

Wigner Measures and Effective Mass Theorems

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Content:

- ① Schrödinger Equation in a Lattice
- ② Floquet-Bloch theory
- ③ Quantifying the lack of dispersion
- ④ Strategy of the proof
- ⑤ Back to Effective Mass Theory

Schrödinger Equation in a Lattice : The equation

The equation:

$$i\hbar\partial_t\Psi + \frac{\hbar^2}{2m}\Delta_x\Psi - Q_{\text{per}}(x)\Psi - Q_{\text{ext}}(x)\Psi = 0, \quad (t, x) \in \mathbb{R} \times \mathbb{R}^d,$$
$$\Psi|_{t=0} = \Psi_0 \in L^2(\mathbb{R}^d),$$

where Q_{per} is a potential periodic with respect to a lattice $\Gamma = \mathbb{Z}^d$.

Let ε be the ratio between the mean spacing of the lattice and the characteristic length scale of variation of Q_{ext} .

$$\varepsilon \ll 1.$$

\implies Change of units and rescaling the external potential and the wave function !
(see [Poupaud & Ringhofer 96]).

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Schrödinger Equation in a Lattice : The scaled equation

The equation:

$$i\partial_t \psi^\varepsilon + \frac{1}{2} \Delta_x \psi^\varepsilon - \frac{1}{\varepsilon^2} V_{\text{per}} \left(\frac{x}{\varepsilon} \right) \psi^\varepsilon - V(x) \psi^\varepsilon = 0, \quad (t, x) \in \mathbb{R} \times \mathbb{R}^d,$$
$$\psi^\varepsilon|_{t=0} = \psi_0^\varepsilon \in L^2(\mathbb{R}^d),$$

where V_{per} is a potential periodic with respect to \mathbb{Z}^d .

Question: Effective Mass Theory consists in showing situations where $\psi^\varepsilon(t)$ can be approximated by the solution of a Effective Mass Equation:

$$i\partial_t \phi(t, x) + \frac{1}{2} \langle M D_x, D_x \rangle \phi(t, x) - V(x) \phi(t, x) = 0.$$

M is a $d \times d$ matrix called the effective mass tensor.

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Schrödinger Equation in a Lattice : Our purpose

The two main questions of the literature :

- Finding initial conditions for which the previous analysis holds,
- Finding the corresponding M .

[Bensoussan, Lions & Papanicolaou 78], [Poupaud & Ringhofer 96], [Allaire & Piatniski 05], [Hoefer & Weinstein 11], [Barletti & Ben Abdallah 11].

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- Clarifying the dependence of M on the parameter of the equation.

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Schrödinger Equation in a Lattice : our strategy

Remark

If v^ε solves the semiclassical Schrödinger equation

$$i\varepsilon\partial_t v^\varepsilon + \frac{\varepsilon^2}{2}\Delta_x v^\varepsilon - V_{\text{per}}\left(\frac{x}{\varepsilon}\right)v^\varepsilon - \varepsilon^2 V(x)v^\varepsilon = 0, \quad v^\varepsilon|_{t=0} = \psi_0^\varepsilon.$$

Then, $\psi^\varepsilon(t, x) = v^\varepsilon\left(\frac{t}{\varepsilon}, x\right)$.

[Gérard], [GMMP] [Poupaud & Ringhofer], [Bechouche, Mauser & Poupaud], [Spohn & Teufel] [Panati, Spohn & Teufel],
[Dimassi, Guillot & Ralston] [Allaire & Palombaro] [Carles & Sparber]

⇒ Perform **simultaneously** the s.c. limit $\varepsilon \rightarrow 0$ with the limit $t/\varepsilon \rightarrow +\infty$.

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Our goal : apply this viewpoint to effective mass theory.

⇒ a **generalized effective mass equation** of Heisenberg type.

