COORDINATE-DEPENDENT DIFFUSION COEFFICIENTS AND DECAY RATE FROM POTENTIAL WELL

Outline

- The master-equation with constant diffusion coefficients
- Coordinate-dependent diffusion coefficients
- Decay rate
- Illustrative calculations
- Summary

Theoretical approach

The master-equation with constant diffusion coefficients describes the dissipative quantum dynamics approximately for anharmonic systems. However, we can expect that the influence of higher order fluctuations on the evolution of systems is large. For more complicated renormalized potential, the potential $\tilde{U}(q)$ near q can be approximated by an local harmonic normal or inverse oscillator potential. Then, one can use the analytical solution for the oscillator.

Model

The Hamiltonian H of the total system:

$$H = H_c + H_b + H_{cb}$$

The reduced density matrix $\hat{\rho}$ for the collective subsystem obeys the following equation ($\hbar$=1)

$$\begin{aligned}\frac{d}{dt}\hat{\rho} &= -i[\tilde{\hat{H}}_c, \hat{\rho}] - \frac{i}{2}\lambda_p[\hat{q}, \{\hat{p}, \hat{\rho}\}] \\ &\quad -D_{pp}[\hat{q}, [\hat{q}, \hat{\rho}]] + D_{pq}[\hat{p}, [\hat{q}, \hat{\rho}]] + [\hat{q}, [\hat{p}, \hat{\rho}]]D_{pq}\end{aligned}$$

where

$\tilde{\hat{H}}_c = \frac{1}{2\mu}\hat{p}^2 + \tilde{U}(\hat{q})$ is renormalized collective Hamiltonian.

Coordinate representation

The master equation for $\hat{\rho}$ in coordinate representation $(\rho(t,x,y) =< x|\hat{\rho}|y >)$

$$\begin{aligned}
\frac{d}{dt}\rho(t,x,y) &= \hat{L}(x,y)\rho(t,x,y), \\
\hat{L}(x,y) &= -i[\frac{1}{2\mu}(\partial_{x,x} - \partial_{y,y}) + (\tilde{U}(x) - \tilde{U}(y))] \\
&- \frac{1}{2}\lambda_p(x-y)(\partial_x - \partial_y) - D_{pp}(x-y)^2 \\
&- i[D_{pq}(\partial_x + \partial_y)(x-y) + (x-y)(\partial_x + \partial_y)]
\end{aligned}$$

Transformation

Making transformation: $x = q + \frac{z}{2}, \quad y = q - \frac{z}{2}$

and expanding the potential in z:

$$\tilde{U}(q + \frac{z}{2}) - \tilde{U}(q - \frac{z}{2}) \approx z\tilde{U}'(q) + \frac{1}{24} z^3 \tilde{U}'''(q)$$

we obtain the transformed equation for $\rho(t, q, z)$:

$$\begin{aligned} \frac{d}{dt}\rho(t, q, z) &= \hat{L}(q, z)\rho(t, q, z), \\ \hat{L}(q, z) &= i\frac{1}{\mu}\partial_{q,z} - iz\tilde{U}'(q) - i\frac{1}{24} z^3 \tilde{U}'''(q) \\ &\quad -\lambda_p z \partial_z - D_{pp} z^2 - i(D_{pq} z \partial_q + \partial_q z D_{pq}). \end{aligned}$$

