Bound State Formation in Open Quantum Systems

Jan Rais

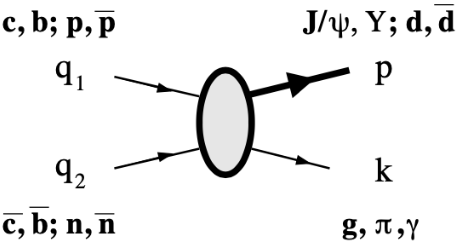
Institut für theoretische Physik,
Universität Frankfurt am Main,
HFHF-Retreat in Castiglione

September 12, 2022

Table of Contents

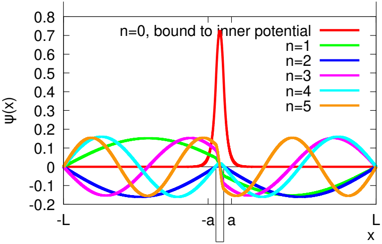
Hadronic bound states in strongly interacting matter in high-energy heavy-ion collisions

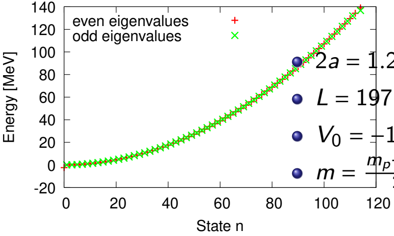
- bound states can be formed and destroyed during specific stages of evolution of the medium
- two important kinds of bound states: heavy quarkonia ($J/\Psi, \Upsilon$ and excited states) and (anti-)deuterons ($d, \bar{d}$); other light nuclei
- 'snowballs in hell': light nuclei appear in the statistical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



Solving the stationary Schrödinger equation with boundary conditions

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(x)\right]\psi(x) = E\psi(x)$$





- $2a = 1.2$ fm
- $L = 197$ fm
- $V_0 = -15$ MeV
- $m = \frac{m_p + m_n}{2}$

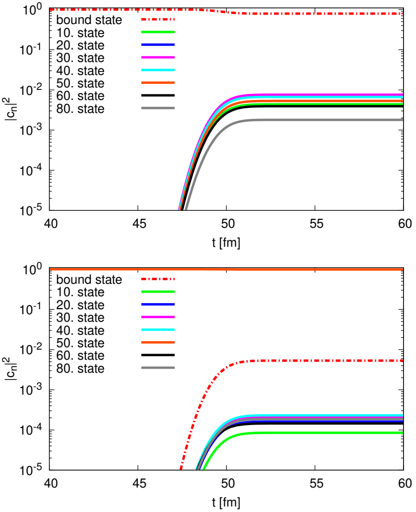
and $i\hbar\partial_t\psi(x,t) = \left[-\frac{\hbar^2}{2m}\partial_x^2 + \hat{V}(x,t)\right]\psi(x,t) = \hat{H}\psi(x,t)$ with $\hat{H} = \hat{H}_0 + V(x,t)$;

$\psi(x,t) = \sum_n c_n(t)\psi_n(x)$ and therefore

$\hat{H}\left|\psi\right\rangle = \sum_n c_n(t)\left[E_n + \hat{V}(t)\right]\left|\psi_n\right\rangle, \qquad \left|\psi_n\right\rangle = \psi_n(x)$ leeds to ODE $\in \mathbb{C}$

$$\boxed{i\dot{\tilde{c}}_j(t) = \sum_n V_{jn}\exp\left(i(E_j - E_n)t\right)\tilde{c}_n(t)} \quad \text{with } \tilde{c}_j = c_j \exp\left(iE_j t\right)$$

$$V(x,t) = V \exp\left(-\frac{(x-x_0)^2}{2\sigma_x^2}\right)\exp\left(-\frac{(t-t_0)^2}{2\sigma_t^2}\right)$$

