Effective density of states of a quantum oscillator coupled to a radiation field

Volker Betz

Mathematics Institute
University of Warwick
Coventry, UK

Orleans, 3rd February 2011

Joint work with **D. P. L. Castrigiano**, TU München

Work supported by EPSRC Advanced Research Fellowship EP/D07181X/1

Quantum particle in a potential

- Hamiltonian: acting in $L^2(\mathbb{R}^3)$, given by

$$H_{\mathrm{p}} = -\frac{\hbar^2}{2m}\Delta + V$$

- Assumption: $V : \mathbb{R}^3 \to \mathbb{R}^3$ continuous, $\lim_{|x|\to\infty} V(x) = +\infty$. Then $\sigma(H_{\mathrm{p}})$ is bounded below, pure point spectrum..

Quantum particle in a potential

- Hamiltonian: acting in $L^2(\mathbb{R}^3)$, given by

$$H_\mathrm{p} = -\frac{\hbar^2}{2m}\Delta + V$$

- Assumption: $V : \mathbb{R}^3 \to \mathbb{R}^3$ continuous, $\lim_{|x|\to\infty} V(x) = +\infty$. Then $\sigma(H_\mathrm{p})$ is bounded below, pure point spectrum..
- Dynamics: $\mathrm{i}\hbar\partial_t\psi(x,t) = H_\mathrm{p}\psi(x,t)$. Therefore: The eigenstates ($H_\mathrm{p}\psi = \lambda\psi$) are stationary.
- H_p could be used to model e.g. an electron in the electric field of a nucleus. The eigenvalues of H_p are the the quantized energy levels.

Quantum particle in a potential

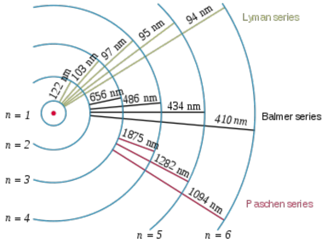
- Hamiltonian: acting in $L^2(\mathbb{R}^3)$, given by

$$H_\mathrm{p} = -\frac{\hbar^2}{2m}\Delta + V$$

- Assumption: $V : \mathbb{R}^3 \to \mathbb{R}^3$ continuous, $\lim_{|x|\to\infty} V(x) = +\infty$. Then $\sigma(H_\mathrm{p})$ is bounded below, pure point spectrum..
- Dynamics: $\mathrm{i}\hbar\partial_t \psi(x,t) = H_\mathrm{p}\psi(x,t)$. Therefore: The eigenstates ($H_\mathrm{p}\psi = \lambda\psi$) are stationary.
- H_p could be used to model e.g. an electron in the electric field of a nucleus. The eigenvalues of H_p are the the quantized energy levels.
- **Problem:** The model cannot describe spontaneous decay to the ground state: an excited state remains excited forever. (No line spectrum!).
- **Solution:** Coupling to the electro-magnetic field (QED).

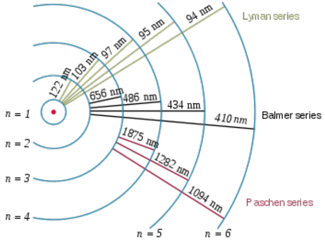
Particle in the radiation field: Spectral lines

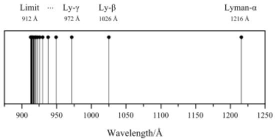
- Evidence for energy quantisation in the hydrogen atom has been found already before the invention of Quantum Mechanics (Balmer 1885, Lyman 1906).
- A photon is absorbed and lifts an electron to its excited state, which later decays and re-emits the photon.
- The frequency corresponds to the energy difference to the energy levels.



Particle in the radiation field: Spectral lines

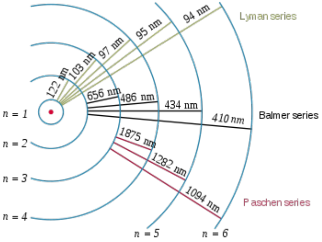
- Evidence for energy quantisation in the hydrogen atom has been found already before the invention of Quantum Mechanics (Balmer 1885, Lyman 1906).
- A photon is absorbed and lifts an electron to its excited state, which later decays and re-emits the photon.
- The frequency corresponds to the energy difference to the energy levels.
- The Lyman-series corresponds precisely to the spectrum of the hydrogen atom $H = -\frac{\hbar^2}{2m}\Delta - 1/|x|$.

