Thermal Ionization for Short-Range Potentials

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Model

- Atom: Schrödinger operator $H_{\mathrm{p}} = -\Delta + V$ on $\mathcal{H}_{\mathrm{p}} := L^2(\mathbb{R}^3)$
- Quantized Field: Weyl algebra $\mathfrak{W}$ over $L^2(\mathbb{R}^3, (1 + |k|^{-1}))$
- GNS Representation w.r.t. a density matrix on $\mathcal{L}(\mathcal{H}_{\mathrm{p}})$ and Araki-Woods representation for inverse temperature $\beta > 0$:

$$\pi^\beta \colon \mathcal{L}(\mathcal{H}_{\mathrm{p}}) \otimes \mathfrak{W} \to \mathcal{L}(\mathcal{H})$$
$$\mathcal{H} := \mathcal{H}_{\mathrm{p}} \otimes \mathcal{H}_{\mathrm{p}} \otimes \mathfrak{F}(L^2(\mathbb{R}^3)) \otimes \mathfrak{F}(L^2(\mathbb{R}^3))$$

$\rightarrow$ von-Neumann algebra $\mathfrak{M}_\beta := (\operatorname{ran} \pi^\beta)'' \subseteq \mathcal{L}(\mathcal{H})$

- **Liouvillian:** self-adjoint (unbounded) operator L_λ on $\mathcal{H}$
- time evolution $\sigma_{t,\lambda}(A) := e^{\mathrm{i}tL_\lambda} A e^{-\mathrm{i}tL_\lambda}$, $t, \lambda \in \mathbb{R}$
- $(\mathfrak{M}_\beta, \sigma_{t,\lambda})$ W^*-dynamical system

Question: $\ker L_\lambda = \{0\} \Rightarrow$ no time-invariant normal states on $\mathfrak{M}_\beta$ (physical interpretation as ionization)

$\rightarrow$ Proof via spectral theory!

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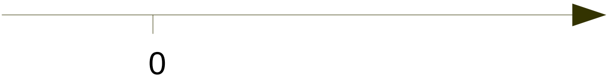

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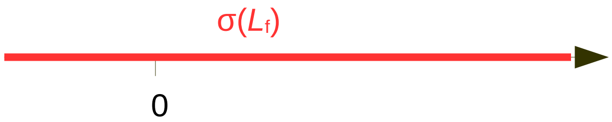

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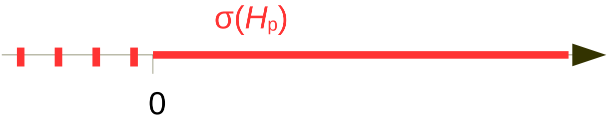

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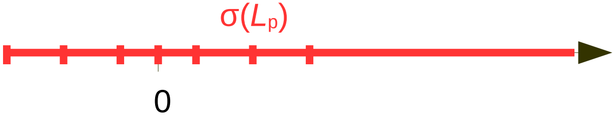

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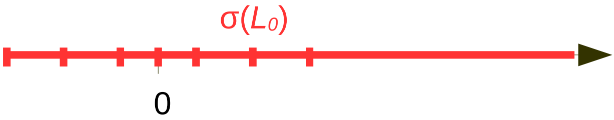

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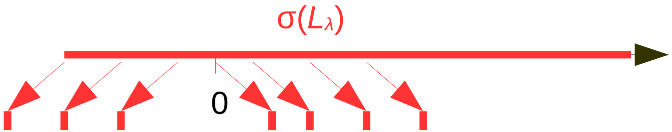

Hypotheses I

Hypothesis (A) on the atom

1. $V \in C_c^\infty(\mathbb{R}^3) \Rightarrow$ finitely many eigenvalues
2. If $\psi \in L^2(\mathbb{R}^3)$ satisfies

$$\psi(x) = -\frac{1}{4\pi} \int \frac{|V(x)|^{1/2} V(y)^{1/2}}{|x-y|} \psi(y) \mathrm{d}y, \quad \text{for almost all } x \in \mathbb{R}^3,$$

where $V^{1/2} := |V|^{1/2} \operatorname{sgn} V$, then $\psi = 0$.