Solution of equation for density matrix

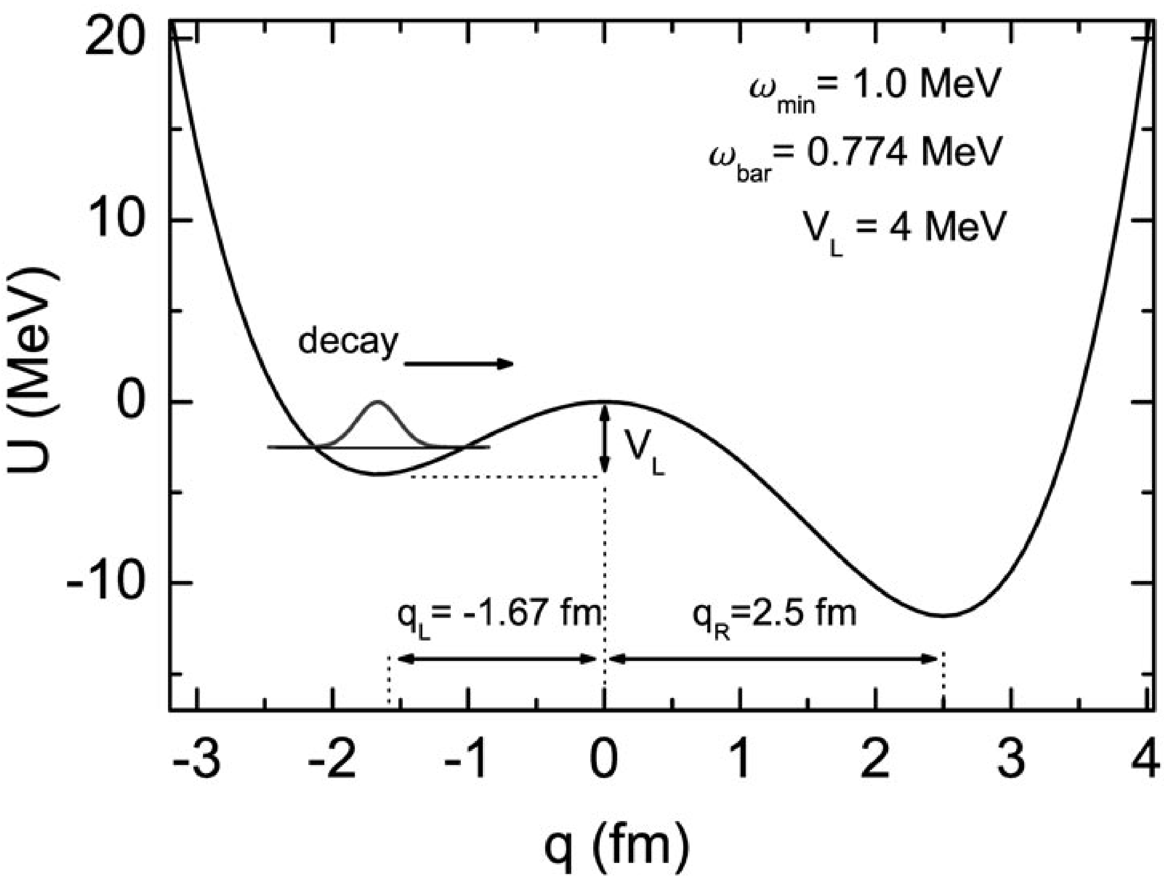
Equation can be solved by using a oscillator basis and expensions

$$
\begin{aligned}
\rho(t,q,z) &= \sum_{k=0}^{n} f_k(t,q) B_k(\sigma,z) \\
B_k(\sigma,z) &= \frac{i^k}{k!}(\frac{k}{2})! e^{-\frac{z^2}{8\sigma^2}} H_k(\frac{z}{2\sigma}).
\end{aligned}
$$

