Partial Semiclassical Limits

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Example: The Schrödinger operator

$$\widehat{H}^{\varepsilon} = -\tfrac{\varepsilon^2}{2}\Delta_x + V(x)$$

is the Weyl-quantization of the symbol

$$H(q,p) = \tfrac{1}{2}p^2 + V(q)\,.$$

In general: Consider an ε-pseudodifferential Operator

$$\widehat{H}^{\varepsilon} = H(x, -\mathrm{i}\varepsilon\nabla_x)\,.$$

We take $\widehat{H}$ to be the ε-Weyl-quantization of a symbol

$$H : \mathbb{R}^{2n} \to \mathbb{R}$$

acting on functions $\psi \in L^2(\mathbb{R}^n)$ as

$$(\widehat{H}^{\varepsilon}\psi)(x) := \frac{1}{(2\pi\varepsilon)^n}\int_{\mathbb{R}^{2n}} \mathrm{e}^{\mathrm{i}p\cdot(x-y)/\varepsilon}\, H\left(\tfrac{1}{2}(x+y), p\right)\, \psi(y)\,\mathrm{d}p\,\mathrm{d}y\,.$$

If $\widehat{H}^\varepsilon$ is self-adjoint, it generates a unitary group

$$U^\varepsilon : \mathbb{R} \to \mathcal{L}(L^2(\mathbb{R}^n)), \quad t \mapsto U^\varepsilon(t) = \mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}$$

and the asymptotic limit $\varepsilon \to 0$ is the **semiclassical limit**.

One way to formulate the semiclassical limit is to look at the way other ε-pseudos transform:

$$\mathrm{e}^{\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}\, \widehat{A}^\varepsilon\, \mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon} = ?$$

Egorov's Theorem 1: Let

$$\Phi^t_{H_0} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$$

be the Hamiltonian flow associated to the principal symbol H_0 of $\widehat{H}^\varepsilon$, then

$$\mathrm{e}^{\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}\, \widehat{A}^\varepsilon\, \mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon} = \widehat{A \circ \Phi^t_{H_0}}^{\,\varepsilon} + \mathcal{O}(\varepsilon)\,.$$

A less commonly known improved version is

Egorov's Theorem 2: Let

$$\Phi^t_{H^\varepsilon} : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$$

be the Hamiltonian flow associated to the symbol $H^\varepsilon = H_0 + \varepsilon H_1$, then

$$\mathrm{e}^{\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}\,\widehat{A}^\varepsilon\,\mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon} = \widehat{A \circ \Phi^t_{H^\varepsilon}}^{\varepsilon} + \mathcal{O}(\varepsilon^2)\,.$$

Remarks:

- For H and A from suitable symbol classes, the approximation holds in norm uniformly on bounded time intervals.
- Theorem 1 holds also on T^*M with M a Riemannian manifold.
- Theorem 2 only holds if M has vanishing curvature.

Consider the Hilbert space

$$L^2(\mathbb{R}^n) \otimes \mathcal{H}_{\mathsf{f}} \cong L^2(\mathbb{R}^n, \mathcal{H}_{\mathsf{f}})\,,$$

where $\mathcal{H}_{\mathsf{f}}$ is the Hilbert space of some quantum mechanical degrees of freedom. For an operator-valued symbol

$$H : \mathbb{R}^{2n} \to \mathcal{L}(\mathcal{H}_{\mathsf{f}})$$

we define $\widehat{H}^\varepsilon$ acting on functions $\psi \in L^2(\mathbb{R}^n, \mathcal{H}_{\mathsf{f}})$ again as

$$(\widehat{H}^\varepsilon \psi)(x) := \frac{1}{(2\pi\varepsilon)^n} \int_{\mathbb{R}^{2n}} \mathrm{e}^{\mathrm{i}p\cdot(x-y)/\varepsilon}\, H\left(\tfrac{1}{2}(x+y), p\right)\, \psi(y)\, \mathrm{d}p\, \mathrm{d}y\,.$$

Example: The molecular Hamiltonian

$$-\tfrac{\varepsilon^2}{2}\Delta_x - \tfrac{1}{2}\Delta_y + V(x,y) = \widehat{H}^\varepsilon \qquad \text{on} \qquad L^2(\mathbb{R}^n_x \times \mathbb{R}^m_y) = L^2(\mathbb{R}^n_x, L^2(\mathbb{R}^m_y))$$

is the Weyl-quantization of the operator-valued symbol

$$H(q,p) = \tfrac{1}{2}p^2 - \tfrac{1}{2}\Delta_y + V(q,y)\,.$$

Since $H(q,p)$ is operator-valued, it does not generate a Hamiltonian flow on T^*M. Can one still prove an Egorov Theorem?