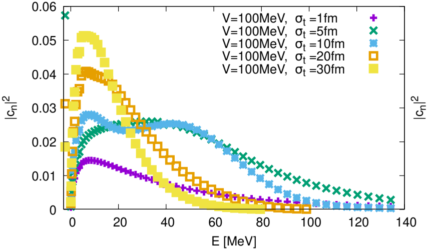


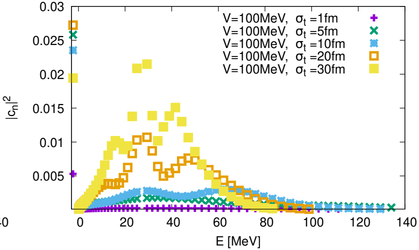
$$\Rightarrow V_{mn} = \int \mathrm{d}x \psi_m^* V(x,t)\psi_n$$

$$\Rightarrow \mathrm{i}\dot{\tilde{c}}_m(t) = \sum_n V_{mn} e^{\mathrm{i}(E_m - E_n)t} \tilde{c}_n(t)$$

- $|c_n(t)|^2$ depends on σ_t, σ_x and V
- since $\partial_t V(x,t) = 0$, $\partial_t |c_n(t)|^2 = 0$
- here $\sigma_t = 1$ fm, $\sigma_x = 1.2$ fm and $V = 100$ MeV

Is Heisenberg's uncertainty relation in energy and time fulfilled ???

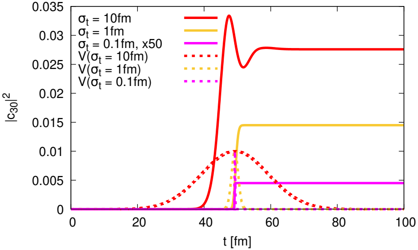




- $\sigma_t = 1, 5, 10, 20, 30$ fm
- $|c_{0,50}(t=0)|^2 = 1$

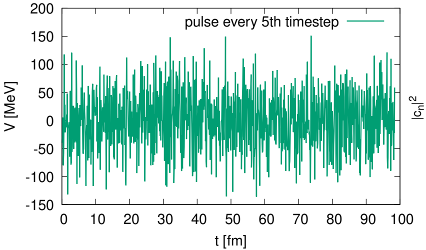
$$\Delta t \Delta E \geq \frac{\hbar}{2} \quad \Leftrightarrow \quad \sigma_t \Delta E \geq \frac{1}{2}$$

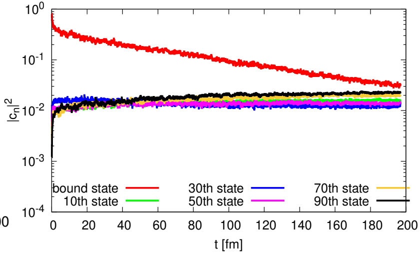
$$\text{"}\tau_{\text{formation}}\text{"} \overset{\lightning}{\neq} \frac{\hbar}{E_B}$$



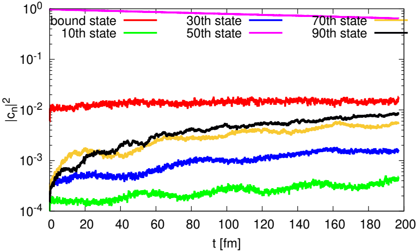
- 2000 pulses with

$$V(x,t) = \sum_{j=1}^{N} V_\xi \exp\left(-\frac{x^2}{2\sigma_x^2}\right)\left[\Theta(t - jn\Delta t) - \Theta(t - j(n+1)\Delta t)\right]$$