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Floquet-Bloch theory : Bloch waves and energies

- We use the Ansatz : $\psi^\varepsilon(t, x) = U^\varepsilon\left(t, x, \frac{x}{\varepsilon}\right)$, where $U^\varepsilon(t, x, y)$ is assumed to be \mathbb{Z}^d -periodic in y and solves

$$i\varepsilon^2 \partial_t U^\varepsilon(t, x, y) = P(\varepsilon D)U^\varepsilon(t, x, y) + \varepsilon^2 V(x)U^\varepsilon(t, x, y), \quad U^\varepsilon|_{t=0} = \psi_0^\varepsilon$$

$$\text{where } P(\xi) = \frac{1}{2}(\xi + D_y)^2 + V_\Gamma(y), \quad y \in \mathbb{T}^d := \mathbb{R}^d \setminus \mathbb{Z}^d.$$

- The Bloch energies are the eigenvalues of the self-adjoint operator on the torus $P(\xi)$:

$$\lambda_1(\xi) \leq \lambda_2(\xi) \leq \dots \leq \lambda_n(\xi) \rightarrow +\infty.$$

They are $2\pi\mathbb{Z}^d$ periodic and smooth in domain where they are of constant multiplicity.

- The Bloch waves are the orthonormal eigenfunctions of $P(\xi)$

$$P(\xi)\varphi_n(\xi, y) = \lambda_n(\xi)\varphi_n(\xi, y), \quad n \in \mathbb{N}, \quad y \in \mathbb{T}^d, \quad \forall \xi \in \mathbb{R}^d.$$

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Floquet Bloch theory : Bloch decomposition

- Consider $(\Pi_n(\xi))_{n \in \mathbb{N}}$ a family of projectors on separated Bloch bands and

$$U_n^\varepsilon(t, x, y) := \Pi_n(\varepsilon D_x) U^\varepsilon(t, x, y) = \int_{\mathbb{R}^d \times \mathbb{R}^d} \Pi_n(\varepsilon \xi) U^\varepsilon(t, w, y) e^{i\xi \cdot (x-w)} \frac{dw d\xi}{(2\pi)^d} dy$$

so that
$$U^\varepsilon(t, x, y) = \sum_{n \in \mathbb{N}} U_n^\varepsilon(t, x, y).$$

- This construction leads to the following representation formula for the solution of the Schrödinger equation

$$\psi^\varepsilon(t, x) = \sum_{n \in \mathbb{N}} U_n^\varepsilon\left(t, x, \frac{x}{\varepsilon}\right).$$

- If $\text{Rk } \Pi_n(\xi) = 1$, $\text{Range } \Pi_n(\xi) = \text{Vect } \varphi_n(\xi, \cdot)$, $P(\xi)\varphi_n(\xi) = \lambda_n(\xi)\varphi_n(\xi)$,

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Quantifying the lack of dispersion : a more general question

- Consider equations of the form

$$\begin{cases} i\varepsilon^2 \partial_t u^\varepsilon(t, x) = \lambda(\varepsilon D_x) u^\varepsilon(t, x) + \varepsilon^2 V(x) u^\varepsilon(t, x), & (t, x) \in \mathbb{R} \times \mathbb{R}^d, \\ u^\varepsilon|_{t=0} = u_0^\varepsilon. \end{cases} \quad (1)$$

This equation ceases to be dispersive as soon as $\lambda(\xi)$ has critical points $\xi \neq 0$, and this is always the case if λ is a Bloch energy.

- Heuristically, dispersive time-evolution \implies smoothing effect
i.e. regularization of the high-frequency effects developed by the initial data.
[Kato 83], [Sjölin 87], [Vega 88], [Constantin & Saut 88], [Kenig, Ponce & Vega 91], [Ben Artzi & Devinatz 91].
- We show that, in the presence of critical points of λ , some of the high-frequency effects developed by the sequence of initial data persist after applying the time evolution.

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Quantifying the lack of dispersion : The assumptions

Assumptions:

H0 The sequence (u_0^ε) is uniformly bounded in $L^2(\mathbb{R}^d)$ and ε -oscillating :

$$\limsup_{\varepsilon \rightarrow 0^+} \int_{|\xi| > R/\varepsilon} |\widehat{u_0^\varepsilon}(\xi)|^2 d\xi \xrightarrow{R \rightarrow +\infty} 0.$$

H1 $V \in C^\infty(\mathbb{R}^d)$ and $\lambda \in C^\infty(\mathbb{R}^d)$ grows at most polynomially; i.e. there exist $C, N > 0$ such that:

$$|\lambda(\xi)| \leq C(1 + |\xi|)^N, \quad \forall \xi \in \mathbb{R}^d.$$

H2 The set $\Lambda := \{\xi \in \mathbb{R}^d : \nabla \lambda(\xi) = 0\}$ is a submanifold of \mathbb{R}^d of codimension $0 < p \leq d$ and the Hessian $\nabla^2 \lambda$ is of maximal rank over Λ . Moreover, each connected component of Λ is compact.

