Thermalization in the Caldeira-Leggett Model

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CRC-TR 211
Strong-interaction matter under extreme conditions

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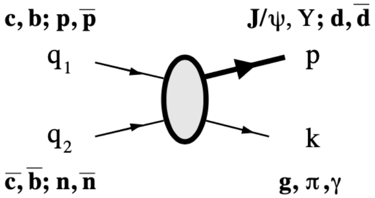
Bound State Formation in HIC's

Hadronic bound states form in high-energy heavy-ion collisions

- bound states can be formed and destroyed during specific stages of evolution of the medium
- two important kinds of bound states: heavy quarkonia (J/Ψ, Υ and excited states) and (anti-)deuterons ($d, \bar{d}$); other light nuclei
- 'snowballs in hell': light nuclei appear in the statistical hadronization model at chemical freeze-out temperature (~ 150 MeV), while binding energy much lower (Deuteron ~ 2.3 MeV)
- $c\bar{c} \leftrightarrow J/\Psi g(\pi), b\bar{b} \leftrightarrow \Upsilon g(\pi), pn \leftrightarrow d\pi(\gamma), \bar{p}\bar{n} \leftrightarrow \bar{d}\pi(\gamma)$



- Focus on Deuteron, because properly described in qm scattering theory in 1-D
- Consider Deuteron as system particle in language of open quantum systems

Equilibration time? Thermalization?

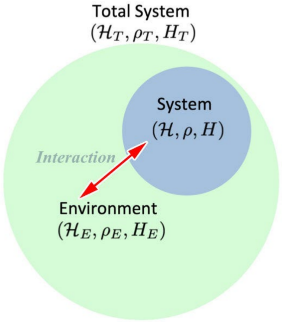
Open Quantum Systems, Dissipative Systems and Irreversibility

Starting point: $\mathrm{i}\dot{\rho}_S = [H, \rho_S]$, ρ_S : reduced density matrix

QM closed systems are invariant under time-reversal + forces derived from a potential

Introducing irreversibility:

- phenomenological equation (e.g. Langevin, Fokker-Planck)
- system-plus-reservoir approach
- modifications of e.o.m. (non-linear Schrödinger equations)



D.o.f. in open quantum system not taken into account explicitly, but effect on the observable macroscopic system.

- environment causes slowing down of motion, described by friction force $\sim v(t), p(t)$
- even if $\langle v(t) \rangle = 0$, the system fulfils rapidly-fluctuating (Brownian) motion, described by $\mathcal{F}(t)$, fluctuation force

Additional assumption (with equipartition theorem):

Final state of system is in thermal equilibrium

Caldeira-Leggett Model as a System-Plus-Reservoir Approach

Caldeira-Leggett-Model: System-to-bath-coupling, (bath: infinitely many d.o.f.) via harmonic oscillators

$$H = H_S + H_R + H_I, \qquad H_S = \frac{p^2}{2m} + V(x)$$
$$H_R = \sum_{i=1}^{N} \left(\frac{p_i^2}{2m_i} + \frac{1}{2} m_i \omega_i^2 q_i^2 \right)$$
$$H_I = -x \sum_i c_i q_i + \Delta V(x)$$

$\Delta V(x)$: "shift of systems potential", "frequency renormalization".

Leads to a coupled set of e.o.m. (classical)

$$m\ddot{x}(t) + m\omega_0^2 x(t) - \sum_{i=1}^{N} c_i \left(q_i(t) - \frac{c_i}{m_i \omega_i^2} x(t) \right) = 0$$
$$m_i \ddot{q}_i(t) + m_i \omega_i^2 q_i(t) - c_i x(t) = 0$$

A technique to solve the Liouville-von Neumann equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = -\mathrm{i}\,[H, \rho(t)] \qquad \rightarrow \qquad \rho(t) = e^{-\mathrm{i}Ht}\rho(t=0)e^{\mathrm{i}Ht}$$

Starting point Schrödinger equation:

$|\psi(t)\rangle = e^{-\mathrm{i}Ht}\,|\psi(0)\rangle$, $\langle x|\psi(t)\rangle = \int \mathrm{d}x' G(x, t; x', t' = 0)\,\langle x'|\psi(0)\rangle$,

where $G(x, t, x', t' = 0) \equiv \langle x|e^{-\mathrm{i}Ht}|x'\rangle$, the propagator.

