SEMICLASSICAL SCALING LIMITS OF QUANTUM DYNAMICS

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Abstract. These are notes for a course given at the RTG summer school "Analysis, PDE's and Mathematical Physics" at the University of Texas at Austin in 2011.

Disclaimer: This is a very sketchy and preliminary version, and might certainly contain many typos. Comments are most welcome.

1. Introduction

Isaac Newton's work in the late 17th century that resulted in the foundations of classical mechanics initiated a tremendous scientific development that was accompanied by a stream of triumphant discoveries in physics, both experimental and theoretical. During the two centuries between Newton's discoveries and the end of the 19th century, numerous classical field and continuum theories, such as electrodynamics, fluid dynamics (Euler and Navier Stokes equations), thermodynamics, kinetic theory (Boltzmann, Vlasov equations), etc, were discovered and have remained extremely active research areas until today. Nowadays, they are the fundamental theories underlying vast areas of technology and engineering, ranging from the design of airplanes and space shuttles, to wireless signal transmission and robotics, to name a tiny number of examples.

The beginning of the 20th century witnessed the discovery of quantum mechanics, which subsequently led to quantum field theory. Those theories describe matter on atomic and subatomic scales; so small that Newton's laws of classical mechanics become inaccurate and incorrect. On the other hand, the beginning of the 20th century also witnessed the discovery of Einstein's theory of General Relativity which describes matter at astronomic scales, where Newton's laws likewise lose their validity.

After many early contributions to quantum theory, the decisive steps completing the transition from classical mechanics to quantum mechanics were accomplished by Schrödinger and Heisenberg, both of whom used intuition from classical mechanics, to devise a "quantization prescription" that yielded the new quantized theory. The discovery of quantum mechanics was preceded by the discovery of a new natural constant, Planck's constant $\hbar \approx 1.054571726... \cdot 10^{-34} \frac{m^2 kg}{sec}$, which turned out to be inseparably tied to any quantum phenomenon. The description of large numbers of interacting quantized particles led to the development of quantum electrodynamics and quantum field theory (with major contributions by Born, Dirac, Heisenberg, Jordan, Pauli, Wigner, among many others). The latter were at first plagued by

severe divergences in perturbation theory, a problem that was resolved with the technique of renormalization developed in the 1940's and 50's (mainly by Bethe, Dyson, Feynman, Tomonaga, Schwinger), and renormalization group theory in the 70's (Kadanoff, Fisher, Wilson, extending early work of Stueckelberg). Nowadays, string theory is studied as a possible framework to unify quantum field theory with general relativity. It is interesting to note that all these developments in quantum theory took place within a human lifetime; the currently (July 2011) oldest living person was born in 1896, one year before the electron was experimentally verified by J. J. Thomson and his collaborators, in 1897.

These lectures are intended for a mathematical audience specializing in areas close to analysis, PDE's, and applied mathematics. Customarily, quantum mechanics and quantum field theory are taught from a historically inspired point of view; that is, one starts with the foundations of classical mechanics and field theory, and subsequently introduces a quantization rule (that depends on $\hbar$) which is in itself not further explainable from any known, more fundamental principles. This point of view places much weight on the quantization procedure; while there is a profound and beautiful mathematical theory of quantization (deformation quantization theory), this aspect is in many instances presented merely as an extrapolation of the heuristics and intuition that led Schrödinger and Heisenberg to their discovery of the equations of quantum mechanics. As a result, this approach often blurs the conceptual relationship between classical and quantum theory, and makes it challenging to grasp for those entering the field.

On the other hand, *conceptually*, it is clear that quantum mechanics and quantum field theory are more fundamental than classical mechanics and field theory (although historically, they were discovered later). Therefore, it may for some (perhaps especially mathematicians, who are used to first identifying the fundamental axioms before deriving higher level theorems) be conceptually more satisfying (while possibly didactically more challenging), to first be introduced to quantum theory without any reference to classical physics, and subsequently to *derive* the equations of classical physics in various *semiclassical limits* where $\hbar \to 0$. The rigorous implementation of such a *derivation of classical physics from quantum theory* leads to profound and beautiful mathematics. Some of the related techniques will be sketched in these lectures. Evidently, we will only be able to offer a few glimpses into this vast area of mathematical research; those will mainly be based on the discussion of a few important example systems.

Contents

These notes are in a very preliminary form, and will be further updated.

2. The Wigner transform

We consider the Schrödinger equation

$$i\partial_t\psi \;=\; -\frac{1}{2}\Delta\psi + V\psi \tag{2.1}$$

with $\psi \in C(\mathbb{R}; L^2_x(\mathbb{R}^d))$, $\psi(0) = \psi_0 \in L^2_x(\mathbb{R}^d)$.

Here, $\psi(t,x)$ is the Schrödinger wave function, and satisfies the normalization condition

$$\|\psi(t)\|^2_{L^2} \;=\; \int |\psi(t,x)|^2 dx \;=\; 1 \tag{2.2}$$

(the L^2-norm is conserved). Accordingly, $\rho(t,x) := |\psi(t,x)|^2$ defines, for any fixed t, a probability measure. The physical interpretation is that if one measures the location of the particle, then $|\psi(t,x)|^2$ is the probability to find it at x, at time t.

On the other hand, the Plancherel identity tells us that

$$\|\psi(t)\|^2_{L^2} \;=\; \int |\widehat{\psi}(t,p)|^2 dp \;=\; 1 \tag{2.3}$$

where $\mu(t,v) := |\widehat{\psi}(t,p)|^2$ defines, for almost every t, a probability measure. The physical interpretation is that if one measures the frequency of the particle, then $|\widehat{\psi}(t,p)|^2$ is the probability to find the measured result that its frequency is p, at time t. De Broglie first realized that the quantum mechanical momentum of a particle coincides with its frequency vector, p. Therefore, the Fourier multiplication operator

$$P \;:=\; i\nabla_x \tag{2.4}$$

with symbol ξ is called the quantum mechanical momentum operator.

Next, let A be a linear operator with domain $\mathrm{dom}(A) \subseteq L^2(\mathbb{R}^d)$. Then, we define

$$\begin{aligned} \big\langle\, A \,\big\rangle_{\psi} \;&:=\; (\,\psi, A\psi\,)_{L^2} \\ &=\; \int \overline{\psi(x)}(A\psi)(x)\,dx \end{aligned} \tag{2.5}$$

for any vector $\psi \in \mathrm{domA}$.

Next, we observe that

$$\widehat{\rho}(t,\xi) \;:=\; \Big\langle e^{-ix\cdot\xi} \Big\rangle_{\psi(t)} \;=\; \int e^{-ix\cdot\xi}|\psi(t,x)|^2 dx \tag{2.6}$$

is the Fourier transform of $\rho(t,x)$, hence $\rho(t,x) = (\widehat{\rho})^\vee(t,x)$.

Also,

$$\widehat{\mu}(t,\eta) \;:=\; \Big\langle e^{-iP\cdot\eta} \Big\rangle_{\psi(t)} \;=\; \int e^{-ip\cdot\eta}|\widehat{\psi}(t,p)|^2 dp \tag{2.7}$$

is the Fourier transform of $\mu(t,p)$, hence $\mu(t,p) = (\widehat{\mu})^\vee(t,p)$.

Evidently, both $e^{-ix\cdot\xi}$ and $e^{-iP\cdot\eta}$ are unitary operators $L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$.

It is important to note that $\rho(t)$ and $\mu(t)$ are *not* mutual Fourier transforms.

In classical mechanics, the state of a point particle is described by its phase space vector (x,p), with the classical momentum $p = mv$. Thus, $p = v$ if $m = 1$.

We would like to determine the phase space content of $\psi(t)$, which gives *simultaneous* information about the (x,p)-space density. To this end, we introduce

$$\begin{aligned}\widehat{W}(t,\xi,\eta) &:= \left\langle e^{-i(x\cdot\xi+P\cdot\eta)}\right\rangle_{\psi(t)} \\ &= \int \overline{\psi(t,x)}(e^{-i(x\cdot\xi+P\cdot\eta)}\psi)(t,x)\,dx\,. \end{aligned} \tag{2.8}$$

Accordingly,

$$W(t,x,p) \,=\, (\widehat{W})^{\vee}(t,x,p) \tag{2.9}$$

corresponds to the phase space density associated to $\psi(t)$.

Definition 2.1. *$W(t,x,v)$ is called the* **Wigner transform** *associated to $\psi(t)$.*

It is in general not positive definite, and thus not a probability density. However, smearing it out with a Gaussian $G(x,p) = Ce^{-|x|^2-|p|^2}$,

$$H(t,x,p) \,:=\, (W(t,\,\cdot\,,\,\cdot\,) \,*\, G)(x,p) \tag{2.10}$$

one does in fact obtain a probability distribution, which is referred to as the *Husimi function* associated to $\psi(t)$.

As we will see, the Wigner transform is ideally suited for the analysis of semiclassical scaling limits of quantum mechanics that are described by kinetic equations.

Lemma 2.2. *The Wigner transform has the form*

$$W(t,x,p) \,=\, \int \overline{\psi(t,x-\frac{y}{2})}\,\psi(t,x+\frac{y}{2})\,e^{ip\cdot y}\,dy\,. \tag{2.11}$$

Proof. We recall the *Baker-Campbell-Hausdorff formula*: Let A, B be two linear operators for which e^A and e^B are well-defined, satisfying that $[A,B] \in \mathbb{C}$ is nonzero, but $[A,[A,B]] = 0 = [B,[A,B]]$. Then,

$$e^{A+B} \,=\, e^A e^B e^{-\frac{1}{2}[A,B]}\,. \tag{2.12}$$

We claim that accordingly,

$$e^{-i(x\cdot\xi+P\cdot\eta)} \,=\, e^{-ix\cdot\xi}e^{-iP\cdot\eta}e^{-\frac{i}{2}\xi\cdot\eta}\,. \tag{2.13}$$

This follows from $[x\cdot\xi, P\cdot\eta] = -i\xi\cdot\eta$.

