kappa = 1$ and $D_{qq} = D_{pq} = 0$ we obtain the 'classic' set of diffusion coefficients which does not preserve the non-negativity of the density matrix at all times [5, 7, 8]. The coupling with the environment, which leads to $\lambda_q \neq 0$, renormalizes the potential barrier and increases the penetrability through the barrier [11, 12]. The penetrability is also very sensitive to the value of D_{qq} [25]. It can be shown straightforwardly that the dissipation rate increases with λ_p and D_{qq}, but decreases with increasing λ_q and D_{pp} [11, 12, 25]. In collisions of heavy ions, surface vibrations and nucleon exchange between the nuclei are responsible for the renormalization of the Coulomb barrier and for the dissipation of the kinetic energy of relative motion [26]. With the effects of the renormalization of potential and the dissipation of the kinetic energy one can obtain $\lambda_p = (1+\kappa)\lambda$ and $\lambda_q = (1-\kappa)\lambda$ (or κ and λ) by fitting the experimental data on the sub-barrier collisions.

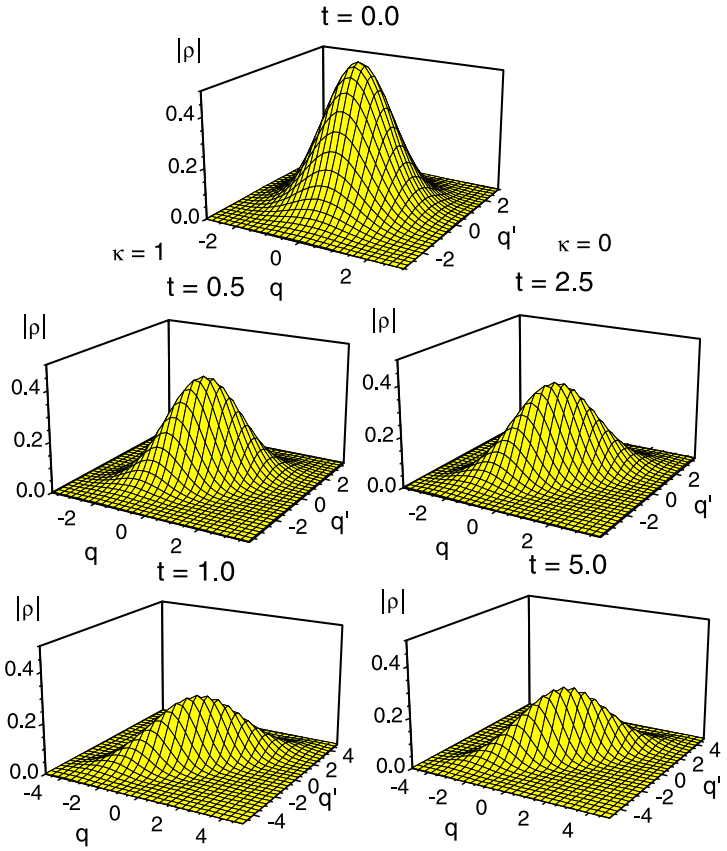

Figure 1. Calculated time dependence of the modulus of the density matrix $|\rho(q, q')|$ in the inverted oscillator potential, reproducing the Coulomb barrier in a ^{76}Ge + ^{170}Er collision, for $\kappa = 1$ (left-hand side) and 0 (right-hand side) in (20), $\lambda_p = (1 + \kappa)\lambda$ and $\lambda_q = (1 - \kappa)\lambda$. The parameters are $\bar{q}(0) = 0$, $\bar{p}(0) = 0$, $\hbar\omega = \hbar\omega_{\rm eff} = 2.0$ MeV, $\sigma_{qq}(0) = 0.7$ fm^2, $m = 53m_0$ (m_0 is the mass of nucleon), $\hbar\lambda = 2$ MeV and $T = 0$ MeV. The initial density matrix is presented at the top. The time is given in units of 6.582×10^{-22} s.

As an example we consider the relative motion of the two nuclei ^{76}Ge and ^{170}Er at the Coulomb barrier which is approximated by the inverted oscillator. Figure 1 shows the time dependence of the density matrix $\rho(q, q')$ for $\kappa = 0$ and 1 in (20), $\lambda_p = (1 + \kappa)\lambda$ and $\lambda_q = (1 - \kappa)\lambda$. Since with $\kappa = 0$ and 1 the density matrix is practically diagonal after a short time interval of about 5×10^{-22} s, semiclassical methods work quite well in heavy ion collisions. The density matrix becomes diagonal faster in the case $\kappa = 1$ than for $\kappa = 0$. The time behaviour of the non-diagonal components of the density matrix is evidently correlated with the time dependence of the decoherence D which is shown in figure 2. After a decrease of D during a short time interval the decoherence increases, indicating a reduction of the interference between different states (trajectories). The decoherence increases slowest for $\kappa = 0$ and more rapidly for higher temperatures. Further, figure 2 shows that the decoherence amplitude decreases with increasing λ_q. This has the consequence that the penetrability through the barrier increases due to a larger interference between different states (trajectories) [11, 12].