"Vernon" Hamilton operator (open quantum system)

$$H \equiv H_S + H_B + H_{SB} \qquad \leftrightarrow \qquad S_{\text{total}} = S_S[q] + S_B[x] + S_{SB}[qx]$$

Assume: system dof's q and bath dof's $x = (x_1, x_2, \ldots, x_n)$

Density matrix $\rho(t)$ in spatial coordinates

$$\langle x, q|\,\rho(t)\,|q', x'\rangle = \int \mathrm{d}q_0\mathrm{d}q_0'\mathrm{d}x_0\mathrm{d}x_0'\,\langle x, q|\,e^{-\mathrm{i}Ht}\,|q_0x_0\rangle\langle x_0q_0|\,\rho(t=0)\,|q_0'x_0'\rangle \times \langle x_0'q_0'|\,e^{\mathrm{i}Ht}\,|q'x'\rangle$$

Assume $\rho(t) = \rho_S \otimes \rho_B$

Trace out bath variables reduced density matrix → partial trace: $\rho_S = \mathrm{Tr}_B \rho$

$$\langle q | \rho_S(t) | q' \rangle = \int \mathrm{d}q_0 \mathrm{d}q_0' \langle q_0 | \rho_S(0) | q_0' \rangle \int_{q_0}^{q} \mathcal{D}q \int_{q_0'}^{q'} \mathcal{D}^* q' \exp\left[\mathrm{i}(S[q] - S[q'])\right] \mathcal{F}[q(t'), q'(t')]$$

with

$$\mathcal{F}[q(t'), q'(t')] = \int \mathrm{d}x_0 \mathrm{d}x_0' \mathrm{d}x \langle x_0 | \rho_B | x_0' \rangle \times \int_{x_0}^{x} \mathcal{D}x \int_{x_0'}^{x} \mathcal{D}^* x' \exp \mathrm{i}\left[(S[x] + S[qx]) - (S[x'] + S[q'x'])\right]$$

From stat. mech. $\rho_B = \frac{e^{-\beta H_B}}{Z}$, $Z = \mathrm{Tr}\, e^{-\beta H_B} = \frac{1}{2\sinh \beta\Omega/2}$,

$$\langle x | \rho_B | x' \rangle = \frac{1}{Z}\sqrt{\frac{M\Omega}{2\pi \sinh \Omega\beta}} \exp\left[\frac{-M\Omega}{2\sinh \beta\Omega}\left[(x^2 + x'^2)\cosh \beta\Omega - 2xx'\right]\right]$$

inserted and solving the Gaussian path integrals leads to

$$\Phi\left[q_{t'}, q'_{t'}\right] = \int_0^t \mathrm{d}t' \int_0^{t'} \mathrm{d}s \left[f[q_{t'}] - f[q'_{t'}]\right]\left[L(t'-s)f[q_s] - L^*(t'-s)f[q'_s]\right]$$

$$L(\tau) = \frac{1}{2M\Omega}\left(\coth\frac{\beta\Omega}{2}\cos\Omega\tau - \mathrm{i}\sin\Omega\tau\right)$$

Input: Caldeira-Leggett Hamiltonian

→ [*canonical quantization,..., Fourier transformation, elimination of the environmental d.o.f., assumption of an Ohmic spectral density, high temperatures, Markovian, etc. ...*]

Leads to *Caldeira-Leggett master equation* (Physica 121A (1983))

$$\frac{\partial}{\partial t}\rho_S = \frac{1}{\mathrm{i}}\mathcal{L}_S\rho_S = \frac{1}{\mathrm{i}\hbar}\left[H'_S, \rho_S\right] - \frac{\gamma}{\hbar}\left\{\frac{mk_BT}{\hbar}\left[x, [x, \rho_S]\right] + \frac{\mathrm{i}}{2}[x, \{p, \rho_S\}]\right\}$$

⇒ eq. is known to violate positivity requirement for density operator

Solution: Kossakowski - Lindblad equations

$$\mathcal{L}[\rho_S] = \frac{1}{\mathrm{i}\hbar}\left[H'_S, \rho_S\right] + \frac{1}{2\hbar}\sum_{i=1}^{\infty}\left([V_i\rho_S, V_i] + [V_i, \rho_S V_i]\right).$$

V-Operators are bounded operators on the $\mathcal{H}$-space of Hamiltonian, usually lin. combination of $\hat{x}$ and $\hat{p}$, and guarantee positivity and norm-conservation.