Next, we note that $e^{-iP\cdot\eta}$ acts as translation by η. Indeed,

$$\begin{aligned} e^{-iP\cdot\eta}f(x) &= e^{\eta\cdot\nabla_x}\int \widehat{f}(\xi)e^{ix\cdot\xi}d\xi \\ &= \int \widehat{f}(\xi)e^{i(x+\eta)\cdot\xi}d\xi \\ &= f(x+\eta)\,. \end{aligned} \tag{2.14}$$

Therefore,

$$\widehat{W}(t,\xi,\eta) \;=\; \int e^{-ix\cdot\xi}\, e^{-\frac{i}{2}\xi\cdot\eta}\, \overline{\psi(t,x)}\psi(t,x+\eta)dx\,, \tag{2.15}$$

and

$$\begin{aligned} W(t,x,p) &= \int d\xi d\eta e^{ix\cdot\xi} e^{ip\cdot\eta} \int e^{-ix'\cdot\xi}\, e^{-\frac{i}{2}\xi\cdot\eta}\, \overline{\psi(t,x')}\, \psi(t,x'+\eta)dx' \\ &= \int e^{i(x-x'-\frac{\eta}{2})\cdot\xi}\, e^{ip\cdot\eta}\, \overline{\psi(t,x')}\, \psi(t,x'+\eta)\, d\xi d\eta dx' \\ &= \int \delta(x-x'-\frac{\eta}{2})\, e^{ip\cdot\eta}\, \overline{\psi(t,x')}\, \psi(t,x'+\eta)\, d\eta dx' \\ &= \int e^{ip\cdot\eta}\, \overline{\psi(t,x-\frac{\eta}{2})}\, \psi(t,x+\frac{\eta}{2})\, d\eta\,, \end{aligned} \tag{2.16}$$

as claimed. □

3. Semiclassical limits and path integrals

This section describes the emergence of classical mechanics from Quantum Mechanics from the path integral point of view.

It is a deep fact in physics that with every new fundamental theory, an associated natural constant is introduced: The speed of light in special relativity, Einstein's gravitational constant in General Relativity, the Boltzmann constant in statistical physics, etc. Quantum Mechanics introduces Planck's constant, $\hbar$. The dimension of $\hbar$ is that of the action functional in classical mechanics,

$$S[T, y', \gamma, y] \,=\, \int_0^T L(q, \dot{q}) dt \tag{3.1}$$

where $\gamma \in C^2([0,T]; \mathbb{R}^d)$ is a path with prescribed endpoints $\gamma(0) = y'$, $\gamma(T) = y$, and $q(t)$ is the coordinate representation of $\gamma(t)$ in the given chart. $L(q, \dot{q})$ is the Lagrange function. Henceforth, we will not distinguish between γ and $q(t)$. We assume the non-degeneracy condition that the matrix of second derivatives in $\dot{q}$,

$$D^2_{\dot{q}} L[q, \dot{q}] \,>\, 0\,, \tag{3.2}$$

is a positive definite $d \times d$ matrix for all $(q, \dot{q})$. For classical mechanics,

$$L[q, \dot{q}] \,=\, E_{kin} - E_{pot} \,=\, \frac{1}{2}\dot{q}^2 - V(q) \tag{3.3}$$

where we set the particle mass equal to 1. The classical Newtonian equations correspond to the stationary point of $S[T, y', \gamma, y]$ with respect to variation of γ, under the above boundary conditions. This is known as Hamilton's *action principle* in classical mechanics. Then, the associated Euler-Lagrange equations are given by

$$\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{q}}\Big) \,-\, \frac{\partial L}{\partial q} \,=\, 0\,, \tag{3.4}$$

They are equivalent to Newton's equations in classical mechanics.

Since $\hbar$ is a natural constant, it is often convenient to use units in which $\hbar = 1$. The Schrödinger equation in general units reads

$$i\hbar \partial_t \psi(t,x) \,=\, -\frac{\hbar^2}{2}\Delta\psi(t,x) \,+\, V(x)\psi(t,x) \tag{3.5}$$

with $\psi(0,x) = \psi_0(x)$. Notably, in metric units, $\hbar \approx 1.054571726 \cdot 10^{-34} \frac{m^2 kg}{sec}$ is an exceedingly small number. As we will see below, the dimensionless quantity $\frac{S[\cdots]}{\hbar}$ is quintessential for quantum mechanics. To put it more poignantly, quantum mechanics is the physical theory describing processes for which the associated classical action functional has values comparable to $\hbar$.

We want to describe how classical mechanics emerges from quantum mechanics in the framework of the *Feynman path integral*. As a preparation, let us first consider the free Schrödinger equation,

$$i\hbar \partial_t \psi(t,x) \,=\, -\frac{\hbar^2}{2}\Delta\psi(t,x) \quad , \quad \psi(0) \,=\, \psi_0\,. \tag{3.6}$$

Recalling that the kernel of the free evolution operator is given by

$$(e^{-it\frac{H_0}{\hbar}})(x,x') \;=\; \Big(\frac{1}{2\pi i\hbar t}\Big)^{\frac{d}{2}} e^{-i\frac{(x-x')^2}{2\hbar t}}\,, \tag{3.7}$$

the solution is given by

$$\psi(t,x) \;=\; \Big(\frac{1}{2\pi i\hbar t}\Big)^{\frac{d}{2}} \int e^{-i\frac{(x-x')^2}{2\hbar t}}\,\psi_0(x')\,dx'\,. \tag{3.8}$$

Instead of using this formula once, we subdivide $[0,t]$ into N intervals $[t_j,t_{j+1}]$ of equal length $\Delta t = \frac{t}{N}$, while setting $q_0 := x'$ and $q_N = x$. Then,

$$\begin{aligned}
\psi(t,x) &= \int (e^{-i\Delta t\frac{H_0}{\hbar}})^n(x,q_0)\psi_0(q_0)\,dq_0 \\
&= \int (e^{-i\Delta t\frac{H_0}{\hbar}})(x,q_{N-1})(e^{-i\Delta t\frac{H_0}{\hbar}})(q_1,q_0)\psi_0(q_0)\,dq_0dq_1\cdots dq_{N-1} \\
&= \Big(\frac{1}{2\pi i\hbar\Delta t}\Big)^{\frac{Nd}{2}} \int \Big[\prod_{j=0}^{N-1} dq_j\Big] \prod_{j=0}^{N-1} e^{-i\frac{(q_{j+1}-q_j)^2}{2\hbar\Delta t}}\psi_0(q_0) \\
&= \int e^{-i\frac{S_{0,N}[t,\underline{q},x]}{\hbar}}\,\psi_0(q_0)\,\mathcal{D}\underline{q}\,,
\end{aligned} \tag{3.9}$$

where we introduced integration variables $\underline{q} := (q_0,\ldots,q_{N-1})$, and

$$\mathcal{D}\underline{q} \;:=\; \Big(\frac{1}{2\pi i\hbar\Delta t}\Big)^{\frac{Nd}{2}} d\underline{q}\,. \tag{3.10}$$

In particular,

$$S_{0,N}[t,q_0,\underline{q},x] \;:=\; \sum_{j=0}^{N-1} \frac{(q_{j+1}-q_j)^2}{2\Delta t^2}\Delta t \tag{3.11}$$

is a discretization of the classical action functional

$$S_0[t,q_0,\gamma,x] \;=\; \int_0^t \frac{(\dot q(s))^2}{2}\,ds \tag{3.12}$$

for a path $\gamma(t) = x$ and $\gamma(0) = q_0$. The coordinates q_j then correspond to sample points $\gamma(t_j)$, where $t_j = j\Delta t$. As $N\to\infty$, we can re-interpret (3.9) as follows: We take arbitrary arbitrary (non-physical) path $q:[0,t]\to\mathbb{R}^d$ connecting q_0 to x, and multiply the phase $e^{-i\frac{S[t,x',\gamma,x]}{\hbar}}$ to $\psi_0(x')$. Then, we "integrate over all such paths", and subsequently over all starting points x'. Thereby, we arrive at the solution of the free Schrödinger equation $\psi(t,x)$. This "integration over paths" is captured by the notion of a *path integral*, as we describe next.

More generally, now including the potential V, the *Feynman path integral* representation of the solution of the above Schrödinger equation is heuristically given by

$$''\quad \psi(t,x) \;=\; \int dx' \int_{\gamma(t)=x,\gamma(0)=x'} e^{-i\frac{S[t,x',\gamma,x]}{\hbar}}\,\psi_0(x')\,\mathcal{D}\gamma\,. \quad '' \tag{3.13}$$

This means that we pick any arbitrary continuous (in general non-physical) path $\gamma:[0,t]\to\mathbb{R}^d$ connecting x' to x, and multiply the phase $e^{-i\frac{S[t,x',\gamma,x]}{\hbar}}$ to $\psi_0(x')$. Then, we "integrate over all such paths", and finally integrate over all starting points x'.

From stationary phase estimates in harmonic analysis, we expect that (putting aside questions for now as to how to define the "complex measure $D\gamma$" for paths γ) as $\hbar \to 0$, the main part of this oscillatory integral stems from the stationary point of $S[\cdots]$, obtained under variation in γ with fixed endpoints. But the latter corresponds to the solutions of the Euler-Lagrange equations (3.4), and thus describe classical trajectories. Thus, the heuristics from the path integral point of view behind the emergence of classical mechanics from quantum mechanics is that for $\hbar > 0$, extremization of the action functional is accomplished approximately via stationary phase principles, while for $\hbar \to 0$, it becomes exact.

We shall now try to be more precise. We again subdivide $[0, t]$ into N intervals $[t_j, t_{j+1}]$ of equal length $\Delta t = \frac{t}{N}$. Given a path $\gamma : [0, T] \mapsto \mathbb{R}^d$, we consider the sample points $q_j := \gamma(t_j)$, setting $q_N = x$. Following the above in reverse direction, we consider the action functional associated to the path q ending at x, and starting at q_0,

$$S[t, q_0, \gamma, x] \;=\; \int_0^t \Big(\frac{(\dot{q}(s))^2}{2} \;-\; V(q(s)) \Big)\, ds\,. \tag{3.14}$$

Its discretization is given by

$$S_N[t, \underline{q}, x] \;:=\; \sum_{j=0}^{N-1} \Big(\frac{(q_{j+1} - q_j)^2}{2(\Delta t)^2} \;-\; V(q_j) \Big) \Delta t\,. \tag{3.15}$$

Then, we define

$$\psi_N(t, x) \;:=\; \int e^{-i\frac{S_N[t,\underline{q},x]}{\hbar}}\, \psi_0(q_0)\, \mathcal{D}\underline{q}\,. \tag{3.16}$$

For finite N, the convergence of this integral follows from stationary phase considerations applied to the phase $S_N[t, \underline{q}, x]$ as a function of the vector $\underline{q} := (q_0, \ldots, q_{N-1})$.

In fact, the following holds:

Lemma 3.1. *The strong limit*

$$s - \lim_{N\to\infty} \psi_N(t, x) \;=\; \psi(t, x) \;=\; (e^{-\frac{itH}{\hbar}} \psi_0)(x) \tag{3.17}$$

holds in $L^2(\mathbb{R}^d)$, as $N \to \infty$.