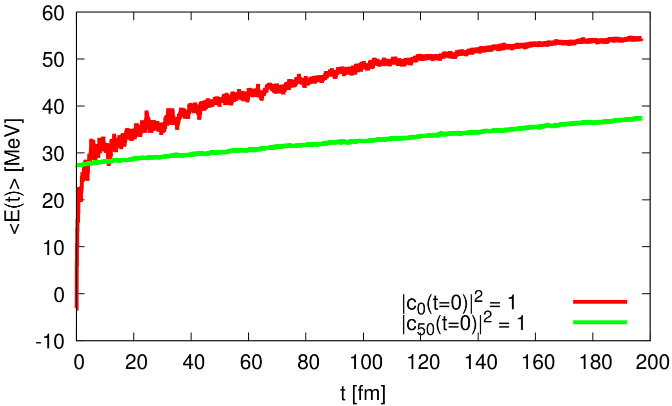




- randomly distributed pulse strength
- formation of states on a long time scale
- initial state destruction on very long time
- no equilibration
- final distribution similar to case with one pulse



Mean Energy, System blows up



Need of an approach, that includes damping

Consider Hamiltonian

$$H(t) = H_S + H_B + H_{\mathrm{I}}(t)$$

where bath is in equilibrium. In terms of density matrices

$$\rho_{SB}(t) = \rho_S \otimes \rho_B$$

Trace out bath variables reduced density matrix → partial trace

$$\mathrm{Tr}_B\left[\rho_{SB}\right] := \sum_j \left(I_S \otimes \langle j|_B\right) \rho_{SB} \left(I_S \otimes |j\rangle_B\right)$$

with $\{|j\rangle\} \in$ ONB for $\mathcal{H}_B$ of subsystem $B \rightarrow \rho_R = \mathrm{Tr}_B\left[\rho_{SB}\right]$. Further need of von Neumann equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho(t) = \mathrm{i}\left[H_I, \rho(t)\right] \quad \text{with} \quad \rho(t) = \rho(0) - \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}s \left[H_{\mathrm{I}}(s), \rho(s)\right]$$

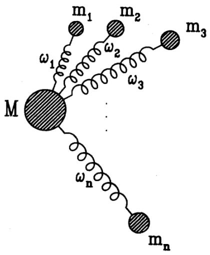
which is inserted to obtain in Schrödinger picture

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\rho_S(t) &= -\frac{\mathrm{i}}{\hbar}\left[H_S, \rho_S\right] - \frac{\mathrm{i}}{\hbar^2}\int_0^t \mathrm{d}\tau \mathrm{tr}_B\left[H_{\mathrm{I}}, \left[H_{\mathrm{I}}(\tau), \rho_S(t) \otimes \rho_B\right]\right] \\ &= -\frac{\mathrm{i}}{\hbar}\left[H_S, \rho_S\right] - \frac{\mathrm{i}}{\hbar^2}\int_0^t \mathrm{d}t \mathrm{tr}_B\left[H_{\mathrm{I}}(t), \left[H_{\mathrm{I}}(t-s), \rho_S(t) \otimes \rho_B\right]\right]\end{aligned}$$

in terms of the system. Born-Markov approximation → $\rho(t) \approx \rho_S(t) \otimes \rho_B(0)$
Substitution of $s \rightarrow \tau = |t-s| \ll \tau_B$. $\Rightarrow$ Redfield equation

Still Hamiltonian

$$H(t) = H_S + H_B + H_I(t)\ (+H_c)$$



with

$$H_S = \frac{1}{2M}p^2 + V(x),$$

$$H_B = \sum_n \left(\frac{1}{2m_n} p_n^2 + \frac{1}{2} m_n \omega_n^2 x_n^2 \right),$$

$$H_I = -x \sum_n \kappa_n x_n \equiv -xB$$

with $B = \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} \left(b_n + b_n^\dagger \right)$ and $H_c = x^2 \sum_n \frac{\kappa_n^2}{2m_n\omega_n^2}$.

