Macroscopic Long-Range Dynamics of Fermions and Quantum Spins on the Lattice

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Historical Remarks

- **1947** – Bogoliubov approximation (boson): $a_0/\sqrt{V} \to c \in \mathbb{C}$ in many-boson Hamiltonians at equilibrium. *Dynamics ?*

- **1957-1984** – BCS theory (fermion): similar kind of approximation at equilibirum. See Bogliubov (1958), Haag (1962), Approx. Hamilt. Method (Bogoliubov Jr., Brankov, Zagrebnov, Kurbatov, Tonchev, 1966-1984). *Dynamics ?*

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- **1967 & 1978** – BCS theory, dynamics: Thirring and Wehrl on a simple BCS-type model (1967), generalization for a general class of models by van Hemmen (1978), at the cost of technical assumptions that are difficult to verify in practice.
- **1973-1992** – Classical effective dynamics from permutation invariant quantum-spin systems with mean-field interactions: Hepp and Lieb (1973), Bóna (1988-1990, “extended quantum mechanics” 2000, 2012).
- **2003-2017** – Dynamics of fermion systems in the continuum with mean-field interactions, by many authors: Bach, Bardos, Benedikter, Breteaux, Elgart, Erdös, Fröhlich, Golse, Gottlieb, Jakšić, Knowles, Mauser, Petrat, Pickl, Porta, Rademacher, Saffirio, Schlein, Yau.

Example of long-range terms: a BCS interaction

Definition

$\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$ is a cubic box (d-dimensional crystal) of volume $|\Lambda_L|$ for $L \in \mathbb{N}$.
$\Lambda_L^* \subseteq [-\pi, \pi)^d$ is the corresponding reciprocal lattice of quasi-momenta.
$a_{x,\mathrm{s}}^*$ (resp. $a_{x,\mathrm{s}}$) creates (resp. annihilates) a fermion with spin $\mathrm{s} \in \{\uparrow, \downarrow\}$ and $x \in \Lambda_L$.
$\tilde{a}_{k,\mathrm{s}}^*$ (resp. $\tilde{a}_{k,\mathrm{s}}$) creates (resp. annihilates) a fermion with spin $\mathrm{s} \in \{\uparrow, \downarrow\}$ and $k \in \Lambda_L^*$.

- Long-range term:

$$-\frac{1}{|\Lambda_L|} \sum_{k,q \in \Lambda_L^*} \tilde{a}_{k,\uparrow}^* \tilde{a}_{-k,\downarrow}^* \tilde{a}_{q,\downarrow} \tilde{a}_{-q,\uparrow} = -\frac{1}{|\Lambda_L|} \sum_{x,y \in \Lambda_L} a_{x,\uparrow}^* a_{x,\downarrow}^* a_{y,\downarrow} a_{y,\uparrow} \ .$$

- Mean-field term:

$$-\frac{1}{|\Lambda_L|} \sum_{x,y \in \Lambda_L} a_{x,\uparrow}^* a_{x,\downarrow}^* a_{y,\downarrow} a_{y,\uparrow} = -\sum_{y \in \Lambda_L} \left(\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} a_{x,\uparrow}^* a_{x,\downarrow}^* \right) a_{y,\downarrow} a_{y,\uparrow} \ .$$

- This is an important, albeit elementary, example of the far more general case we study in a series of papers (B. and de Siqueira Pedra, 2019).

Example of the Strong-Coupling BCS-Hubbard Model

Definition (Strong-coupling BCS-Hubbard model)

$$\mathrm{H}_L \doteq \underbrace{\sum_{x\in\Lambda_L} \left(2\lambda n_{x,\uparrow} n_{x,\downarrow} - \mu \left(n_{x,\uparrow} + n_{x,\downarrow}\right)\right)}_{H_{\mathrm{short-range}}} \underbrace{- \frac{\gamma}{|\Lambda_L|} \sum_{x,y\in\Lambda_L} a^*_{x,\uparrow} a^*_{x,\downarrow} a_{y,\downarrow} a_{y,\uparrow}}_{H_{\mathrm{long-range}}}$$

for $L \in \mathbb{N}_0$, $\mu \in \mathbb{R}$ and $\lambda, \gamma \geq 0$, acting on the fermion Fock space

$$\mathcal{F}_{\Lambda_L} \doteq \bigwedge \mathbb{C}^{\Lambda_L \times \{\uparrow,\downarrow\}} \equiv \mathbb{C}^{2^{\Lambda_L \times \{\uparrow,\downarrow\}}} .$$

