Schrödinger evolution in a low-density random potential - Convergence to solutions of the linear Boltzmann equation

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High frequency analysis: from operator algebras to PDEs

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Schrödinger evolution in microscopic coordinates

Consider the Schrödinger opereator

$$H_{\lambda,1} = -\tfrac{1}{2}\Delta_X + \lambda W(X),$$

where $-\Delta_X$ is the positive Laplacian, $\lambda > 0$ is a coupling constant and $W(X)$ is the potential.

We have the associated time dependent Schrödinger equation

$$\begin{cases} i\partial_T \varphi(T,X) = H_{\lambda,1}\varphi(T,X) \\ \varphi(0,X) = \varphi(X) \end{cases}$$

with suitable initial data φ.

Schrödinger evolution in macroscopic coordinates

We call (X, T) the microscopic coordinates and define the macroscopic coordinates (x, t) to be

$$(x\hbar, t\hbar) = (X, T).$$

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The time dependent Schrödinger equation is given by

$$\begin{cases} i\hbar\partial_t\varphi_\hbar(t,x) = H_{\lambda,\hbar}\varphi_\hbar(t,x) \\ \varphi_\hbar(0,x) = \varphi_\hbar(x) \end{cases}$$

with suitable initial data $\varphi_\hbar$.

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with suitable initial data $\varphi_\hbar$.

Assume that $\sup_{\hbar\in(0,1]}\|\varphi_\hbar\|_{L^2(\mathbb{R}^d)} < \infty$. Then along some subsequence $\{\hbar_j\}_{j\in\mathbb{N}}$ we have

$$\langle \mathrm{Op}_\hbar^{\mathrm{w}}(a)\varphi_{\hbar_j}(t,x), \varphi_{\hbar_j}(t,x)\rangle \to \int_{\mathbb{R}^{2d}} a(x,p)\, d\mu_t(x,p)$$

for all $a \in \mathcal{S}(\mathbb{R}^{2d})$.

The model we consider

Let $\mathcal{X}$ be a Poisson point process with intensity 1 and assume V is a positive Schwartz function. We are interested in solutions to the Schrödinger equation

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$$H_{\lambda,\hbar} = -\frac{\hbar^2}{2}\Delta + \lambda \sum_{x_j\in\mathcal{X}} V\left(\frac{x-\hbar^{1-1/d}x_j}{\hbar}\right).$$

Under these assumption we have that $H_{\lambda,\hbar}$ is self-adjoint and the solutions is given by

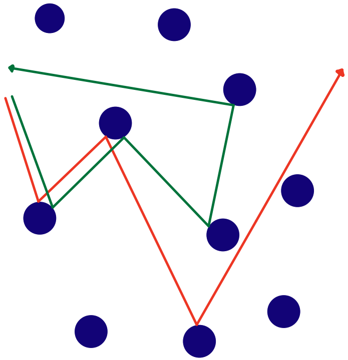
$$\varphi_\hbar(t,x) = U_{\lambda,\hbar}(t)\varphi_\hbar(x) = e^{-it\hbar^{-1}H_{\lambda,\hbar}}\varphi_\hbar(x).$$

To investigate the behaviour as $\hbar \to 0$ we will consider the expectations

$$\mathbb{E}[\langle \mathrm{Op}_\hbar^{\mathrm{w}}(a)U_{\lambda,\hbar}(t)\varphi_\hbar, U_{\lambda,\hbar}(t)\varphi_\hbar\rangle],$$

where $a \in \mathcal{S}(\mathbb{R}^{2d})$ is some observable.

The Lorentz gas and linear Boltzmann equation



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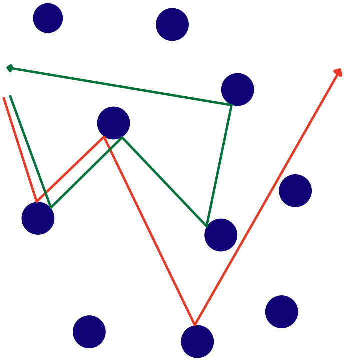

Time evolution of a particle cloud with density $f \in L^1(\mathbb{R}^{2d})$ is given by

$$f_t^{(r)}(x,p) = f(\Phi_r^{-t}(x,p)).$$

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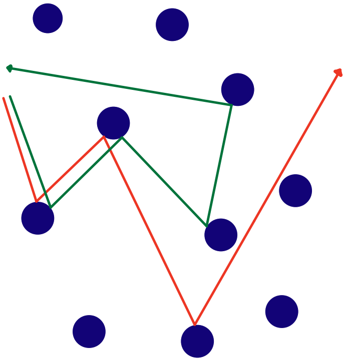

