Some results about the dynamics of an electron in a crystal

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Quantum Hall effect and Topological Phases

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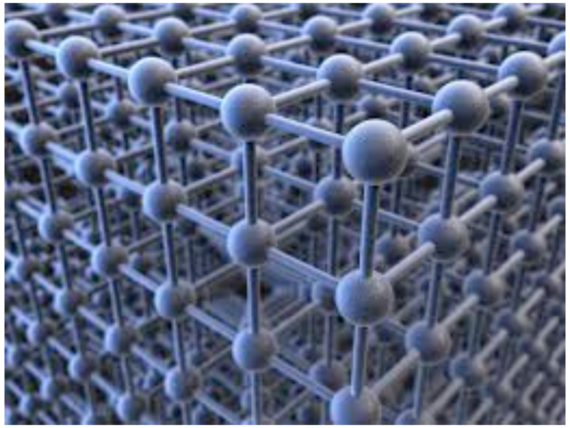
The Schrödinger equation



$$\begin{cases} i\partial_t \psi^\varepsilon(t,x) + \frac{1}{2}\Delta_x \psi^\varepsilon(t,x) - \frac{1}{\varepsilon^2} V_{per}\left(\frac{x}{\varepsilon}\right) \psi^\varepsilon(t,x) - V_{ext}(t,x)\,\psi^\varepsilon(t,x) = 0 \\ \psi^\varepsilon_{|t=0} = \psi^\varepsilon_0 \end{cases}$$

Semi-classical parameter :

$$\boxed{\varepsilon = \frac{\lambda}{L} \ll 1}$$

The aim : Describe the weak limits of the measure $|\psi^\varepsilon(t,x)|^2 \, dx \, dt$

Ref: [Poupaud-Ringhofer] CPDE 1995

Two-scale Analysis/Bloch-Floquet Analysis

Fact : We look for solutions of the form

$$\psi^\varepsilon(t,x) = U^\varepsilon\Big(t, x, \frac{x}{\varepsilon}\Big), \qquad U^\varepsilon(t) \in L^2(\mathbb{R}^d \times \mathbb{T}^d)$$

$\psi^\varepsilon(t,x)$ is solution of the semi-classical Schrod. eq. if and only if $U^\varepsilon(t,x,y)$ solves

$$\begin{cases} i\varepsilon^2 \partial_t U^\varepsilon(t,x,y) = P(\varepsilon D_x) U^\varepsilon(t,x,y) + \varepsilon^2 V_{\text{ext}}(t,x) U^\varepsilon(t,x,y) \\ U^\varepsilon|_{t=0} = U_0^\varepsilon \end{cases}$$

for adequate choice of U_0^ε $\quad (e.g.\ \ U_0^\varepsilon(x,y) = \psi_0^\varepsilon(x) \mathbf{1}_{y \in \mathbb{T}^d})$.

Schrödinger operator on the torus :

$$\boxed{P(\xi) = -\frac{1}{2}|\xi + D_y|^2 + V_{per}(y), \ \ y \in \mathbb{T}^d}$$

Bloch modes and Bloch waves

Spectral resolution : For all $\xi \in \mathbb{R}^d$, $P(\xi)$ is self-adjoint in $L^2(\mathbb{T}^d)$, has domain $H^2(\mathbb{T}^d)$ and compact resolvent

Bloch modes : The spectrum of $P(\xi)$ is a non-decreasing sequence of eigenvalues:

$$\varrho_1(\xi) \leq \varrho_2(\xi) \leq \cdots \leq \varrho_n(\xi) \leq \varrho_{n+1}(\xi) \leq \cdots \qquad n \in \mathbb{N}$$

➡ The functions $\xi \mapsto \varrho_n(\xi)$ are $(2\pi\mathbb{Z})^d$ periodic.