However: "choice is *guided by intuition*" (Gao, PRL 82, 3377)

Caldeira-Leggett Master Equation for a Harmonic Oscillator

$V = \frac{m\omega_0^2 x^2}{2}$ allows wider repertoire of CLME

$$\mathrm{i}\frac{\partial \rho_S}{\partial t} = \left[\frac{p^2}{2} + \frac{\omega_0^2 x^2}{2}, \rho_S\right] - \mathrm{i}D_{pp}\left[x, [x, \rho_S]\right] + \gamma\,[x, \{p, \rho_S\}] - 2\mathrm{i}D_{px}\left[x, [p, \rho_S]\right]$$

or in coordinate space, $\langle x|[\ldots]|y\rangle$

$$\mathrm{i}\frac{\partial}{\partial t}\rho(x, y, t) = \left[\frac{1}{2m}\left(\frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial x^2}\right) + \frac{m\omega^2}{2}(x^2 - y^2) - \mathrm{i}D_{pp}(x-y)^2 \right.$$
$$\left. - \mathrm{i}\gamma(x-y)\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right) - 2D_{px}(x-y)\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)\right]\rho(x, y, t)$$

where

Case	D_{pp}	D_{px}
I; CL	$2\gamma m k_B T/\hbar^2$	0
II; Breuer, Petruccione	$2\gamma m k_B T/\hbar^2$	$\frac{-\gamma k_B T}{\hbar^2 \Omega}$
III; Diosi	$2\gamma m k_B T/\hbar^2$	$\frac{\Omega\gamma}{6\pi k_B T}$

Analytical Solutions of the Harmonic Oscillator

CLME can be solved by Fourier transformation and taking the limit $t \to \infty$

$$\rho(x, y, \infty) = \frac{\sqrt{\gamma} m\omega}{\hbar\sqrt{\pi}\sqrt{D_{pp} - 4\gamma m D_{px}}} \exp\left\{-\frac{\gamma\left[m\omega(x+y)\right]^2}{4\hbar^2\left(D_{pp} - 4\gamma m D_{px}\right)} - \frac{D_{pp}(x-y)^2}{4\gamma}\right\}$$

To show thermalization we need $\rho_{nn}(t)$ from

$$\rho(x, y, t) = \sum_{nm} \rho_{nm}(t)\phi_n(x)\phi_m(y)$$

$$\phi_n(x) \neq \phi_{\text{initial system harm. oscillator,n}}(x)$$

To find the wave functions one starts (Homa, Bernad, Csirik, Eur. Phys. J. D (2018))

$$\int_{-\infty}^{\infty} \rho(x, y, \infty)\phi_n(y)\mathrm{d}y = \epsilon_n \phi_n(x).$$

Is solved by $\phi_n(x) = H_n\left(x, \frac{1}{4\sqrt{AC}}\right)\exp\left\{-2\sqrt{AC}x^2\right\}$ with $\epsilon_n = \epsilon_0\epsilon^n$, where

$$\epsilon_0 = \frac{2\sqrt{C}}{\sqrt{A}+\sqrt{C}}, \qquad \epsilon = \frac{\sqrt{A}-\sqrt{C}}{\sqrt{A}+\sqrt{C}}, \qquad A = \frac{D_{pp}}{4\gamma}, \qquad C = \frac{\gamma(m\omega)^2}{4\hbar^2\left(D_{pp} - 4\gamma m D_{px}\right)}$$

Analytical Solutions of the Harmonic Oscillator

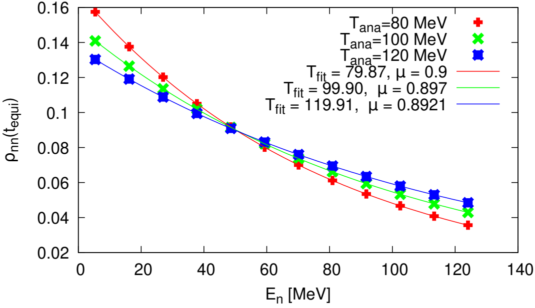
The model is physical if (Homa, Bernad, Lisztes, Eur. Phys. J. D (2019))

$$A \geq C \qquad \text{or} \qquad \hbar^2 \frac{D_{pp}^2 - 4\gamma m D_{pp} D_{px}}{\gamma^2 m^2 \omega^2} \geq 1$$

If this inequality is not satisfied then the stationary density operator has negative eigenvalues for every odd state.

