Quantum Statistical Mechanics

$\psi_t \in \mathcal{H} = L^2\left(\mathbb{R}^{3N}, (\mathbb{C}^d)^{\otimes N}\right)$ Hilbert space

$$\psi_{\dots s_i \dots s_j \dots}(\dots q_i \dots q_j \dots) =$$

$$\gamma\, \psi_{\dots s_j \dots s_i \dots}(\dots q_j \dots q_i \dots)$$

$$\gamma = \begin{cases} +1 & \text{bosons, spin } 0, 1, 2, \dots \\ -1 & \text{fermions, spin } \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \dots \end{cases}$$

$$S(\mathcal{H}) = \{\psi \in \mathcal{H} : \|\psi\| = 1\}$$ unit sphere

$\hbar = 1$

$$i \frac{d\psi_t}{dt} = H\psi_t$$ Schrödinger eq.

$$\Rightarrow \quad \psi_t = e^{-iHt}\psi_0 = U_t \psi_0$$

unitary, i.e., bijective and

$$\langle U_t \phi | U_t \psi \rangle = \langle \phi | \psi \rangle$$

$\Leftrightarrow$ bij. and $U_t^{-1} = U_t^{+}$.

$H = H^{+}$ self-adjoint.

$\{ U : \mathcal{H} \to \mathcal{H} \text{ unitary} \} = \mathcal{U}(\mathcal{H})$

unitary group.

$\{ \phi_n : n \in \mathbb{N} \}$ ONB of $\mathcal{H}$.

$\{ U\phi_n : n \in \mathbb{N} \}$ another ONB

$$\{ \text{ONBs} \} \xleftrightarrow{1:1} \mathcal{U}(\mathcal{H})$$

Haar measure

uniform distr. over $\mathcal{U}(\mathcal{H})$

and thus over $\{\text{ONBs}\}$.

group G, $\mu(gB) = \mu(B)$ $B \subseteq G$

invariance under left multiplication

$\forall g \in G$

$\mu(Bg) = \mu(B)$ right

locally compact

$G = U(\mathcal{H})$ locally compact $\iff$ $\dim \mathcal{H} < \infty$.

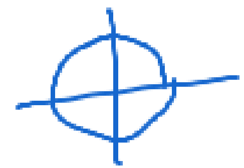
compact $\iff$

<u>Thm</u>

G locally comp. $\Rightarrow$ $\exists_1$ μ left inv.

& regularity conditions, called left Haar measure.

G compact $\cancel{\iff}$ $\Rightarrow$ Haar measure is left <u>AND</u> right inv., AND finite.

<u>Ex</u> $U(1)$, $U(n) = U(\mathbb{C}^n)$. 

Alfred Haar (1885 - 1933) 1933

Adolf Hurwitz (1859 - 1919) 1897

uniform distr. over $\{ONB_s\}$: $(\dim \mathcal{H} < \infty)$

1) choose $\phi_1 \in \mathcal{S}(\mathcal{H})$

$$\phi_1 \sim \mathcal{U}_{\mathcal{S}(\mathcal{H})}$$

2) $(\mathbb{C}\phi_1)^\perp$

$$\mathcal{K}^\perp = \{\psi \in \mathcal{H} : \forall x \in \mathcal{K} \ \langle \psi | x \rangle = 0\}$$

choose $\phi_2 \sim \mathcal{U}_{\mathcal{S}((\mathbb{C}\phi_1)^\perp)}$

3) $\phi_3 \sim \mathcal{U}_{\mathbb{S}}(\mathrm{span}\{\phi_1, \phi_2\}^{\perp})$

$\vdots$

$\dim \mathcal{H} = d$) $\phi_d \sim \mathcal{U}_{\mathbb{S}}(\mathrm{span}\{\phi_1 \dots \phi_{d-1}\}^{\perp})$.

Then $\{\phi_1 \dots \phi_d\} \sim \mathcal{U}_{ONB} \longleftrightarrow$ Haar measure.

Schrödinger Hamiltonians

$$H = -\frac{1}{2m}\Delta + V,$$

compact 3-volume $\Lambda \subset \mathbb{R}^3$

b.c. or compact 3-manifold Λ.

<u>Rule</u> compact Λ, "reasonable" interactions

$\Longrightarrow$ H has purely discrete spectrum

and $E_1 \leq E_2 \leq E_3 \leq \dots \longrightarrow \infty$

and dim eigenspace$(E_n) < \infty$.