Bloch waves : The eigenvectors of $P(\xi)$ form an orthonormal basis of $L^2(\mathbb{T}^d)$

$$P(\xi)\varphi_n(y,\xi) = \varrho_n(\xi)\varphi_n(y,\xi), \quad y \in \mathbb{T}^d.$$

➡ $$\varphi_n(y+k,\xi) = e^{-2i\pi y\cdot k}\varphi_n(y,\xi), \quad k \in \mathbb{Z}^d, \quad \xi \in \mathbb{R}^d \ \ y \in \mathbb{T}^d.$$

Bloch - Floquet decomposition

$$\psi^\varepsilon(t,x) = \sum_{n\in\mathbb{N}} \psi_n^\varepsilon(t,x), \qquad \psi_n^\varepsilon(t,x) = \varphi_n\Big(\frac{x}{\varepsilon}, \varepsilon D_x\Big) \int_{\mathbb{T}^d} \overline{\varphi_n}(y, \varepsilon D_x) U^\varepsilon(t,x,y)dy$$

The functions $\psi_n^\varepsilon(t,x)$ solve the equations

$$\begin{cases} i\varepsilon^2\partial_t \psi_n^\varepsilon(t,x) = \varrho_n(\varepsilon D)\,\psi_n^\varepsilon(t,x) + \varepsilon^2 V_{ext}(t,x)\,\psi_n^\varepsilon(t,x) + \varepsilon^2 f_n^\varepsilon(t,x) \\ \psi_n^\varepsilon(0,x) = \psi_{n,0}^\varepsilon(x) \end{cases}$$

with $\quad f_n^\varepsilon(t,x) = \displaystyle\int_{\mathbb{T}^d} \Big[\varphi_n\big(\frac{x}{\varepsilon}, \varepsilon D_x\big)\overline{\varphi}_n(y,\varepsilon D)\,,\, V_{\text{ext}}(t,x)\Big] U^\varepsilon(t,x,y)dy$

Structure of Bloch modes

Lemme: If $d = 1$, the critical points of Bloch modes are in πZ, they are all non-degenerate.
The crossing set associated with two consecutive Bloch modes does not contain any critical points, crossing points are conical

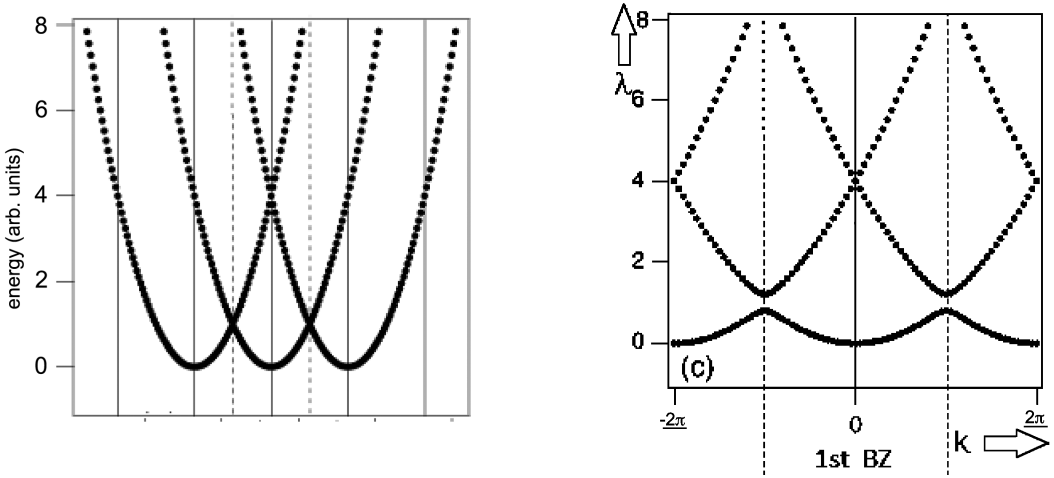


Fig 1 : Bloch modes
with $V = 0$ (left) and V small (right)