$H(q,p)$ is self-adjoint for each $(q,p) \in \mathbb{R}^{2n}$. Its eigenvalues $E(q,p)$ are real-valued and thus define Hamiltonian functions on phase space.

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Adiabatic perturbation theory:

(Littlejohn-Flynn, Emmrich-Weinstein, Brummelhuis-Nourrigat, Martinez-Nenciu-Sordoni, Panati-Spohn-T.)

If $H_0(q,p)$ has an eigenvalue $E(q,p)$ with spectral projection $P(q,p)$ that is separated by a gap from the remainder of the spectrum of $H_0(q,p)$, then there exists a unique symbol

$$P^\varepsilon(q,p) \qquad \text{with} \qquad P^\varepsilon(q,p) = P(q,p) + \mathcal{O}(\varepsilon)$$

such that $\widehat{P}^\varepsilon$ is an orthogonal projection, i.e.

$$(\widehat{P}^\varepsilon)^2 = \widehat{P}^\varepsilon \qquad \text{and} \qquad (\widehat{P}^\varepsilon)^* = \widehat{P}^\varepsilon\,,$$

that commutes with the Hamiltonian $\widehat{H}^\varepsilon$ up to small errors,

$$[\widehat{H}^\varepsilon, \widehat{P}^\varepsilon] = \mathcal{O}(\varepsilon^\infty)\,.$$

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$$[\widehat{H}^\varepsilon, \widehat{P}^\varepsilon] = \mathcal{O}(\varepsilon^\infty)\,.$$

Hence $\mathrm{Ran}\widehat{P}^\varepsilon$ is almost invariant under the group $\mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}$,

$$[\mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}, \widehat{P}^\varepsilon] = \mathcal{O}(\varepsilon^\infty|t|)$$

and

$$\widehat{H}^\varepsilon\widehat{P}^\varepsilon = \widehat{E}^\varepsilon\widehat{P}^\varepsilon + \mathcal{O}(\varepsilon)\,.$$

Egorov's Theorem 3: Let

$$\Phi_E^t : \mathbb{R}^{2n} \to \mathbb{R}^{2n}$$

be the Hamiltonian flow associated to the eigenvalue E of H_0, then

$$\mathrm{e}^{\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}\, \widehat{P}^\varepsilon\, \widehat{A}^\varepsilon\, \widehat{P}^\varepsilon\, \mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon} = \widehat{P}^\varepsilon\, \widehat{a \circ \Phi_E^t}^{\,\varepsilon}\, \widehat{P}^\varepsilon + \mathcal{O}(\varepsilon)$$

for any observable $\widehat{A}^\varepsilon$ with principle symbol of the form

$$A_0(q,p) = a(q,p) \otimes \mathbf{1}_{\mathcal{H}_\mathsf{f}}\,.$$

Idea of the proof (PST 2003): Construct a unitary mapping

$$\widehat{U}^\varepsilon : \widehat{P}^\varepsilon L^2(\mathbb{R}^n, \mathcal{H}_\mathsf{f}) \to L^2(\mathbb{R}^n, \mathbb{C})$$

and apply the standard Egorov Theorem to the effective Hamiltonian

$$\widehat{H}^\varepsilon_{\mathsf{eff}} := \widehat{U}^\varepsilon\, \widehat{P}^\varepsilon\, \widehat{H}^\varepsilon\, \widehat{P}^\varepsilon\, \widehat{U}^{\varepsilon\,*} = \widehat{E}^\varepsilon + \mathcal{O}(\varepsilon)\,.$$

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Problem: The construction of this unitary requires the choice of a family of normalized eigenvectors

$$\varphi(q,p) \in P(q,p)\,\mathcal{H}_{\mathsf{f}}$$

depending smoothly on $(q,p) \in \mathbb{R}^{2n}$.

Put differently, the line bundle over $\mathbb{R}^{2n}$ defined by the eigenspaces $P(q,p)\mathcal{H}_{\mathsf{f}}$ needs to be trivializable!

In important applications, like periodic potentials in strong magnetic fields, the corresponding bundle is not trivializable and this fact has important physical consequences, like the integer quantum Hall effect.