Proof. To prove this, we invoke the Trotter product formula,

$$\begin{aligned} e^{-it\frac{H_0+V}{\hbar}} \;&=\; s - \lim_{N\to\infty} \Big(e^{-i\frac{t}{N}\frac{H_0}{\hbar}} e^{-i\frac{t}{N}\frac{V}{\hbar}} \Big)^N \\ &=\; s - \lim_{N\to\infty} \Big(e^{-i\Delta t\frac{H_0}{\hbar}} e^{-i\Delta t\frac{V}{\hbar}} \Big)^N . \end{aligned} \tag{3.18}$$

Therefore,

$$\begin{aligned} & e^{-it\frac{H_0+V}{\hbar}}(x, q_0) \\ &\quad=\; s - \lim_{N\to\infty} \int (e^{-i\Delta t\frac{H_0}{\hbar}})(x, q_{N-1}) e^{-i\Delta t\frac{V(q_{N-1})}{\hbar}} (e^{-i\Delta t\frac{H_0}{\hbar}})(q_{N-1}, q_{N-2}) \\ &\qquad\qquad \cdots\cdots\, (e^{-i\Delta t\frac{H_0}{\hbar}})(q_1, q_0) e^{-i\Delta t\frac{V(q_0)}{\hbar}}\, dq_1 \cdots dq_{N-1}\,, \end{aligned} \tag{3.19}$$

letting $H_0 := -\frac{\hbar^2}{2}\Delta$. Using that

$$e^{-i\Delta t\frac{H_0}{\hbar}}(q_j, q_{j-1}) \;=\; \Big(\frac{1}{2\pi i\hbar\Delta t}\Big)^{\frac{d}{2}} e^{-i\frac{(q_j-q_{j-1})^2}{2\hbar\Delta t}}\,, \tag{3.20}$$

we immediately arrive at the right hand side of (3.16). The limit then follows from the Trotter product formula. For more details, see for instance [33]. □

We recall that for sufficiently regular $\Phi(x)$ and $\psi_0(x)$, with $x \in \mathbb{R}^n$, we have the *stationary phase* formula

$$\begin{aligned}&\int e^{-i\frac{\Phi(x)}{\hbar}}\psi_0(x)dx \qquad\qquad (3.21)\\ &\quad= \big(2\pi\hbar\big)^{\frac{n}{2}}\Big|\det(D^2\Phi(x^*))\Big|^{-\frac{1}{2}} e^{-i\frac{\pi}{4}\mathrm{sign}(D^2\Phi(x^*))}\, e^{-i\frac{\Phi(x^*)}{\hbar}}\psi_0(x^*) \,+\, o_\hbar(1)\end{aligned}$$

provided that there is a single stationary point x^*, solving $(\nabla_x\Phi)(x^*) = 0$, and that the Hessian $\det(D^2\Phi(x^*))$ is non-degenerate. Its signature $\mathrm{sign}(D^2\Phi(x^*))$ is defined as the difference between the numbers of positive and negative eigenvalues.

That is, we determine the stationary point $\underline{q}^*$ of $S_N[t, \underline{q}]$,

$$(\nabla_{\widetilde{\underline{q}}}S)[t, \underline{q}^*, x] \;=\; 0\,, \tag{3.22}$$

with $\widetilde{\underline{q}} := (q_1, \ldots, q_{N-1})$, with q_0^* and $q_N^* = x$ fixed. One easily verifies that the Hessian is given by

$$\begin{aligned}\mathrm{Hess}(S_N[t, \underline{q}^*]) \;&=\; (D^2_{\widetilde{\underline{q}}}S_N)[t, \underline{q}^*] \qquad\qquad (3.23)\\ &=\; \frac{1}{\Delta t}\begin{bmatrix} 2\mathbf{1}_d & -\mathbf{1}_d & 0 & \cdots & 0\\ -\mathbf{1}_d & 2\mathbf{1}_d & -\mathbf{1}_d & \cdots & 0\\ 0 & -\mathbf{1}_d & 2\mathbf{1}_d & \cdots & 0\\ \cdots & \cdots & \cdots & \cdots & \cdots\\ 0 & \cdots & 0 & -\mathbf{1}_d & 2\mathbf{1}_d \end{bmatrix} + (D^2_{\underline{q}}V)(\underline{q}^*)\,\Delta t\\ &=:\; \frac{1}{\Delta t}M_{N,d} \,+\, (D^2_{\underline{q}}V)(\underline{q}^*)\,\Delta t \qquad\qquad (3.24)\end{aligned}$$

is non-degenerate at the critical point $\underline{q}^*$, with q_0^* and $q_N^* = x$ fixed, if $V \in C^2(\mathbb{R}^d)$, and Δt sufficiently small. We note that $M_{N,d}$ is invertible.

On the other hand, we note that criticality of the discretized action (3.22) yields

$$\frac{-q^*_{j+1} + 2q^*_j - q^*_{j-1}}{\Delta t^2} \;=\; -\,\nabla_{q^*_j}V(q^*_j)\,, \tag{3.25}$$

for $j = 1, \ldots, N-1$. As expected from the action principle, these corresponds to the discretized Newton equations. Hence, $\underline{q}^* = (q_0^*, \ldots, q_{N-1}^*, x)$ is a discrete approximation to the classical solution $q^*(t)$ of Newton's equations of motion for the given Lagrangian, connecting q_0^* to x.

The stationary phase analysis sketched above (after integrating out the variables $q_1, \ldots, q_{N-1}$) implies that

$$\psi_N(t, x) \;=\; \int K_N(t, q_0^*, \widetilde{\underline{q}}^*, x)\,\psi_0(q_0^*)\,dq_0^* \,+\, o_\hbar(1)\,. \tag{3.26}$$

where

$$\begin{aligned} K_N(t,q_0^*,\underline{\widetilde{q}}^*,x) &:= \Big(\frac{1}{2\pi i\hbar\Delta t}\Big)^{\frac{Nd}{2}} (2\pi i\hbar)^{\frac{Nd}{2}} \Big|\det\Big(D^2_{\underline{\widetilde{q}}}(S_N[t,\underline{q}^*,x])\Big)\Big|^{-\frac{1}{2}} e^{-i\frac{S[t,\underline{q}^*,x]}{\hbar}} \\ &= \Big|\det\Big(\Delta t\, D^2_{\underline{\widetilde{q}}}(S_N[t,\underline{q}^*,x])\Big)\Big|^{-\frac{1}{2}} e^{-i\frac{S[t,\underline{q}^*,x]}{\hbar}} \\ &= \Big|\det\Big(M_{N,d} + (D^2_{\underline{q}}V)(\underline{q}^*)\Delta t^2\Big)\Big|^{-\frac{1}{2}} e^{-i\frac{S[t,\underline{q}^*,x]}{\hbar}} . \end{aligned} \tag{3.27}$$

So far, we have little control on this determinant as $N \to \infty$.

However, this can be remedied by making the following observation. We notice that for the free evolution with potential $V = 0$, we have the following kernel for the same initial and end point, $q_0^* = x$ (so that $q_j^* = x$ along the classical trajectory, for $j = 0, 1, \ldots, N$, and $S_N[t, x, x, \ldots, x] = 0$),

$$\begin{aligned} \Big(\frac{1}{2\pi i\hbar t}\Big)^{\frac{d}{2}} &= \Big(\frac{1}{2\pi i\hbar t}\Big)^{\frac{d}{2}} e^{-i\frac{|x-x|^2}{2t}} \\ &= K_{0,N}(t,x,x,\ldots,x) \\ &= \Big|\det\Big(M_{N,d}\Big)\Big|^{-\frac{1}{2}} e^{-i\frac{S_{0,N}[t,x,x,\ldots,x]}{\hbar}} + o_\hbar(1)\,. \end{aligned} \tag{3.28}$$

To pass to the third line, we applied similar considerations as above to (3.9) (which is an exact identity), using stationary phase estimates. This implies that

$$\psi_N(t,x) = \Big(\frac{1}{2\pi i\hbar t}\Big)^{\frac{d}{2}} \int G_N(t,y,\underline{\widetilde{q}}^*,x)\, e^{-i\frac{S[t,y,\underline{\widetilde{q}}^*,x]}{\hbar}}\, \psi_0(y)\, dy + o_\hbar(1)\,, \tag{3.29}$$

where $q_0^* = y$, and

$$\begin{aligned} G_N(t,y,\underline{\widetilde{q}}^*,x) &:= \frac{\Big|\det\Big(M_{N,d}\Big)\Big|^{\frac{1}{2}}}{\Big|\det\Big(M_{N,d} + (D^2_{\underline{q}}V)(\underline{q}^*)\,\Delta t^2\Big)\Big|^{\frac{1}{2}}} \\ &= \Big|\det\Big(\mathbf{1}_{Nd} + M_{N,d}^{-\frac{1}{2}}\,(D^2_{\underline{q}}V)(\underline{q}^*)\,M_{N,d}^{-\frac{1}{2}}\;\Delta t^2\Big)\Big|^{-\frac{1}{2}} . \end{aligned} \tag{3.30}$$

Assuming that the limits $G_N \to G$ and $\psi_N(t,x) \to \psi(t,x)$ can be controlled as $N \to \infty$, one finds

$$\psi(t,x) = \Big(\frac{1}{2\pi i\hbar t}\Big)^{\frac{d}{2}} \int G(t,y,\gamma^*,x)\, e^{-i\frac{S[t,y,\gamma^*,x]}{\hbar}}\, \psi_0(y)\, dy + o_\hbar(1)\,, \tag{3.31}$$

where γ^* is the classical solution of Newton's equation with endpoints $\gamma^*(0) = y$ and $\gamma^*(t) = x$. In particular, the phase is obtained from the classical action functional evaluated for the solution of Newton's equation connecting y to x. A more detailed discussion can be found in [33].

We also note the similarity of (3.16) to the Feynman-Kac formula for diffusion processes in probability theory. The *crucial* difference here is the presence of the imaginary unit in the exponent in the case of quantum mechanics, due to which the problem here is of oscillatory type.

4. Wigner transform and convergence to Liouville equations

We have seen how the path integral interpretation, combined with stationary phase estimates, explains how classical mechanics is related to quantum mechanics in the limit $\hbar \to 0$. We now want to address a method that allows us to grasp such concepts in a manner more readily accessible to methods of PDE's. This brings us back to the use of the Wigner transform.

Let us assume that $V \in C^2(\mathbb{R}^d)$. We consider the Schrödinger equation

$$i\epsilon\partial_t\psi^\epsilon(t,x) \,=\, -\,\frac{\epsilon^2}{2}\Delta\psi^\epsilon(t,x) \,+\, V(x)\psi^\epsilon(t,x) \tag{4.1}$$

We want to study the limit $\hbar \to 0$, but $\hbar$ is a number with a fixed value (a natural constant); this is why we write ϵ instead.