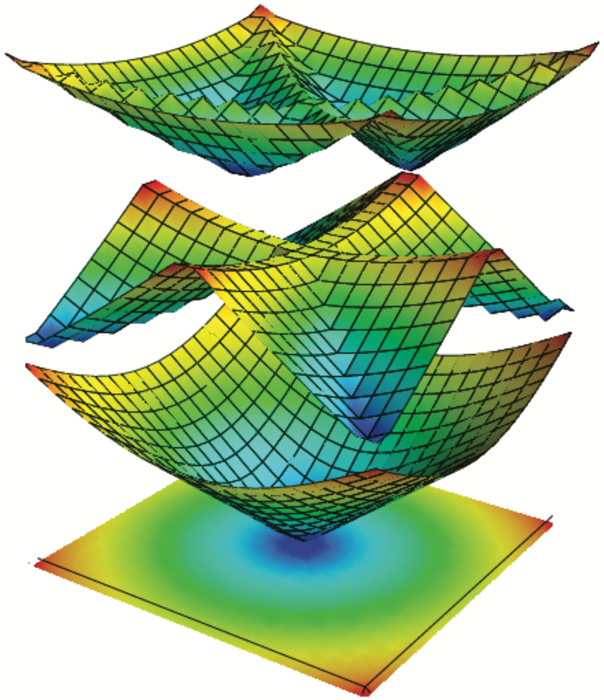


Fig 2 : Example of Bloch surfaces

Ref: [Kuchment] Bull. Amer. Math. Soc. 2016

Well-prepared initial data

Assumption: $\psi_0^\varepsilon(x) = e^{-\frac{i}{\varepsilon}x\cdot\xi_0}\,\varphi\Big(\frac{x}{\varepsilon},\xi_0\Big)\,u_0(x)$ with $u_0 \in L^2(\mathbb{R}^d)$

$P(\xi_0)\,\varphi(y,\xi_0) = \varrho(\xi_0)\,\varphi(y,\xi_0)$ for all $y \in \mathbb{T}^d$

$\varrho(\xi)$ an isolated simple Bloch mode and ξ_0 a non-degenerate critical point of $\xi \mapsto \varrho(\xi)$

Theorem: [Allaire - Piatniski] Comm. Math. Phys. 2005 & [Allaire - Palombaro] SIAM J. Math. Anal. 2006

As ε goes to 0, $\psi^\varepsilon(t,x) = e^{-\frac{i}{\varepsilon^2}t\,\varrho(\xi_0) - \frac{i}{\varepsilon}x\cdot\xi_0}\,\varphi\Big(\frac{x}{\varepsilon},\xi_0\Big)u(t,x) + o(1)$

where $u(t,x)$ satisfies the Effective mass equation

$$\begin{cases} i\partial_t u(t,x) = \dfrac{1}{2}\mathrm{Hess}\,\varrho(\xi_0)D\cdot D\,u(t,x) + V_{ext}(t,x)\,u(t,x) \\ u(0,x) = u_0 \end{cases}$$

The questions !

Data: What can be said for more general data ? Not so well prepared ?

Conical intersections: They are unavoidable, even in d=1... so ?

Do they trap the energy like critical points ?

Degenerate critical points: Is-it possible to extend the result to sets Λ of critical points provided a generic assumption (Morse-Bott) such as

$$\mathrm{Rk}\,(\mathrm{Hess}\,\varrho)_{|\Lambda} = \mathrm{Codim}\,\Lambda$$

Some questions !

Data: What can be said for more general data ? Not so well prepared ?

$$\|(1-\varepsilon^2\Delta)^s\psi_0^\varepsilon\|_{L^2} \le C \quad s > \frac{d}{2}$$

Conical intersections: They are unavoidable, even in 1-d... so ?

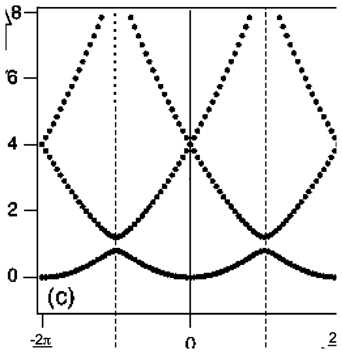
Do they trap the energy like critical points ? No!

Degenerate critical points: Is-it possible to extend the result to sets Λ of critical points provided a generic assumption such as

$$\text{Rank}\,(\text{Hess}\,\varrho)_\Lambda = \text{Codim}\,\Lambda$$

Yes!

Effective mass equations of Heisenberg type !