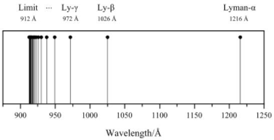


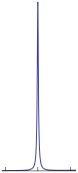


Particle in the radiation field: Spectral lines

- Evidence for energy quantisation in the hydrogen atom has been found already before the invention of Quantum Mechanics (Balmer 1885, Lyman 1906).
- A photon is absorbed and lifts an electron to its excited state, which later decays and re-emits the photon.
- The frequency corresponds to the energy difference to the energy levels.
- The Lyman-series corresponds precisely to the spectrum of the hydrogen atom $H = -\frac{\hbar^2}{2m}\Delta - 1/|x|$.
- Line broadening:







Particle and radiation field: Pauli-Fierz model

Hilbert space: $L^2(\mathbb{R}^3) \otimes \mathcal{F}^{\otimes 2}$, $\mathcal{F}$ is the bosonic Fock space.

$$\mathcal{F} = \bigoplus_{n=0}^{\infty} \mathcal{F}^{(n)}, \quad \mathcal{F}^{(n)} = L^2_{\mathrm{symm}}(\mathbb{R}^{3n}).$$

Hamiltonian: $H = \frac{1}{2m}(p - eA_\varphi(q))^2 + V + H_{\mathrm{f}}$ with

- $p = -\mathrm{i}\hbar\nabla_q$ particle momentum, $V(q)$ particle potential
- Energy of the free field ($\omega(k) = |k|$ dispersion relation):

$$H_{\mathrm{f}} = \sum_{\lambda=1,2} \int \mathrm{d}^3k \hbar\omega(k) a^*(k,\lambda) a(k,\lambda)$$

- Coupling operator:

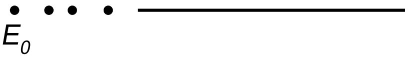
$$A_\varphi(q) = \sum_{\lambda=1,2} \int \mathrm{d}^3k \sqrt{\frac{\hbar}{2\omega(k)}} e_\lambda(k) \Big(\mathrm{e}^{\mathrm{i}q\cdot k}\, \hat{\varphi}(k) a(k,\lambda) + \mathrm{e}^{-\mathrm{i}q\cdot k}\, \hat{\varphi}^*(k) a^*(k,\lambda) \Big)$$

e_λ transversal vector field, φ form factor with UV cutoff.

Pauli-Fierz Hamniltonian: spectrum

$$H = \frac{1}{2m}(p - eA_\varphi(q))^2 + V + H_\mathrm{f}$$

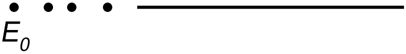
- Spectrum of $H_\mathrm{p} = -\frac{\hbar^2}{2m}\Delta + V$:



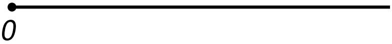
Pauli-Fierz Hamniltonian: spectrum

$$H = \frac{1}{2m}(p - eA_\varphi(q))^2 + V + H_\mathrm{f}$$

- Spectrum of $H_\mathrm{p} = -\frac{\hbar^2}{2m}\Delta + V$:



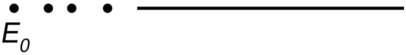
- Spectrum of the free field H_f



Pauli-Fierz Hamniltonian: spectrum

$$H = \frac{1}{2m}(p - eA_\varphi(q))^2 + V + H_\mathrm{f}$$

- Spectrum of $H_\mathrm{p} = -\frac{\hbar^2}{2m}\Delta + V$:



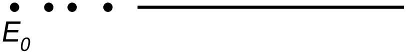
- Spectrum of the free field H_f

- Spectrum of the coupled system:

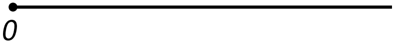
Pauli-Fierz Hamnltonian: spectrum

$$H = \frac{1}{2m}(p - eA_\varphi(q))^2 + V + H_{\mathrm{f}}$$

- Spectrum of $H_{\mathrm{p}} = -\frac{\hbar^2}{2m}\Delta + V$:



- Spectrum of the free field H_{f}



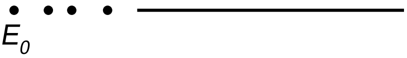
- Spectrum of the coupled system:

- In the coupled system, the higher eigenvalues disappear and become **resonances**.

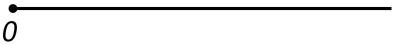
Pauli-Fierz Hamniltonian: spectrum

$$H = \frac{1}{2m}(p - eA_\varphi(q))^2 + V + H_\mathrm{f}$$

- Spectrum of $H_\mathrm{p} = -\frac{\hbar^2}{2m}\Delta + V$:



- Spectrum of the free field H_f



- Spectrum of the coupled system:

- In the coupled system, the higher eigenvalues disappear and become **resonances**.
- [Hunziker 1990]: Connection between resonances and metastability.
- [Bach, Fröhlich, Sigal 1998]: Found resonances in the PF model.

Resonances: Definitions

$$H = H_0 + eH_{\mathrm{I}}$$

Traditional definition: (e.g. Reed-Simon)

$$R^{(u)}(z) = \langle u, (H - z)^{-1} u \rangle, \quad R_0^{(u)}(z) = \langle u, (H_0 - z)^{-1} u \rangle$$

Assumption: For a dense subset of vectors u, $R^{(u)}$ and $R_0^{(u)}$ can be continued analytically into the lower half plane, up to the point $p \in \mathbb{C}$, $\mathrm{Im}(p) < 0$.

p is a resonance of H if $R^{(u)}$ is singular and $R_0^{(u)}$ is regular at p for at least one u.