Here, $d \in \mathbb{N}$, $\Lambda_L \doteq \{\mathbb{Z} \cap [-L, L]\}^d$ and $n_{x,\mathrm{s}} \doteq a^*_{x,\mathrm{s}} a_{x,\mathrm{s}}$ is the particle number operator.

1. The first term with $\lambda \geq 0$ is the (screened) Coulomb repulsion as in the Hubbard model.
2. The second with chemical potential $\mu \in \mathbb{R}$ represents the strong-coupling limit of the kinetic energy.
3. The third with $\gamma \geq 0$ is the BCS interaction, written in the x-space.

Cooper Pair Condensate Density (B-Pedra, 2010)

At fixed $L \in \mathbb{N}_0$ and inverse temperature $\beta > 0$, the Gibbs states $\omega^{(L)}$ is defined by

$$\omega^{(L)}(A) \doteq \mathrm{Trace}_{\mathcal{F}_{\Lambda_L}}\left(A \frac{\mathrm{e}^{-\beta \mathrm{H}_L}}{\mathrm{Trace}_{\mathcal{F}_{\Lambda_L}}(\mathrm{e}^{-\beta \mathrm{H}_L})}\right) , \qquad A \in \mathcal{B}(\mathcal{F}_{\Lambda_L}) .$$

For $\mu \in \mathbb{R}$ and $\lambda, \gamma \geq 0$, let $\mathrm{r}_\beta \geq 0$ be such that $\sup_{r \geq 0} f(r) = f(\mathrm{r}_\beta)$ with

$$f(r) \doteq -\gamma r + \beta^{-1} \ln\left(1 + e^{-\lambda\beta} \cosh\left(\beta\sqrt{(\mu-\lambda)^2 + \gamma^2 r}\right)\right).$$

Theorem (Cooper pair condensate density)

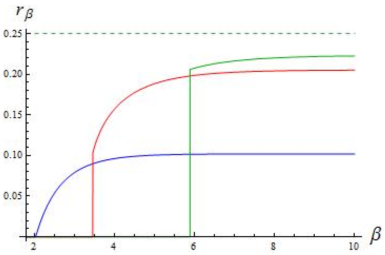
Outside any critical point, the Cooper pair condensate density equals

$$\lim_{L\to\infty}\left\{\frac{1}{|\Lambda_L|}\omega^{(L)}(\mathfrak{c}_0^*\mathfrak{c}_0)\right\} = \mathrm{r}_\beta \leq \max\{0, 1/4\}$$

with

$$\mathfrak{c}_0 \doteq \frac{1}{\sqrt{|\Lambda_L|}}\sum_{x\in\Lambda_L} a_{x,\downarrow}a_{x,\uparrow} = \frac{1}{\sqrt{|\Lambda_L|}}\sum_{k\in\Lambda_L^*} \tilde{a}_{k,\downarrow}\tilde{a}_{-k,\uparrow}.$$

Existence of a Superconducting Phase (B-Pedra, 2010)



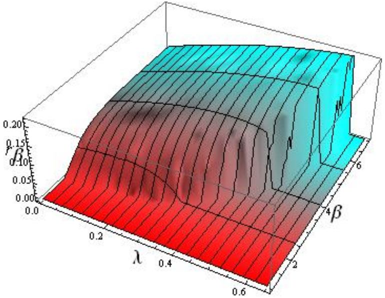


Figure: On the left, we have three illustrations of the Cooper pair condensate density r_β as a function of the inverse temperature β for $\lambda = 0$ (blue line), $\lambda = 0.45$ (red line) and $\lambda = 0.575$ (green line).

On the right, the Cooper pair condensate density r_β is given as a function of λ and β.

In all figures, $\mu = 1$ and $\gamma = 2.6$.