Case	D_{pp}	D_{px}	Condition
I; CL	$2\gamma m k_B T/\hbar^2$	0	$T \geq \frac{\hbar\omega}{2k_B}$
II; Breuer, Petruccione	$2\gamma m k_B T/\hbar^2$	$\frac{-\gamma k_B T}{\hbar^2 \Omega}$	$T \geq \frac{\hbar\omega}{2k_B\sqrt{1+2\gamma/\Omega}}$, $\Omega \gg \gamma$
III; Diosi	$2\gamma m k_B T/\hbar^2$	$\frac{\Omega\gamma}{6\pi k_B T}$	$T \geq \frac{\hbar\omega}{2k_B}\sqrt{1+\frac{2\Omega\gamma}{3\pi\omega^2}}$, $\hbar\Omega \gg k_B T \gg \hbar\omega$

Results of the Analytic Solution of the Harmonic Oscillator

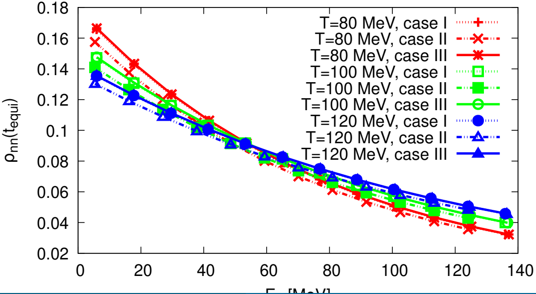


- $\gamma = 12$ MeV, therefore $\tau_{\text{rel}} \approx \frac{1}{\gamma} \approx 16 - 17$ fm
- thermal fit $\sim \exp\left[-\frac{1}{T}\,(E-\mu)\right]$
- other parameters:
  $m = 470$ MeV,
  $\Omega = 100$ MeV,
  $\omega = 0.06$ fm^{-1}

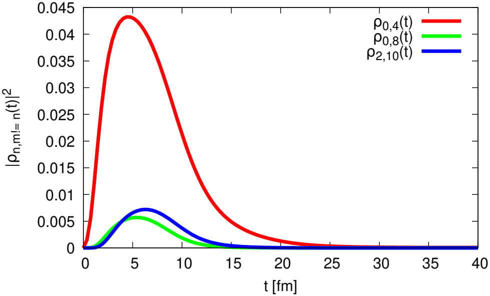
Impact of different combinations for cases I-III,

$$D_{pp} = 2\gamma m k_B T/\hbar^2,$$

$$D_{px} = \begin{cases} 0, & \text{case } I \\ \frac{-\gamma k_B T}{\hbar^2 \Omega}, & \text{case } II \\ \frac{\Omega\gamma}{6\pi k_B T}, & \text{case } III \end{cases}$$



- Interaction of open quantum system with its surroundings creates correlations between the states of the system and of the environment
- Environment carries information on the open system in the form of these correlations
- Dynamical destruction of quantum coherence is called decoherence.
- Define decoherence function $\Gamma_{nm}(t) \leq 0$, $|\langle \phi_n(t)|\phi_m(t)\rangle| = \exp\left[\Gamma_{nm}(t)\right]$



- Calculation directly from path integral (Müller, Ayyar, *J. Modern Phys. E, 22, 1350016 (2012))*, non-Markovian, same parameters
- Showing $\rho_{0,2}(t)$, $\rho_{0,8}(t)$, $\rho_{2,10}(t)$
- Equilibrium after all non-diagonal elements vanish
- initial condition:

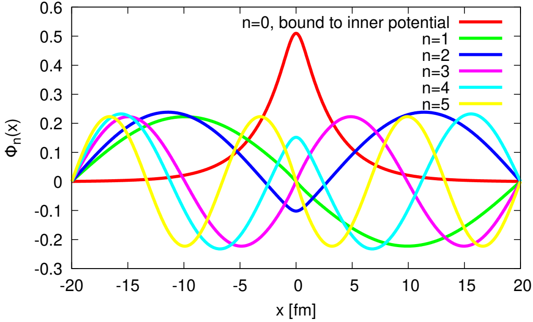
$$\rho(x, y, 0) = \sqrt{\frac{M\omega}{\pi}} \exp\left[-\frac{M\omega}{2}\left(x^2 + y^2\right)\right]$$

Application on Model with Bound State

To mimic a bound state in 1-D, we chose

$$V = \begin{cases} \frac{V_0}{\cosh^2(ax)}, & x \in [-20\text{fm}, 20\text{fm}] \\ \infty, & \text{else} \end{cases}$$

where $V_0 = -25$ MeV, and $a = 1.47$ fm, similar to deuteron parameters, cf. Rais, Phys. Rev. C 106, 064004 (2022)