Resonances: Definitions

$$H = H_0 + eH_{\mathrm{I}}$$

Traditional definition: (e.g. Reed-Simon)

$$R^{(u)}(z) = \langle u, (H - z)^{-1} u \rangle, \quad R_0^{(u)}(z) = \langle u, (H_0 - z)^{-1} u \rangle$$

Assumption: For a dense subset of vectors u, $R^{(u)}$ and $R_0^{(u)}$ can be continued analytically into the lower half plane, up to the point $p \in \mathbb{C}$, $\mathrm{Im}(p) < 0$.

p is a resonance of H if $R^{(u)}$ is singular and $R_0^{(u)}$ is regular at p for at least one u.

Equivalent definition: [BC 11]

$$\mu^{(u)}(\Delta) = \langle u, E(\Delta) u \rangle \quad \text{scalar spectral measure of } H$$

Assumption: For a dense subset of vectors u, the Lebesgue-density $\phi^{(u)}$ of $\mu^{(u)}$, and of $\phi_0^{(u)}$, can be analytically continued up to the point $p \in \mathbb{C}$.

p is a resonance if $\phi_0^{(u)}$ is regular and $\phi^{(u)}$ is singular at p.

Resonances and Lorenz profiles

$\phi^{(u)}$ scalar spectrale density, $\quad p \in \mathbb{C}$ resonance

- Simplest case: $\phi^{(u)}$ has a simple pole at p.
- Since $\phi^{(u)}$ is real analytic (on an interval), we also know $\phi^{(u)}(\overline{z}) = \overline{\phi^{(u)}(z)}$.
- If no other poles are nearby, we have

$$\phi^{(u)}(z) = \frac{\varphi^{(u)}(z)}{(z-p)(z-\overline{p})} \quad \text{mit } \varphi^{(u)} \text{ holomorph.}$$

Resonances and Lorenz profiles

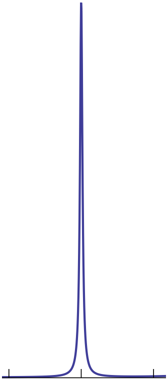
$\phi^{(u)}$ scalar spectrale density, $\quad p \in \mathbb{C}$ resonance

- Simplest case: $\phi^{(u)}$ has a simple pole at p.
- Since $\phi^{(u)}$ is real analytic (on an interval), we also know $\phi^{(u)}(\overline{z}) = \overline{\phi^{(u)}(z)}$.
- If no other poles are nearby, we have

$$\phi^{(u)}(z) = \frac{\varphi^{(u)}(z)}{(z-p)(z-\overline{p})} \quad \text{mit } \varphi^{(u)} \text{ holomorph.}$$

- Sei $p = \hat{\omega} - \mathrm{i}\gamma/2$. On the real axis, this produces a Lorenz profile:

$$\phi^{(u)}(\omega) \simeq C \frac{\gamma/2}{(\omega - \hat{\omega})^2 + \gamma^2/4}.$$



Resonances and Lorenz profiles

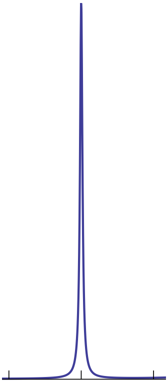
$\phi^{(u)}$ scalar spectrale density, $\quad p \in \mathbb{C}$ resonance

- Simplest case: $\phi^{(u)}$ has a simple pole at p.
- Since $\phi^{(u)}$ is real analytic (on an interval), we also know $\phi^{(u)}(\overline{z}) = \overline{\phi^{(u)}(z)}$.
- If no other poles are nearby, we have

$$\phi^{(u)}(z) = \frac{\varphi^{(u)}(z)}{(z-p)(z-\overline{p})} \quad \text{mit } \varphi^{(u)} \text{ holomorph.}$$

- Sei $p = \hat{\omega} - \mathrm{i}\gamma/2$. On the real axis, this produces a Lorenz profile:

$$\phi^{(u)}(\omega) \simeq C \frac{\gamma/2}{(\omega - \hat{\omega})^2 + \gamma^2/4}.$$



- In the full Pauli-Fierz model, the precise complex structure of the resolvent is unknown.

Open quantum systmes: basics

- We want an effective description for the particle in the radiation field, treating the field as an environment.
- Method of choice: open quantum systems.
- Simplest case: Hamiltonian H is such that $\mathrm{e}^{-\beta H}$ is trace class.
- The state at inverse temperature β is given by the density matrix $\frac{1}{Z(\beta)} \mathrm{e}^{-\beta H}$.
- Partition function: $Z(\beta) = \mathrm{Tr}\, \mathrm{e}^{-\beta H}$.

