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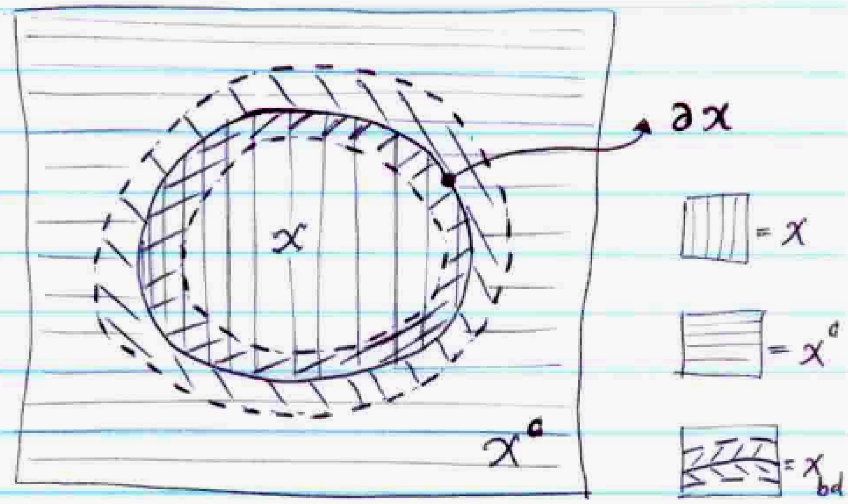
"Approximating Ground-States of Gapped Hamiltonians"

① Relevant picture:



② THEOREM: $\| P_{\mathcal{X}_{bd}(3\ell)} P_{\mathcal{X}} P_{\mathcal{X}^c} - P_0 \| \leq C_{R,J} |\partial\mathcal{X}|^2 \, \ell^{7/2} \, e^{-\ell/2\xi}$

with $\frac{1}{\xi} = \frac{1}{2}\left(\frac{\mu\gamma^2}{\mu^2 v^2 + \gamma^2}\right)$, some constant, $\mu \geq 2\mu_0$.

③ Explaining ...: (i) $P_{\mathcal{X}} \in \mathcal{A}_{\mathcal{X}}$ and $P_{\mathcal{X}^c} \in \mathcal{A}_{\mathcal{X}^c}$, are projections and $P_{\mathcal{X}_{bd}} \in \mathcal{A}_{\mathcal{X}_{bd}(3\ell)}$ satisfies $\|P_{\mathcal{X}_{bd}}\| \leq 1$.

(ii) $P_{\mathcal{X}} \in \mathcal{A}_{\mathcal{X}}$ means $P_{\mathcal{X}}$ acts non-trivially on subset $\mathcal{X}$ of the space of interactions and is $\otimes \mathbb{1}$ everywhere else.

$\Rightarrow P_{\mathcal{X}} P_{\mathcal{X}^c} = P_{\mathcal{X}} \otimes P_{\mathcal{X}^c}$

(iii) $\mathcal{X}_{bd}(3\ell) = \{ s \in V : d(s, \partial\mathcal{X}) < 3\ell \}$.

Continue ③: (iv) Hamiltonian $H_V = \sum'_{Z \in V} \Phi(Z)$, satisfies $V \cong \mathbb{Z}^n$, $\operatorname{diam}(Z) > R \Rightarrow \Phi(Z) = 0$ and $\sup_{s \in V} \sum'_{Z \ni s} \|\Phi(Z)\| \leq J$.

(Finite range + finite strength interactions)

(v) H_V has unique g.s. $|\Psi_0\rangle$ with projection P_0 and spectral gap $\gamma > 0$.

(vi) v is the Lieb-Robinson velocity of H_V and depends only on R, J and $\mathbb{Z}^{(n)}$, while $\mu = \frac{1}{R}$ is the usual choice, since $v \sim e^{\mu R}$...