- (2) excludes bound and 'half-bound' states at energy zero
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Hypothesis (B) on the interaction

$G(k)$ multiplication with a function $x \mapsto G(k)(x)$

1. 3 times differentiable in $|k|$, infinitely often in x
2. UV cutoff (superpolynomial decay for large k)
3. sufficient IR regularity ($\sim |k|^p$, $p \in \{-1/2, 1/2, 3/2\} \cup (2, \infty)$)
4. Spatial decay (in x) like a Schwartz function

Example (non-relativistic QED)

$$G(k)(x) = \kappa(|k|)e^{ikx}\chi(x), \qquad k, x \in \mathbb{R}^3,$$

$0 \neq \chi \in \mathcal{S}(\mathbb{R}^3)$, and κ non-vanishing function on $\mathbb{R}_+$, satisfying the UV and IR conditions

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Main Result

Definition (Levelshift operator)

For $E \in \sigma_{\mathrm{d}}(H_{\mathrm{p}})$, $\varepsilon > 0$ let

$$F_{G,\beta}(E,\varepsilon) := \int_{\mathbb{R}^3} \frac{1}{1-e^{-\beta\omega(k)}} G(k)^* \frac{P_{\mathrm{ess}}(H_{\mathrm{p}})}{(H_{\mathrm{p}} - E + \omega(k))^2 + \varepsilon^2} G(k) \mathrm{d}k \geq 0$$

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In example: $\inf_{\beta>0} \gamma_\beta(\varepsilon) > 0$ for all $\varepsilon > 0$

Theorem (Hasler, S. '21)

Assume that Hypotheses (A) and (B) are satisfied. Let $\beta_0 > 0$ and $\varepsilon > 0$. Then there exists $C > 0$ such that zero is not an eigenvalue of L_λ for all $\beta \geq \beta_0$ and $0 < |\lambda| < C \min\{1, \gamma_\beta(\varepsilon)^2\}$. In particular, there are no $\sigma_{t,\lambda}$-invariant normal states on $\mathfrak{M}_\beta$.

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Positive Commutators - Basic Principle

Goal: Self-adjoint operator L has no eigenvalues.

A self-adjoint operator (*conjugate operator*) and E eigenvalue with eigenvector ψ:

$$\langle \psi, [L, A]\psi \rangle = \langle L\psi, A\psi \rangle - \langle A\psi, L\psi \rangle = E \langle \psi, A\psi \rangle - E \langle A\psi, \psi \rangle = 0$$

$\Rightarrow$ self-adjoint operator $\mathrm{i}[L, A]$ has eigenvalue zero
But if $\mathrm{i}[L, A] > 0 \Rightarrow$ **Contradiction!**

Two major challenges:

- Positivity
- Virial theorem

In our case on the atom: generator of dilations in the space of scattering functions

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In our case on the atom: generator of dilations in the space of scattering functions

Positive Commutators - Basic Principle

Goal: Self-adjoint operator L has no eigenvalues.

A self-adjoint operator (*conjugate operator*) and E eigenvalue with eigenvector ψ:

$$\langle\psi, [L, A]\psi\rangle = \langle L\psi, A\psi\rangle - \langle A\psi, L\psi\rangle = E\langle\psi, A\psi\rangle - E\langle A\psi, \psi\rangle = 0$$

$\Rightarrow$ self-adjoint operator $\mathrm{i}[L, A]$ has eigenvalue zero
But if $\mathrm{i}[L, A] > 0 \Rightarrow$ **Contradiction!**

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Previous work in this setting:

- (Fröhlich, Merkli '04) - for abstract operator H_{p}
  - diagonal w.r.t. energy and with one bound state
  - abstract virial theorem
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Related problem: *Return to Equilibrium*

- if $\operatorname{tr} e^{-\beta H_{\mathrm{p}}} < \infty$ (no continuous spectrum in H_{p}, e.g. $\mathcal{H}_{\mathrm{p}}$ finite-dimensional) $\Rightarrow$ Gibbs state exists
- $\dim \ker L_\lambda = 1$ - eigenvalue zero corresponds to equilibrium state
- many papers by (Jakšic, Pillet '95 –'97), (Bach, Fröhlich, Sigal '00), (Merkli '01), (Dereziński, Jakšic '01,'03) and others

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