We consider the Wigner transform

$$W^\epsilon(t,x,p) \,=\, \int \overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy\,. \tag{4.2}$$

Then, using

$$\partial_t\psi^\epsilon(t,x) \,=\, \frac{i\epsilon}{2}\Delta\psi^\epsilon(t,x) \,-\, \frac{i}{\epsilon}V(x)\psi^\epsilon(t,x)\,, \tag{4.3}$$

we obtain

$$\partial_t W^\epsilon(t,x,p) \,=\, (I) \,+\, (II) \tag{4.4}$$

with

$$\begin{aligned}
(I) \;&:=\; \frac{i\epsilon}{2}\int \overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\Delta_x\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy \\
&\quad -\frac{i\epsilon}{2}\int \overline{\Delta_x\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy \\
&=\; i\int \nabla_x\cdot\nabla_y\Big(\overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\Delta_x\psi^\epsilon(t,x+\frac{\epsilon y}{2})\Big)\,e^{iy\cdot p}\,dy \\
&=\; p\cdot\nabla_x\int \overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\Delta_x\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy \\
&=\; p\cdot\nabla_x W^\epsilon(t,x,p)\,,
\end{aligned} \tag{4.5}$$

where we used integration by parts in y to pass to the third line. Moreover,

$$\begin{aligned}
(II) \;&:=\; -\frac{i}{\epsilon}\int \big(\,V(x+\frac{\epsilon y}{2})-V(x-\frac{\epsilon y}{2})\,\big)\overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy \\
&=\; -i\int \nabla_x V(x)\cdot y\;\overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy \,+\, R^\epsilon \\
&=\; -\nabla_x V(x)\cdot\nabla_p\int \overline{\psi^\epsilon(t,x-\frac{\epsilon y}{2})}\,\psi^\epsilon(t,x+\frac{\epsilon y}{2})\,e^{iy\cdot p}\,dy \,+\, R^\epsilon \\
&=\; -\nabla_x V(x)\cdot\nabla_p W^\epsilon(t,x,p) \,+\, R^\epsilon\,,
\end{aligned} \tag{4.6}$$

where the error term R^ϵ can be shown to tend to zero weakly as $\epsilon \to 0$. We note that for $V \in C^2$, the error term can be expressed via the Taylor remainder term of

degree 2 of V. In particular, it can be proved that W^ϵ converges weakly, along a subsequence (ϵ_k), to a distribution $\mu(t,x,p)$ which satisfies the Liouville equation

$$\partial_t \mu(t,x,p) \,+\, p\cdot\nabla_x\mu(t,x,p) \,-\, \nabla_x V(x)\cdot\nabla_p\mu(t,x,p) \,=\, 0\,. \tag{4.7}$$

In this sense, the Wigner transform of the solution of a Schrödinger equation converges to a solution of a classical Liouville equation. We shall not address any details about the proofs here, and instead refer to [30, 31, 32]. There are many works concerned with the proof of such limits under weaker assumptions on V.

The meaning of the Liouville equation in classical mechanics is as follows. We first address the Hamiltonian formulation of classical mechanics. Given the Lagrangian $L(q,v)$, we define

$$p(q,v) \,:=\, \frac{\partial L}{\partial v}(q,v)\,. \tag{4.8}$$

Given the non-degeneracy condition (3.2) on the Lagrangian, this equation can be solved for $v = v(q,p)$. Then,

$$H(q,p) \,:=\, p\cdot v(q,p) \,-\, L(q,v(q,p)) \tag{4.9}$$

is the *Hamiltonian*.

As a matter of fact, (3.2) is a rather strong condition that we used for the stationary phase arguments related to the path integral approach. For the construction of the Hamiltonian, it suffices to impose the weaker conditions that $L(q,v)$ is convex in v, and that $\lim_{|v|\to\infty}\frac{L(q,v)}{|v|} = \infty$ (these properties follow immediately from (3.2)). Then, the Legendre transform of the Lagrangian,

$$H(q,p) \,=\, \sup_v \big(\, p\cdot v \,-\, L(q,v)\,\big) \tag{4.10}$$

is well-defined for every $p\in\mathbb{R}^d$, and gives an alternative construction of the Hamiltonian. If (3.2) is satisfied, both approaches result in the same expression for the Hamiltonian, as it should be.

The action functional for a path $x(s) = (q(s),p(s)) \in \mathbb{R}^{2d}$ in phase space corresponds to

$$S[t,x(\cdot)] \,=\, \int_0^t \left(p(s)\cdot\dot q(s) - H(q(s),p(s))\right) ds \tag{4.11}$$

with fixed initial and end points $q(0)$ and $q(t)$ of the projection $x(s)\to q(s)$.

Variation in $x(\cdot)$ with fixed end points of $q(s)$ yields the Hamiltonian equations of motion,

$$\begin{aligned} \dot q &= \nabla_p H(q,p) \\ \dot p &= -\nabla_q H(q,p)\,. \end{aligned} \tag{4.12}$$

Letting $x = (q,p)\in\mathbb{R}^{2d}$ denote the phase space variable, we have the ODE

$$\dot x \,=\, J\,\nabla_x H(x) \,=\, X_H(x) \tag{4.13}$$

where X_H is the Hamiltonian vector field, and $J = \begin{bmatrix} 0 & \mathbf{1}_d \\ -\mathbf{1}_d & 0 \end{bmatrix}$. The flow Φ_t generated by X_H is called the Hamiltonian flow. In particular, it is symplectic, $D\Phi_t^T J D\Phi_t = J$, and preserves the volume dx.

Instead of a single orbit $\Phi_t(x)$ (passing through x at $t = 0$), we now ask how a distribution given by $f_0(x)$ at $t = 0$ evolves in time, that is,

$$f(t, x) \,=\, f_0(\Phi_{-t}(x))\,. \tag{4.14}$$

We note that (4.14) is the solution of

$$\partial_t f(t, x) \,+\, X_H(x) \cdot (\nabla_x f)(t, x) \,=\, 0 \tag{4.15}$$

obtained from the method of characteristics. In components $x = (q, p)$,

$$\partial_t f(t, q, p) \,+\, \nabla_p H(q, p) \cdot \nabla_q f(t, q, p) \,-\, \nabla_q H(q, p) \cdot \nabla_p f(t, q, p) \,=\, 0\,, \tag{4.16}$$

which is the general form of the Liouville equation.

For the Hamiltonian of a point particle in the potential V,

$$H(q, p) \,=\, \frac{p^2}{2} \,+\, V(q)\,, \tag{4.17}$$

we obtain

$$\partial_t f(t, q, p) \,+\, p \cdot \nabla_q f(t, q, p) \,-\, \nabla_q V(q) \cdot \nabla_p f(t, q, p) \,=\, 0\,, \tag{4.18}$$

which is the Liouville equation (4.7) obtained from the semiclassical limit of the Wigner transform associated to ψ^ϵ.

5. The Boltzmann limit for the weakly disordered Anderson model

We will now discuss a model in quantum mechanics for which a semiclassical scaling limit can be rigorously performed, in such a way that the Wigner transform converges in a suitable way to the solution of a Boltzmann equation.

We let $\Lambda_L := [-L, L]^d \cap \mathbb{Z}^d$ denote a box with side length $L \gg 1$ which we will eventually send to infinity. Let $\Lambda_L^* := \frac{1}{L}\Lambda_L$ denote the associated dual lattice.

We consider the *discrete* Schrödinger equation

$$i\partial_t \psi(t,x) \;=\; \Delta\psi(t,x) \;+\; \eta\, V_\omega(x)\psi(t,x) \tag{5.1}$$

for $x \in \Lambda_L$ and $\psi(t) \in \ell^2(\Lambda_L)$, where $\eta > 0$ is a small parameter.

Here, $\Delta = -\Delta$ is the centered nearest neighbor Laplacian,

$$(\Delta\psi)(x) \;=\; \sum_{x',\, |x-x'|=1} \psi(x')\,. \tag{5.2}$$

(we discard the diagonal term in the discrete Laplacian by a shift of the spectrum of the Hamiltonian). Its spectrum is given by $\operatorname{spec}\Delta \;=\; [-2d, 2d] \cap \frac{1}{L^d}\mathbb{Z}$.

Furthermore, we assign to each lattice site x a random variable ω_x, for instance with Gaussian distribution, and assume that $(\omega_x)_{x\in\Lambda_L}$ are independent, identically distributed. Moreover, we assume zero mean, $\mathbb{E}[\omega_x] = 0$, and normalized variance, $\mathbb{E}[\omega_x^2] = 1$. Then, V_ω is a random potential which acts as a multiplication operator $V_\omega(x)\psi(x) = \omega_x\psi(x)$.

The lattice Hamiltonian

$$H_\omega \;=\; \Delta \;+\; \eta\, V_\omega(x) \tag{5.3}$$

defines the so-called *Anderson model*. It is one of the most widely studied models for the dynamics of electrons in disordered materials such as semiconductors. For any $L < \infty$, H_ω is almost surely selfadjoint on $\ell^2(\Lambda_L)$.

The discrete Fourier transform is given by

$$\widehat{f}(p) \;:=\; \sum_{x\in\Lambda_L} e^{-2\pi i p\cdot x}\, f(x)\,, \tag{5.4}$$

where $p \in \Lambda_L^*$, and its inverse

$$f(x) \;=\; \frac{1}{L^d} \sum_{p\in\Lambda_L^*} e^{2\pi i p\cdot x}\, \widehat{f}(p)\,. \tag{5.5}$$

For brevity, we will use the notation

$$\int dp \;\equiv\; \frac{1}{L^d} \sum_{p\in\Lambda_L^*} \tag{5.6}$$

in the sequel, which recovers its usual meaning in the thermodynamic limit $L \to \infty$.

The nearest neighbor lattice laplacian is a Fourier multiplication operator

$$\widehat{\Delta\psi}\,(k) \;=\; e_\Delta(k)\,\widehat{\psi}(k)$$

whose symbol

$$e_\Delta(k) \;=\; \sum_{i=1}^{d} 2\cos(2\pi k_i)$$

is the kinetic energy of the quantum mechanical electron.

The *Schrödinger equation* for the Anderson model on $\ell^2(\Lambda_L)$ is given by

$$i\,\partial_t\,\psi_t(x) \;=\; H_\omega\,\psi_t(x)$$
$$\psi_0 \;\in\; \ell^2(\Lambda_L)$$

The solution to this Cauchy problem is given by the unitary flow generated by H_ω, that is, $\psi_t \,=\, e^{-itH_\omega}\,\psi_0$.

5.1. **A little background on the Anderson model.** The absence of electron transport (*Anderson localization*, electric insulators) for large $|\eta| \gg 1$, is a classical mathematical result that is nowadays well understood, [2, 29]. On the other hand, the weak disorder regime, $|\eta| \ll 1$, poses some very prominent open problems. Only in dimension $d = 1$, it is known that Anderson localization occurs for all values of $|\eta| > 0$, [13]. In $d = 2$, it is conjectured that even for small $|\eta| \ll 1$, Anderson localization persists. In $d \geq 3$, it is conjectured that there exists a component of absolutely continuous spectrum, associated to delocalized states and electric conduction. For a kinetic scaling determined by macroscopic time and space coordinates $(T, X) = \eta^2(t, x)$, it is proven that, as $\eta \to 0$, the semiclassical dynamics is determined by a linear Boltzmann equation in [22, 27, 47]; see also [14, 15, 16]. It is proven in [23, 24, 26, 25] that for $d \geq 3$, the dynamics predicted by the Anderson model is diffusive, in a scaling limit that corresponds to large but finite microscopic times. It is expected that diffusive transport holds for all times, thus explaining electric conductivity, and the delocalization of electron wave functions in the relevant energy regimes. See also [3, 9, 10, 11, 17, 18, 21, 34, 35, 36, 37, 38, 39, 40, 43, 44, 46].