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In 1905 Lorentz proposed that $f_t^{(r)}(x,p)$ is governed, as $r \to 0$, by the linear Boltzmann equation given by

$$\partial_t f(t,x,p) + \langle p, \nabla_x f(t,x,p)\rangle$$
$$= \int_{\mathbb{R}^d} [\Sigma(p,q) f(t,x,q) - \Sigma(q,p) f(t,x,p)]\, dq$$

with initial condition $f(0,x,p) = f(x,p)$, and where $\Sigma(p,q)$ is the collision kernel (differential cross section) of the individual scatterer.

Collision series for solutions to the linear Boltzmann equation

The solution of the linear Boltzmann equation can be expressed as the collision series

$$f(t,x,p) = \sum_{n=0}^{\infty} f^{(n)}(t,x,p),$$

where

$$f^{(n)}(t,x,q_0) = \int_{[0,t]^n_{\leq}} \int_{\mathbb{R}^{nd}} \prod_{i=1}^{n} \Sigma(q_i, q_{i-1}) \prod_{i=1}^{n+1} e^{-(s_{i-1}-s_i)\Sigma_{\text{tot}}(q_i)}$$
$$\times f_0(x - tq_0 - \sum_{i=1}^{n} s_i(q_i - q_{i-1}), q_n)\, d\boldsymbol{q}_{1,n} d\boldsymbol{s}_{n,1},$$

with the convention $s_0 = t$, $s_{n+1} = 0$, the notation

$$[0,t]^n_{\leq} = \{s_n \leq \cdots \leq s_1 \mid s_i \in [0,t]\},$$

and the total scattering cross section

$$\Sigma_{\text{tot}}(q) = \int_{\mathbb{R}^d} \Sigma(p,q)\, dp.$$

Measures solving the linear Boltzmann equation

The solution to the linear Boltzmann equation defines a semigroup $\{\mathcal{L}_t\}_{t\geq 0}$ of linear operators $\mathcal{L}_t : L^1(\mathbb{R}^{2d}) \to L^1(\mathbb{R}^{2d})$ so that

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We define the adjoint $\mathcal{L}_t^*$ by

$$\int a(x,p) f(t,x,p)\,dx\,dp = \int [\mathcal{L}_t^* a](x,p) f_0(x,p)\,dx\,dp.$$

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Given a Borel measure μ_0 on $\mathbb{R}^{2d}$, we define the measure μ_t by

$$\int a(x,p)\, d\mu_t(x,p) = \int [\mathcal{L}_t^* a](x,p)\, d\mu_0(x,p).$$

We will say *the family of measures $\{\mu_t\}_{t\geq 0}$ is a solution of the linear Boltzmann equation with initial data μ_0.*

T-operator and scattering matrix

The T-operator $T(E)$ for the quantum mechanical scattering in the single-site potential V is defined as the limit

$$T(E) = \lim_{\gamma \to 0_+} T^\gamma(E), \qquad T^\gamma(E) = \lambda V + \lambda^2 V \frac{1}{E - (-\frac{1}{2}\Delta + \lambda V) + i\gamma} V. \qquad (1)$$

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An important quantity is the kernel of $T(E)$ in momentum representation with $E = \frac{1}{2}p^2$, which we denote by $\hat{T}(p,q)$. This "T-matrix" is related to the scattering matrix $S(p,q)$ by the relation

$$S(p,q) = \delta(p-q) - 2\pi i\, \delta(\tfrac{1}{2}p^2 - \tfrac{1}{2}q^2)\, \hat{T}(p,q). \tag{2}$$

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From the resolvent formalism we obtain the formal series expansion given by

$$T^\gamma(E) = \lambda V \sum_{n=0}^{\infty} [\lambda \frac{1}{E - (-\frac{1}{2}\Delta) + i\gamma} V]^n.$$

Main theorem

Theorem (M. 2022)

Let $\mathcal{X}$ be a Poisson point process with intensity 1 and assume V is a positive Schwartz function. We assume $\lambda > 0$ is small enough and let

$$H_{\lambda,\hbar} = -\frac{\hbar^2}{2}\Delta + \lambda \sum_{x_j \in \mathcal{X}} V\left(\frac{x - \hbar^{1-1/d} x_j}{\hbar}\right).$$