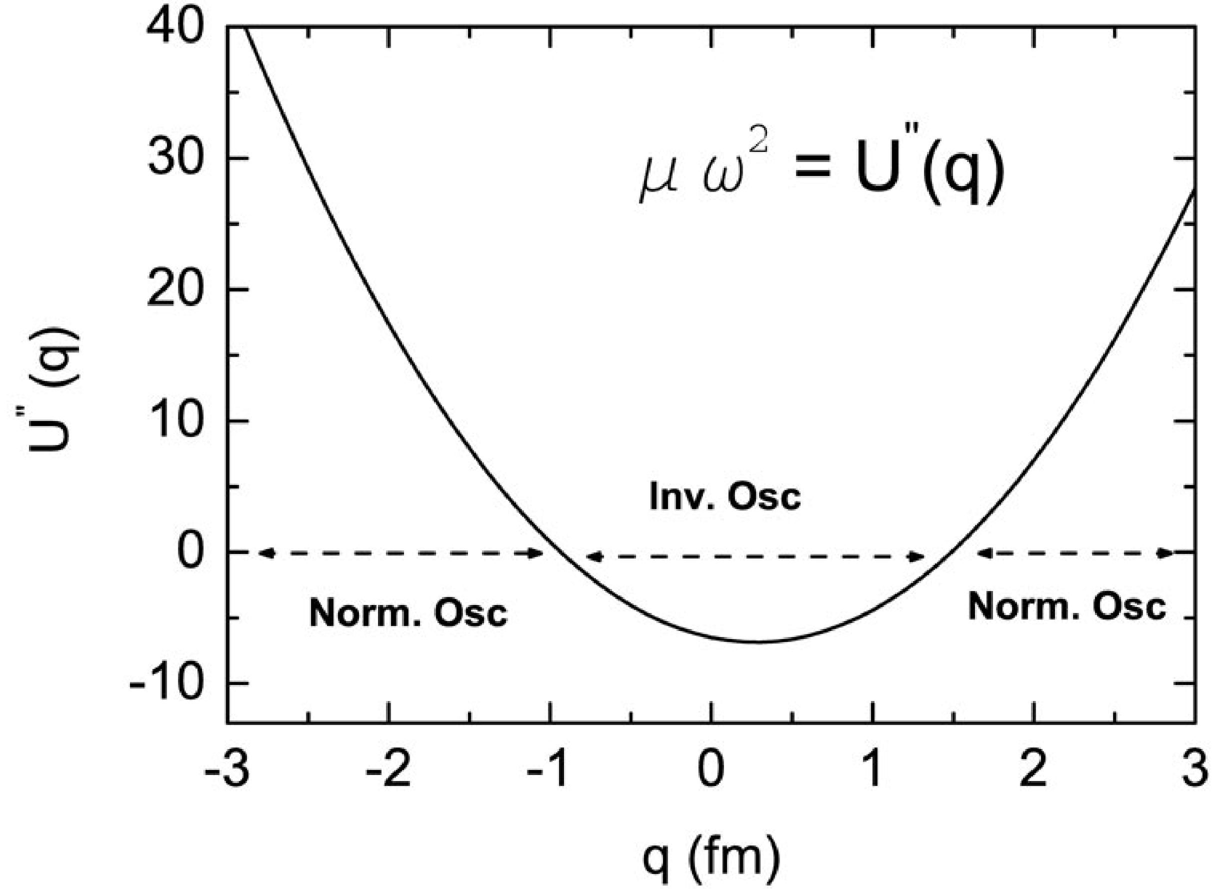
$B_k(\sigma,0)$=1 if k=0,2,4,... and $B_k(\sigma,0)$=0 if k=1,3,5,....

Asymmetric bistable potential

$$\tilde{U}(q) = -\frac{6q_R V_L}{q_L^2(2q_R - q_L)}q^2 - \frac{4(q_L + q_R)V_L}{q_L^3(q_L - 2q_R)}q^3 - \frac{3V_L}{q_L^3(2q_R - q_L)}q^4$$



The second derivative of Potential and Stiffness



Asymptotic expressions of time-dependent microscopic diffusion coefficients

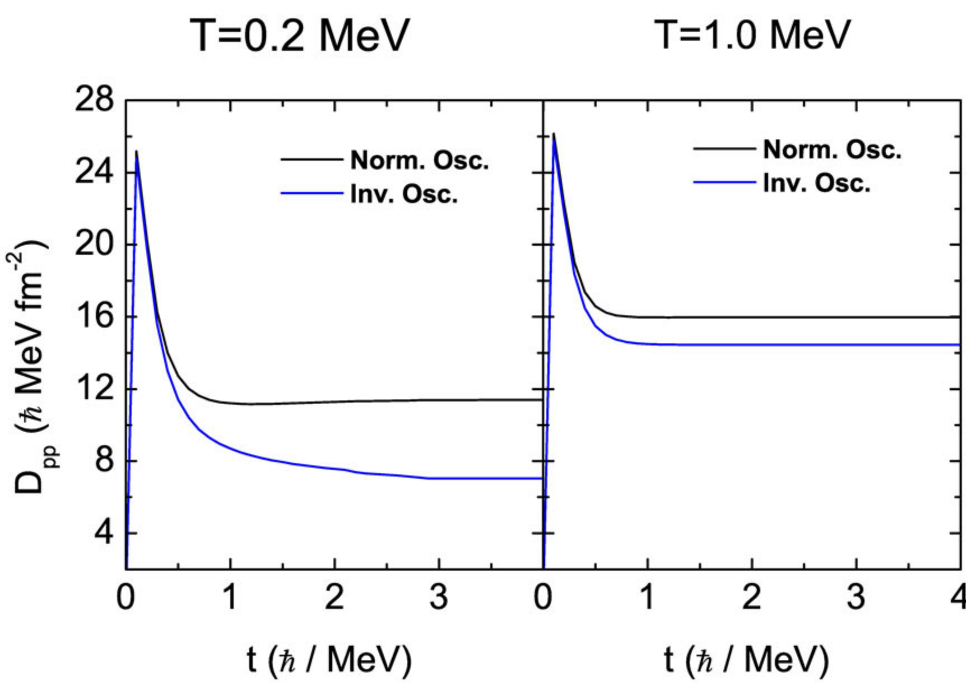
$$
\begin{aligned}
D_{pp} &= \frac{T\mu\gamma^2\lambda_p}{\gamma(\gamma+\lambda_p) \pm \tilde{\omega}^2} \\
&\quad \left(1 + 2\sum_{k=1}^{\infty} \frac{\nu_k\gamma\lambda_p \pm \tilde{\omega}^2(\gamma+\nu_k)}{(\gamma+\nu_k)(\nu_k(\nu_k+\lambda_p) \pm \tilde{\omega}^2)}\right), \\
D_{qp} &= \frac{T\gamma\lambda_p}{2(\gamma(\gamma+\lambda_p) \pm \tilde{\omega}^2)} \\
&\quad \left(1 + 2\gamma\sum_{k=1}^{\infty} \frac{-\nu_k\gamma \pm \tilde{\omega}^2}{(\gamma+\nu_k)(\nu_k(\nu_k+\lambda_p) \pm \tilde{\omega}^2)}\right).
\end{aligned}
$$