5.2. **Kinetic scaling limits for small disorders $\eta \ll 1$.** We will next show that the quantum dynamics in the weakly disordered Anderson model is, in a sense that we will make precise, governed by a linear Boltzmann equation. This is based on work in [14, 23, 24, 25, 49]; see also [36, 37].

We consider the Wigner transform of $\psi_t = e^{-itH_\omega}\psi_0$

$$W_t(x, v) \;=\; 8 \sum_{\substack{y,z\in\Lambda_L\\ y+z=2x}} \overline{\psi_t(y)}\;\psi_t(z)\;e^{2\pi i v(y-z)}\,.$$

Next, we introduce macroscopic time and space variables, $(T, X) = \eta^2(t, x)$. Because both t and x scale with the same constant, this is referred to as a *kinetic scaling* (suggesting a dynamics where particles propagate freely between collisions).

To understand that η^2 is the correct factor for our considerations, we think of the following heuristics. The assumption of vanishing mean implies that the average effect of the random potential on the dynamics of μ_t in a time interval $[0, t]$ is proportional to its variance, of size $O(\eta^2 t)$. This suggests that the strength of the interaction with the random potential becomes significant (of order $O(1)$) once the

time is of order $t = O(\eta^{-2})$. Until then, the solution will propagate like a small perturbation of the free evolution ("*ballistically*").

In addition, we make the following heuristic observation. If for a moment, we think of Δ as being the Laplacian on $\mathbb{R}^3$ (instead of being the lattice Laplacian), then we would have

$$\eta^2 \partial_T \psi^\eta(T,X) \;=\; -\,\eta^4 \Delta \psi^\eta(T,X) \;+\; \eta V_\omega(X/\eta^2)\,\psi^\eta(T,X) \tag{5.7}$$

in macroscopic space-time coordinates, where

$$\psi^\eta(T,X) \;:=\; \psi(T/\eta^2, X/\eta^2)\,. \tag{5.8}$$

Comparing with our previous discussion, this means that η^2 plays the rôle of $\hbar$.

Accordingly, we consider rescaled Wigner transform

$$W_T^{(\eta)}(X,V) \;=\; \left(\frac{1}{\eta^2}\right)^3 W_{T/\eta^2}(X/\eta^2, V)\,,$$

and intend to control the limit as $\eta \to 0$. Then, the Boltzmann limit holds in the sense of weak convergence in expectation.

Theorem 5.1. [27, 14] *For $\mu > 0$, let*

$$\phi_0^\mu(x) \;:=\; \mu^{\frac{3}{2}}\, \frac{h(\mu x)\, e^{2\pi i \frac{S(\mu x)}{\mu}}}{\|h\|_{\ell^2(\mu\mathbb{Z}^3)}}\,, \tag{5.9}$$

with $h, S \in \mathcal{S}(\mathbb{R}^3, \mathbb{R})$ of Schwartz class, and $\|h\|_{L^2(\mathbb{R}^3)} = 1$. Assume L sufficiently large that $\phi_0^\mu\Big|_{\Lambda_L} = \phi_0^\mu$. Let ϕ_t^μ be the solution of the random Schrödinger equation

$$i\,\partial_t \phi_t^\mu \;=\; H_\omega\, \phi_t^\mu \tag{5.10}$$

on $\ell^2(\Lambda_L)$ with initial condition ϕ_0^μ, and let

$$W_T^{(\mu)}(X,V) \;:=\; W^\mu_{\phi^\mu_{\mu^{-1}T}}(X,V) \tag{5.11}$$

denote the corresponding rescaled Wigner transform.

Choosing

$$\mu \;=\; \eta^2\,, \tag{5.12}$$

where η is the coupling constant in (5.1)*, it follows that*

$$\lim_{\eta\to 0} \lim_{L\to\infty} \mathbb{E}\big[\,\langle\, J\,,\, W_T^{(\eta^2)}\,\rangle\,\big] \;=\; \langle\, J\,,\, F_T\,\rangle\,, \tag{5.13}$$

where $F_T(X,V)$ solves the linear Boltzmann equation

$$\begin{aligned} \partial_T F_T(X,V) \;+\; 2\pi\, \nabla_V e_\Delta(V) \cdot \nabla_X F_T(X,V) \\ \;=\; \int_{\mathbb{T}^3} dU\, \sigma(U,V)\, [F_T(X,U) \;-\; F_T(X,V)] \end{aligned} \tag{5.14}$$

with initial condition

$$\begin{aligned} F_0(X,V) \;&=\; w - \lim_{\mu\to 0} W^\mu_{\phi_0^\mu} \\ &=\; |h(X)|^2\, \delta(V \;-\; \nabla S(X))\,, \end{aligned} \tag{5.15}$$

and where

$$\sigma(U,V) \;:=\; 2\pi\, \delta(e_\Delta(U) \;-\; e_\Delta(V))$$

denotes the collision kernel.

The convergence proven here is weakly, and in expectation. In [15], it was proven that it actually holds in the weak sense, and in higher mean $\mathcal{L}^r$ with respect to the randomness, for any $1 \leq r < \infty$, and therefore, also in probability. This means that the average dynamics is also typical.

The proof Theorem 5.1 due to Erdös and Yau, [27], and further developed in [14, 15, 24, 37], involves the following main steps, some of which are profoundly inspired by techniques of Quantum Field Theory. We shall now sketch the main steps.

5.3. **Step 1: Resolvent expansion.** As a starting point, we represent the time evolution operator of the random Schrödinger equation by use of the spectral theorem,

$$\psi_t \;=\; \frac{1}{2\pi i}\int_{\mathbb{R}+i\epsilon} dz\, e^{-itz}\,\frac{1}{H_\omega - z}\,\psi_0$$

and apply a truncated Neumann series exansion to the resolvent,

$$\psi_t \;=\; \sum_{n=0}^{N}\psi_t^{(n)} \;+\; R_t^{(N)}$$

$$\psi_t^{(n)} \;=\; \frac{(-\eta)^n}{2\pi i}\,e^{\epsilon t}\int_{\mathbb{R}} dE\, e^{-itE}\left(\frac{1}{\Delta - E - i\epsilon}\,V_\omega\right)^n \frac{1}{\Delta - E - i\epsilon}\,\psi_0\,.$$

This infers a decomposition of the Wigner transform into

$$W_t \;=\; \sum_{n,\widetilde{n}=0}^{N+1} W_t^{(n,\widetilde{n})}\,.$$

We then note that

$$\begin{aligned}
&\int J(X,V)W^{(\eta^2)}(t,X,V)\,dX\,dV\\
&\quad= \int J_{\eta^2}(x,v)W(t,x,v)\,dx\,dv\\
&\quad= \int \widehat{J}_{\eta^2}(\xi,v)\overline{\widehat{\psi}(t,v-\frac{\xi}{2})}\,\widehat{\psi}(t,v+\frac{\xi}{2})\,d\xi\,dv \qquad (5.16)
\end{aligned}$$

where we define $J_\mu(x,v) := J(\mu x, v)$, so that $\widehat{J}_\mu(\xi,v) = \mu^{-3}\widehat{J}(\mu^{-1}\xi, v)$ corresponds to the Fourier transform in the first argument.

Taking the expectation with respect to the random potential, one obtains an expansion of the form

$$\begin{aligned}
\mathbb{E}[\,\langle\, W_t\,,\, J_{\eta^2}\,\rangle\,] \;&=\; \sum_{n,\widetilde{n}=0}^{N+1}\mathbb{E}[\,\langle\, W_t^{(n,\widetilde{n})}\,,\, J_{\eta^2}\,\rangle\,]\\
&=\; \sum_{n,\widetilde{n}=0}^{N+1}\;\sum_{\pi\in\Gamma_{n,\widetilde{n}}}\mathrm{Amp}_{J_{\eta^2}}(\pi)
\end{aligned}$$

where the resulting terms are organized by use of *Feynman graphs*. By $\Gamma_{n,\widetilde{n}}$, we are denoting the set of *Feynman graphs* on $n+\widetilde{n}$ vertices corresponding to copies of V_ω, and one distinguished vertex corresponding to J_{η^2}, see the next section.

The number of graphs is given by $|\Gamma_{n,\widetilde{n}}| \sim (n+\widetilde{n})!$

5.4. **Step 2: Graph expansion.** The elements of the set of *Feynman graphs* $\Gamma_{n,\widetilde{n}}$, with $n+\widetilde{n} \in 2\mathbb{N}$, are defined as follows. We consider two horizontal solid lines, which we refer to as *particle lines*, joined by a distinguished vertex which we refer to as the J-vertex (corresponding to the the integration against the rescaled test function J_{η^2}. On the line on its left, we introduce n vertices, and on the line on its right, we insert $\widetilde{n}$ vertices. We refer to those vertices as *interaction vertices*, and enumerate them from 1 to $2\bar{n}$ starting from the left. The edges between the interaction vertices are referred to as *propagator lines*. We label them by the momentum variables u_0, ..., $u_{2\bar{n}+1}$, increasingly indexed starting from the left. To the j-th propagator line, we associate the resolvent $\frac{1}{E(u_j)-\alpha-i\epsilon}$ if $0 \leq j \leq n$, and $\frac{1}{E(u_j)-\widetilde{\alpha}+i\epsilon}$ if $n+1 \leq j \leq 2\bar{n}+1$. To the ℓ-th interaction vertex (adjacent to the edges labeled by $u_{\ell-1}$ and u_ℓ), we associate the random potential $\widehat{V}_\omega(u_\ell - u_{\ell-1})$, where $1 \leq \ell \leq 2\bar{n}+1$.

A *contraction graph* associated to the above pair of particle lines joined by the ρ_0-vertex, and decorated by $n+\widetilde{n}$ interaction vertices, is the graph obtained by pairwise connecting interaction vertices by dashed *contraction lines*. We denote the set of all such contraction graphs by $\Gamma_{n,\widetilde{n}}$; it contains

$$|\Gamma_{n,\widetilde{n}}| \;=\; (2\bar{n}-1)(2\bar{n}-3)\cdots 3\cdot 1 \;=\; \frac{(2\bar{n})!}{\bar{n}!2^{\bar{n}}} \;=\; O(\bar{n}!) \tag{5.17}$$

elements.