Let $\{\varphi_\hbar\}_{\hbar \in I}$ be a uniform semiclassical family in $H^{20}_\hbar(\mathbb{R}^3)$ with Wigner measure μ_0, and let $\varphi_\hbar(t) = U_{\lambda,\hbar}(t)\varphi_\hbar$. Then, for any $t > 0$, $a \in \mathcal{S}(\mathbb{R}^{2d})$, we have that

$$\mathbb{E}\langle \mathrm{Op}^{\mathrm{w}}_\hbar(a)\varphi_\hbar(t), \varphi_\hbar(t)\rangle \to \int_{\mathbb{R}^{2d}} a(x,p)\, d\mu_t(x,p), \tag{3}$$

for $\hbar \to 0$ in I, where μ_t is a solution of the linear Boltzmann equation with initial data μ_0 and collision kernel

$$\Sigma(p,q) = (2\pi)^{d+1} \rho\, \delta(\tfrac{1}{2}p^2 - \tfrac{1}{2}q^2)|\hat{T}(p,q)|^2. \tag{4}$$

Previous known results

L. Erdős and H.-T. Yau.
Linear Boltzmann equation as the weak coupling limit of a random Schrödinger equation.
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D. Eng and L. Erdős.
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J. Griffin and J. Marklof.
Quantum transport in a low-density periodic potential: homogenisation via homogeneous flows.
Pure Appl. Anal., 1(4):571–614, 2019.

J. Griffin and J. Marklof.
Quantum transport in a crystal with short-range interactions: the Boltzmann-Grad limit.
J. Stat. Phys., 184(2):Paper No. 16, 46, 2021.

J. Griffin.
Derivation of the linear boltzmann equation from the damped quantum lorentz gas with a general scatterer configuration.
Annales Henri Poincaré, 2022.

Duhamel expansion

The proof is based on the following expansion

$$\begin{aligned} U_{\lambda,\hbar}(-t)U_{\hbar,0}(t) - I &= \frac{i\lambda}{\hbar}\int_0^t U_{\lambda,\hbar}(-t_1)W_\hbar U_{\hbar,0}(-t_1)\,d\boldsymbol{t}_1 \\ &= \frac{i\lambda}{\hbar}\int_0^t U_{\lambda,\hbar}(-t_1)U_{\hbar,0}(-t_1)W_\hbar^{t_1}\,d\boldsymbol{t}_1, \end{aligned}$$

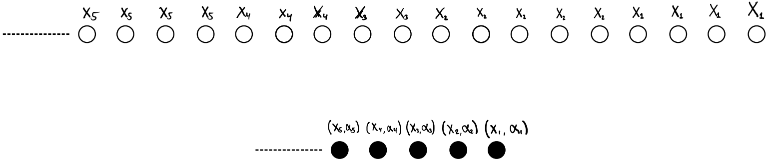
where

$$W_\hbar^{t_1} = U_{\hbar,0}(t_1)W_\hbar U_{\hbar,0}(-t_1)$$

In each step we sort the terms in diagonal and off diagonal terms

$$W_\hbar^{t_2}W_\hbar^{t_1} = \sum_{x\in\mathcal{X}} V_{\hbar,x}^{t_2}\sum_{x\in\mathcal{X}} V_{\hbar,x}^{t_1} = \sum_{x\in\mathcal{X}} V_{\hbar,x_j}^{t_2}V_{\hbar,x_j}^{t_1} + \sum_{(x_1,x_2)\in\mathcal{X}^2_{\neq}} V_{\hbar,x_2}^{t_2}V_{\hbar,x_1}^{t_1}.$$

Duhamel expansion II



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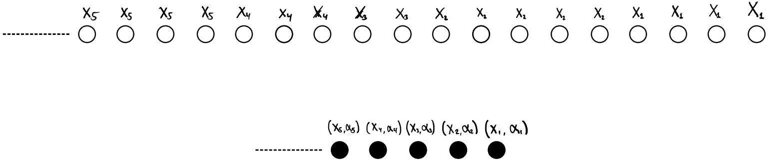