Approximating Hamiltonians

$$\begin{aligned} \mathrm{H}_L(c) &\doteq \sum_{x\in\Lambda_L}\left(2\lambda n_{x,\uparrow}n_{x,\downarrow} - \mu\left(n_{x,\uparrow}+n_{x,\downarrow}\right) - \gamma\left(c a_{x,\uparrow}^{*}a_{x,\downarrow}^{*} + \bar{c}a_{x,\downarrow}a_{x,\uparrow}\right)\right) \\ F(c) &\doteq -\gamma|c|^2 + \lim_{L\to\infty}\left\{\frac{1}{\beta\left|\Lambda_L\right|}\ln \mathrm{Trace}_{\mathcal{F}_{\Lambda_L}}\left(\mathrm{e}^{-\beta \mathrm{H}_L(c)}\right)\right\} \end{aligned}$$

for $c\in\mathbb{C}$. Heuristically, $\gamma\left|\Lambda_L\right|\left|c\right|^2 + \mathrm{H}_L(c) - \mathrm{H}_L = \gamma\left|\mathfrak{c}_0 - \sqrt{|\Lambda_L|}c\right|^2 \geq 0$.

Approximating Hamiltonians

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$$F(c) \doteq -\gamma|c|^2 + \lim_{L\to\infty}\left\{\frac{1}{\beta|\Lambda_L|}\ln \mathrm{Trace}_{\mathcal{F}_{\Lambda_L}}\left(\mathrm{e}^{-\beta\mathrm{H}_L(c)}\right)\right\}$$

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1. **Pressure in the thermodynamic limit (cf. Approx. Hamilt. Method):**

$$\lim_{L\to\infty}\frac{1}{\beta|\Lambda_L|}\ln\mathrm{Trace}_{\mathcal{F}_{\Lambda_L}}\left(\mathrm{e}^{-\beta\mathrm{H}_L}\right) = \sup_{c\in\mathbb{C}} F(c) = \beta^{-1}\ln 2 + \mu + \sup_{r\geq 0} f(r)$$

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2. **Gibbs state in the thermodynamic limit (B-Pedra, 2010):** The Gibbs state $\omega^{(L)}$ (weak*) converges to a convex combination of the limit of the Gibbs state $\omega^{(L,\mathfrak{d})}$ associated with $\mathrm{H}_L(\mathfrak{d})$, where $\mathfrak{d} = \mathrm{r}_\beta \mathrm{e}^{i\theta}$, $\theta\in[0,2\pi)$ and $\sup_{c\in\mathbb{C}} F(c) = F(\mathfrak{d})$.

   Recall that the Cooper pair condensate density equals

$$\lim_{L\to\infty}\left\{\frac{1}{|\Lambda_L|}\omega^{(L)}\left(\mathfrak{c}_0^*\mathfrak{c}_0\right)\right\} = \mathrm{r}_\beta = |\mathfrak{d}|^2 \qquad \text{with} \qquad \mathfrak{c}_0 \doteq \frac{1}{\sqrt{|\Lambda_L|}}\sum_{x\in\Lambda_L} a_{x,\downarrow}a_{x,\uparrow}.$$

Dynamical Problem in the Thermodynamic Limit

Finite-volume dynamics (Heisenberg picture of QM).

$$\tau_t^{(L)}(A) = \exp(it\delta_L)(A) \doteq \mathrm{e}^{it\mathrm{H}_L} A \mathrm{e}^{-it\mathrm{H}_L} , \qquad A \in \mathcal{B}(\mathcal{F}_{\Lambda_L}),\ L \in \mathbb{N}_0,\ t \in \mathbb{R} .$$

The generator is the linear operator δ_L defined on $\mathcal{B}(\mathcal{F}_{\Lambda_L})$ by

$$\delta_L(A) \doteq i[\mathrm{H}_L, A] \doteq i(\mathrm{H}_L A - A\mathrm{H}_L) , \qquad A \in \mathcal{B}(\mathcal{F}_{\Lambda_L}) .$$

Infinite-volume dynamics ($L \to \infty$).