④ Useful Tools:

(i) Lieb-Robinson Bound: Let $A \in \mathcal{A}_X$, $B \in \mathcal{A}_Y$ with $X, Y \subset V$ and $X \cap Y = \phi$. Define the dynamics

$$\tau_t^{H_V}(A) = e^{itH_V} A e^{-itH_V}.$$ Then,

$$\|[\tau_t^{H_V}(A), B]\| \leq 2 \|A\| \cdot \|B\| \min\{|\partial X|, |\partial Y|\} \cdot \boxed{e^{-\frac{d(X,Y)}{R} + v|t|}}$$

(a) v is L-R velocity and looks like $\sim R^3 J$ for $\mathbb{Z}^2$

(b) $|\partial X| = \{s \in X : \exists Y \in V, s \in Y, Y \cap X^c \neq 0$ and $\Phi(Y) \neq 0\}$.

Continue ④ : (iii) Ground-state candidate :

$$P_0(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{i(H_v - E_0)t} e^{-\alpha t^2} dt$$

Let $H_v \Psi_m\rangle = E_m \Psi_m\rangle$, eigenvectors, with $E_m - E_0 \geq \gamma$, for $m \geq 1$.

Note that $\langle \Psi_m, (P_0(\alpha) - P_0) \Psi_n \rangle =$

$$\delta_{m,n} \left(\sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha t^2} e^{i(E_m - E_0)t} dt - \delta_{m,0} \right)$$

So, only $\langle \Psi_m, (P_0(\alpha) - P_0) \Psi_m \rangle \neq 0$, for $m \geq 1$.

But, then $\langle \Psi_m, (P_0(\alpha) - P_0) \Psi_m \rangle = e^{-(E_m - E_0)^2/4\alpha}$

$$\leq e^{-\gamma^2/4\alpha}, \text{ for } \alpha > 0.$$

Comments on energy selection: The use of the Gaussian $\sqrt{\frac{\alpha}{\pi}} e^{-\alpha t^2}$ is not the only choice for effective energy selection in Fourier space. In fact, one may use the so-called C^∞- bump functions (such as powers of the $\operatorname{sinc}(x) = \frac{\sin(\pi x)}{\pi x}$), to get exact truncation with no exponentially decaying tails ($e^{-\gamma^2/4\alpha}$).

The trade-off is in the use of Lieb-Robinson bounds later on.

Continue ④ : (iii) Energy selection:

Let $A \in \mathcal{A}_X$, $X \subset V$.

Define $$(A)(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} T_t^{H_V}(A)\, e^{-\alpha t^2}\, dt - \langle \Psi_0, A \Psi_0 \rangle$$

(a) $\langle \Psi_0, A(\alpha)\, \Psi_0 \rangle = 0$, since $\langle \Psi_0, T_t^{H_V}(A) \Psi_0 \rangle = \langle \Psi_0, A\, \Psi_0 \rangle$.

(b) $$\langle \Psi_m, A(\alpha)\, \Psi_0 \rangle \overset{m \neq 0}{=} \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{-\alpha t^2} e^{i(E_m - E_0)t}\, dt \; \langle \Psi_m, A\, \Psi_0 \rangle$$

$$= e^{-(E_m - E_0)^2/4\alpha} \langle \Psi_m, A\, \Psi_0 \rangle \quad \text{(from Gaussian F.T.)}$$

for any eigenvector $|\Psi_m\rangle$ of H_V : $H_V |\Psi_m\rangle = E_m |\Psi_m\rangle$, $m \neq 0$.

From $\langle \Psi_m, A(\alpha)\, \Psi_0 \rangle = e^{-(E_m - E_0)^2/4\alpha} \langle \Psi_m, A \Psi_0 \rangle$

$$\Rightarrow \langle \Psi_0, A(\alpha)\, \Psi_m \rangle\langle \Psi_m\, A(\alpha)\, \Psi_0 \rangle = e^{-(E_m - E_0)^2/2\alpha} \langle \Psi_0, A\, \Psi_m \rangle\langle \Psi_m\, A \Psi_0 \rangle$$