Lemma

Let $H_{\lambda,\hbar} = -\frac{\hbar^2}{2}\Delta + \lambda W_\hbar(x)$, *where* $\hbar \in (0,\hbar_0]$, $W_\hbar$ *and* λ *satisfy assumption of the main theorem and let* $U_{\lambda,\hbar}(t) = e^{-it\hbar^{-1}H_{\lambda,\hbar}}$. *Then for any* $\tau_0 \in \mathbb{N}$ *and* $k_0 \in \mathbb{N}$ *we have that*

$$U_{\lambda,\hbar}(-t) = U_{\hbar,0}(-t) + \sum_{i=0}^{2}\sum_{k=k_i}^{k_0}\sum_{\boldsymbol{x}\in\mathcal{X}_{\neq}^{k-i}} \mathcal{I}_i(k,\boldsymbol{x},t;\hbar) + \mathcal{R}^{\mathrm{rec}}(k_0;\hbar) + \mathcal{R}^{k_0,\tau_0}(N;\hbar)$$

where $k_0 = 1$, $k_1 = 3$, *and* $k_2 = 4$.

Duhamel expansion III

The operators from the previous lemma are given “explicitly”. For the operator $\mathcal{I}_0(k, \boldsymbol{x}, t; \hbar)$ we have

$$\mathcal{I}_0(k, \boldsymbol{x}, t; \hbar) = \sum_{\alpha \in \mathbb{N}^k} (i\lambda)^{|\alpha|} \int_{[0,t]^k_{\leq}} \prod_{m=1}^{k} \Theta_{\alpha_m}(s_{m-1}, s_m, x_m; V, \hbar)\, d\boldsymbol{s}_{k,1} U_{\hbar,0}(-t),$$

where the operators $\Theta_m(s_1, s_2, z; V, \hbar)$ are given by

$$\frac{1}{\hbar} \int_{\mathbb{R}_+^{m-1}} \mathbf{1}_{[0,\hbar^{-1}(s_1 - s_2)]}(\boldsymbol{t}^+_{1,m-1}) U_{\hbar,0}(-s_2) V_{\hbar,z} \times \Big\{ \prod_{i=1}^{m-1} U_{\hbar,0}(-t_i) V_{\hbar,z} \Big\} U_{\hbar,0}(\boldsymbol{t}^+_{1,m-1} + s_2)\, d\boldsymbol{t}_{1,m-1},$$

with

$$V_{\hbar,z}(x) = V\Big(\frac{x - \hbar^{1-1/d} z}{\hbar}\Big).$$

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with

$$V_{\hbar,z}(x) = V\left(\frac{x - \hbar^{1-1/d} z}{\hbar} \right).$$

Note that the kernel of $\Theta_m(s_1, s_2, z; V, \hbar)$ in momentum representation is given by

$$(p_m, p_0) \mapsto \frac{1}{\hbar} e^{-i\hbar^{-1/d}\langle z, p_m - p_0\rangle} e^{is_2 \hbar^{-1} \frac{1}{2}(p_m^2 - p_0^2)} \Psi_m(p_m, p_0, \hbar^{-1}(s_1 - s_2); V).$$

Convergence of the Duhamel expansion?

Assume $\varphi \in H^{20}_{\hbar}(\mathbb{R}^3)$ and consider the expansion

$$U_{\lambda,\hbar}(-t)\varphi = U_{\hbar,0}(-t)\varphi + \sum_{i=0}^{2}\sum_{k=k_i}^{k_0}\sum_{\boldsymbol{x}\in\mathcal{X}_{\neq}^{k-i}} \mathcal{I}_i(k,\boldsymbol{x},t;\hbar)\varphi + \mathcal{R}^{\text{rec}}(k_0;\hbar)\varphi + \mathcal{R}^{k_0,\tau_0}(N;\hbar)\varphi$$

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A key step in the proof of the main theorem is to prove that this series converge on average in L^2. For fixed $i=0$ and k one of these norms is

$$\mathbb{E}\Big[\Big\|\sum_{\boldsymbol{x}\in\mathcal{X}_{\neq}^{k}} \mathcal{I}_0(k,\boldsymbol{x},t;\hbar)\varphi\Big\|_{L^2(\mathbb{R}^d)}^2\Big] = \mathbb{E}\Big[\sum_{\boldsymbol{x}\in\mathcal{X}_{\neq}^{k}}\sum_{\tilde{\boldsymbol{x}}\in\mathcal{X}_{\neq}^{k}} \langle \mathcal{I}_0(k,\boldsymbol{x},t;\hbar)\varphi, \mathcal{I}_0(k,\tilde{\boldsymbol{x}},t;\hbar)\varphi\rangle_{L^2(\mathbb{R}^d)}\Big].$$

Convergence of the Duhamel expansion?