- No long-range part ($\gamma = 0$): the (strong) limit $L \to \infty$ of $\{\tau_t^{(L)}\}_{t\in\mathbb{R}}$ exist as a C_0-group $\{\tau_t\}_{t\in\mathbb{R}}$ of $*$-automorphisms of the CAR C^*-algebra of the infinite lattice.
- With long-range part ($\gamma > 0$): One may approximate $\{\tau_t^{(L)}\}_{t\in\mathbb{R}}$ by

  $$\tau_t^{(L,c)}(A) \doteq \mathrm{e}^{it\mathrm{H}_L(c)} A \mathrm{e}^{-it\mathrm{H}_L(c)} , \qquad A \in \mathcal{B}(\mathcal{F}_{\Lambda_L}),\ t \in \mathbb{R} .$$

  A natural choice for $c \in \mathbb{C}$ would be a solution $\mathfrak{d}$ to $\sup_{c\in\mathbb{C}} F(c) = F(\mathfrak{d})$, but what about if the solution is not unique ?

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- With long-range part ($\gamma > 0$):

Dynamical Problem

As a matter of fact, the finite-volume dynamics $\{\tau_t^{(L)}\}_{t\in\mathbb{R}}$ does not converge within the CAR C^*-algebra of the infinite lattice for $\gamma > 0$, even if $\mathfrak{d} = 0$ would be the unique solution to the variational problem!

Self-Consistency Equations

- One-site Fermion Fock space: $\mathcal{F}_{\{0\}} \doteq \bigwedge \mathbb{C}^{\{0\}\times\{\uparrow,\downarrow\}} \equiv \mathbb{C}^4$.
- A state $\rho : \mathcal{B}(\mathcal{F}_{\{0\}}) \to \mathbb{C}$ is a positive normalized linear functional.
- For any continuous family $\omega \doteq (\omega_t)_{t\in\mathbb{R}}$ of states acting on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$ and $s,t \in \mathbb{R}$,

$$\tau^{\omega}_{t,s} \equiv \text{“}\exp\left(\int_s^t \delta_0^{\omega_u}\mathrm{d}u\right)\text{”} \doteq \mathbf{1}_{\mathcal{B}(\mathcal{F}_{\{0\}})} + \sum_{k\in\mathbb{N}} \int_s^t \mathrm{d}t_1 \cdots \int_s^{t_{k-1}} \mathrm{d}t_k \delta_0^{\omega_{t_k}} \circ \cdots \circ \delta_0^{\omega_{t_1}}$$

where, for any state ρ acting on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$ and $c_\rho \doteq \rho(a_{0,\uparrow}a_{0,\downarrow})$,

$$\delta_0^{\rho}(A) \doteq i[\mathrm{H}_0(c_\rho), A] , \qquad A \in \mathcal{B}(\mathcal{F}_{\{0\}}).$$

Theorem (Self-consistency equations)

For any fixed initial (even) state ρ on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$ at $t=0$, there is a unique family $(\varpi(t;\rho))_{t\in\mathbb{R}}$ of on-site states acting on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$ such that

$$\varpi(t;\rho) = \rho \circ \tau_{t,0}^{\varpi(\cdot;\rho)} , \qquad t \in \mathbb{R}.$$

Infinite-Volume Dynamics of Product States

- Recall that
$$\tau_t^{(L)}(A) \doteq \mathrm{e}^{it\mathrm{H}_L} A \mathrm{e}^{-it\mathrm{H}_L}\ , \qquad A \in \mathcal{B}(\mathcal{F}_{\Lambda_L}),\ t \in \mathbb{R}.$$
- For any continuous family $\omega \doteq (\omega_t)_{t\in\mathbb{R}}$ of states acting on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$ and $s, t \in \mathbb{R}$,
$$\tau_{t,s}^{\omega} \equiv \text{“}\exp\left(\int_s^t \delta_L^{\omega_u} \mathrm{d}u\right)\text{”} \doteq \mathbf{1}_{\mathcal{B}(\mathcal{F}_{\{0\}})} + \sum_{k\in\mathbb{N}} \int_s^t \mathrm{d}t_1 \cdots \int_s^{t_{k-1}} \mathrm{d}t_k \delta_L^{\omega_{t_k}} \circ \cdots \circ \delta_L^{\omega_{t_1}}$$
(can be defined for $L = \infty$) where, for any state ρ and $c_\rho \doteq \rho(a_{0,\uparrow} a_{0,\downarrow})$,
$$\delta_L^\rho \doteq i\left[\mathrm{H}_L(c_\rho),\ \cdot\ \right] = \sum_{x\in\Lambda_L} i\left[\mathrm{H}_0(c_\rho),\ \cdot\ \right]$$