The limits of the energy density (d=1)

Assumption: Assume $\|(1-\varepsilon^2\Delta)^s\psi_0^\varepsilon\|_{L^2} \leq C,\ s > 1/2$

Theorem [FCM]: There exists $\varepsilon_\ell \to 0$ such that for all $\phi \in \mathscr{C}_0^\infty(\mathbb{R}^d),\ \ \theta \in L^1(\mathbb{R})$

$$\lim_{\ell\to\infty}\int_{\mathbb{R}}\int_{\mathbb{R}^d}\theta(t)\,\phi(x)\,|\,\psi^{\varepsilon_\ell}(t,x)\,|^2\,dxdt = \sum_{n\in\mathbb{N}^*}\ \sum_{\xi\in\Lambda_n}\int_{\mathbb{R}}\int_{\mathbb{R}^d}\theta(t)\,\phi(x)\,|\,\psi_\xi^{(n)}(t,x)\,|^2\,dxdt$$

where $\psi_\xi^{(n)}(t)$ solves the effective mass equation

$$i\partial_t\psi_\xi^{(n)}(t,x) = \frac{1}{2}\partial_\xi^2\varrho_n(\xi)\,\partial_x^2\psi_\xi^{(n)}(t,x) + V_{\text{ext}}(t,x)\,\psi_\xi^{(n)}(t,x)$$

with initial data $\psi_\xi^{(n)}(0)$ is a weak limit in $L^2(\mathbb{R})$ of $\left(\mathrm{e}^{\frac{i}{\varepsilon_\ell}\xi x}\,\Pi_n(\varepsilon_\ell D_x)(\psi_0^{\varepsilon_\ell}\otimes \mathbf{1}_{y\in\mathbb{T}})\right)$

N.B. $\Pi_n(\xi)$ is the orthogonal projector on $\mathrm{Ker}\Big(P(\xi)-\varrho_n(\xi)\mathrm{Id}\Big)$

Λ_n is the set of critical points of ϱ_n

Semi-classical analysis

Wigner transform : Replace the measure $|\psi^\varepsilon(t,x)|^2 dxdt$ by the distribution

$$W^\varepsilon(t,x,\xi) = (2\pi)^{-d} \int_{\mathbb{R}^d} e^{iv\cdot\xi}\, \psi^\varepsilon(t, x+\varepsilon v/2)\, \overline{\psi}^\varepsilon(t, x-\varepsilon v/2)\, dv$$

Wigner measure: Assume $\psi_0^\varepsilon \in H^s_\varepsilon,\ s > \dfrac{d}{2}$ (uniform control))

$\mu(t,x,\xi) \in L^\infty(\mathbb{R}, \mathscr{M}^+(\mathbb{R}^{2d}))$ a weak limit of $W^\varepsilon(t,x,\xi)$ in $L^1(\mathbb{R}, \mathscr{D}'(\mathbb{R}^{2d}))$, then

$$\mathrm{w} - \lim_{\varepsilon\to 0} |\psi^\varepsilon(t,x)|^2\, dx\, dt = \int_{\mathbb{R}^{2d}} \mu(t,x,d\xi)$$

Wigner measures for Bloch components

Recall $\psi^\varepsilon(t,x) = \sum_{n\in\mathbb{N}} \psi_n^\varepsilon(t,x)$ with

$$i\varepsilon^2\partial_t \psi_n^\varepsilon(t,x) = \varrho_n(\varepsilon D)\,\psi_n^\varepsilon(t,x) + \varepsilon^2 V_{ext}(t,x)\,\psi_n^\varepsilon(t,x) + \varepsilon^2 f_n^\varepsilon(t,x)$$

Set $w_{n,n'}^\varepsilon(t,x,\xi) = (2\pi)^{-d}\int_{\mathbb{R}^d} e^{iv\cdot\xi}\,\psi_n^\varepsilon(t,x+\varepsilon v/2)\,\overline{\psi}_{n'}^\varepsilon(t,x-\varepsilon v/2)\,dv$

Lemme: There exists a subsequence realizing all weak limits $\mu(t,x,\xi)$ and $\mu_{n,n'}(t,x,\xi)$ for $n,n'\in\mathbb{N}$ and

(i) for a. e. $t\in\mathbb{R}$, $\mu(t) = \sum_{n,n'\in\mathbb{N}} \mu_{n,n'}(t)$,

(ii) $\mu_{n,n'}(t) = \overline{\mu_{n',n}(t)} \ll \mu_{n,n}(t)$

(iii) if $\varrho_n \in \mathscr{C}^{1,1}$ and $\nabla\varrho_n \neq 0$ on Ω, $\mu_{n,n}(t)(\mathbb{R}^d\times\Omega) = 0$