Need of spectral density

$$J(\omega) = \sum_n \frac{\kappa_n^2}{2m_n\omega_n} \delta(\omega - \omega_n) \rightarrow \frac{2m\gamma}{\pi} \omega \frac{\Omega^2}{\Omega^2 + \omega^2} \qquad \text{(Lorentz-Drude cutoff)}$$

For Brownian motion define correlation functions

$$\langle B(0)B(-\tau)\rangle_B = \underbrace{\int_0^\infty \mathrm{d}\omega J(\omega) \coth\left(\frac{\hbar\omega}{2k_B T}\right) cos(\omega\tau)}_{\text{noise kernel}} - \mathrm{i} \underbrace{\int_0^\infty \mathrm{d}\omega J(\omega) \sin(\omega\tau)}_{\text{dissipation kernel}}$$

which finally leads to

$$\begin{aligned}\dot{\rho}_S(t) &= -\frac{\mathrm{i}}{\hbar}\left[H_S + H_c, \rho_S\right] - \frac{1}{\hbar^2}\int_0^\infty \mathrm{d}\tau \mathrm{tr}_B\left[H_I, \left[H_I(\tau), \rho_S(t)\otimes\rho_B\right]\right] \\ &= -\frac{\mathrm{i}}{\hbar}\left[H_S + H_c, \rho_S\right] + \frac{\mathrm{i}}{\hbar}\left[H_c, \rho_S\right] - \frac{\mathrm{i}\gamma}{\hbar}\left[x, \{p, \rho_S(t)\}\right] - \frac{2mk_BT\gamma}{\hbar^2}\left[x, \left[x, \rho_S(t)\right]\right] \\ &= \underbrace{-\frac{\mathrm{i}}{\hbar}\left[H_S, \rho_S\right]}_{\text{free coherent dynamics}} \underbrace{-\frac{\mathrm{i}\gamma}{\hbar}\left[x, \{p, \rho_S(t)\}\right]}_{\text{dissipation } \sim D(\tau)} - \underbrace{\frac{2mk_BT\gamma}{\hbar^2}\left[x, \left[x, \rho_S(t)\right]\right]}_{\text{thermal fluctuations } (\textit{decoherence})}\end{aligned}$$

- $\gamma = \eta/2m$, characteristic damping rate of oscillator with m and H
  $\eta \in$ friction coefficient
- Fokker-Planck equation, $k_B T/\hbar \gg \Omega \gg \omega \Rightarrow$ Caldeira-Leggett limit
- Satisfies $\langle F(t+\tau)F(t)\rangle = 2\gamma k_B T$

Problems of the Caldeira-Leggett Master equation

- $\lambda_{dB} = \frac{\hbar}{\sqrt{4Mk_BT}}$; the coherent length pertaining to state ρ_{nn} must always be greater than λ_{dB}; otherwise ME tends to violate the positivity of ρ
- Particular coarse-graining of CLME lead to Lindblad form
- not a priori norm-conserving

Has similarity to Lindblad equation (Markovian process)

$$\mathcal{L}\rho_S = -\mathrm{i}\left[\mathcal{H},\rho_S\right] + \sum_{ij=1}^{N^2-1} a_{ij}\left(F_i\rho_S F_j^\dagger - \frac{1}{2}F_j^\dagger F_i\rho_S - \frac{1}{2}\rho_S F_j^\dagger F_i\right)$$

with Lindblad Operators $F_1 = x$ and $F_2 = \mathrm{i}p$ and $a_{ij} = \begin{pmatrix} \frac{4m\gamma k_B T}{\hbar^2} & \gamma/\hbar \\ \gamma/\hbar & \frac{\gamma}{4mk_B T} \end{pmatrix}$

$$\boxed{\dot{\rho}_S(t) = -\frac{\mathrm{i}}{\hbar}\left[\mathcal{H},\rho_S\right] - \mathrm{i}a_{12}\left[x,\{p,\rho_S(t)\}\right] - \frac{a_{11}}{2}\left[x,\left[x,\rho_S(t)\right]\right] - a_{22}\left[p,\left[p,\rho_S\right]\right]}$$