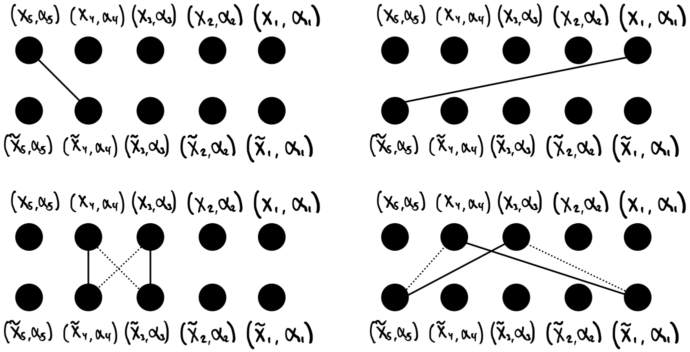
We have the expression

$$\mathbb{E}\Big[\sum_{\boldsymbol{x}\in\mathcal{X}^k_{\neq}}\sum_{\tilde{\boldsymbol{x}}\in\mathcal{X}^k_{\neq}}\langle\mathcal{I}_0(k,\boldsymbol{x},t;\hbar)\varphi,\mathcal{I}_0(k,\tilde{\boldsymbol{x}},t;\hbar)\varphi\rangle_{L^2(\mathbb{R}^d)}\Big].$$

What is the combinatorics?

n = 1

n = 2



This indicates that there is a combinatoric challenge in estimating these norms.

What remains

After having established the convergence of the Duhamel expansion what remain is to establish the limits of the terms

$$\sum_{i=0}^{2}\sum_{j=0}^{2}\sum_{k=k_i}^{k_0}\sum_{\tilde{k}=k_j}^{k_0}\mathbb{E}\Big[\sum_{\boldsymbol{x}\in\mathcal{X}_{\neq}^{k-i}}\sum_{\tilde{\boldsymbol{x}}\in\mathcal{X}_{\neq}^{k-j}}\langle \mathrm{Op}_{\hbar}^{\mathrm{w}}(a)\mathcal{I}_i(k,\boldsymbol{x},t;\hbar)\varphi,\mathcal{I}_j(\tilde{k},\tilde{\boldsymbol{x}},t;\hbar)\varphi\rangle_{L^2(\mathbb{R}^d)}\Big].$$

This is done in a number of steps:

1. Firstly when either $i>0$ or $j>0$ we can prove the average converges to zero.

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This is done in a number of steps:

1. Firstly when either $i>0$ or $j>0$ we can prove the average converges to zero.
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3. For the ladder terms a number of "regulations" of the terms are needed. That is we replace Ψ_{α_m} and $\Psi_{\tilde{\alpha}_m}$ with regularised versions $\Psi_{\alpha_m}^{\gamma}$ and $\Psi_{\tilde{\alpha}_m}^{\gamma}$ depending on a parameter γ. These regularised versions will satisfy

$$\hat{T}^{\gamma}(p,p_0)=-i\sum_{n=1}^{\infty}(i\lambda)^n\Psi_n^{\gamma}(p,p_0,\infty;V). \tag{5}$$

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4. Then in the end one can prove convergence.

Thank you for your attention.

Examples of semiclassical Wigner measures

Type	$\psi_\hbar(x)$	$d\mu(x,p)$
Lagrangian	$w(x)\exp(i\hbar^{-1}\langle x, p_0\rangle)$	$\lvert w(x)\rvert^2\delta(p-p_0)\,dx\,dp$
Lagrangian	$\hbar^{-d/2}w(\hbar^{-1}(x-x_0))$	$\delta(x-x_0)\lvert\hat{w}(p)\rvert^2\,dx\,dp$
WKB	$w(x)\exp(i\hbar^{-1}S(x))$	$\lvert w(x)\rvert^2\delta(p-\partial_x S(x))\,dx\,dp$
Coherent	$(\pi\hbar)^{-d/4}\exp(i\hbar^{-1}\langle x-x_0, p_0+i2(x-x_0)\rangle)$	$\delta(x-x_0)\delta(p-p_0)\,dx\,dp$