If in a given graph $\pi \in \Gamma_{n,\widetilde{n}}$, the ℓ-th and the ℓ'-th vertex are joined by a contraction line, we write

$$\ell \sim_\pi \ell' \,, \tag{5.18}$$

and we associate the delta distribution

$$\delta(u_\ell - u_{\ell-1} - (u_{\ell'} - u_{\ell'-1})) \;=\; \mathbb{E}[\,\widehat{V}_\omega(\,u_\ell - u_{\ell-1}\,)\,\widehat{V}_\omega(\,u_{\ell'} - u_{\ell'-1}\,)\,] \tag{5.19}$$

to this contraction line.

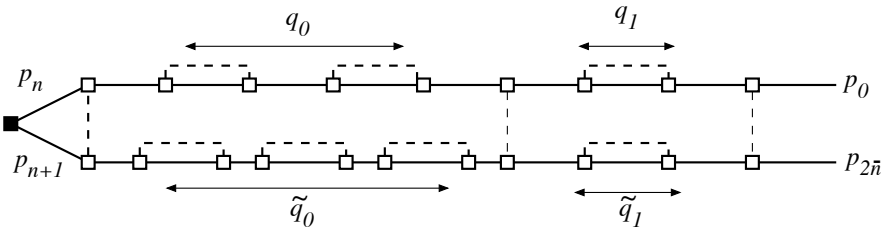

Figure 1. An example of a Feynman graph, $\pi \in \Gamma_{n,\widetilde{n}}$.

We consider the following classification of Feynman graphs, [27].

- A subgraph consisting of one propagator line adjacent to a pair of vertices ℓ and $\ell+1$, and a contraction line connecting them, i.e., $\ell \sim_\pi \ell+1$, where both ℓ, $\ell+1$ are either $\leq n$ or $\geq n+1$, is called an *immediate recollision*.
- The graph $\pi \in \Gamma_{n,n}$ (i.e., $n = \widetilde{n} = \bar{n}$) with $\ell \sim_\pi 2n-\ell$ for all $\ell = 1, \ldots, n$, is called a *basic ladder* diagram. The contraction lines are called *rungs* of the ladder. We note that a rung contraction always has the form $\ell \sim_\pi \ell'$ with $\ell \leq n$ and $\ell' \geq n+1$. Moreover, in a basic ladder diagram one always has that if $\ell_1 \sim_\pi \ell_1'$ and $\ell_2 \sim_\pi \ell_2'$ with $\ell_1 < \ell_2$, then $\ell_2' < \ell_1'$.
- A diagram $\pi \in \Gamma_{n,\widetilde{n}}$ is called a *decorated ladder* if any contraction is either an immediate recollision, or a rung contraction $\ell_j \sim_\pi \ell_j'$ with $\ell_j \leq n$ and $\ell_j' \geq n$ for $j = 1, \ldots, k$, and $\ell_1 < \cdots < \ell_k$, $\ell_1' > \cdots > \ell_k'$. Evidently, a basic ladder diagram is the special case of a decorated ladder which contains no immediate recollisions (so that necessarily, $n = \widetilde{n}$).
- A diagram $\pi \in \Gamma_{n,\widetilde{n}}$ is called *crossing* if there is a pair of contractions $\ell \sim_\pi \ell'$, $j \sim_\pi j'$, with $\ell < \ell'$ and $j < j'$, such that $\ell < j$.
- A diagram $\pi \in \Gamma_{n,\widetilde{n}}$ is called *nesting* if there is a subdiagram with $\ell \sim_\pi \ell + 2k$, with $k \geq 1$, and either $\ell \geq n+1$ or $\ell + 2k \leq n$, with $j \sim_\pi j+1$ for $j = \ell+1, \ell+3, \ldots, \ell+2k-1$. The latter corresponds to a progression of $k-1$ immediate recollisions.

We note that any diagram that is not a decorated ladder contains at least a crossing or a nesting subdiagram.

To each Feynman graph, $\pi \in \Gamma_{m,n}$, we associate its Feynman amplitude,

$$\begin{aligned} \mathrm{Amp}_{J_{\eta^2}}(\pi) \;=\; & \frac{\eta^{2\bar{n}}}{(2\pi)^2} \;\; e^{2\epsilon t} \;\; \int_{\mathbb{R}^2} dE\, dE' \;\; e^{-it(E-E')} \\ & \int du_0 \cdots du_{2\bar{n}+1} \;\; \overline{\widehat{\psi}_0(u_0)}\, \widehat{\psi}_0(u_{2\bar{n}+1}) \;\; \frac{1}{\eta^6}\, \widehat{J}\left(\frac{u_{n+1}-u_n}{\eta^2}, \frac{u_{n+1}+u_n}{2} \right) \\ & \delta_\pi(\underline{u}) \;\; \left[\prod_{j=0}^{n} \frac{1}{e_\Delta(u_j) - E - i\epsilon} \right] \;\; \left[\prod_{\ell=n+1}^{2\bar{n}+1} \frac{1}{e_\Delta(u_\ell) - E' + i\epsilon} \right] \end{aligned} \tag{5.20}$$

for $\pi \in \Pi_{m,n}$ and $\bar{n} = \frac{m+n}{2}$ (zero if $m+n \notin 2\mathbb{N}$). We set

$$\epsilon \;=\; \frac{1}{t} \;=\; \frac{\eta^2}{T} \tag{5.21}$$

so that the overall exponential factor $e^{2\epsilon t}$ remains bounded. Here, δ_π denotes the product of the delta distributions associated to all contractions between random potentials in π.

5.5. **Step 3: Control of error estimates.** The following estimates are the main ingredients of the argument:

• *A priori bound:* One verifies that for every Feynman graph π, the a priori bound

$$\left| \mathrm{Amp}_{J_{\eta^2}}(\pi) \right| \;\leq\; \left(\log \frac{1}{\eta} \right)^3 \;\left(c\, T \log \frac{1}{\eta} \right)^{\bar{n}}$$

holds. To obtain this bound, one chooses a suitable spanning tree T_π with $\bar{n}+2$ edges for every given Feynman graph $\pi \in \Gamma_{n,\widetilde{n}}$. The edges contained in T_π are called

tree edges, and accordingly, the momentum variables and resolvents supported on them are called tree momenta and tree resolvents, respectively. The edges in π not contained in T_π are referred to as loop edges (because adding them to T_π produces loop subdiagrams), and correspondingly, they carry loop momenta and loop resolvents. A spanning tree T_π is admissible if it contains all contraction lines, and precisely one edge adjacent to the distinguished vertex.

Associated to an admissible choice of T_π, one integrates out all delta distributions using the tree momenta, whereby the tree momenta are substituted by linear combinations of loop momenta. Next, one applies the L^∞-bound to the resolvents supported on $\bar{n}$ edges of T_π,

$$\Big\| \frac{1}{e_\Delta(\,\cdot\,) - E + i\epsilon} \Big\|_{L^\infty(\mathbb{T}^d)} \lesssim \frac{1}{\epsilon} \tag{5.22}$$

and L^1-estimates on the $\bar{n}$ loop resolvents,

$$\Big\| \frac{1}{e_\Delta(\,\cdot\,) - E + i\epsilon} \Big\|_{L^1(\mathbb{T}^d)} \lesssim \log \frac{1}{\epsilon}\,. \tag{5.23}$$

Moreover, the integrals over the spectral parameters E, E' can be controlled by applying

$$\Big\| \int dE \frac{1}{|e_\Delta(\,\cdot\,) - E + i\epsilon|} \Big\|_{L^\infty(\mathbb{T}^d)} \lesssim \log \frac{1}{\epsilon} \tag{5.24}$$

to the two remaining tree resolvents. The a priori bound then follows.

• *Dominant diagrams:* The dominant contributions to the expansion are obtained from decorated ladder diagrams, where

$$\Big| \operatorname{Amp}_{J_{\eta^2}}(\pi_{ladder}) \Big| \;\leq\; \frac{(cT)^{\bar{n}}}{\sqrt{\bar{n}!}}$$

is *summable* in $\bar{n}$, uniformly in η.

The scaling limit of decorated ladder diagrams gives the solution $F_T(X,V)$ of the linear Boltzmann equation.

• *Nesting and crossing diagrams:* For every Feynman graph π that contains a crossing or a nesting diagram, one obtains the upper bound

$$\Big| \operatorname{Amp}_{J_{\eta^2}}(\pi_{crossing/nesting}) \Big| \;\leq\; \eta^{\frac{2}{5}} \underbrace{\Big(\log \frac{1}{\eta}\Big)^3 \Big(\, cT \log \frac{1}{\eta} \,\Big)^{\bar{n}}}_{\text{a priori bound}}$$

where the gain of a factor $\eta^{\frac{2}{5}}$ over the a priori bound is crucial. The number of graphs exhibiting a crossing or a nesting is $O(\bar{n}!)$.

Choosing the truncation of the resolvent expansion at

$$N \;\approx\; \frac{\log \frac{1}{\eta}}{\log\log \frac{1}{\eta}}\,,$$

one obtains that

$$\sum_{m,n=1}^{N} \sum_{\Gamma_{m,n}} \Big| \operatorname{Amp}_{J_{\eta^2}}(\pi_{crossing/nesting}) \Big| \;\lesssim\; \eta^\delta$$

for some $\delta > 0$.

• *Terms involving the remainder term $R_t^{(N)}$:* If n and/or $\widetilde{n} = N + 1$, the corresponding term in the expansion for the Wigner transform involves the remainder term $R_t^{(N)}$ of the resolvent expansion. It can be proven that the sum of these contributions are also bounded by $\lesssim \eta^\delta$ for the given choice of N, [27, 14]. We will not discuss the fairly technical proof of this result in this survey.

In conclusion, collecting all of the above estimates, and letting $\eta \to 0$, we have proven the asserted Boltzmann limit. □

5.6. **Step 4: Crossing estimates.** The most delicate part in the analysis is the proof of smallness of the Feynman amplitudes associated with crossing diagrams. Amplitudes of nesting graphs, on the other hand, can be straightforwardly controlled by use of analyticity arguments. For every crossing diagram, it is possible to choose a spanning tree for which the associated bound on the Feynman amplitude contains a factor of the form

$$\int_{\mathbb{T}^3\times\mathbb{T}^3} dp\, dq\, \frac{1}{|e_\Delta(p) - E - i\epsilon|}\, \frac{1}{|e_\Delta(q) - E' + i\epsilon|}\, \frac{1}{|e_\Delta(p+q-u) - E - i\epsilon|} \tag{5.25}$$

which can be trivally bounded by

$$\lesssim \frac{(\log \frac{1}{\epsilon})^2}{\epsilon} \tag{5.26}$$

Here, p, q are loop momenta which appear only on the subgraph associated to this expression, and u is a linear combination of loop momenta in π independent of p, q. The bound (5.26) is insufficient for our purposes because it does not improve on the a priori bound.