Open quantum systmes: basics

- We want an effective description for the particle in the radiation field, treating the field as an environment.
- Method of choice: open quantum systems.
- Simplest case: Hamiltonian H is such that $\mathrm{e}^{-\beta H}$ is trace class.
- The state at inverse temperature β is given by the density matrix $\frac{1}{Z(\beta)}\,\mathrm{e}^{-\beta H}$.
- Partition function: $Z(\beta) = \mathrm{Tr}\ \mathrm{e}^{-\beta H}$.
- The inverse Laplace transform of $Z(\beta)$ is a positive measure, namely $\mu = \sum_j N_j \delta_{\lambda_j}$. **Measure of states**
- $\mu^{(\beta)} := \frac{1}{Z(\beta)}\,\mathrm{e}^{-\beta(\cdot)}\,\mu$, then

$$\mu^{(\beta)}(\Delta) = \frac{1}{Z(\beta)} \mathrm{Tr}\,(\,\mathrm{e}^{-\beta H}\,E(\Delta))$$

is the probability of measuring a value for the energy that lies within Δ.

Spectral discretisation

In many interesting cases (e.g. in the Pauli Fierz model), $\mathrm{e}^{-\beta H}$ is not trace class, and even has absolutely continuous spectrum. We use a slight generalization of a standard technique from random Schrödinger operators.

Definition

Let H be a self-adjoint operator in the Hilbert space $\mathcal{H}$, and let (P_n) be a family of orthogonal projections on $\mathcal{H}$. Put
$H_n = P_n H P_n$.
We call H_n a **spectral discretization** of H (wrt. P_n) if:

(i) $P_n D(H) \subset D(H)$

(ii) $\lim_{n\to\infty} P_n = 1$ strongly.

(iii) The spectrum of H_n (defined on $P_n\mathcal{H}$) consists of eigenvalues of finite multiplicity, and $\mathrm{e}^{-\beta H_n}$ is trace class for all n.

Effective description of a subsystem

$$H = H_1 \otimes 1 + 1 \otimes H_2 + H_{\mathrm{I}}, \quad \text{auf } \mathcal{H}_1 \otimes \mathcal{H}_2$$

- $\mathcal{H}_1$ Hilbert space of the small system, $\mathcal{H}_2$ HS of the large one.
- Assume: $\mathrm{Tr}\ \mathrm{e}^{-\beta H}$ exists, and so do those of H_1, H_2.
- Assume: The large system is in thermal equilibrium and is not influenced by the small one (heat bath).

Effective description of a subsystem

$$H = H_1 \otimes 1 + 1 \otimes H_2 + H_\mathrm{I}, \quad \text{auf } \mathcal{H}_1 \otimes \mathcal{H}_2$$

- $\mathcal{H}_1$ Hilbert space of the small system, $\mathcal{H}_2$ HS of the large one.
- Assume: $\mathrm{Tr}\ \mathrm{e}^{-\beta H}$ exists, and so do those of H_1, H_2.
- Assume: The large system is in thermal equilibrium and is not influenced by the small one (heat bath).
- The effective (un-normed) density matrix for the small system is then given by

$$W(\beta) := (\mathrm{Tr}\ \mathrm{e}^{-\beta H_2})^{-1} \mathrm{Tr}_2\, \mathrm{e}^{-\beta H}$$

- In the uncoupled system: $W(\beta) = \mathrm{e}^{-\beta H_1}$.
- Effective partition function: $Z(\beta) = \mathrm{Tr}\, W(\beta) = \dfrac{\mathrm{Tr}\ \mathrm{e}^{-\beta H}}{\mathrm{Tr}\ \mathrm{e}^{-\beta H_2}}$.

Effective description of a subsystem

$$H = H_1 \otimes 1 + 1 \otimes H_2 + H_{\mathrm{I}}, \quad \text{auf } \mathcal{H}_1 \otimes \mathcal{H}_2$$

- $\mathcal{H}_1$ Hilbert space of the small system, $\mathcal{H}_2$ HS of the large one.
- Assume: $\mathrm{Tr}\ \mathrm{e}^{-\beta H}$ exists, and so do those of H_1, H_2.
- Assume: The large system is in thermal equilibrium and is not influenced by the small one (heat bath).
- The effective (un-normed) density matrix for the small system is then given by

$$W(\beta) := (\mathrm{Tr}\ \mathrm{e}^{-\beta H_2})^{-1} \mathrm{Tr}_2\, \mathrm{e}^{-\beta H}$$

- In the uncoupled system: $W(\beta) = \mathrm{e}^{-\beta H_1}$.
- Effective partition function: $Z(\beta) = \mathrm{Tr}\, W(\beta) = \dfrac{\mathrm{Tr}\ \mathrm{e}^{-\beta H}}{\mathrm{Tr}\ \mathrm{e}^{-\beta H_2}}$.
- Idea: the inverse Laplace transform of $Z(\beta)$ is the effective measure of states of the open small system.
- But for this, it has to be a positive measure on $\mathbb{R}$.