Remark

If all critical points of λ are non-degenerate, then Λ is a discrete set in \mathbb{R}^d . If moreover one has that λ is \mathbb{Z}^d -periodic, this set is finite modulo \mathbb{Z}^d .

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Quantifying the lack of dispersion : non-degenerate case

Theorem (Obstruction to smoothing effects in presence of critical points)

Assume **H0 & H1** and that all critical points of λ are non-degenerate.

Then there exists a subsequence $(u_0^{\varepsilon_k})$ such that $\forall a < b$ and $\forall \phi \in \mathcal{C}_c(\mathbb{R}^d)$:

$$\lim_{k \rightarrow \infty} \int_a^b \int_{\mathbb{R}^d} \phi(x) |u^{\varepsilon_k}(t, x)|^2 dx dt = \sum_{\xi \in \Lambda} \int_a^b \int_{\mathbb{R}^d} \phi(x) |u_\xi(t, x)|^2 dx dt,$$

where u_ξ solves the Schrödinger equation:

$$i\partial_t u_\xi(t, x) = \nabla^2 \lambda(\xi) D_x \cdot D_x u_\xi(t, x) + V(x) u_\xi(t, x),$$

with initial data $u_\xi|_{t=0}$ which is the weak limit in $L^2(\mathbb{R}^d)$ of $(e^{-i\xi/\varepsilon_k \cdot x} u_0^{\varepsilon_k})$.
If $\Lambda = \emptyset$ then the right-hand side above is equal to zero.

Example : If $u_0^\varepsilon(x) = \frac{1}{\varepsilon^{d/4}} \rho\left(\frac{x-x_0}{\sqrt{\varepsilon}}\right) e^{i\xi_0/\varepsilon \cdot x}$, then $u_\xi = 0$ for all ξ and the

Theorem yields that (u^ε) converge to zero in $L^2_{loc}(\mathbb{R} \times \mathbb{R}^d)$.

Related work : [Ruzhanski & Sugimoto 16]

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Related work : [Ruzhanski & Sugimoto 16]

Quantifying the lack of dispersion : degenerate case

- When the non-degeneracy of the critical points is replaced by H2, we obtain a similar result which requires some geometric preliminaries.

- Define the tangent bundle of Λ as the union of all tangent spaces to Λ ,

$$T\Lambda := \{(x, \xi) \in \mathbb{R}^d \times \Lambda : x \in T_\xi \Lambda\}.$$

- The normal bundle of Λ is the union of linear subspaces normal to Λ :

$$N\Lambda := \{(y, \xi) \in \mathbb{R}^d \times \Lambda : y \in N_\xi \Lambda = (T_\xi \Lambda)^\perp\}.$$

Every point $x \in \mathbb{R}^d$ can be uniquely written as $x = z + y$, where $z \in T_\xi \Lambda$ and $y \in N_\xi \Lambda$.

- Given a function $\phi \in L^\infty(\mathbb{R}^d)$, we write $m_\phi(z, \xi)$, where $z \in T_\xi \Lambda$, to denote the operator acting on $L^2(N_\xi \Lambda)$ by multiplication by $\phi(z + \cdot)$.
- We use the notation Δ_E to denote the Laplacian acting on functions defined on a linear subspace $E \subset \mathbb{R}^d$.

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Every point $x \in \mathbb{R}^d$ can be uniquely written as $x = z + y$, where $z \in T_\xi \Lambda$ and $y \in N_\xi \Lambda$.

- Given a function $\phi \in L^\infty(\mathbb{R}^d)$, we write $m_\phi(z, \xi)$, where $z \in T_\xi \Lambda$, to denote the operator acting on $L^2(N_\xi \Lambda)$ by multiplication by $\phi(z + \cdot)$.
- We use the notation Δ_E to denote the Laplacian acting on functions defined on a linear subspace $E \subset \mathbb{R}^d$.