with $\mathcal{H} = H_S - \gamma xp$

- ME's of Lindblad class do not violate positivity
- Lindblad operator has vanishing trace $\Rightarrow$ norm-conserving
- $\dot{\rho} = \mathcal{L}\rho$, from Liouville equation $\dot{\rho} = \frac{1}{\mathrm{i}\hbar}\left[H,\rho\right]$
- $p-$commutator term comes from Markovian approximation; memory kernel is $M\gamma\delta(\tau - s)$ which leads to $\Omega \gg \omega_R$, characteristic frequency of the particle dynamics and $kT \gg \hbar\Omega$ (*Diosi, Europhys. Lett, 22 (1), pp. 1-3 (1993)*)

To solve $\rho_S(t)$ we need ansatz

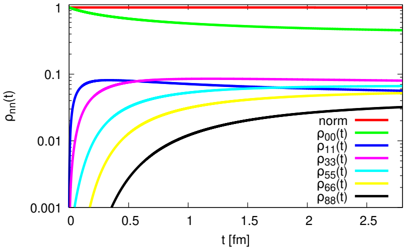
$$\rho_S(x,x',t) = \sum_{mn} \rho_{mn}(t)\Phi_m(x)\Phi_n(x'), \text{ where } \quad \rho_{mn}(t) = \tilde{\rho}_{mn}(t)\exp\left(\mathrm{i}\frac{E_m - E_n}{\hbar}t\right)$$

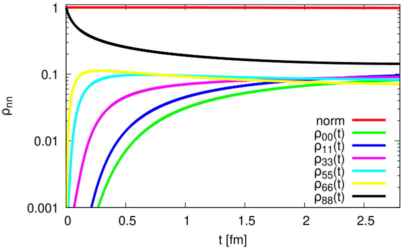
insert and multiply $\int_{-L}^{L} dx' \int_{-L}^{L} dx \Phi_k(x)\Phi_l(x')$ from left to CL-master equation to obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_{kl}(t) = \sum_{mn}\left[-\frac{\mathrm{i}}{\hbar}\mathcal{A}_{kl,mn} + \gamma\mathcal{B}_{kl,mn} - \frac{2mk_B T\gamma}{\hbar^2}C_{kl,mn} + \frac{\gamma\hbar^2}{4mk_B T}\mathcal{D}_{kl,mn}\right]\rho_{mn}(t)$$

- Runge-Kutta solver 4th order to solve differential equation
- Dependence on γ and T
- Comparison Caldeira Leggett to Lindblad equation
- Discontinuities in 2nd derivatives!!

(above) T=40 MeV, $\gamma = 0.1\ fm^{-1}$, *left* $\rho_{00}(t=0) = 1$, *right* $\rho_{88}(t=0) = 1$

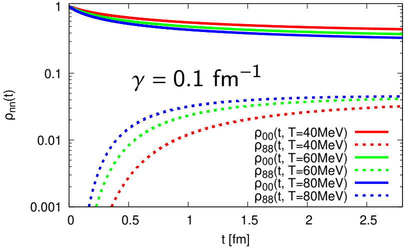


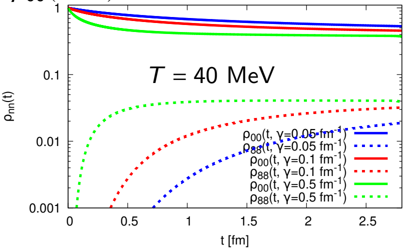


- bound state initially populated
- 8^{th} state init. populated ≈ 25 MeV

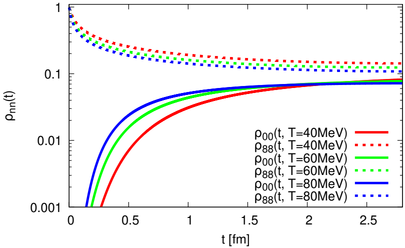
Depopulation of an originally populated bound state, T and γ dependent:

Initial condition $\rho_{00}(t=0) = 1$

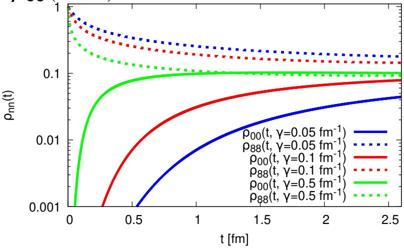




Initial condition $\rho_{88}(t = 0) = 1$



- different T, $\gamma = 0.1$ fm^{-1}

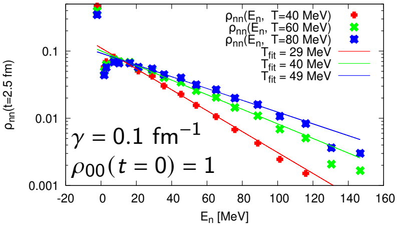


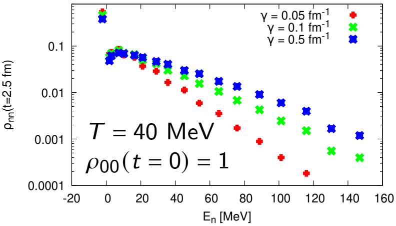
- different γ, $T = 40$ MeV

- 8^{th} corresponds to ≈ 25 MeV
- population of bound state faster, if T is higher
- population of bound state faster, if γ is higher

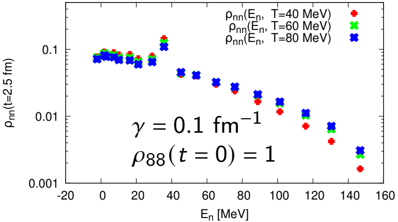
Equilibration after $\approx 2 - 3$ fm??

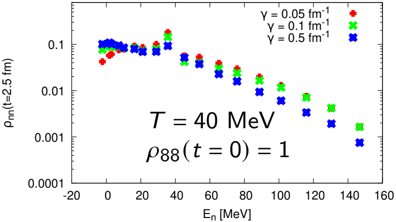
- Bound state initially populated (above), 8th initially populated (below),





- $\rho_{nn} \sim \exp(-\frac{1}{T}(E_n - \mu))$
- the higher the friction, the higher states are populated

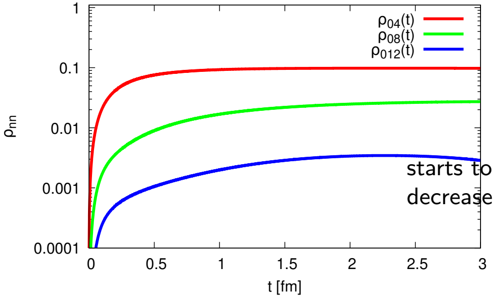




- depopulation of an originally populated bound state, T and γ dependent

- 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. Counteracts the superposition principle in the Hilbert space of the open system.
- define decoherence function $\Gamma_{nm}(t) \leq 0$, $|\langle \phi_n(t)|\phi_m(t)\rangle = \exp\left[\Gamma_{nm}(t)\right]$

- Showing 0th row, $q = 4, 8, 12 \rightarrow \rho_{n,m\neq q} = 0$
- Correlation of higher frequencies start to decrease
- Equilibrium after all non-diagonal elements vanish



Conclusions:

- states populate immediately with appearance of potential
- Heisenberg's uncertainty relation in distribution of states
- Damping introduced via Caldeira-Leggett master equation
- This leads to an equilibrated system, T and γ dependent
- Equilibrium not reached after $1/\gamma \rightarrow$ violates assumption
- try Lindblad formalism

Outlook:

- Will Lindblad be numerically advantageous over Caldeira Leggett?
- Extension to three dimensions
- Damping/Bath Temperature/Oscillator Spectrum
- Introducing Fermions??
- Smooth the potential