Egorov's Theorem 4: (Stiepan-T.)
There is a flow

$$\Phi_\varepsilon^t : T^*M \to T^*M$$

(M either $\mathbb{R}^n$ or $\mathbb{T}^n$) such that

$$\mathrm{e}^{\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon}\,\widehat{P}^\varepsilon\,\widehat{A}^\varepsilon\,\widehat{P}^\varepsilon\,\mathrm{e}^{-\mathrm{i}\widehat{H}^\varepsilon t/\varepsilon} = \widehat{P}^\varepsilon\,\widehat{a \circ \Phi_\varepsilon^t}^{\,\varepsilon}\,\widehat{P}^\varepsilon + \mathcal{O}(\varepsilon^2)$$

for any observable $\widehat{A}^\varepsilon$ with principle symbol of the form

$$A_0(q,p) = a(q,p) \otimes \mathbf{1}_{\mathcal{H}_\mathrm{f}}\,.$$

Here Φ_ε^t is the Hamiltonian flow of

$$H^\varepsilon_{\mathrm{eff}} := E + \varepsilon\,\tfrac{\mathrm{i}}{2}\,\mathrm{tr}\left(P\left\{P, H_0 - E, P\right\}\right) =: E + \varepsilon M$$

with respect to the symplectic form

$$\omega := \begin{pmatrix} 0 & \mathbf{1}_n \\ -\mathbf{1}_n & 0 \end{pmatrix} + \varepsilon \begin{pmatrix} \Omega^{qq} & \Omega^{pq} \\ \Omega^{qp} & \Omega^{pp} \end{pmatrix}.$$

Here

$$\begin{pmatrix} \Omega^{qq} & \Omega^{pq} \\ \Omega^{qp} & \Omega^{pp} \end{pmatrix} = \begin{pmatrix} \mathrm{i}\,\mathrm{tr}(P[\nabla_q P, (\nabla_q P)^{\mathsf{T}}]) & \mathrm{i}\,\mathrm{tr}(P[\nabla_q P, (\nabla_p P)^{\mathsf{T}}]) \\ \mathrm{i}\,\mathrm{tr}(P[\nabla_p P, (\nabla_q P)^{\mathsf{T}}]) & \mathrm{i}\,\mathrm{tr}(P[\nabla_p P, (\nabla_p P)^{\mathsf{T}}]) \end{pmatrix}$$

or shorter

$$\Omega_{ij} = \mathrm{i}\,\mathrm{tr} P[\partial_i P, \partial_j P]$$

is the curvature 2-form of the Berry connection.

The Hamiltonian equations of motion have the form

$$\begin{aligned} \dot{q} &= \nabla_p(E + \varepsilon M) + \varepsilon(\Omega^{qq}\nabla_q E + \Omega^{pq}\nabla_p E) \\ \dot{p} &= -\nabla_q(E + \varepsilon M) + \varepsilon(\Omega^{qp}\nabla_q E + \Omega^{pp}\nabla_p E) \end{aligned}$$

or alternatively

$$\begin{aligned} \dot{q} &= \nabla_p(E + \varepsilon M) - \varepsilon(\Omega^{qq}\dot{p} - \Omega^{pq}\dot{q}) + \mathcal{O}(\varepsilon^2) \\ \dot{p} &= -\nabla_q(E + \varepsilon M) - \varepsilon(\Omega^{qp}\dot{p} - \Omega^{pp}\dot{q}) + \mathcal{O}(\varepsilon^2)\,. \end{aligned}$$

As a Corollary we obtain the formula

$$\mathrm{Tr}\left(\widehat{\rho}\,\widehat{P}^{\varepsilon}\,\widehat{A}^{\varepsilon}(t)\,\widehat{P}^{\varepsilon}\right) = \int_{T^*M} \rho(q,p)\,\left(a \circ \Phi^t_{\varepsilon}\right)(q,p)\,\mathrm{d}\omega + \mathcal{O}(\varepsilon^2)$$

where $\mathrm{d}\omega$ denotes integration with respect to the volume measure induced by the symplectic form ω,

$$\mathrm{d}\omega = \Big(1 - \mathrm{i}\varepsilon\,\mathrm{tr}\,(P\{P,P\})\Big)\,\mathrm{d}q\,\mathrm{d}p\,.$$