Ergodic Components

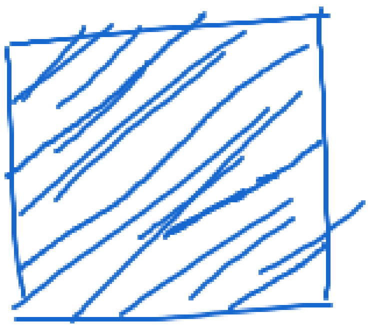
Suppose H has pure point spectrum,

$$H = \sum_{\alpha} \underset{\substack{\uparrow \\ \text{e.value}}}{E_\alpha} |\alpha\rangle\langle\alpha| \quad \leftarrow \text{e. vector} \quad \phi_\alpha = |\alpha\rangle$$

$$\psi_0 = \sum_{\alpha} c_\alpha |\alpha\rangle$$

$$\psi_t = \sum_{\alpha} \overbrace{e^{-itE_\alpha} c_\alpha}^{c_\alpha(t)} |\alpha\rangle$$

$|c_\alpha|$ conserved quantity.



generically, ergodic on the torus $\{ \sum c_\alpha |\alpha\rangle :$
$|c_\alpha| = \text{given} \}$

Main theorem about POVMs

$\forall$ experiment with outcome Z,

$$\mathbb{P}(Z=z) = \langle\psi|E_z|\psi\rangle$$

$$\text{POVM}\begin{cases}\text{with } E_z = E_z^\dagger,\ \ \text{spectrum}(E_z) \subseteq [0,1] \\ E_z \geq 0,\ \ \sum_z E_z = I\end{cases}$$

positive-operator-valued measure

<u>Random wave fct</u> $\psi \in S(\mathcal{H})$

prob. measure μ over $S(\mathcal{H})$

$$\mathbb{P}(Z=z) = \int_{S(\mathcal{H})} \mu(d\psi) \langle\psi|E_z|\psi\rangle$$

$$= \int_{S(\mathcal{H})} \mu(d\psi)\, \mathrm{tr}\left(E_z |\psi\rangle\langle\psi|\right)$$

$$= \mathrm{tr}\left(\int_{S(\mathcal{H})} \mu(d\psi)\, E_z |\psi\rangle\langle\psi|\right)$$

$$= \mathrm{tr}\left(E_z \rho_\mu\right)$$

with $\rho_\mu = \int_{S(\mathcal{H})} \mu(d\psi) \; |\psi\rangle\langle\psi|$

density matrix of μ.

<u>Thm</u> For every prob measure μ on $S(\mathcal{H})$,

$\exists \rho_\mu$.

Properties: $\operatorname{tr} \rho_\mu = 1$, $\rho_\mu \geq 0$, $\rho_\mu^\dagger = \rho_\mu$

$$\| \rho_1 - \rho_2 \|_{tr}$$

$$\|T\|_{tr} := tr\,|T| := tr\sqrt{T^\dagger T}$$

$T \in$ trace class $\Leftrightarrow \|T\|_{tr} < \infty$.

distinguish ρ_1, ρ_2

$$\mathbb{P}_1(Z=z) - \mathbb{P}_2(Z=z) = tr(\rho_1 E_z) - tr(\rho_2 E_z)$$

$$= tr\left((\rho_1 - \rho_2) E_z\right).$$

$$T = \rho_1 - \rho_2 = \sum_\alpha \tau_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$$

$$\sum_\alpha \tau_\alpha = 0 \,, \quad E_2 = \sum_\alpha \varepsilon_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$$

$$P_1 - P_2 = \mathrm{tr}(T E_2) = \sum_\alpha \tau_\alpha \varepsilon_\alpha$$

$$\text{maximal} = \sum_{\alpha : \tau_\alpha > 0} \tau_\alpha$$

$$\|T\|_{tr} = \sum_\alpha |\tau_\alpha| = \sum_{\tau_\alpha>0} \tau_\alpha + \overbrace{\sum_{\tau_\alpha<0} -\tau_\alpha}^{= \sum_{\tau_\alpha>0} \tau_\alpha} = 2 \sum_{\tau_\alpha>0} \tau_\alpha$$

Thus, $\max\limits_{\text{experiments}} \mathbb{P}_1 - \mathbb{P}_2 = \frac{1}{2} \| \rho_1 - \rho_2 \|_{tr}$.

Reduced density matrix

$\psi \in \mathcal{H}_a \otimes \mathcal{H}_b$ bipartite

experiment on a: $E_z \otimes I_b$

$\mathbb{P}(Z=z) = \langle \psi | E_z \otimes I_b | \psi \rangle = \mathrm{tr}\left(E_z \rho_a \right)$

with $\rho_a = \mathrm{tr}_b \, |\psi\rangle\langle\psi|$ partial trace so $\rho_a : \mathcal{H}_a \to \mathcal{H}_a$

$\rho_a \geq 0, \quad \operatorname{tr} \rho_a = 1.$