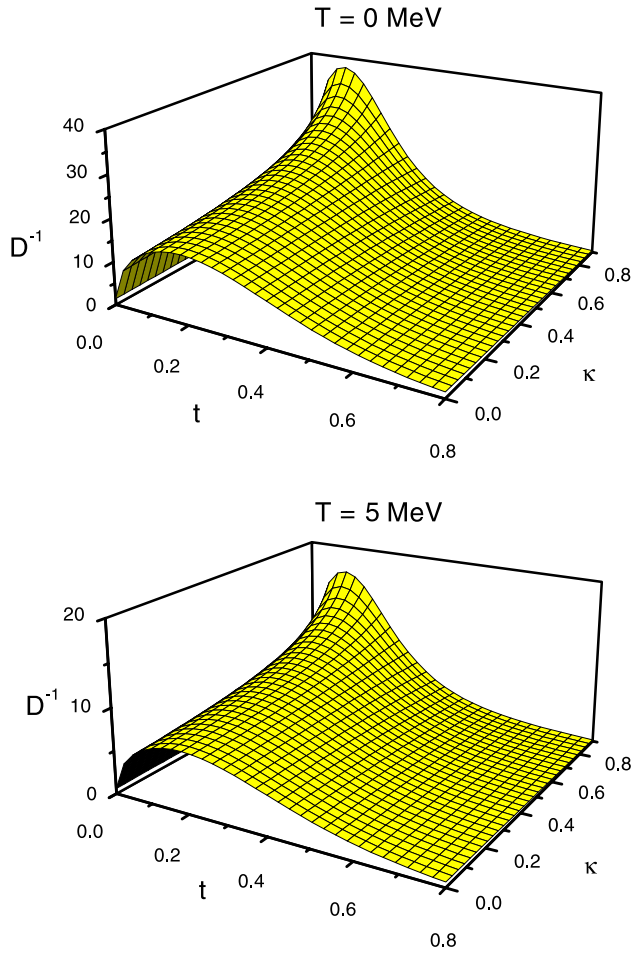

Figure 2. Dependence of the inverse decoherence D^{-1} (in units of $\hbar^{-1/2}$) on time and κ, used in the definitions of D_{pp} and D_{qq} in (20), $\lambda_p = (1+\kappa)\lambda$ and $\lambda_q = (1-\kappa)\lambda$ at $T = 0$ and 5 MeV. The initial values are $q(0) - q'(0) = 0.01$ fm and $p(0) = p'(0) = 0$. The other parameters are the same as in figure 1. The time is given in units of 6.582×10^{-22} s.

In order to show the role of D_{qq} in distorting the coherence between states, we compare the time dependence of D in figure 3 for $\kappa = 0$, 0.5 and 1 in (20) with $\lambda_p = 2\lambda$ and $\lambda_q = 0$. For times $t > 5 \times 10^{-22}$ s, which are of interest for physical observables, the decoherence increases quickly for $D_{qq} = 0$ ($\kappa = 1$). With $D_{qq} \neq 0$ ($\kappa < 1$) the interference between different states survives a longer time.

Equation (1) can also be solved by rewriting it in a system of equations for the matrix elements of $\hat{\rho}$ in some basis [25]. These equations can be treated numerically for arbitrary potentials. With complete orthogonal set of basis functions $|n\rangle$ we obtain from equation (1) the system of equations for the matrix elements of density matrix $\hat{\rho}$:

$$\frac{\mathrm{d}\rho_{mn}}{\mathrm{d}t} = \sum_l \left\{ -\frac{\mathrm{i}}{\hbar}(\langle m|\hat{H}_0|l\rangle\rho_{ln} - \langle l|\hat{H}_0|n\rangle\rho_{ml}) + \rho_{ml}B_{ln} + \rho_{ln}C_{ml} + \sum_{l'}\rho_{ll'}A_{mll'n} \right\} \tag{21}$$