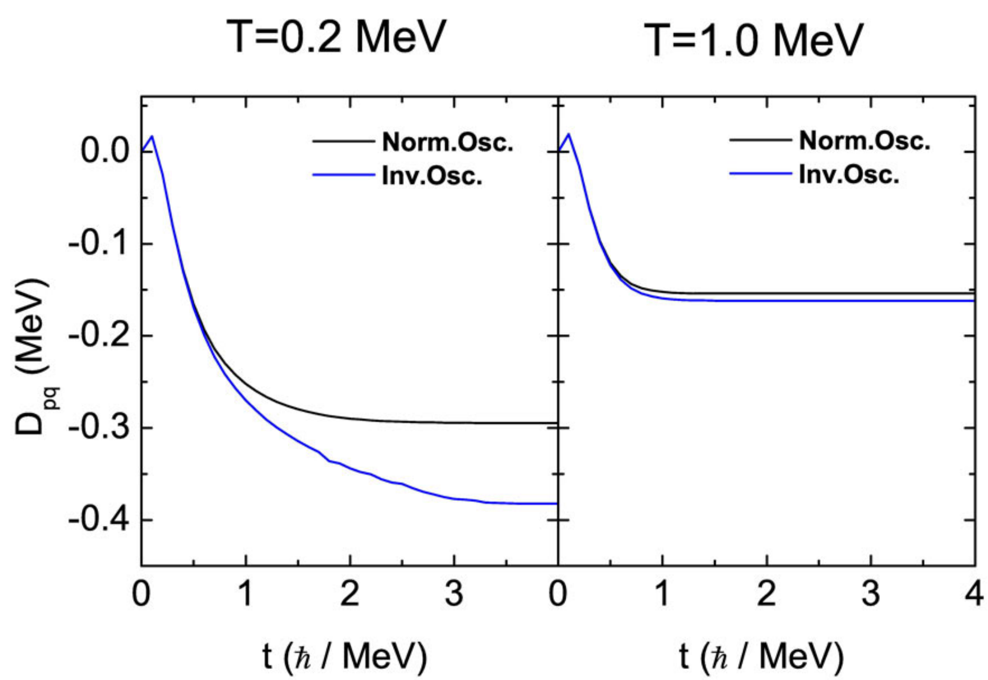
where $\nu_k = 2\pi T k$.

Time-dependent diffusion coefficients

We set parameters:

$$\mu = 450 m_0,\ \hbar\lambda_p(\infty) = 1 \text{ MeV},\ \hbar\omega(\infty) = 1 \text{ MeV}.$$