Consider the Hamiltonian

$$H = \tfrac{1}{2}\Big(-\mathrm{i}\nabla_x + A_0(x) + A(\varepsilon x)\Big)^2 + V_\Gamma(x) - \phi(\varepsilon x) \qquad \text{on} \qquad L^2(\mathbb{R}^3)$$

with a Γ-periodic potential V_Γ, smooth electromagnetic potentials A and ϕ and the vector potential of a constant rational magnetic field B_0,

$$A_0(x) = \tfrac{1}{2} B_0\, x^\perp\,.$$

After a suitable Bloch-Floquet transformation this operator takes the form

$$\widehat{H}^\varepsilon = \tfrac{1}{2}\Big(-\mathrm{i}\nabla_y + k + A_0(y) + A(\mathrm{i}\varepsilon\nabla_k^\tau)\Big)^2 + V_\Gamma(y) - \phi(\mathrm{i}\varepsilon\nabla_k^\tau)$$

acting on

$$L^2(M_k, L^2(T_y)) =: L^2(M_k, \mathcal{H}_\mathrm{f})\,.$$

$\widehat{H}^\varepsilon$ is the Weyl-quantization of the operator-valued symbol

$$H(k,r) = \tfrac{1}{2}\Big(-\mathrm{i}\nabla_y + k + A_0(y) + A(r)\Big)^2 + V_\Gamma(y) - \phi(r)$$

with $H : T^*M \to \mathcal{L}(L^2(T_y))$.

The eigenvalues $E_n(k)$ of the periodic Hamiltonian

$$H_0(k) = \frac{1}{2}\Big(-\mathrm{i}\nabla_y + k + A_0(y)\Big)^2 + V_\Gamma(y)$$

are known as the magnetic Bloch bands and the corresponding spectral projections $P_n(k)$ define the magnetic Bloch bundle over the torus M. This bundle has in general nonvanishing Chern number and is thus not trivializable. Hence the standard techniques can not be applied.

Our general Egorov Theorem applied to magnetic Bloch Hamiltonians yields

$$M_n(k,r) = B(r)\,\mathcal{M}_n(k - A(r))$$

with

$$\mathcal{M}_n(k) := \tfrac{\mathrm{i}}{2}\,\mathrm{tr}\left(P_n(k)\nabla P_n(k)\cdot\Big(H_0(k) - E_n(k)\Big)\nabla P_n(k)^{\perp}\right)$$

and

$$\Omega_n^{kk}(k,r) = \Omega_n(k - A(r)) \quad \text{and} \quad \Omega_n^{kr} = \Omega_n^{rr} = 0\,,$$

with

$$\Omega_n(k) = \mathrm{i}\,\mathrm{tr}\left(P_n(k)\nabla P_n(k)\cdot\nabla P_n(k)^{\perp}\right)\,.$$

Introducing the kinetic momentum $\kappa := k - A(r)$ we obtain

$$\begin{aligned}\dot r &= \nabla_\kappa\Big(E_n(\kappa) + \varepsilon B(r)\mathcal{M}_n(\kappa)\Big) - \varepsilon\,\Omega(\kappa)\,\dot\kappa^{\perp}\\ \dot\kappa &= -\nabla_r\Big(\phi(r) + \varepsilon B(r)\mathcal{M}_n(\kappa)\Big) - B(r)\,\dot r^{\perp}\,.\end{aligned}$$

Introducing the kinetic momentum $\kappa := k - A(r)$ we obtain

$$\begin{aligned}\dot{r} &= \nabla_\kappa \Big(E_n(\kappa) + \varepsilon B(r) \mathcal{M}_n(\kappa) \Big) - \varepsilon\, \Omega(\kappa)\, \dot{\kappa}^\perp \\ \dot{\kappa} &= -\nabla_r \Big(\phi(r) + \varepsilon B(r) \mathcal{M}_n(\kappa) \Big) - B(r)\, \dot{r}^\perp .\end{aligned}$$