(iv) if $\varrho_n \neq \varrho_{n'}$ on Ω, $\mu_{n,n'}(t)(\mathbb{R}^d\times\Omega) = 0$

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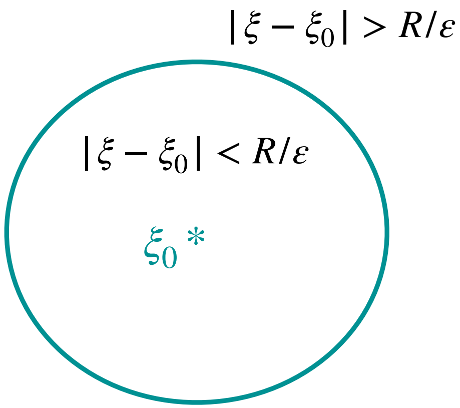
(iv) if $\varrho_n - \varrho_{n'} \neq 0$ on Ω, $\mu_{n,n'}(t)(\mathbb{R}^d\times\Omega) = 0$

Critical points !

Crossing points !

2-scale analysis of the concentration on a point



$$\psi_n^\varepsilon(t,x) = \chi\left(\frac{\varepsilon D-\xi_0}{R\varepsilon}\right)\psi_n^\varepsilon(t,x) + \left(1-\chi\left(\frac{\varepsilon D-\xi_0}{R\varepsilon}\right)\right)\psi_n^\varepsilon(t,x), \qquad \chi\in\mathscr{C}_0^\infty(\mathbb{R}^d)$$

$(1) \longrightarrow_{\varepsilon_\ell\to 0} \Psi_{\xi_0}^{(n)}(t,x)$

(2) generates a Wigner measure $\nu_n(t,x,\omega)$ sur $\mathbb{R}^d\times\mathbb{S}^{d-1}$ in the limit $\varepsilon\to 0,\ R\to+\infty$

Decomposition of the Wigner measure:

$$\mu_{n,n}(t,x,\xi)\mathbf{1}_{\xi=\xi_0} = \delta(\xi-\xi_0)\otimes\left(\left|\Psi_{\xi_0}^{(n)}(t,x)\right|^2 dxdt + \int_{\mathbb{S}^{d-1}}\nu_n(t,x,d\omega)\right)$$

Remark: Similar description when the set of observation larger than a point (d>1).

→ Trace-class operator-valued + measure

Two-scale Wigner measures

$$\mu_{n,n}(t,x,\xi)\mathbf{1}_{\xi=\xi_0} = \left|\Psi^{(n)}_{\xi_0}(t,x)\right|^2 dxdt + \delta(\xi-\xi_0)\otimes\int_{\mathbb{S}^{d-1}} \nu_n(t,x,d\omega)$$

d=1

Critical points : $\Psi^{\xi}_n(t)$ satisfies the effective mass equation

$\nu_n(t)$ satisfies invariance through $(x,\omega)\mapsto(x+s\mathrm{Hess}\,\varrho_n(\xi)\,\omega,\omega)$

$\Rightarrow$ $\nu_n(t)=0$

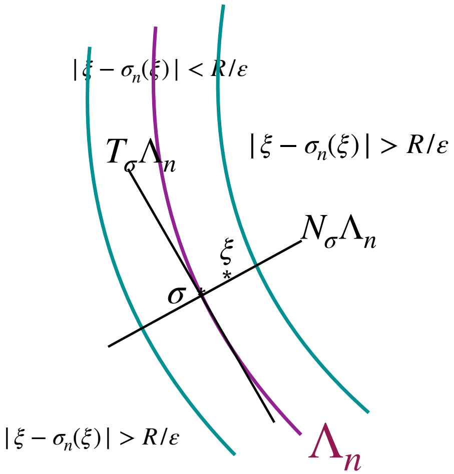
Crossing points : $\widetilde{\Psi}^{\xi}_n(t)$ satisfies an equation of the form $|D|\,\widetilde{\psi}^{\xi}_n(t)=0$

$\Rightarrow$ $\widetilde{\psi}^{\xi}_n(t)=0$

$\widetilde{\nu}_n(t)$ satisfies invariance through $(x,\omega)\mapsto(x+s\omega,\omega)$