To improve on this bound, we observe that the singular integrand in (5.25) is concentrated on the intersection of the ϵ-tubular neighborhoods of isoenergy surfaces

$$\Sigma_E = \{p \in \mathbb{T}^3 \,|\, e_\Delta(p) = E\}\,. \tag{5.27}$$

The idea is to exploit the smallness of the intersection measure, in order to improve on the trivial bound (5.26).

As a matter of fact, improving (5.26) by a factor ϵ^δ for any arbitrary $\delta > 0$ suffices for our purposes.

We remark that in the case of the continuum, $\mathbb{R}^d$, the surfaces Σ_E are spheres, and it is easy to control the size of their ϵ-thickened intersections, [27].

• *The geometry of level surfaces for lattice models:* In the case of lattice models, the geometry of the isoenergy surfaces is necessarily more complicated than in the continuum case. The prototypical situation is given by the case of the nearest neighbor laplacian which acts as a Fourier multiplication operator with symbol

$$e_\Delta(p) \;=\; 2\cos(2\pi p_1) \;+\; 2\cos(2\pi p_2) \;+\; 2\cos(2\pi p_3) \tag{5.28}$$

in $d = 3$. The surface $\Sigma_E = \{p \in \mathbb{T}^3 \,|\, e_\Delta(p) = E\}$ is non-convex, and exhibits *lines of vanishing Gauss curvature.*

Naturally, one might ask if this problem can be circumvented by a different choice of the kinetic energy operator than the nearest neighbor Laplacian Δ. However, this problem cannot be avoided by a different choice of the kinetic energy operator, due to the topology of $(\mathbb{Z}^d)^* \cong \mathbb{T}^d$. The reason is that at best, the kinetic energy $e_\Delta : \mathbb{T}^d \to [-2d, 2d]$ is a (perfect) Morse function (which is the case for the nearest neighbor laplacian). In $d = 3$, the Morse inequalities enforce a transition of Σ_E between a topological sphere and a surface of genus at least 3, depending on the paramter E. This is because the Betti numbers b_p of $\mathbb{T}^3$ are $b_0 = 1 = b_3$, and $b_1 = 3 = b_2$.

In [23], Erdös and Salmhofer have obtained a gain of $\epsilon^{\frac{1}{4}}$ upon the a priori bound (5.26) via a direct parametrization of level surfaces in $3D$. Their result is obtained from a very involved analysis and holds in greater generality than only for (5.28).

In [14], an improvement of $\epsilon^{\frac{1}{5}}$ upon (5.26) is obtained by a short argument related to restriction estimates in harmonic analysis, involving dimensional reduction. It holds for a smaller class of energy functions than those admitted in [23], since it exploits the addititive structure of $e_\Delta(p)$ in (5.28) with respect to coordinate components. Due to its simplicity, we briefly sketch the argument. We rewrite the 3-dimensional integral into a parametrized 2-D integral,

$$\int_{\mathbb{T}\times\mathbb{T}} dp_3\, dq_3 \int_{\mathbb{T}^2\times\mathbb{T}^2} d\underline{p}\, d\underline{q}\, \frac{1}{|\widetilde{e_\Delta}(\underline{p}) - E(p_3) - i\epsilon|} \\ \frac{1}{|\widetilde{e_\Delta}(\underline{q}) - E'(q_3) + i\epsilon|}\, \frac{1}{|\widetilde{e_\Delta}(\underline{p}+\underline{q}-\underline{u}) - E(p_3+q_3-u_3) - i\epsilon|}$$

where $p = (p_1, p_2, p_3)$ and $\underline{p} := (p_1, p_2)$, and similarly for q and $\underline{q}$. Moreover,

$$\widetilde{e_\Delta}(\underline{p}) \;:=\; 2\cos(2\pi p_1) \;+\; 2\cos(2\pi p_2) \tag{5.29}$$

and

$$E(p_3) \;:=\; E - 2\cos(2\pi p_3)\,, \tag{5.30}$$

et cetera. We note that there exists exactly one critical value $E_{crit} = 0$, for which the isoenergy curve $\{\underline{p} \in \mathbb{T}^2 | \widetilde{e_\Delta}(\underline{p}) = E_{crit}\}$ is a union of straight lines, and thus has vanishing curvature. The idea is to exploit the fact that for a (p_3, q_3)-set of large measure, the level lines of the 2-dimensional problem parametrized by $\underline{p}, \underline{q}$ have a curvature sufficiently bounded away from zero.

Let, for brevity, $E_1 := E(p_3)$, $E_2 := E(q_3)$, and $E_3 := E(p_3 + q_3 - u_3)$.

We focus on the most singular part of

$$\widetilde{R}_i(\underline{p}) \;:=\; \frac{1}{|\widetilde{e_\Delta}(\underline{p}) - E_i - i\epsilon|} \tag{5.31}$$

which can be estimated by

$$R_i^\nu(\underline{p}) \;:=\; \chi_i^\nu(\underline{p})\, \frac{1}{|\widetilde{e_\Delta}(\underline{p}) - E_i - i\epsilon|} \;\lesssim\; \frac{\nu}{\epsilon}\, \delta_i^\nu(\underline{p}) \tag{5.32}$$

where

$$\chi_i^\nu(\underline{p}) \;:=\; \chi_{\{\underline{p}\,|\,|\widetilde{e_\Delta}(\underline{p}) - E_i| < \nu\}}(\underline{p}) \tag{5.33}$$

and

$$\delta_i^\nu(\underline{p}) := \frac{1}{\nu}\chi_i^\nu(\underline{p}) \tag{5.34}$$

for some choice of $\nu > 0$ which remains to be optimized, and χ a smooth characteristic function. Then,

$$(\delta_i^\nu)^\vee(\underline{x}) = \int d\underline{p}\, e^{-2\pi i \underline{p}\cdot\underline{x}}\, \delta_i^\nu(\underline{p}) \tag{5.35}$$

has a decay

$$|(\delta_i^\nu)^\vee(\underline{x})| \lesssim \tau^{-1/2}\,|x|^{-1/2}\, e^{-\nu\,|x|} \tag{5.36}$$

for $|E_i - E_{crit}| > \tau$ where E_{crit} is the critical energy value for which the level line has zero curvature. This curvature induced decay in $\underline{x}$-space is proven with a stationary phase estimate.

If $|E_i - E_{crit}| > \tau$ for $i = 1, 2, 3$, the contribution to the crossing integral can be estimated by

$$\begin{aligned}
\left\langle R_1^\nu * R_2^\nu\,,\, R_3^\nu\right\rangle &\lesssim (\frac{\nu}{\epsilon})^3 \sum_{\underline{x}} (\delta_1^\nu)^\vee(\underline{x})\,(\delta_2^\nu)^\vee(\underline{x})\,(\delta_3^\nu)^\vee(\underline{x}) &(5.37)\\
&\lesssim (\frac{\nu}{\epsilon})^3 \sum_{0<|\underline{x}|\lesssim\frac{1}{\nu}} \tau^{-3/2}|\underline{x}|^{-3/2} &(5.38)\\
&= (\frac{\nu}{\epsilon})^3 \tau^{-3/2}\nu^{-1/2}\,. &(5.39)
\end{aligned}$$

On the other hand, the measure of the set of (p_3, q_3)-values for which there exists at least one index $i \in \{1, 2, 3\}$ such that $|E_i - E_{crit}| \le \tau$ is small, of order $O(\tau^{1/2})$ (for the choice of the cosine function, as it appears in $\widetilde{e_\Delta}$). On this (p_3, q_3)-set, the level lines have small curvature $\le \tau$, and we only get

$$\left\langle R_1^\nu * R_2^\nu\,,\, R_3^\nu\right\rangle \le \frac{1}{\epsilon}(\log\frac{1}{\epsilon})^2\,. \tag{5.40}$$

Finally, for the non-singular contribution where $|\widetilde{e_\Delta}(\underline{p}) - E_i| > C\nu$ for at least one value of i, we get a contribution of size

$$\left|\left\langle \widetilde{R}_1 * \widetilde{R}_2\,,\, \widetilde{R}_3\right\rangle - \left\langle R_1^\nu * R_2^\nu\,,\, R_3^\nu\right\rangle\right| \lesssim \frac{1}{\nu}(\log\frac{1}{\epsilon})^2 \tag{5.41}$$

to (5.25).

Combining the bounds for the two (p_3, q_3)-regions discussed above, we find the upper bound

$$\int dp_3\, dq_3 \left\langle \widetilde{R}_1 * \widetilde{R}_2\,,\, \widetilde{R}_3\right\rangle \lesssim (\frac{\nu}{\epsilon})^3\tau^{-3/2}\nu^{-1/2} + (\frac{1}{\nu} + \frac{\tau^{1/2}}{\epsilon})(\log\frac{1}{\epsilon})^2 \tag{5.42}$$

and choosing $\nu = \epsilon^{4/5}$ and $\tau = \epsilon^{2/5}$, one obtains

$$\begin{aligned}
\int_{\mathbb{T}^3\times\mathbb{T}^3} dp\, dq\, &\frac{1}{|e_\Delta(p) - E - i\epsilon|}\,\frac{1}{|e_\Delta(q) - E' + i\epsilon|}\,\frac{1}{|e_\Delta(p+q-u) - E - i\epsilon|}\\
&\lesssim \frac{(\log\frac{1}{\epsilon})^2}{\epsilon^{4/5}}\,,
\end{aligned}$$

which improves (5.26) by a factor $\epsilon^{1/5} = O(\eta^{2/5})$. □

6. The Vlasov limit for interacting Fermi gases

In this section, we study the combination of a semiclassical limit with a *mean field limit* for a gas of electrons. Electrons are *fermions*. Accordingly, the Schrödinger wave function for N electrons is totally antisymmetric in all arguments,

$$\psi_N(x_{\pi(1)},\dots,x_{\pi(N)}) \,=\, (-1)^{\mathrm{sign}(\pi)}\psi_N(x_1,\dots,x_N) \tag{6.1}$$

where $\pi \in S_N$ is an element of the N-th symmetric group. We will largely describe the classic work of Narnhofer and Sewell in [41] (but with a notation not entirely matching theirs).

The Schrödinger equation for N fermions which interact with a pair potential V is given by

$$\begin{aligned} &i\hbar\partial_t\psi_N(t,x_1,\dots,x_N) \\ &\quad = \Big(-\frac{\hbar^2}{2}\sum_{j=1}^N \Delta_{x_j} \,+\, \sum_{1\le i<j\le N} V(x_i-x_j)\Big)\,\psi_N(t,x_1,\dots,x_N) \end{aligned} \tag{6.2}$$

We assume that V is real analytic with Fourier transform $\widehat{V} \in C_0$ (continuous with compact support).