Quantifying the lack of dispersion : degenerate case

- When the non-degeneracy of the critical points is replaced by H2, we obtain a similar result which requires some geometric preliminaries.
- Define the tangent bundle of Λ as the union of all tangent spaces to Λ ,

$$T\Lambda := \{(x, \xi) \in \mathbb{R}^d \times \Lambda : x \in T_\xi \Lambda\}.$$

- The normal bundle of Λ is the union of linear subspaces normal to Λ :

$$N\Lambda := \{(y, \xi) \in \mathbb{R}^d \times \Lambda : y \in N_\xi \Lambda = (T_\xi \Lambda)^\perp\}.$$

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Quantifying the lack of dispersion : degenerate case

Theorem

Assume **H0**, **H1** & **H2**. Then there exist a subsequence $(u_0^{\varepsilon_k})$, a positive measure $\gamma \in \mathcal{M}_+(T\Lambda)$ and a measurable fami. of s.-adj., positive, trace-class operators

$$M_0 : T_\xi\Lambda \ni (z, \xi) \longmapsto M_0(z, \xi) \in \mathcal{L}_+^1(L^2(N_\xi\Lambda)), \quad \text{Tr}_{L^2(N_\xi\Lambda)} M_0(z, \xi) = 1,$$

such that for every $a < b$ and every $\phi \in \mathcal{C}_c(\mathbb{R}^d)$ one has:

$$\begin{aligned} \lim_{k \rightarrow \infty} \int_a^b \int_{\mathbb{R}^d} \phi(x) |u^{\varepsilon_k}(t, x)|^2 dx dt \\ = \int_a^b \int_{T\Lambda} \text{Tr}_{L^2(N_\xi\Lambda)} [m_\phi(z, \xi) M(t, z, \xi)] \gamma(dz, d\xi) dt, \end{aligned}$$

where $M(\cdot, z, \xi) \in \mathcal{C}(\mathbb{R}; \mathcal{L}_+^1(L^2(N_\xi\Lambda)))$ solves the following Heisenberg equation:

$$i\partial_t M(t, z, \xi) + \left[\frac{1}{2} \Delta_{N_\xi\Lambda} + m_V(z, \xi), M(t, z, \xi) \right] = 0, \quad M|_{t=0} = M_0.$$

Quantifying the lack of dispersions : comments

- The measure γ and the family of operators $M_0(z, \xi)$, for $z \in T_\xi \Lambda$, only depend on the subsequence of initial data $(u_0^{\varepsilon_k})$.
- When Λ is a set of isolated critical points, both Theorems are equivalent : $T\Lambda = \{0\} \times \Lambda$ and

$$\gamma = \sum_{\xi \in \Lambda} \gamma_\xi \delta_\xi, \quad \text{where } \gamma_\xi = \|u_\xi|_{t=0}\|_{L^2(\mathbb{R}^d)}^2.$$

In addition, $N_\xi \Lambda = \mathbb{R}^d$ and $M(t, \xi)$ is the orth. proj. onto $u_\xi(t, \cdot)$.

- A consequence of this Theorem is that the weak- \star limit of the densities $|u^{\varepsilon_k}|^2$ is absolutely continuous with respect to the Lebesgue measure $dxdt$ and can be expressed as a superposition of position densities associated to solutions to the family of p -dimensional Schrödinger evolutions:

$$i\partial_t v_{z,\xi}(t, y) + \frac{1}{2}\Delta_y v_{z,\xi}(t, y) + V(z + y)v_{z,\xi}(t, y) = 0, \quad (t, y) \in \mathbb{R} \times N_\xi \Lambda.$$

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Strategy of the proof : phase space analysis

- **Phase space analysis:** Let $W(u^\varepsilon)$ be the **Wigner transform** of (u^ε) ,

$$W^\varepsilon(t, x, \xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} \bar{u}^\varepsilon \left(t, x + \varepsilon \frac{v}{2} \right) u^\varepsilon \left(t, x - \varepsilon \frac{v}{2} \right) e^{iv \cdot \xi} dv.$$