$\Rightarrow$ $\widetilde{\nu}_n(t)=0$

Analysis of the concentration on a sub-manifold



In Ω, $\quad \xi = \sigma(\xi) + \eta(\xi) \quad \sigma(\xi) \in \Lambda_n$ et $\eta(\xi) \in N_{\sigma(\xi)}\Lambda_n$

$$\psi_n^\varepsilon(t,x) = \chi\left(\frac{\varepsilon D - \sigma(\varepsilon D)}{R\varepsilon}\right)\psi_n^\varepsilon(t,x) + \left(1 - \left(\frac{\varepsilon D - \sigma(\varepsilon D)}{R\varepsilon}\right)\right)\psi_n^\varepsilon(t,x), \qquad \chi \in \mathscr{C}_0^\infty(\mathbb{R}^d)$$

(1) generates a measure on $T\Lambda_n$ and a family of trace-class positive operators on $T\Lambda_n$

(2) generates a Wigner measure ν_n sur $S_\sigma\Lambda_n = N_\sigma\Lambda_n / R_+^*$ in the limit $\varepsilon \to 0,\ R \to +\infty$

Decomposition of the Wigner measure:

$$\mu(t,x,\sigma)\mathbf{1}_{\sigma\in\Lambda_n} = \int_{T_\sigma\Lambda_n} \mathrm{Tr}_{L^2(N_\sigma\Lambda_n)} M^t(\sigma,v)\, d\gamma_n(t,\sigma,dv) + \int_{S_\sigma\Lambda_n} \nu_n(t,\sigma,d\omega)$$

Conical crossing sets

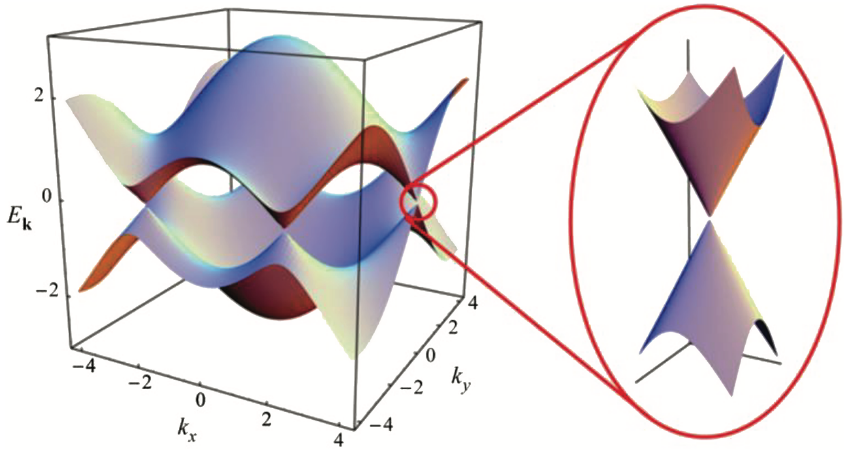
Define : $g_n(\sigma,\eta) := \frac{1}{2}\left(\varrho_{n+1}(\sigma+\eta) - \varrho_n(\sigma+\eta)\right), \quad \lambda_n = \frac{1}{2}\left(\varrho_{n+1}(\sigma+\eta) + \varrho_n(\sigma+\eta)\right)$

Definition: $\Sigma_n = \{\varrho_n(\xi) = \varrho_{n+1}(\xi)\}$ is said conical. if for $\sigma \in \Sigma_n, \quad \eta \in N_\sigma\Sigma_n$

$$g_n(\sigma,\eta) > c\,|\eta|$$

Theorem [CFM:]

Assume $\nabla\lambda_n(\sigma) \pm \nabla_\eta g_n(\sigma,\eta) \neq 0$
Then $\nu_n = 0, \quad \gamma_n = 0$



Why ? $(\lambda_n = 0)$

ν_n is invariant by $(\sigma,\omega) \mapsto (\sigma - t\,\nabla_\eta g_n(\sigma,\omega), \omega)$

M_n satisfies $[M_n(\sigma,v)\,, g_n(\sigma,D)] = 0, \;\; \forall(\sigma,v) \in T\Sigma_n$