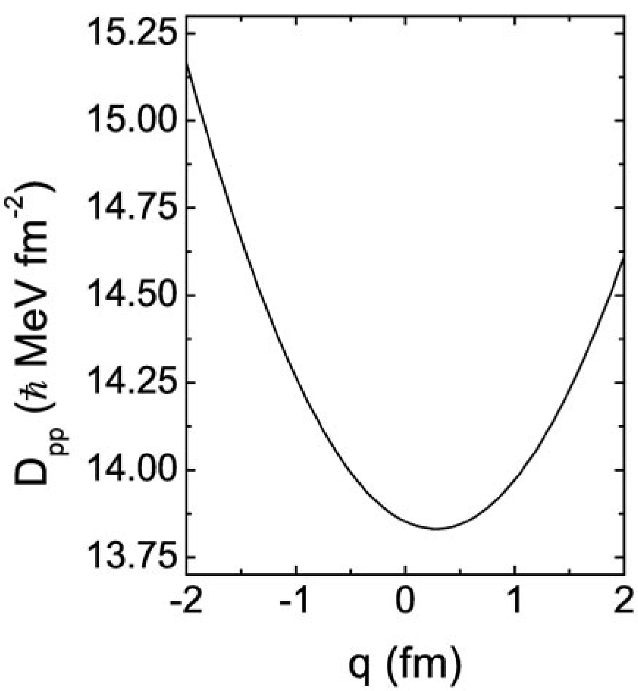


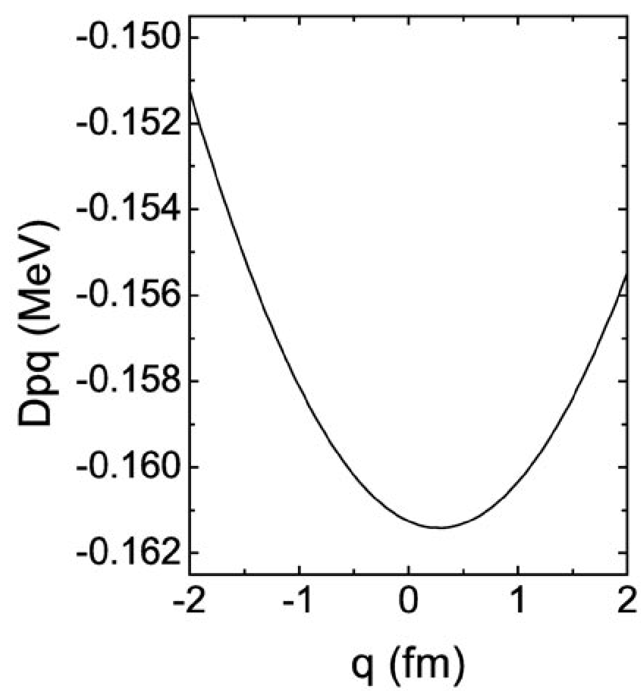


Coordinate-dependent diffusion coefficients

We set parameters:

$\mu = 450m_0$, $\hbar\lambda_p(\infty) = 1$ MeV, $T = 1$MeV.





Decay rate

Probability of penetrability

$$P(t) = \int_{q_b}^{\infty} \rho(t,q,0) = \sum_{k=0,2,4,\ldots} \int_{q_b}^{\infty} f_k(t,q)dq$$

Dacey rate

$$\begin{aligned}\Lambda(t) &= \frac{1}{1-P(t)}\frac{dP(t)}{dt} \\ &= \frac{1}{1-P(t)}\frac{1}{M}\sum_k f_k(t,q_b)(-i\partial_z)B_k(\sigma,z=0)\end{aligned}$$

Decay rate with different sets of diffusion coefficients

I — microscopical diffusion coefficients: $D_{pp}(q)$ and $D_{pq}(q)$

II — "Classical" diffusion coefficient: $D^{cl}_{pp}(q)$

$(D^{cl}_{pp} = \frac{1}{2}\mu\lambda_p\omega\coth[\frac{\omega}{2T}])$

III — microscopical diffusion coefficients:

$D_{pp}(q = q_w)$=$const$ and $D_{pq}(q = q_w)$=$const$

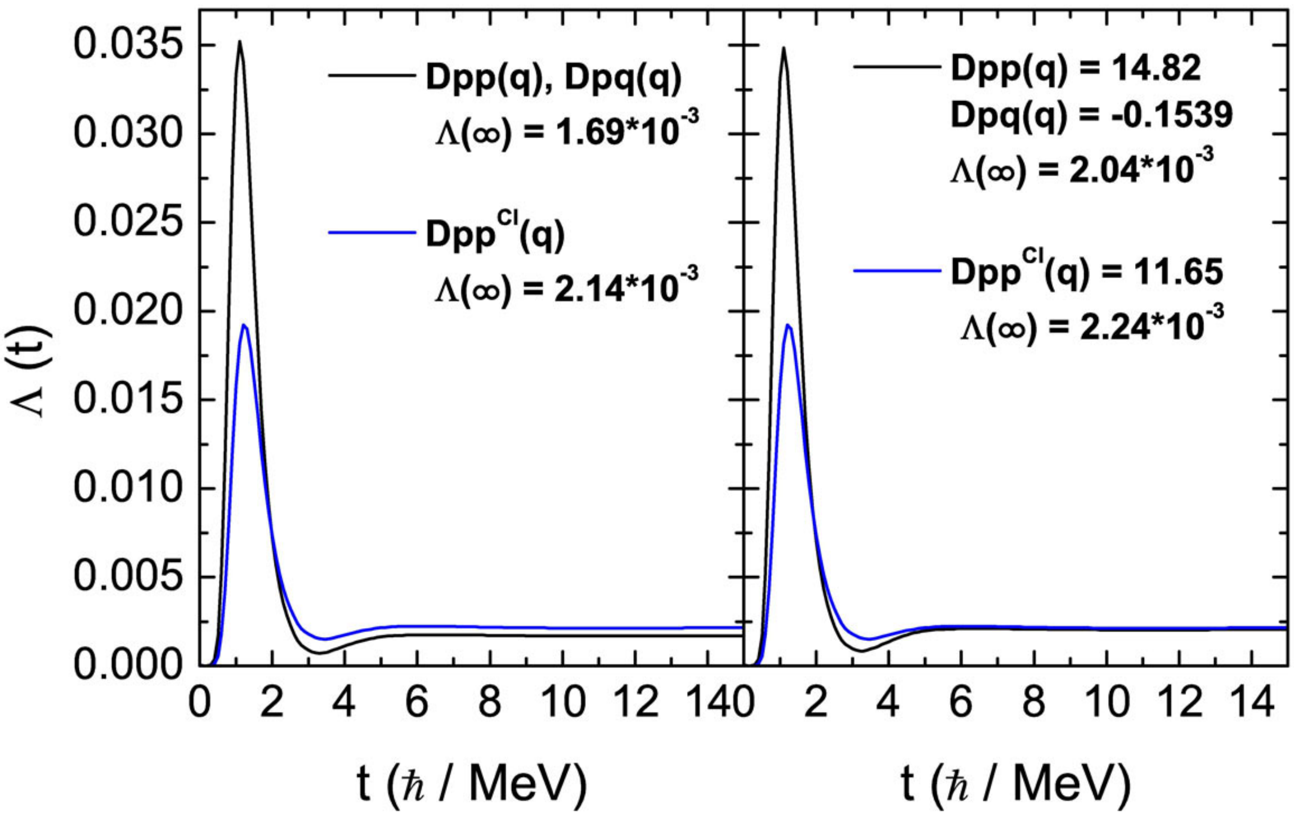
IV — "Classical" diffusion coefficient: $D^{cl}_{pp}(q = b_w)$=$const$

V — microscopical diffusion coefficients: $D_{pp}(q)$ and D_{pq}=0

Decay rate at temperature T=1.0 MeV

We use parameters:

$\mu = 450 m_0$, $\hbar\lambda_p(\infty) = 1$ MeV, $T = 1.0$MeV.



Calculation data at temperature T=1.0 MeV

	D_{pp} w	b	D_{pq} w	b	$\Lambda_{(\infty)}$
I	14.82	13.85	-0.154	-0.161	$1.69 * 10^{-3}$
II	11.65	10.27	—	—	$1.75 * 10^{-3}$
III	14.82	14.82	-0.154	-0.154	$2.04 * 10^{-3}$
IV	11.65	11.65	—	—	$2.14 * 10^{-3}$
V	14.82	13.85	0	0	$4.47 * 10^{-3}$