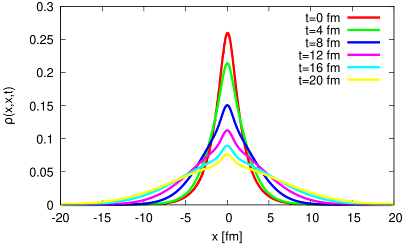


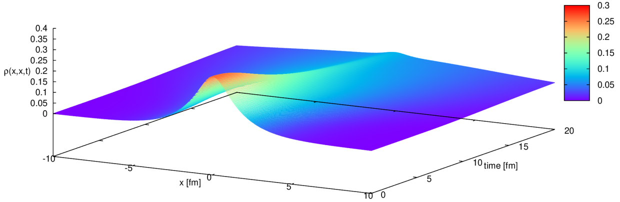
$$V = \frac{V_0}{\cosh^2(ax)},$$
$x \in [-20\text{fm}, 20\text{fm}]$ with

- $V_0 = -25$ MeV,
- $a = 1.47$ fm, $m = 938/2$ MeV
- $V_{\text{bind}} = -2.32$ MeV
- The wave functions are computed with a shooting method

$$\mathrm{i}\frac{\partial}{\partial t}\rho(x,y,t) = \left[H(y) - H(x) - \mathrm{i}D_{pp}(x-y)^2 - \mathrm{i}\gamma(x-y)\left(\frac{\partial}{\partial x} - \frac{\partial}{\partial y}\right)\right]\rho(x,y,t)$$

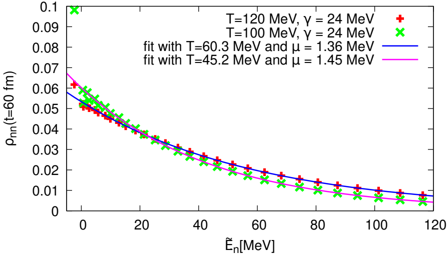
- Solved numerically by Crank-Nicholson method, to obtain $\rho(x,y,t)$ in coordinate representation.
- Here $\gamma = 12$ MeV, $\Omega = T = 120$ MeV

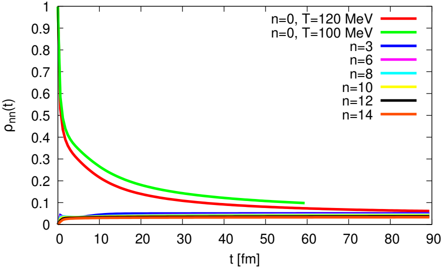




Evolution of $\rho(t)$

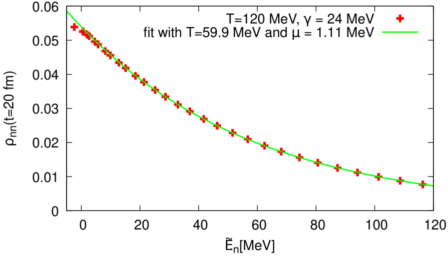
- Results can be evolved in the basis of the wave functions, but therefore do not correspond to the energy eigenvalues of the system.
- Equilibration time is too large for HIC (3-6 fm) (numerics), $1/\gamma \approx 9$ fm

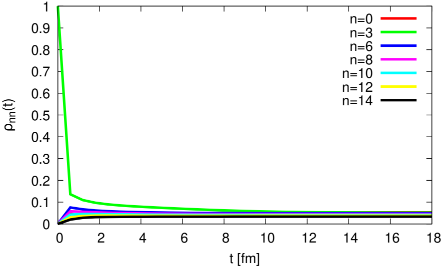




- $\sim \exp\left[-\frac{1}{T}\left(E-\mu\right)\right]$ fit. Very weak damping (system still not in equilibrium!!!)
- Fitted temperature only approx. half T_{bath} because of shifts in the modes
- t_{equi} faster for higher T, ($t_{\text{equi}} > 50$fm)

n=3 Populated as Initial Condition





- Fitted temperature only approx. half T_{bath} because of shifts in the modes
- t_{equi} much higher, if higher state is initial condition ($t_{\text{equi}} \approx 9$fm)

Conclusions and Outlook

Conclusions:

- The CL-model is common to describe the influence of a environment with a temperature on a system
- Lindblad-Form of the CLME satisfies positivity and norm-conservation
- Further temperature-dependent extends are done in the literature
- Decomposition of density matrix not valid for constant wave functions. The modes of the wave function are changing during the interaction with the environment ($k_n \to k_n(t)$)
- Therefore thermalization can be shown only indirectly through expectation values of total energy

Outlook:

- Testing for different initial conditions
- Shift of modes k_n has to be understood deeper
- Testing for different Ω, γ, T, estimating critical values
- Matching with Kadanoff-Baym approach of Tim Neidig, arXiv:2308.07659