The limit of an infinitely large system

$$H = H_1 \otimes 1 + 1 \otimes H_2 + H_{\mathrm{I}}, \quad \text{in } \mathcal{H}_1 \otimes \mathcal{H}_2$$

- In our case, $\mathrm{e}^{-\beta H_2}$ is not trace class.
- Spectral discretizations: $H_{2,n}, H_n$.
- Define

$$Z_n(\beta) = \frac{\mathrm{Tr}\ \mathrm{e}^{-\beta H_n}}{\mathrm{Tr}\ \mathrm{e}^{-\beta H_{2,n}}}.$$

The limit of an infinitely large system

$$H = H_1 \otimes 1 + 1 \otimes H_2 + H_\mathrm{I}, \quad \text{in } \mathcal{H}_1 \otimes \mathcal{H}_2$$

- In our case, $\mathrm{e}^{-\beta H_2}$ is not trace class.
- Spectral discretizations: $H_{2,n}, H_n$.
- Define

$$Z_n(\beta) = \frac{\mathrm{Tr}\ \mathrm{e}^{-\beta H_n}}{\mathrm{Tr}\ \mathrm{e}^{-\beta H_{2,n}}}.$$

- We will show that $\lim_{n\to\infty} Z_n$ exists, and that the inverse Laplace transform is a positive Borel measure μ.
- Interpretation: μ is the **effective measure of states**:

$$\mu^{(\beta)} = \frac{1}{Z(\beta)} \mathrm{e}^{-\beta(\cdot)} \mu$$

determines the probability for energy measurements at temperature $1/\beta$.
- The Lebesgue-density of μ is the **effective density of states**.

Pauli-Fierz model: dipole approximation

$$H = (H_{\mathrm{p}} + H_{\mathrm{r}}) \otimes 1 + 1 \otimes H_{\mathrm{f}} + H_{\mathrm{I}} \text{ in } L^2(\mathbb{R}^3) \otimes \mathcal{F}^{\otimes 2}$$

with

$$H_{\mathrm{p}} = -\hbar^2 \frac{m}{2} \eta^2 \Delta_q + \frac{1}{2m} q^2, \qquad \text{particle Hamiltonian in } L^2(\mathbb{R}^3),$$

$$H_{\mathrm{f}} = H_{\mathrm{f},1} \otimes 1 + 1 \otimes \mathrm{H}_{\mathrm{f},2} \text{ and } \mathrm{H}_{\mathrm{f},\sigma} = \hbar \int \omega(\mathrm{k}) \mathrm{a}^*(\mathrm{k},\sigma) \mathrm{a}(\mathrm{k},\sigma) \, \mathrm{dk}.$$

Furthermore, $H_{\mathrm{I}} = H_{\mathrm{I},1} \otimes 1 + 1 \otimes H_{\mathrm{I},2}$ with

$$H_{\mathrm{I},\sigma} = \frac{e}{m} \int \chi_c(k) \sqrt{\frac{\hbar}{4\pi^2 \omega(k)}} (q \cdot u_\sigma(k)) \Big(a^*(k,\sigma) + a(k,\sigma) \Big) \mathrm{d}k,$$

and UV-cutoff $\chi_c = 1_{\{|k| < C\}}$, $\omega(k) = c|k|$, c speed of light.

H_{r} in $L^2(\mathbb{R}^3)$ contains mass and energy renormalisation.

Pauli-Fierz model: Spectral discretization

- For $N \in \mathbb{N}$ let $\Lambda_j,\, j \in \mathbb{N}$ be the half-open cube with volume $V = N^{-3}$ and corners in $(\frac{1}{N}\mathbb{Z})^3 \subset \mathbb{R}^3$.
- Orthogonal projections:

$$P_N(j) : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \quad f \mapsto \langle h_j, f \rangle h_j \text{ mit } h_j := \frac{1}{\sqrt{V}} 1_{\Lambda_j}.$$

Pauli-Fierz model: Spectral discretization

- For $N \in \mathbb{N}$ let Λ_j, $j \in \mathbb{N}$ be the half-open cube with volume $V = N^{-3}$ and corners in $(\frac{1}{N}\mathbb{Z})^3 \subset \mathbb{R}^3$.
- Orthogonal projections:

$$P_N(j) : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \quad f \mapsto \langle h_j, f \rangle h_j \text{ mit } h_j := \frac{1}{\sqrt{V}} 1_{\Lambda_j}.$$

- Put $J_N = \{j \in \mathbb{N} : \Lambda_j \cap B(0, N) \neq \emptyset\}$.
- $P_N = \sum_{j \in J_N} P_N(j)$ is also an orthogonal projection.
- Let $\boldsymbol{P}_N$ be the second quantisation of P_N. $\boldsymbol{P}_N$ ist also OP.