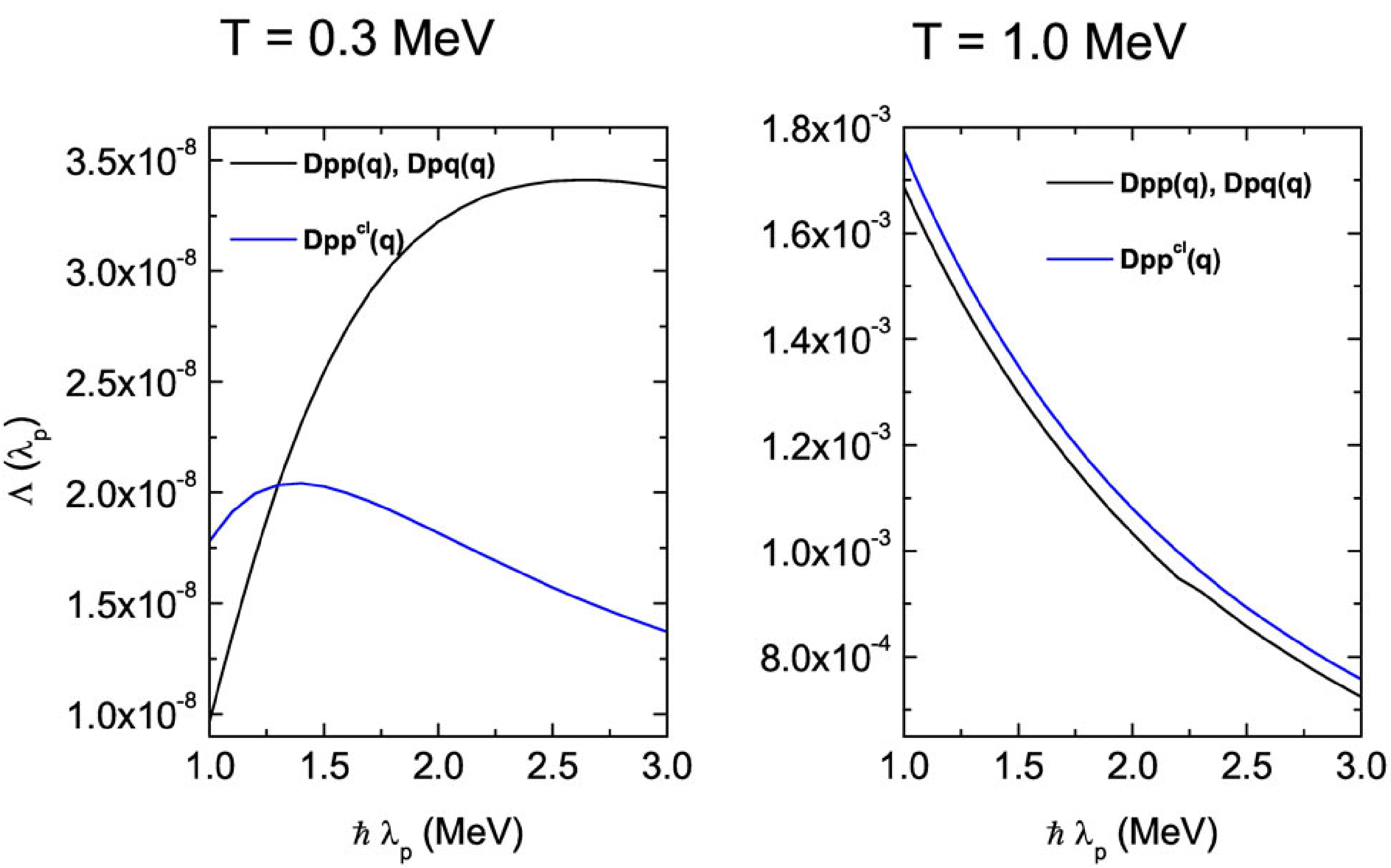
Calculation data at temperature T=0.3 MeV

	D_{pp}		D_{pq}		$\Lambda_{(\infty)}$
	w	b	w	b	
I	10.85	8.43	-0.264	-0.304	$9.70 * 10^{-9}$
II	5.19	1.65	–	–	$1.78 * 10^{-8}$
III	10.85	10.85	-0.264	-0.264	$1.30 * 10^{-5}$
IV	5.19	5.19	–	–	$1.36 * 10^{-5}$
V	10.85	8.43	0	0	$1.00 * 10^{-3}$

Dependence on friction

We use parameters:

$\mu = 450 m_0$, $\hbar\omega = 1$MeV.



Summary

- We obtain coordinate-dependent diffusion coefficients, and solve the master-equation for reduced density matrix with these coefficients.
- We study the influence of diffusion coefficients on decay rate, and compare the decay rates obtained with microscopical and classical diffusion coefficients.
- The obtained dependences of the decay probability on the friction and diffusion at low temperatures proves that the coordinate dependence of the diffusion coefficients should be taken into consideration for nonlinear systems.
- At low temperature the friction promotes the penetrability through barrier.