$$\Rightarrow \langle \Psi_0, A(\alpha)^2\, \Psi_0 \rangle = \sum_{m \geq 0} e^{-(E_m - E_0)^2/2\alpha} \langle \Psi_0, A\, P_m A \Psi_0 \rangle$$

$$\leq e^{-\gamma^2/2\alpha} \langle \Psi_0, A^2\, \Psi_0 \rangle$$

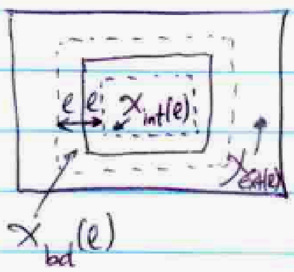
$$\Rightarrow \| A(\alpha)\, \Psi_0 \rangle \| \leq e^{-\gamma^2/4\alpha} \underbrace{\| A\, \Psi_0 \rangle \|}$$

For $A_0 = \langle \Psi_0, A \Psi_0 \rangle$, the above bound may be written $\|(A - A_0)\, \Psi_0 \rangle \|$.

Proof: ① Split $H_V = H^b_{X_{int}(\ell)} + H_{X_{bd}(\ell)} + H^b_{X_{ext}(\ell)}$

where $H^b_{X_{int}(\ell)} = \sum'_{Z \cap X_{int} \neq \phi} \Phi(Z)$, $H_{X_{bd}(\ell)} = \sum'_{Z \subset X_{bd}(\ell)} \Phi(Z)$

and $H^b_{X_{ext}(\ell)} = \sum'_{Z \cap X_{ext}(\ell) \neq \phi} \Phi(Z)$ (b-superscript stands for terms crossing boundary of X).



② $H_V = H^b_{X_{int}}(\alpha) + H_{X_{bd}}(\alpha) + H^b_{X_{ext}}(\alpha)$, where

$A(\alpha)$ is the operator defined in 4 (iii).

The above identity follows from $H_V = H_V(\alpha)$,

assuming $H_V \Psi_0 \rangle = 0$ w.l.o.g.

At this point, we have split H_V into three region of interactions (each spread over all of V, due to $T_t^{H_V}(A)$ evolution).

Continuing proof: (3) We use Lieb-Robinson bounds to localize each of the components $H^b_{X_{int}(\ell)}(\alpha)$, $H_{X_{bd}(\ell)}(\alpha)$ and $H_{X_{ext}(\ell)}(\alpha)$ as follows:

Define $$M_X(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} T_t^{H_X}\left(H^b_{X_{int}}\right) e^{-\alpha t^2}\, dt$$

$$M_{X_{bd}(2\ell)}(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} T_t^{H_{X_{bd}(2\ell)}}\left(H_{X_{bd}(\ell)}\right) e^{-\alpha t^2}\, dt$$

and $$M_{X^c}(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} T_t^{H_{X^c}}\left(H_{X_{ext}(\ell)}\right) e^{-\alpha t^2}\, dt$$

NOTE: (a) $M_X(\alpha) \in \mathcal{A}_X$, $M_{X_{bd}(2\ell)}(\alpha) \in \mathcal{A}_{X_{bd}(2\ell)}$ and $M_{X^c}(\alpha) \in \mathcal{A}_{X^c}$.

(b) $$\left\| H^b_{X_{int}(\ell)}(\alpha) - M_X(\alpha) \right\| \le \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} \left\| T_t^{H_V}(H_{X_{int}}) - T_t^{H_X}(H_{X_{int}}) \right\| e^{-\alpha t^2}\, dt.$$

For $|t| \le T_0$, Lieb-Robinson bounds give good upper bound on $\left\| T_t^{H_V}(H_{X_{int}}) - T_t^{H_X}(H_{X_{int}}) \right\| \le \int_0^t \left\| \left[\overset{H_V - H_X}{H^b_{X^c}}, T_t^{H_X}(H_{X_{int}}) \right] \right\|$

For $|t| > T_0$, we use the bound $\| T_t^{H_V}(A) - T_t^{H_\alpha}(A) \| \leq 2\|A\|$ and exploit the fast decay of the Gaussian $e^{-\alpha t^2}$, to get a bound of the form:

$$\| H^b_{X_{int}(\ell)}(\alpha) - M_X(\alpha) \| \leq K\, |\partial X|\, \ell^{3/2}\, e^{-\ell/\xi}, \text{ for}$$

ξ defined in ② (Theorem).