Theorem (Infinite-volume dynamics of product states)

For any even state ρ on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$ and $t \in \mathbb{R}$, in the weak*-topology,
$$\lim_{L\to\infty} (\otimes_{\Lambda_L}\rho) \circ \tau_t^{(L)} = (\otimes_{\mathbb{Z}^d}\rho) \circ \tau_{t,0}^{\varpi(\cdot;\rho)} \doteq \rho_t. \qquad P.S. \quad \rho_t|_{\mathcal{B}(\mathcal{F}_{\{0\}})} = \varpi(t;\rho).$$

Dynamics of Cooper-Field Densities

In the thermodynamic limit $L \to \infty$, $(\otimes_{\Lambda_L} \rho) \circ \tau_t^{(L)}$ converges to $\rho_t \doteq (\otimes_{\mathbb{Z}^d} \rho) \circ \tau_{t,0}^{\varpi(\cdot;\rho)}$.

Lemma (Electron and Cooper-field densities)

Fix any even state ρ on $\mathcal{B}\left(\mathcal{F}_{\{0\}}\right)$. Then the electron density is constant:

$$\mathrm{d}(\rho) \doteq \rho\left(n_{0,\uparrow} + n_{0,\downarrow}\right) = \rho_{t=0}\left(n_{0,\uparrow} + n_{0,\downarrow}\right) = \rho_t\left(n_{0,\uparrow} + n_{0,\downarrow}\right) \in [0,2],$$

while, for any $t \in \mathbb{R}$,

$$\rho_t\left(a_{0,\downarrow} a_{0,\uparrow}\right) = \left|\rho\left(a_{0,\downarrow} a_{0,\uparrow}\right)\right| \mathrm{e}^{i\left(t\nu(\rho)+\theta_\rho\right)} \quad \textit{with} \quad \nu\left(\rho\right) \doteq 2\left(\mu - \lambda\right) + \gamma\left(1 - \mathrm{d}(\rho)\right) \ .$$

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Define the 3D vector $(\Omega_1(t), \Omega_2(t), \Omega_3(t))$ by $\rho_t\left(a_{0,\downarrow} a_{0,\uparrow}\right) = \Omega_1(t) + i\Omega_2(t)$ and $\Omega_3(t) \doteq 2(\mu - \lambda) + \gamma\left(1 - \rho_t\left(n_{0,\uparrow} + n_{0,\downarrow}\right)\right)$. Then, for any time $t \in \mathbb{R}$,

$$\begin{cases} \dot{\Omega}_1(t) = -\Omega_3(t)\,\Omega_2(t) \ , \\ \dot{\Omega}_2(t) = \Omega_3(t)\,\Omega_1(t) \ , \\ \dot{\Omega}_3(t) = 0 \ , \end{cases}$$

$\Rightarrow$ time evolution of the angular momentum of a symmetric rotor in classical mechanics.

From Quantum to Classical Mechanics

- In the thermodynamic limit, $(\otimes_{\Lambda_L}\rho) \circ \tau_t^{(L)}$ converges to $\rho_t \doteq (\otimes_{\mathbb{Z}^d}\rho) \circ \tau_{t,0}^{\varpi(\cdot;\rho)}$.
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$$\Downarrow$$

Not an accident: One can define a Poisson bracket on the state space and derive Liouville's equation.

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$$\Downarrow$$

Macroscopic long-range dynamics are, in general, equivalent to an intricate combinations of classical and quantum short-range dynamics.

Our contribution with de Siqueira Pedra (2019)

In a series of papers we mathematically study the macroscopic long-range, or mean-field, dynamics of lattice-fermion or quantum-spin systems. Results beyond previous ones:

- The short-range part $H_{\mathrm{short-range}}$ of the corresponding Hamiltonian

$$H = H_{\mathrm{short-range}} + H_{\mathrm{long-range}}$$

  is very general since only a sufficiently strong polynomial decay of its interactions and a translation invariance are necessary.