Application: Integer quantum Hall effect

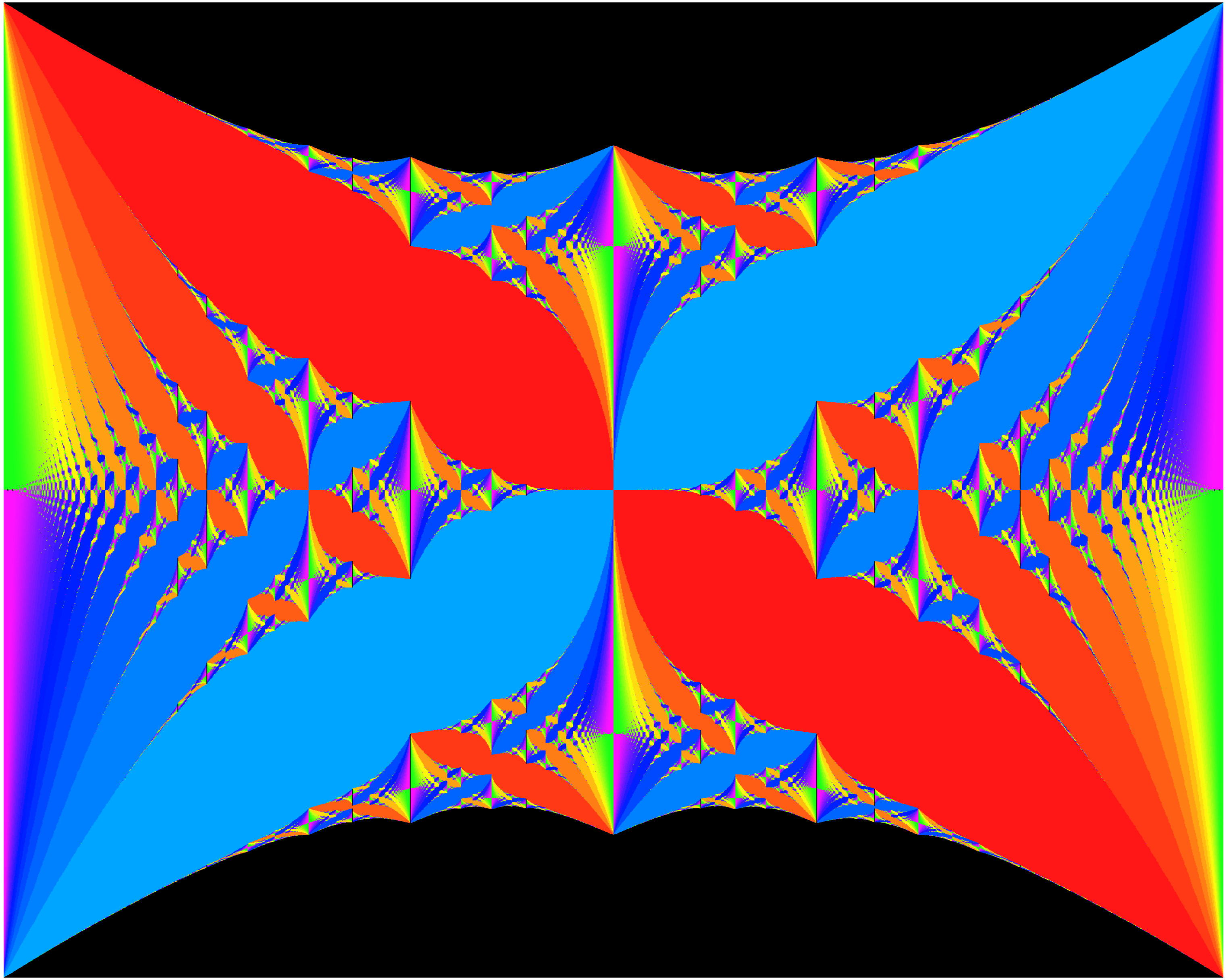
Let $A = \frac{1}{2} B\, r^\perp$ and $\phi(r) = -\mathcal{E} \cdot r$ then $\dot{\kappa} = \mathcal{E} - B\, \dot{r}^\perp$ and

$$\dot{r} = \frac{\nabla_\kappa (E_n(\kappa) + \varepsilon B \mathcal{M}_n(\kappa)) - \varepsilon\, \mathcal{E}^\perp \Omega_n(\kappa)}{1 + \varepsilon B \Omega} .$$

Averaging the velocity over M yields the equilibrium current density:

$$j = \frac{1}{\varepsilon (2\pi)^2} \int_M \dot{r}(\kappa)\, \mathrm{d}\omega = -\mathcal{E}^\perp \frac{1}{(2\pi)^2} \underbrace{\int_M \Omega_n(\kappa)\, \mathrm{d}\kappa}_{\in 2\pi\mathbb{Z}} = \mathcal{E}^\perp \sigma_{\mathrm{H}} .$$

Thus the Hall conductivity σ_{H} of a filled band is quantized.



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Adiabatic approximation:

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Thank you!