Note that T_0 is chosen optimally by matching the bounds from Lieb-Robinson application for $|t| \leq T_0$ and Gaussian decay for $|t| > T_0$.

<u>Proof</u> : ④ $\| H_V - (M_X(\alpha) + M_{X_{bd}(2\ell)}(\alpha) + M_{X^c}(\alpha)) \| \leq K' |\partial X|\, \ell^{3/2}\, e^{-\ell/\xi}$

Moreover, $\| M_X(\alpha)\, \Psi_0 \rangle \| \leq \mathcal{O}(e^{-\ell/\xi} + e^{-\gamma^2/4\alpha})$

$\hookrightarrow \leq \| (M_X(\alpha) - H^b_{X_{int}(\ell)}(\alpha))\, \Psi_0 \rangle \| + \| H_{X_{int}(\ell)}(\alpha)\, \Psi_0 \rangle \|$

$\leq \ell^{3/2}\, e^{-\ell/\xi}\, (K\, |\partial X|)$

and, also $\| M_{X^c}(\alpha)\, \Psi_0 \rangle \| \leq \mathcal{O}(e^{-\ell/\xi} + e^{-\gamma^2/4\alpha})$, so we choose $\alpha \sim 1/\ell$.

Proof ⑤ : Recall $P_0(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{itH_V} e^{-\alpha t^2} dt$, where we assume $\langle \Psi_0, H_V \Psi_0 \rangle = 0$, w.l.o.g.

We had $\| P_0(\alpha) - P_0 \| \leq e^{-\gamma^2/4\alpha}$.

Now, from $\| \mathbb{1} - e^{-it(H^b_{X_{int}}(\alpha) + H^b_{X_{ext}}(\alpha))} e^{it(M_X(\alpha) + M_{X^c}(\alpha))} \| \leq$

$$\int_0^{|t|} \{ \| M_X(\alpha) - H^b_{X_{int}}(\alpha) \| + \| M_{X^c}(\alpha) - H^b_{X_{ext}}(\alpha) \| \} dt$$

$$\leq |t| \cdot \mathcal{O}(e^{-\ell/\xi})$$

we get the next good approximation to the ground-state:

$$P_0^{(1)}(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{itH_V} e^{-it(H_V - H_{X_{bd}}(\alpha))} e^{it(M_X(\alpha) + M_{X^c}(\alpha))} e^{-\alpha t^2} dt$$

since $\| P_0^{(1)}(\alpha) - P_0(\alpha) \| \leq \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} |t| e^{-\alpha t^2} dt \; (\ell^{3/2} e^{-\ell/\xi})$

$$\leq \sqrt{\frac{1}{\alpha\pi}} \ell^{3/2} e^{-\ell/\xi} \sim \ell^2 e^{-\ell/\xi}$$, since $\frac{1}{\sqrt{\alpha}} \sim \sqrt{\ell}$

DEFINING P_X and P_{X^c} :

⑥ Now, let P_X be the projection onto eigenvalues of $M_X(\alpha)$ ~~[illegible]~~ less than $\delta \leq \ell^{3/2} e^{-\ell/2\xi}$ ⊛, and equivalently for P_{X^c} and $M_{X^c}(\alpha)$. Why do this?

⊛ in absolute value

Continuing proof: ⑥ In general, we have

$$\| (1-P_x)\,\psi_0\rangle \| \le \frac{1}{\delta}\, \| M_x\, \psi_0\rangle \| \le K\, |\partial x|\, e^{-\ell/2\xi}$$

where we used $M_x^2 \ge \delta^2 (1-P_x)$ and the bound from step ④ of the proof.