- The long-range part $H_{\mathrm{long-range}}$ is also very general, being an infinite sum (over n) of mean-field terms of order $n \in \mathbb{N}$ constructed from translation-invariant interactions. Even for permutation-invariant systems, the class of long-range interactions we are able to handle is much larger than what was previously studied.

- The initial state is only required to be periodic. The set of all such initial states is (weak*) dense within the set of all even states, the physically relevant ones.

From Product to Permutation-Invariant Initial States

- Any permutation-invariant state can be written (or approximated to be more precise) as a convex combination of product states.
- If $\rho^{(1)}, \ldots, \rho^{(n)}$ are $n \in \mathbb{N}$ product states and $u_1, \ldots, u_n \in [0,1]$ such that $u_1 + \cdots + u_n = 1$, then, in the weak* topology,

$$\lim_{L\to\infty} \left(\sum_{j=1}^{n} u_j \rho^{(j)} \right) \circ \tau_t^{(L)} = \sum_{j=1}^{n} u_j \rho^{(j)} \circ \tau_{t,0}^{\varpi(\cdot;\rho^{(j)})} \doteq \rho_t \ ,$$

where, by a slight abuse of notation, $\varpi(\cdot;\rho) = \varpi(\cdot;\rho|_{\mathcal{B}(\mathcal{F}_{\{0\}})})$.

- For instance, for any $t \in \mathbb{R}$,

$$\rho_t\left(a_{0,\downarrow}a_{0,\uparrow}\right) = \sum_{j=1}^{n} u_j |\rho^{(j)}\left(a_{0,\downarrow}a_{0,\uparrow}\right)| \mathrm{e}^{i\left(t\nu(\rho^{(j)})+\theta_{\rho^{(j)}}\right)}$$

with $\theta_{\rho^{(j)}} \doteq \arg \rho^{(j)}\left(a_{0,\downarrow}a_{0,\uparrow}\right)$ and

$$\nu(\rho^{(j)}) \doteq 2\left(\mu - \lambda\right) + \gamma\left(1 - \rho^{(j)}\left(n_{0,\uparrow} + n_{0,\downarrow}\right)\right)$$

$\Rightarrow$ **The Cooper pair condensate density is not anymore necessarly constant.**

Long-Range Dynamics for Periodic Initial States

- Fix $\vec{\ell} \in \mathbb{N}^d$ and let $E_{\vec{\ell}}$ be the weak*-compact convex set of $\vec{\ell}$-*periodic* states on the CAR C^*-algebra of the infinite lattice $\mathbb{Z}^d$.

- Let $\mathcal{E}(E_{\vec{\ell}})$ be the (non-empty) set of extreme point of $E_{\vec{\ell}}$, by the Krein-Milman theorem. For any $\rho \in E_{\vec{\ell}}$, there is a unique probability measure μ_ρ on $E_{\vec{\ell}}$ such that

$$\mu_\rho \left(\mathcal{E}(E_{\vec{\ell}})\right) = 1 \qquad \text{and} \qquad \rho = \int_{\mathcal{E}(E_{\vec{\ell}})} \hat{\rho} \, \mathrm{d}\mu_\rho (\hat{\rho}) \ ,$$

  by the Choquet theorem.

- For any $\rho \in \mathcal{E}(E_{\vec{\ell}})$, there is a unique family $(\varpi(t;\rho))_{t\in\mathbb{R}}$ of states such that

$$\varpi(t;\rho) = \rho \circ \tau_{t,0}^{\varpi(\cdot;\rho)} \ , \qquad t \in \mathbb{R},$$

  by ergodicity of extreme states.

- For any $\rho \in E_{\vec{\ell}}$, in the weak*-topology,

$$\lim_{L\to\infty} \rho \circ \tau_t^{(L)} = \int_{\mathcal{E}_{\vec{\ell}}} \varpi^{\mathrm{m}} (t;\hat{\rho}) \ \mathrm{d}\mu_\rho (\hat{\rho}) \doteq \rho_t,$$

  by using the theory of direct integrals and Lieb-Robinson bounds.