We observe that evidently, no two fermions can be at the same place, $x_i = x_j$, because then, $\psi_N = 0$. Also, no two fermions can have the same momentum $\xi_i = \xi_j$, because then, $\widehat{\psi}_N = 0$.

Next, we determine the scaling of terms with respect to powers of N. To this end, we think of N fermions in a box $[-L,L]^3$ with wave function $\psi_N(x_1,\dots,x_N)$. The Fourier transform is given by $\widehat{\psi}_N(\xi_1,\dots,\xi_N)$ with $\xi \in \frac{1}{2\pi L}\mathbb{Z}^3$. We would like to know, first of all for $V = 0$, what the lowest energy configuration is for N electrons (the free ground state). For a state with Fourier transform of the form

$$\begin{aligned} \widehat{\psi}_N(\xi_1,\dots,\xi_N) \;&=\; (\delta_{k_1}\wedge\cdots\wedge\delta_{k_N})(\xi_1,\dots,\xi_N) \\ &=\; \frac{1}{N!}\sum_{\pi\in S_N}(-1)^{\mathrm{sign}(\pi)}\prod_{j=1}^N \delta_{k_j}(\xi_{\pi(j)})\,, \end{aligned} \tag{6.3}$$

(where δ_k are Kronecker delta functions) the kinetic energy is given by

$$\frac{\hbar^2}{2}\sum_{j=1}^N k_j^2\,. \tag{6.4}$$

By antisymmetry, all values of k_j are mutually unequal; hence, minimizing this sum, we start by picking $k_0 = 0$, and subsequently fill out the smallest possible approximate ball centered at the origin. Its radius is evidently $O(N^{\frac{1}{3}})$. The total kinetic energy corresponds to the sum of k^2 over all values inside this ball (referred to as the *Fermi sea*), and is $O(N^{\frac{5}{3}})$. Typically, we will consider solutions of the Schrödinger equation for which the kinetic energy is $O(N^{\frac{5}{3}})$.

On the other hand, when we now include the pair interactions between all fermions, the potential energy $\sum_{1\le i<j\le N} V(x_i-x_j)$ contains $O(N^2)$ terms.

We would like to understand the dynamics of the system in a situation when the kinetic energy and the potential energy balance one another. This will typically lead to a so-called mean field limit. In the current system, this is achieved in the following way. We let $\hbar_N := N^{-\frac{1}{3}}$, and assume that the interactions between fermions are *weak*, of order $O(N^{-1})$. The resulting Schrödinger equation is given by

$$\frac{i}{N^{\frac{1}{3}}}\partial_t\psi_N(t,x_1,\ldots,x_N) \tag{6.5}$$
$$= \Big(-\frac{1}{2N^{\frac{2}{3}}}\sum_{j=1}^N \Delta_{x_j} + \frac{1}{N}\sum_{1\leq i<j\leq N} V(x_i-x_j)\Big)\psi_N(t,x_1,\ldots,x_N)\,.$$

The power counting now tells us that both the total kinetic energy, and the total potential energy (with associated powers of $\frac{1}{N}$ included), are of the same order $O(N)$.

The semiclassical limit is obtained as $\hbar_N = N^{-\frac{1}{3}} \to 0$. Similar to the approach described before, we introduce the Wigner transform associated to ψ_N,

$$W_N(t,\underline{x}_N,\underline{p}_N) = \int \overline{\psi_N\big(\underline{x}_N - \frac{N^{-\frac{1}{3}}\underline{y}_N}{2}\big)}\psi_N\big(\underline{x}_N + \frac{N^{-\frac{1}{3}}\underline{y}_N}{2}\big)\, e^{-i\sum_{j=1}^N y_j\cdot p_j}\, d\underline{y}_N \tag{6.6}$$

which is now defined for N particles instead of only one. Here, $\underline{x}_N := (x_1,\ldots,x_N)$, $\underline{p}_N = (p_1,\ldots,p_N)$, etc. One can also check that

$$\widehat{W}_N(t,\underline{\xi}_N,\underline{\eta}_N) = \Big(\psi_N(t)\,,\, e^{-i\sum_{j=1}^N(x_j\cdot\xi_j + N^{-\frac{1}{3}}P_j\cdot\eta_j)}\,\psi_N(t)\Big)_{L^2} \tag{6.7}$$

according to Section 2.

Next, we ask how a subsystem of $n < N$ particles behaves if the interactions with the remaining $N-n$ particles are integrated out. For this purpose, we define the so-called n-particle marginals

$$\widehat{\mu}_N^{(n)}(t,\underline{\xi}_n,\underline{\eta}_n) := \Big(\psi_N(t)\,,\, e^{-i\sum_{j=1}^n(x_j\cdot\xi_j + N^{-\frac{1}{3}}P_j\cdot\eta_j)}\,\psi_N(t)\Big) \tag{6.8}$$

and one can verify that alternatively, this is equivalent to

$$\mu_N^{(n)}(t;\underline{x}_n;\underline{p}_n) = \int W_N(t,\underline{x}_N,\underline{p}_N)\,dx_{n+1}\cdots dx_N dp_{n+1}\cdots dp_N \tag{6.9}$$

(we note that in the notation of [41], the rôles of ξ_j and η_j are exchanged). The n-particle marginals satisfy the equations

$$\partial_t\widehat{\mu}_N^{(n)}(t;\underline{\xi}_n;\underline{\eta}_n) = \sum_{j=1}^N \xi_j\cdot\nabla_{\eta_j}\widehat{\mu}_N^{(n)}(t;\underline{\xi}_n;\underline{\eta}_n) \tag{6.10}$$
$$+\frac{1}{N}\sum_{1\leq i<j\leq n}\int dq\,\widehat{V}(q)\Big(2N^{\frac{1}{3}}\sin\big(\frac{1}{2}N^{-\frac{1}{3}}q\cdot(\eta_i-\eta_j)\big)\Big)\widehat{\mu}_N^{(n)}(t;\underline{\xi}_n;\underline{\eta}_n) \tag{6.11}$$
$$+\frac{N-n}{N}\sum_{1\leq j\leq n}\int dq\,\widehat{V}(q)\Big(2N^{\frac{1}{3}}\sin\big(\frac{1}{2}N^{-\frac{1}{3}}q\cdot\eta_j\big)\Big) \tag{6.12}$$
$$\widehat{\mu}_N^{(n)}(t;\xi_1,\ldots,\xi_j+q,\ldots,\xi_n,-q;\underline{\eta}_n,0)\,.$$

We note that the equation for the n-th marginal involves the $(n+1)$-st marginal. This hierarchical system of partial differential equations is referred to as the *BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) hierarchy* associated to the Wigner transform of the N-fermion system in discussion.

Next, we note that the sum (6.11) contains $O(\frac{n^2}{N})$ terms, and in an appropriate topology, it will converge to zero in the limit $N \to \infty$, for every fixed n. Furthermore, the sum (6.12) contains $O(n)$ terms, and it will survive in the limit $N \to \infty$. In fact, the following holds.

Theorem 6.1. *(H. Narnhofer, G. Sewell, [41]) Assume that $\widehat{V} \in C_0$, and that the initial states $(\widehat{\mu}_N^{(n)})(t=0)$ satisfy the second moment condition*

$$\int \big(x_j^2 \,+\, N^{-\frac{2}{3}} p_j^2 \big) \mu_N^{(n)}(0; \underline{x}_n; \underline{p}_n)\, d\underline{x}_n\, d\underline{p}_n \,<\, C\,, \tag{6.13}$$

for $j = 1, \ldots, n$, and a constant C independent of N.

Then, for every n, $\widehat{\mu}_N^{(n)}(t) \to \widehat{\mu}^{(n)}(t)$ converges pointwise in $(t, \underline{\xi}_n, \underline{\eta}_n)$ to the characteristic function (Fourier transform) of a probability measure m_t on $\mathbb{R}^{3n} \times \mathbb{R}^{3n}$, as $N \to \infty$ along a subsequence of integers $(N_j)_{j\in\mathbb{N}}$. In particular, the infinite sequence of marginals $(\widehat{\mu}_N^{(n)})$ satisfies

$$\begin{aligned} \partial_t \widehat{\mu}^{(n)}(t; \underline{\xi}_n; \underline{\eta}_n) \,&=\, \sum_{j=1}^{N} \xi_j \cdot \nabla_{\eta_j} \widehat{\mu}^{(n)}(t; \underline{\xi}_n; \underline{\eta}_n) \\ &+ \sum_{1\le j\le n} \int dq\, \widehat{V}(q)\, q \cdot \eta_j\, \widehat{\mu}^{(n+1)}(t; \xi_1, \ldots, \xi_j + q, \ldots, \xi_n, -q; \underline{\eta}_n, 0)\,. \end{aligned} \tag{6.14}$$

This is the so-called Vlasov hierarchy*.*

We note that by applying the inverse Fourier transform, we obtain

$$\begin{aligned} \partial_t \mu^{(n)}(t; \underline{x}_n; \underline{p}_n) \,&=\, -\sum_{j=1}^{N} p_j \cdot \nabla_{x_j} \mu^{(n)}(t; \underline{x}_n; \underline{p}_n) \\ &+ \sum_{1\le j\le n} \int (\nabla V)(x_j - x_{n+1}) \cdot \nabla_{p_j}\, \mu^{(n+1)}(t; \underline{x}_{n+1}; \underline{p}_{n+1})\, dx_{n+1}\, dp_{n+1}\,. \end{aligned} \tag{6.15}$$

In particular, if we choose *factorized initial data*

$$\mu^{(n)}(0; \underline{x}_n; \underline{p}_n) \,=\, \prod_{j=1}^{n} \mu^{(1)}(0; x_j; p_j)\,, \tag{6.16}$$

one can verify that the solution of the Vlasov hierarchy at $t > 0$ remains factorized,

$$\mu^{(n)}(t; \underline{x}_n; \underline{p}_n) \,=\, \prod_{j=1}^{n} \mu^{(1)}(t; x_j; p_j)\,, \tag{6.17}$$

and that $\mu^{(1)}(t; x; p)$ satisfies

$$\partial_t \mu^{(1)}(t; x; p) + p \cdot \nabla_x \mu^{(1)}(t; x; p) - ((\nabla V) * \rho_t)(x) \cdot \nabla_p\, \mu^{(1)}(t; x; p) \,=\, 0\,, \tag{6.18}$$

where $\rho_t(x) := \int \mu^{(1)}(t; x; p) dp$. This is the *Vlasov equation.*

In this sense, the classical Vlasov equation describes the joint mean field and semiclassical scaling limit for a weakly interacting gas of fermions. It is similar to the Liouville equation (4.18), but the interaction is now *nonlinear* in $\mu^{(1)}$.

There is a large literature on the derivation of the Vlasov equation from interacting classical particle systems which we will not address here. An important early work proving such a result is [12].

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