Similarly, $\| (1-P_{X^c})\,\psi_0\rangle \| \le K\, |\partial x|\, e^{-\ell/2\xi}$.

Using the above observations, we have:

$$\| P_0 (1 - P_x P_{X^c}) \| \le \| P_0 (1-P_x) \| + \| P_0 (1 - P_{X^c}) \| \le O(e^{-\ell/2\xi})$$

where we used $1 - P_x P_{X^c} = \frac{1}{2} \left\{ (1-P_x)(1+P_{X^c}) + (1-P_{X^c})(1+P_x) \right\}$.

Moreover, $\| P_0^{(1)}(\alpha)\, P_x P_{X^c} - P_0 \| \le \| (P_0^{(1)}(\alpha) - P_0)\, P_x P_{X^c} \| +$

$$\| P_0 (1 - P_x P_{X^c}) \|$$

$$\le O(e^{-\ell/2\xi}) \; \blacksquare .$$

But, $\| e^{it(M_X(\alpha) + M_{X^c}(\alpha))} P_X P_{X^c} - P_X P_{X^c} \| =$

$$\| (e^{itM_X(\alpha)} P_X) \otimes (e^{itM_{X^c}(\alpha)} P_{X^c}) - P_X \otimes P_{X^c} \| \le$$

$$\| e^{itM_X(\alpha)} P_X - P_X \| + \| e^{itM_{X^c}(\alpha)} P_{X^c} - P_{X^c} \| \le 2\xi\delta|t|\, \ell^{3/2} e^{-\ell/2\xi} \rightarrow$$

Step ⑦ : From ⑥, we get that

$$\mathbb{P}_0^{(\ell)}(\alpha) = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{itH_V} e^{-it(H_V - H_{X_{bd}}^{(\alpha)})} e^{-\alpha t^2} dt \quad P_X P_{X^c}$$

satisfies : $\| P_0^{(\ell)}(\alpha) - P_0 \| \leq_{K|\partial X|} e^{-\ell/23}$

It remains to show that $\sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{itH_V} e^{-it(H_V - H_{X_{bd}}^{(\alpha)})} e^{-\alpha t^2} dt$

can be localized (up to $e^{-\ell/23}$ error) on $\mathcal{A}_{X_{bd}(3\ell)}$.

Note that $\frac{\partial}{\partial t} \underbrace{e^{itH_V} e^{-it(H_V - H_{X_{bd}}(\alpha))}}_{U(t)} = i\, T_t^{H_V}(H_{X_{bd}(\ell)}^{(\alpha)}) \cdot U(t)$

So, we want to localize the generator $T_t^{H_V}(H_{X_{bd}(\ell)}^{(\alpha)}) \in \mathcal{A}_{X_{bd}(3\ell)}$

First, we sub $M_{X_{bd}(2\ell)}^{(\alpha)}$ for $H_{X_{bd}(\ell)}^{(\alpha)}$ and then we truncate

the dynamics $T_t^{H_V}(M_{X_{bd}(2\ell)}^{(\alpha)}) \rightarrow T_t^{H_{X_{bd}(3\ell)}}(M_{X_{bd}(2\ell)}^{(\alpha)})$.

Using the bound $\| U_0^{+}(t) \cdot U_1(t) - \mathbb{1} \| \leq \| \int_0^t U_0^{+}(s) (G_0(s) - G_1(s)) U_1(s) ds \|$

$\leq |t| \sup_{s \in [0,t]} \| G_0(s) - G_1(s) \|$, we

where $\partial_t U_0(t) = i\, G_0(t)\, U_0(t)$

$\partial_t U_1(t) = i\, G_1(t)\, U_1(t)$

see that $P_{X_{bd}(3\ell)} = \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} e^{it H_{X_{bd}(3\ell)}} e^{-it(H_{X_{bd}(3\ell)} - M_{X_{bd}(2\ell)}^{(\alpha)})} e^{-\alpha t^2} dt$.