The Wigner transform plays the role of a generalised energy density since

$$|u^\varepsilon(t, x)|^2 = \int_{\mathbb{R}^d} W^\varepsilon(t, x, \xi) d\xi.$$

- **Wigner measures** of (u^ε) are positive measures $\mu(t)$ satisfying for some subsequence ε_k and for all $a < b, c \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$,

$$\lim_{k \rightarrow \infty} \int_a^b \int_{\mathbb{R}^{2d}} c(x, \xi) W^{\varepsilon_k}(t, x, \xi) dx d\xi dt = \int_a^b \int_{\mathbb{R}^{2d}} c(x, \xi) \mu(t, dx, d\xi) dt.$$

- Besides, ε -oscillation \implies

$$\lim_{k \rightarrow \infty} \int_a^b \int_{\mathbb{R}^d} \phi(x) |u^{\varepsilon_k}(t, x)|^2 dx dt = \int_a^b \int_{\mathbb{R}^{2d}} \phi(x) \mu(t, dx, d\xi) dt.$$

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Set for $\chi \in \mathcal{C}_0(\mathbb{R})$ and $c \in \mathcal{C}_0^\infty(\mathbb{R}^{2d})$,

$$I^\varepsilon(\chi, c) = \int_{\mathbb{R}} \int_{\mathbb{R}^{2d}} \chi(t) c(x, \xi) W^{\varepsilon_k}(t, x, \xi) dx d\xi dt.$$

- Invariance of Wigner measure : Egorov's theorem \implies

Proposition

Any μ_t is invariant by the flow $\phi_s^1 : s \mapsto (x + s\nabla\lambda(\xi), \xi)$.

- Localization of Wigner measures

Corollary

$$\text{Supp}(\mu_t) \subset \{(x, \xi) \in \mathbb{R}^{2d}, \nabla\lambda(\xi) = 0\}.$$

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Strategy of the proof : Two scale observables

We add to the phase space \mathbb{R}^{2d} a new variable $\eta \in \overline{\mathbb{R}^d}$.

[CK], [Nier], [Miller], [FFK & Gérard], [Laser & Teufel], [Harris, Lukkarinen, Teufel & Theil], [Macia], [Anantharaman & Macia]

With $c = c(x, \xi, \eta) \in C^\infty(\mathbb{R}^{3d})$ satisfying additional properties, which satisfy :

- 1 there exists a compact K such that for all $\eta \in \mathbb{R}^d$, $(x, \xi) \mapsto c(x, \xi, \eta)$ is a smooth function compactly supported in K ;
- 2 there exists a function $c_\infty(x, \xi, \omega)$ defined on $\mathbb{R}^{2d} \times \mathbf{S}^{d-1}$ and $R_0 > 0$ such that if $|\eta| > R_0$, then $c(x, \xi, \eta) = c_\infty(x, \xi, \eta/|\eta|)$.

Assume $\Lambda = \xi_0 + 2\pi\mathbb{Z}^d$. We associate with such c , the two-scale observable

$$c_\varepsilon^\sharp(x, \xi) = c\left(x, \xi, \frac{\xi - \xi_0}{\varepsilon}\right).$$

Remarks : 1) If $c \in C_0^\infty(\mathbb{R}^{2d})$, c is admissible.

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Strategy of the proof : Two scale Wigner measures

Theorem

There exist, $\varepsilon_n \xrightarrow[n \rightarrow +\infty]{} 0$, $\nu \in L^\infty(\mathbb{R}, \mathcal{M}^+(\mathbb{R}^d \times \mathbf{S}^{d-1}))$, $\Phi \in C^0(\mathbb{R}, L^2(\mathbb{R}^d))$ such that

$$I^{\varepsilon_n}(\chi, c_{\varepsilon_n}^\#) \xrightarrow[n \rightarrow +\infty]{} \int_{\mathbb{R}} \chi(t) (a(x, \xi_0, D)\Phi(t), \Phi(t)) dt + \int_{\mathbb{R}} \chi(t) \langle a_\infty(\cdot, \xi_0, \cdot), \nu_t \rangle dt.$$

① Φ solves the effective mass equation

$$i\partial_t \Phi = \text{Hess } \lambda(\xi_0) D \cdot D \Phi + V_{\text{ext}}(x)\Phi, \quad \Phi(0) = \Phi_0,$$

where Φ_0 is a weak limit in $L^2(\mathbb{R}^d)$ of the sequence $x \mapsto e^{\frac{i}{\varepsilon}\xi_0 \cdot x} u_\varepsilon^\varepsilon(x)$.