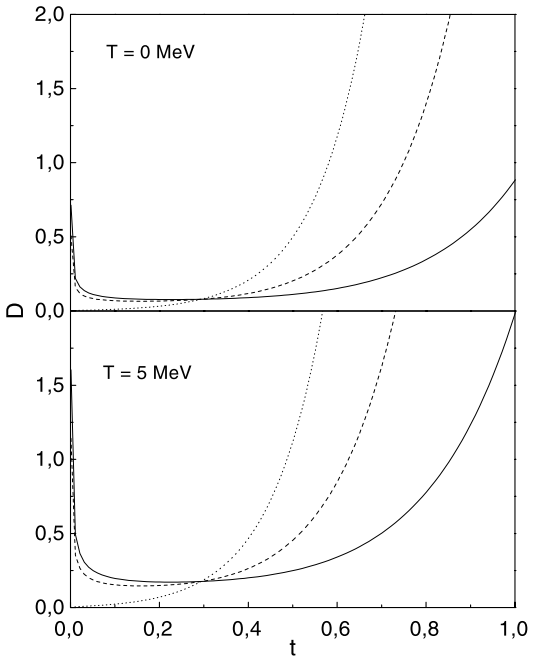

Figure 3. Time dependence of the decoherence D (in units of $\hbar^{1/2}$) for $\lambda_p = 2\lambda$, $\lambda_q = 0$, $T = 0$ and 5 MeV, and $\kappa = 0$ (full curves), 0.5 (broken curves) and 1 (dotted curves). The initial values are $q(0) - q'(0) = 0.01$ fm and $p(0) = p'(0) = 0$. The other parameters are the same as in figure 1. The time is given in units of 6.582×10^{-22} s.

where the coefficients are defined as follows:

$$B_{ln} = \sum_{l'}(D_1^- \Delta_{ll'}^+ \Delta_{l'n}^+ + D_1^{+*} \Delta_{ll'}^- \Delta_{l'n}^- - D_2^- \Delta_{ll'}^- \Delta_{l'n}^+ - D_2^+ \Delta_{ll'}^+ \Delta_{l'n}^-)$$
$$C_{ml} = \sum_{l'}(D_1^+ \Delta_{l'l}^+ \Delta_{ml'}^+ + D_1^{+*} \Delta_{l'l}^- \Delta_{ml'}^- - D_2^+ \Delta_{l'l}^- \Delta_{ml'}^+ - D_2^- \Delta_{l'l}^+ \Delta_{ml'}^-) \tag{22}$$
$$A_{mll'n} = -(D_1^- + D_1^+)\Delta_{ml}^+ \Delta_{l'n}^+ - (D_1^{-*} + D_1^{+*})\Delta_{ml}^- \Delta_{l'n}^- + 2D_2^- \Delta_{ml}^+ \Delta_{l'n}^- + 2D_2^+ \Delta_{ml}^- \Delta_{l'n}^+.$$

Here, $\Delta_{mn}^- = \langle m|a|n\rangle$ and $\Delta_{mn}^+ = \langle m|a^+|n\rangle$ are the matrix elements of the creation a^+ and annihilation a operators, and $D_1^\pm = 0.5(D_1 \pm 0.5(\lambda_p - \lambda_q))$, $D_2^\pm = 0.5(D_2 \pm 0.5(\lambda_p + \lambda_q))$. For the basis related to the eigenfunctions of harmonic oscillator with the frequency ω, $D_1 = (m\omega D_{qq} - D_{pp}/m\omega + 2\mathrm{i}D_{pq})/\hbar$ and $D_2 = (m\omega D_{qq} + D_{pp}/m\omega)/\hbar$. It was shown in [20] that in the weak-coupling limit the time coarse graining leads to a generalized master equation for strong damping of Lindblad form (21) where $(m\omega)^2 D_{qq} = D_{pp}$, $D_{pq} = 0$ and $\lambda_p = \lambda_q$ (or $\mu = 0$).

Either the eigenfunctions of the harmonic oscillator or the eigenfunctions of the potential $U(\hat{q})$ are convenient as a complete orthogonal set of basis functions $|n\rangle$. The initial density matrix is calculated as $\rho_{mn}(t = 0) = \langle m|\Psi\rangle\langle\Psi|n\rangle$ where the initial state of the open system is determined by the wavefunction $\Psi(q)$. Then we can solve equation (21) and find the time dependence of the average value $F = \mathrm{Tr}(\hat{\rho}(t)\hat{F})$ of any operator $\hat{F}$ and of the diagonal and non-diagonal elements of the density matrix.