Pauli-Fierz model: Spectral discretization

- For $N \in \mathbb{N}$ let $\Lambda_j,\ j \in \mathbb{N}$ be the half-open cube with volume $V = N^{-3}$ and corners in $(\frac{1}{N}\mathbb{Z})^3 \subset \mathbb{R}^3$.
- Orthogonal projections:

$$P_N(j) : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3), \quad f \mapsto \langle h_j, f \rangle h_j \text{ mit } h_j := \frac{1}{\sqrt{V}} 1_{\Lambda_j}.$$

- Put $J_N = \{j \in \mathbb{N} : \Lambda_j \cap B(0,N) \neq \emptyset\}$.
- $P_N = \sum_{j \in J_N} P_N(j)$ is also an orthogonal projection.
- Let $\boldsymbol{P}_N$ be the second quantisation of P_N. $\boldsymbol{P}_N$ ist also OP.
- Put

$$H_{\mathrm{f},N} := (\boldsymbol{P}_N \otimes \boldsymbol{P}_N)\, H_{\mathrm{f}}\, (\boldsymbol{P}_N \otimes \boldsymbol{P}_N),$$
$$H_N := (1 \otimes \boldsymbol{P}_N \otimes \boldsymbol{P}_N)\, H\, (1 \otimes \boldsymbol{P}_N \otimes \boldsymbol{P}_N).$$

- **Thm:** $H_{\mathrm{f},N}$ and H_N are spectral discretizations of H_{f} und H.

Effective partition function: finite UV cutoff

Theorem:
$\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_N}$ and $\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_{\mathrm{f},N}}$ exist for all $N \in \mathbb{N}$ and all $\beta > 0$.
$Z(\beta;\gamma) := \lim_{N\to\infty}(\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_N})/(\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_{\mathrm{f,N}}})$ exists for all $\beta > 0$, and

$$Z(\beta;\gamma) = \left[2\pi\rho\ \mathrm{e}^{-2\rho\ln(1+\gamma)\sin\varphi}\prod_{l=1}^{\infty}\left(1+\frac{\rho^2}{l^2}+\frac{4}{\pi}\frac{\rho}{l}\sin(\varphi)\arctan\left(\gamma\frac{\rho}{l}\right)\right)\right]^{-3}.$$

Above, $\sin\phi \sim e,\ \ \rho \sim \beta,\ \ \gamma \sim C$.

Effective partition function: finite UV cutoff

Theorem:
$\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_N}$ and $\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_{\mathrm{f},N}}$ exist for all $N \in \mathbb{N}$ and all $\beta > 0$.
$Z(\beta;\gamma) := \lim_{N\to\infty}(\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_N})/(\mathrm{Tr}\ \mathrm{e}^{-\frac{\beta}{\hbar}H_{\mathrm{f,N}}})$ exists for all $\beta > 0$, and

$$Z(\beta;\gamma) = \left[2\pi\rho\ \mathrm{e}^{-2\rho\ln(1+\gamma)\sin\varphi}\prod_{l=1}^{\infty}\left(1+\frac{\rho^2}{l^2}+\frac{4}{\pi}\frac{\rho}{l}\sin(\varphi)\arctan\left(\gamma\frac{\rho}{l}\right)\right)\right]^{-3}.$$

Above, $\sin\phi \sim e,\ \ \rho \sim \beta,\ \ \gamma \sim C$.

Sketch of proof: Write H_N as a system of $n = 2|J_N| + 3$ coupled quantum oscillators; potential $\sum_{i,j} A_{ij}X_iX_j$; $A > 0$ matrix with entries λ_j. Use

$$\mathrm{Tr}\ \mathrm{e}^{-\beta H} = \prod_{i=1}^{n}\left(2\sinh(\frac{\beta}{2}\sqrt{\lambda_i})\right)^{-1} = \det\left(2\ \sinh\left(\frac{\beta}{2}A^{\frac{1}{2}}\right)\right)^{-1} =$$

$$= \beta^{-n}\det(A)^{-\frac{1}{2}}\prod_{l=1}^{\infty}\det\left(I_n + (\frac{\beta}{2\pi l})^2 A\right)^{-1}.$$

Effective density of states without UV cutoff

Theorem:

For all $\beta > 0$, $Z(\beta) := \lim_{\gamma\to\infty} Z(\beta;\gamma)$ exists, and

$$Z(\beta) = \Big[\frac{\rho}{2\pi}\,\mathrm{e}^{-2\rho\ln(\rho)\sin\varphi}\,\big|\Gamma(\mathrm{i}\rho\,\mathrm{e}^{-\mathrm{i}\varphi})\big|^2\Big]^3.$$

Also, $\beta \mapsto Z(\beta)$ is the Laplace transform of a positive measure.

Effective density of states without UV cutoff

Theorem:

For all $\beta > 0$, $Z(\beta) := \lim_{\gamma\to\infty} Z(\beta;\gamma)$ exists, and

$$Z(\beta) = \Big[\frac{\rho}{2\pi}\,\mathrm{e}^{-2\rho\ln(\rho)\sin\varphi}\,\big|\Gamma(\mathrm{i}\rho\,\mathrm{e}^{-\mathrm{i}\varphi})\big|^2\Big]^3 .$$

Also, $\beta \mapsto Z(\beta)$ is the Laplace transform of a positive measure.