② ν^t is invariant by the flow $\phi_s^2 : (x, \omega) \mapsto (x + s\text{Hess } \lambda(\xi_0)\omega, \omega)$.

Corollary

If $\text{Hess } \lambda(\xi_0)$ is non degenerated, then $\nu_t = 0$ and $\mu_t(x, \xi) \mathbf{1}_{\xi=\xi_0} = |\Phi(t, x)|^2 dx$.

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Back to effective mass theory : assumptions on the initial data

Let $I \subset \mathbb{N}$, a set of indices n such that the multiplicity of the Bloch energy $\lambda_n(\xi)$ is constant for every $\xi \in \mathbb{R}^d$

- Assume that **H2** holds for any λ_n , $n \in I$
- Assume that ψ_0^ε is ε -oscillating and

$$\psi_0^\varepsilon = \sum_{n \in I} \psi_{n,0}^\varepsilon, \quad \psi_{n,0}^\varepsilon = U_n^\varepsilon \left(0, x, \frac{x}{\varepsilon} \right),$$

where $\widehat{U}_n^\varepsilon(0, \xi)$ is in the eigenspace of $\lambda_n(\xi)$.

Back to effective mass theory : application of the Theorem

Then, if (ψ^ε) is the solution to the Schrödinger equation issued for data (ψ_0^ε) ,

- For every $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$, the family $(\phi\psi^\varepsilon(t))$ is ε -oscillating.
- $\psi^\varepsilon(t, x) = \sum_{n \in I} \psi_n^\varepsilon(t, x)$ with $\psi_n^\varepsilon(t, x) = U_n^\varepsilon\left(t, x, \frac{x}{\varepsilon}\right)$, For each $n \in \mathbb{N}$,

$$\begin{cases} i\varepsilon^2 \partial_t \psi_n^\varepsilon(t, x) = \lambda_n(\varepsilon D_x) \psi_n^\varepsilon(t, x) + \varepsilon^2 V(x) \psi_n^\varepsilon(t, x) + \varepsilon^2 f_n^\varepsilon(t, x), \\ \|f_n^\varepsilon(t, \cdot)\|_{L^2(\mathbb{R}^d)} \leq C\varepsilon, \quad t \in \mathbb{R},. \end{cases}$$

- There exist a subsequence ε_k such that, for every $a < b$, $\phi \in \mathcal{C}_0^\infty(\mathbb{R}^d)$,

$$\lim_{k \rightarrow \infty} \int_a^b \int_{\mathbb{R}^d} \phi(x) |\psi^\varepsilon(t, x)|^2 dx dt = \sum_{n \in I} \int_a^b \int_{\mathbb{R}^d} |\phi(x)|^2 \mu_t^n(dx) dt,$$

where, for each $n \in \mathbb{N}$, the measures $\mu_t^n \in \mathcal{M}_+(\mathbb{R}^d \times \mathbb{R}^d)$ are Wigner measures of (ψ_n^ε) .

Conclusion

- **Second microlocalisation** along Λ has led to a complete description of the mechanism for any (ε -oscillating) initial data.
- In non standard cases (when Λ is a submanifold with H2), we have introduced a **generalized effective mass equation** with an operator-valued macroscopic item satisfying a **Heisenberg equation** (instead of a function satisfying a Schrödinger equation).
- In those non standard cases, the second microlocalisation does not concern “all the variable ξ ” and the remaining part is responsible of the **quantum feature at macroscopic level** in the derived effective mass equation which becomes a Heisenberg equation.
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Conclusion

- **Second microlocalisation** along Λ has led to a complete description of the mechanism for any (ε -oscillating) initial data.
- In non standard cases (when Λ is a submanifold with **H2**), we have introduced a **generalized effective mass equation** with an operator-valued macroscopic item satisfying a **Heisenberg equation** (instead of a function satisfying a Schrödinger equation).
- In those non standard cases, the second microlocalisation does not concern “all the variable ξ ” and the remaining part is responsible of the **quantum feature at macroscopic level** in the derived effective mass equation which becomes a Heisenberg equation.
- The next step should consist in treating a Bloch band containing two eigenvalues presenting a **conical intersection** (work in progress).

Thank you for your attention !