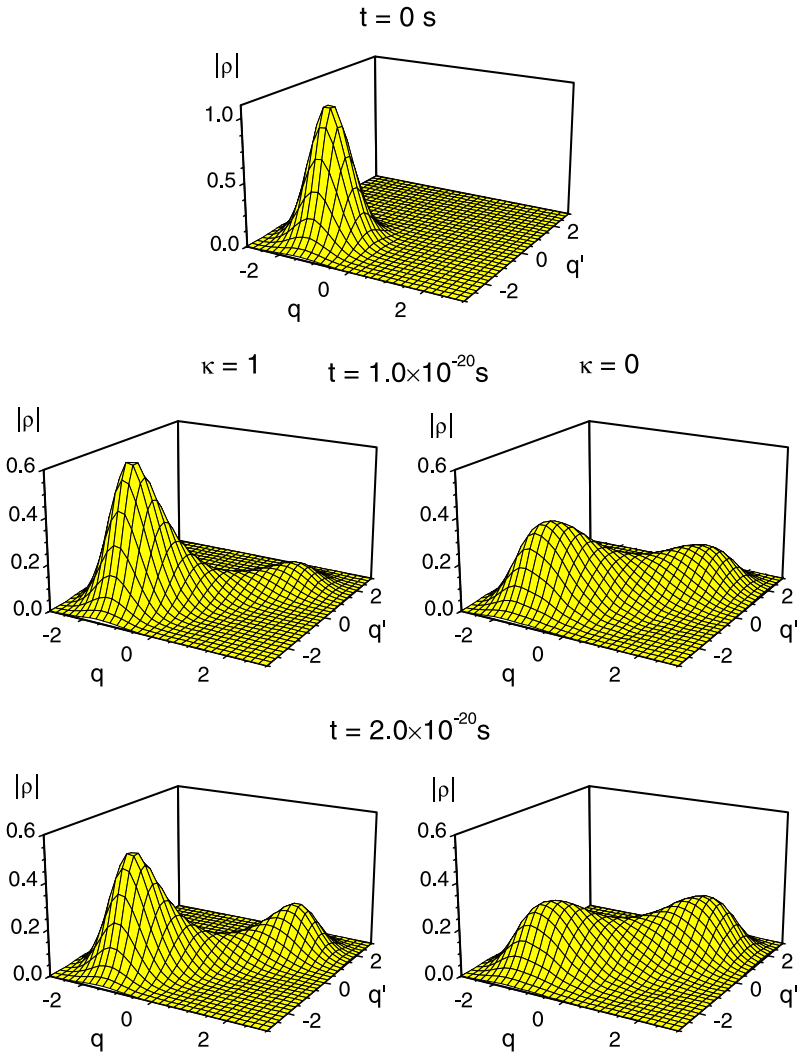

Figure 4. Calculated time dependence of the modulus of the density matrix $|\rho(q, q')|$ in a double-well potential (see text) for $\kappa = 1$ (left-hand side) and 0 (right-hand side) in (20) at $T = 0$ MeV and $\lambda_p = 2\lambda$, $\lambda_q = 0$. The initial Gaussian distribution (top part) with $\sigma_{qq}(0) = 0.14$ fm^2, $\bar{p}(0) = 0$ starts with $\bar{q} = -1.5$ fm in the left-hand well. The further parameters are $\hbar\omega_{\rm eff} = 2.0$ MeV, $\hbar\lambda = 2$ MeV and $m = 53m_0$. The time is indicated.

Let us consider a system with mass $m = 53m_0$ (m_0 is the mass of a nucleon) in a symmetric double-well potential

$$U(q) = -\frac{8\Delta U}{L^2}q^2 + \frac{16\Delta U}{L^4}q^4 \tag{23}$$

with $\Delta U = 1.5$ MeV, $L = 3$ fm and start with an initial Gaussian state for the density matrix with a variance $\sigma_{qq}(0) = 0.14$ fm^2 in the left-hand well at $\bar{q}(0) = -1.5$ fm. The calculated time dependence of $\rho(q, q')$ is presented in figure 4 for $\kappa = 1$ and $\kappa = 0$ in (20) with $\lambda_p = 2\lambda$ and $\lambda_q = 0$. The transition of the system to the right-hand well mainly occurs along the direction $q = q'$. At the same time the non-diagonal part of the density matrix is larger with

$D_{qq} \neq 0$ than with $D_{qq} = 0$. For $D_{qq} \neq 0$, the distribution in the right-hand well is wider and the transition rate between the two wells is larger [25, 27].

4. Summary

Using the path-integral method for master equations of general Lindblad form for Markovian open quantum systems, we obtained an analytical expression for the propagator of the density matrix of a general quadratic Hamiltonian coupled linearly (in coordinate and momentum) with the environment. The time-dependent diagonal and non-diagonal elements of the density matrix in a coordinate representation were calculated as a function of different sets of transport coefficients for the inverted oscillator and double-well potentials. At times of interest for heavy ion collisions at the Coulomb barrier, the density matrix is practically diagonal which justifies the use of semiclassical methods. The time behaviour of the decoherence crucially depends on the choice of the friction and diffusion coefficients. With diffusion coefficients preserving the non-negativity of the density matrix at any time, the decoherence increases slower than in the classical case with $D_{qq} = 0$. Therefore, the penetrability of a barrier is larger in the case of $D_{qq} \neq 0$ due to a stronger coherence between different states.

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