Sketch of proof: Convergence and computation of the limit with hard analysis. For the inverse Laplace transform: Using Binet's formula,

$$\ln\Gamma(z) = \int_0^\infty \frac{\mathrm{e}^{-tz}}{t}\left(\frac{1}{1-\mathrm{e}^{-t}} - \frac{1}{t} - \frac{1}{2}\right)\mathrm{d}t + \frac{\ln(2\pi)}{2} + (z - \tfrac{1}{2})\ln(z) - z$$

we find, with $\tau = \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\varphi}\,t$ and $t_\varphi := 6(\sin\varphi + (\frac{\pi}{2} - \varphi)\cos\varphi)$,

$$\ln Z(\beta) = \int_0^\infty \mathrm{e}^{-t\rho}\,g(t)\,\mathrm{d}t - t_\varphi\,\rho, \quad g(t) := \frac{6}{t}\,\mathrm{Re}\left(\frac{1}{1-\mathrm{e}^{-\tau}} - \frac{1}{\tau} - \frac{1}{2}\right).$$

We show $g(t) \geqslant 0$ for $t \geqslant 0$. Thus $\ln Z(\beta)$ is completely monotone, and so is $Z(\beta)$.

Effective density of states: inverse Laplace tranfsorm

$$Z(\beta) = \Big[\frac{\rho}{2\pi} \, \mathrm{e}^{-2\rho \ln(\rho) \sin\varphi} \, \big| \Gamma(\mathrm{i}\rho \, \mathrm{e}^{-\mathrm{i}\varphi}) \big|^2 \Big]^3 .$$

Effective density of states: inverse Laplace tranfsorm

$$Z(\beta) = \mathrm{e}^{\int_0^\infty \mathrm{e}^{-t\rho} \, g(t) \, \mathrm{d}t \; - t_\varphi \, \rho}, \quad g(t) := \frac{6}{t} \, \mathrm{Re} \left(\frac{1}{1 - \mathrm{e}^{-\tau}} - \frac{1}{\tau} - \frac{1}{2} \right).$$

Effective density of states: inverse Laplace tranfsorm

$$Z(\beta) = \mathrm{e}^{\int_0^\infty \mathrm{e}^{-t\rho} g(t)\,\mathrm{d}t \; - t_\varphi \rho}, \quad g(t) := \frac{6}{t}\,\mathrm{Re}\,\left(\frac{1}{1 - \mathrm{e}^{-\tau}} - \frac{1}{\tau} - \frac{1}{2} \right).$$

- Crucial observation: $Z(\beta) = Y(\rho)\,\mathrm{e}^{-t_\varphi \rho}$, and

$$Y(\rho) = \exp \mathfrak{L} g(\rho) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \mathfrak{L} g^{*n}(\rho).$$

- Above, $h * k\,(x) = \int_0^x h(t)k(x-t)\,\mathrm{d}t$.

Effective density of states: inverse Laplace tranfsorm

$$Z(\beta) = \mathrm{e}^{\int_0^\infty \mathrm{e}^{-t\rho}\, g(t)\,\mathrm{d}t \; - t_\varphi\,\rho}, \quad g(t) := \frac{6}{t}\,\mathrm{Re}\,\left(\frac{1}{1 - \mathrm{e}^{-\tau}} - \frac{1}{\tau} - \frac{1}{2}\right).$$

- Crucial observation: $Z(\beta) = Y(\rho)\,\mathrm{e}^{-t_\varphi \rho}$, and

$$Y(\rho) = \exp \mathfrak{L}g(\rho) = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \mathfrak{L}g^{*n}(\rho).$$

- Above, $h * k\,(x) = \int_0^x h(t)k(x-t)\,\mathrm{d}t$.
- Thus

$$\mathfrak{L}^{-1} Y = \delta_0 + \sum_{n=1}^{\infty} \frac{1}{n!}\, g^{*n}$$

- Up to translation and scaling, this is the effective density of states!

Effective density of states: complex structure

$$\varrho = \mathfrak{L}^{-1} Y = \delta_0 + \sum_{n=1}^{\infty} \frac{1}{n!} g^{*n}$$

Lemma: g is meromorphic with simple poles at

$$q_j = 2\pi j \, \mathrm{e}^{-\mathrm{i}\varphi} \quad \text{und} \quad \overline{q_j} = 2\pi j \, \mathrm{e}^{\mathrm{i}\varphi}, \qquad j \in \mathbb{Z} \setminus \{0\}.$$

The residues are $\mathrm{Res}(g; q_j) = \frac{3\mathrm{i}}{2\pi j}$, $\mathrm{Res}(g; \overline{q_j}) = \frac{-3\mathrm{i}}{2\pi j}$.

A first analysis of the singularities of the convolution products leads to

Theorem: The effective density of states ϕ is continuous and positive for $\omega \geqslant \omega_\varphi$. ϕ is real analytic, and can be continued to an analytic function up to singularities at the points

$$p_j = \omega_\varphi + j\eta \, \mathrm{e}^{-\mathrm{i}\varphi} \text{ and } \overline{p_j} = \omega_\varphi + j\eta \, \mathrm{e}^{\mathrm{i}\varphi}, \qquad j \in \mathbb{Z} \setminus \{0\},$$

and branch cuts along $z = \omega_\varphi + s \, \mathrm{e}^{\pm \mathrm{i}\varphi}$ for $s \in \mathbb{R}$, $|s| \geqslant \eta$.