Ref: [Kuchment] Bull. Amer. Math. Soc. 2016

Effective mass equations of Heisenberg type

Theorem [CFM]:

If $\mathrm{Hess}\,\varrho_n$ is of maximal rank on Λ_n and the crossing sets conical with $\nabla\lambda_n(\sigma) \pm \nabla_\eta g_n(\sigma,\eta) \neq 0$,

then any Wigner measure $\mu_{n,n}$ satisfies

$$\mu_{n,n}(t,x,\sigma)\mathbf{1}_{\sigma\in\Lambda_n} = \int_{T_\sigma\Lambda_n} \mathrm{Tr}_{L^2(N_\sigma\Lambda_n)} M_n^t(\sigma,v)\,d\gamma_n(t,\sigma,dv) + \int_{S_\sigma\Lambda_n} \nu_n(t,\sigma,d\omega)$$

with: $\gamma_n(t) = \gamma_n(0)$

$M_n(\sigma,v)$ solves

$$i\partial_t M_n^t(\sigma,v) = \left[\frac{1}{2}\mathrm{Hess}\,\varrho_n(\sigma)D_z\cdot D_z + m_{V_{\mathrm{ext}}}^{\Lambda_n}(v,\sigma)\ ,\ M_n^t(\sigma,v)\right]$$

ν_n invariant by the flow $(x,\omega)\mapsto(x+t\,\mathrm{Hess}\,\varrho_n(\xi_0)\,\omega,\omega)$, whence ν_n= 0

5.4 **Remark :** $\mathrm{Ker}\,\mathrm{Hess}\,\varrho_n(\sigma) = T_\sigma\Lambda_n,\ \ \sigma\in\Lambda_n$

Conclusion

- Description of the weak limits of the energy density with rather general assumptions
  on the data
  on the geometry of the critical & crossing sets for $d > 1$ (Morse-Bott).

- Operator-valued effective mass equations when the critical set is larger than a point.

- For degenerate crossing points, interactions between Bloch modes are possible.

- Question : What about the structure of the Bloch modes in dimension larger than 1 ?

Thank you for your attention !

Analysis of the concentration on a critical point

Theorem (critical points) [CFM]:

Il ξ_0 is a non-degenerate critical point of ϱ_n any Wigner measure $\mu_{n,n}$ satisfies

$$\mu_{n,n}(t,x,\xi)\mathbf{1}_{\xi=\xi_0} = \left|\Psi^{(n)}_{\xi_0}(t,x)\right|^2 dxdt + \delta(\xi-\xi_0)\otimes\int_{\mathbb{S}^{d-1}} \nu_n(t,x,d\omega)$$

with $\Psi^{(n)}_{\xi_0}$ solution to the effective mass equation

ν_n invariant by the flow $(x,\omega)\mapsto(x+t\,\mathrm{Hess}\,\varrho_n(\xi_0)\,\omega,\omega)$, whence $\nu_n = 0$

Remark: Similar statement when d>1, with the condition that the Hessian is of maximal rank on the set of critical points. ($\mathrm{Ker\,Hess}\,\varrho_n(\sigma) = T_\sigma\Lambda_n,\ \ \sigma\in\Lambda_n$)

Regularity spaces

Weighted Sobolev spaces: $\psi \in H^s_\varepsilon(\mathbb{R}^d \times \mathbb{T}^d)$ iff. $\exists C, \varepsilon_0 > 0$

$$\forall \varepsilon \in (0,\varepsilon_0), \quad \|\psi\|^2_{H^s_\varepsilon(\mathbb{R}^d)} := \int_{\mathbb{R}^d} (1 + |\varepsilon\xi|^2)^s |\widehat{\psi}(\xi)|^2 d\xi \leq C$$

Lemma:

Assume $\|\psi_0^\varepsilon\|_{H^s_\varepsilon} < C_0$ for some $C_0 > 0$, $s > \dfrac{d}{2}$, then, for all $t \in \mathbb{R}$

$$\limsup_{\varepsilon \to 0^+} \Big\| \sum_{n>N} \psi_n^\varepsilon(t, \cdot) \Big\|_{L^2(\mathbb{R}^d)} \longrightarrow_{N \to 0} 0$$