Effective density of states: Lorenz profiles

Define the normed Lorenz profile $\ell_j(z) := \frac{-1}{2\pi \mathrm{i}(z-p_j)} + \frac{1}{2\pi \mathrm{i}(z-\overline{p_j})}$.

Theorem: Let $N \in \mathbb{N}$ and $z = \omega_\varphi + s\,\mathrm{e}^{\mathrm{i}\chi}$ for $0 < s < N\eta$ and $|\chi| < \frac{\pi}{2}$. Then

$$\phi(z) = \begin{cases} \sum_{j=1}^{N} \binom{j+2}{2} \ell_j(z) + h_N(z) & \text{for } |\chi| < \varphi, \\ -\sum_{j=1}^{3} (-1)^j \binom{3}{j} \ell_j(z) + \tilde{h}_N(z) & \text{for } |\chi| > \varphi. \end{cases}$$

h_N and $\tilde{h}_N$ are analytic up to singularities at p_j, $\overline{p_j}$ and cuts along $z = \omega_\varphi + s\,\mathrm{e}^{\pm\mathrm{i}\varphi}$, $s \geqslant \eta$. Moreover, there exists a constant $C = C(N)$, so that h_N (and also $\tilde{h}_N$) satisfies the inequality $|h_N(z)| \leqslant C(1 + |\ln(\varphi - |\chi|)|^{\eta N})$ for $|\chi| < \varphi$.

Effective density of states: Lorenz profiles

Define the normed Lorenz profile $\ell_j(z) := \frac{-1}{2\pi \mathrm{i}(z-p_j)} + \frac{1}{2\pi \mathrm{i}(z-\overline{p_j})}$.

Theorem: Let $N \in \mathbb{N}$ and $z = \omega_\varphi + s\,\mathrm{e}^{\mathrm{i}\chi}$ for $0 < s < N\eta$ and $|\chi| < \frac{\pi}{2}$. Then

$$\phi(z) = \begin{cases} \displaystyle\sum_{j=1}^{N} \binom{j+2}{2} \ell_j(z) + h_N(z) & \text{for } |\chi| < \varphi, \\ \displaystyle -\sum_{j=1}^{3} (-1)^j \binom{3}{j} \ell_j(z) + \tilde{h}_N(z) & \text{for } |\chi| > \varphi. \end{cases}$$

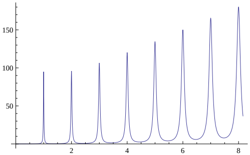
h_N and $\tilde{h}_N$ are analytic up to singularities at p_j, $\overline{p_j}$ and cuts along $z = \omega_\varphi + s\,\mathrm{e}^{\pm \mathrm{i}\varphi}$, $s \geqslant \eta$. Moreover, there exists a constant $C = C(N)$, so that h_N (and also $\tilde{h}_N$) satisfies the inequality $|h_N(z)| \leqslant C(1 + |\ln(\varphi - |\chi|)|^{\eta N})$ for $|\chi| < \varphi$.

Compare with $\mu_0 = \sum_{j=0}^{\infty} \binom{j+2}{2} \delta_{(j+3/2)\eta}$ (uncoupled oscillator).

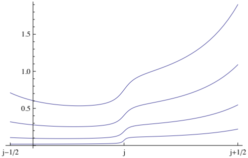
Summary and open problems

- The effective density of states close to $\mathbb{R}$ is

$$\phi(z) \approx \sum_j \binom{j+2}{2} \ell_j(z).$$



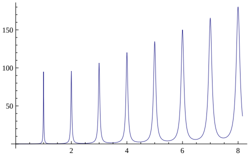
- The mass in each Lorenz profile corresponds to the multiplicity of the eigenvalues of the uncoupled oscillator.
- Complex singularities are first order poles plus a small perturbation.
- **Definition:** resonances of the effective system are the complex singularities of the effective density of states.
- Metastability: $Z(\beta)^{-1}\,\mathrm{e}^{-\beta\cdot}\,\mu$ gives the probability for energy measurements at temperature $1/\beta$.



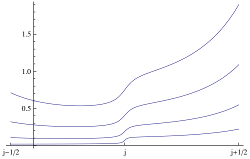
Summary and open problems

- The effective density of states close to $\mathbb{R}$ is

$$\phi(z) \approx \sum_j \binom{j+2}{2} \ell_j(z).$$



- The mass in each Lorenz profile corresponds to the multiplicity of the eigenvalues of the uncoupled oscillator.
- Complex singularities are first order poles plus a small perturbation.



- **Definition:** resonances of the effective system are the complex singularities of the effective density of states.
- Metastability: $Z(\beta)^{-1} \, \mathrm{e}^{-\beta \cdot} \, \mu$ gives the probability for energy measurements at temperature $1/\beta$.

Open questions:

- how about other systems: spin-boson, hydrogen atom, ...
- Connection with Hunzikers theory of resonances (Bach/Fröhlich/Sigal).
- Connection with works about return to equilibrium (Merkli/Sigal).