Semiclassical analysis for periodic media

Summary

Ingo Witt
(Georg-August-Universität Göttingen)

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1 Introduction

Semiclassical analysis involves a small parameter $h > 0$ and statements are in the limit as $h \to 0$. Notice that we now move from an operator-theoretic level in terms of abstract spectral theory of selfadjoint operators to the level of concretely realized linear, bounded operators acting on $\mathscr{S}'(\mathbb{R}^d)$ (and leaving $\mathscr{S}(\mathbb{R}^d)$ invariant), where then the domain of the operator under study can be specified as appropriate. An additional point is a symbolic calculus which provides control of the operators under investigation up to neglectable terms. It is the combination of both approaches that yields the best results (known to date).

In the first two lectures, we will lay the groundwork for later applications. These applications concern the spectral theory for perturbed periodic media and will be dealt with in the remaining two lectures.

2 Semiclassical operators

Semiclassical operators $P(h)$ are families of operators depending on $h \in (0, h_0]$ for a suitable $h_0 > 0$. The example to keep in mind is the **Schrödinger operator** $P(h) = -h^2\Delta + V(x)$ realized as a selfadjoint operator in $L^2(\mathbb{R}^d)$, where the potential V satisfies (at least) $V \in \mathscr{C}^\infty(\mathbb{R}^d)$, $\inf V > -\infty$, and $V(x) = O(\langle x\rangle^N)$ for some $N > 0$. The principal symbol of this operator family as a semiclassical operator is $|\xi|^2 + V(x)$ which is the classical energy. If, in addition, $|\partial_x^\alpha V(x)| \le C_\alpha\,(C + V(x))$ for all $\alpha \in \mathbb{N}_0^d$, where $C + \inf V > 0$, then $C + |\xi|^2 + V(x)$ can be taken for an admissible weight function.

The semiclassical operators $P(h) = p^{\mathrm{W}}(x, hD_x; h)$ considered below generalize differential operators as well as their parametrices (i.e., almost inverses, where 'almost' has to be made precise) in the elliptic case.

Admissible weight functions $M \in \mathscr{C}^\infty(\mathbb{R}^{2d})$, where

- $0 < M(x,\xi) \le C\,\langle x,\xi\rangle^N$ for some $N > 0$,
- $|\partial_x^\alpha \partial_\xi^\beta M(x,\xi)| \le C_{\alpha\beta}\, M(x,\xi)$ for all $\alpha, \beta \in \mathbb{N}_0^d$.

Amplitude functions $a = a(x,\xi;h) \in S(M)$ if $a(\cdot,\cdot;h) \in \mathscr{C}^\infty(\mathbb{R}^{2d})$ for each $h \in (0,h_0]$, $|\partial_x^\alpha \partial_\xi^\beta a(x,\xi;h)| \le C_{\alpha\beta}\, M(x,\xi)$ for all $\alpha, \beta \in \mathbb{N}_0^d$ uniformly in $h \in (0,h_0]$.

Regular amplitude functions $a \in S^{\mathrm{reg}}(M)$ if there exists a sequence $\{a_j\}_{j\in\mathbb{N}_0} \subset S(M)$ of h-independent amplitudes such that $a(x,\xi;h) \sim \sum_{j\ge 0} h^j\, a_j(x,\xi)$ in the sense that, for all $J \in \mathbb{N}_0$,

$$a(x,\xi;h) - \sum_{0\le j<J} h^j\, a_j(x,\xi) \in h^J\, S(M).$$

a_0 – principal symbol, a_1 – subprincipal symbol.

Weyl quantization For $a \in S(M)$,

$$a^{\mathrm{W}}(x, hD; h) = \mathscr{F}_h^{-1}\, a\Big(\frac{x+y}{2}, \xi; h\Big)\, \mathscr{F}_h,$$

where $\mathscr{F}_h u(\xi) = \int_{\mathbb{R}^d} e^{-i(x-y)\xi/h} u(x)\, dx$, $\mathscr{F}_h^{-1} v(x) = (2\pi h)^{-d} \int_{\mathbb{R}^d} e^{i(x-y)\xi/h} v(\xi)\, d\xi$.

Note that

$$a^{\mathrm{W}} \colon \mathscr{S}(\mathbb{R}^d) \to \mathscr{S}(\mathbb{R}^d), \qquad a^{\mathrm{W}} \colon \mathscr{S}'(\mathbb{R}^d) \to \mathscr{S}'(\mathbb{R}^d)$$

continuously.

Composition $a \in S(M)$, $b \in S(M')$ implies $a \sharp b \in S(MM')$, where

$$a^{\mathrm{W}}(x, hD; h) \circ b^{\mathrm{W}}(x, hD; h) = (a \sharp b)^{\mathrm{W}}(x, hD; h)$$

and

$$\begin{aligned}(a \sharp b)(x, \xi; h) &= e^{i\, h(D_x D_\eta - D_y D_\xi)} \big(a(x, \xi; h)\, b(y, \eta; h)\big)\Big|_{\substack{y=x,\\ \eta=\xi}} \\ &\sim \sum_{\alpha, \beta \in \mathbb{N}_0^d} \frac{i^{|\alpha|-|\beta|} h^{|\alpha|+|\beta|}}{2^{|\alpha|+|\beta|} \alpha! \beta!} \big(\partial_x^\alpha \partial_\xi^\beta a\big)(x, \xi; h) \big(\partial_x^\beta \partial_\xi^\alpha b\big)(x, \xi; h) \quad \text{in } S(MM').\end{aligned}$$

For $a \in S^{\mathrm{reg}}(M)$, $b \in S^{\mathrm{reg}}(M')$,

$$a \sharp b - a_0 b_0 - h\Big(a_0 b_1 + a_1 b_0 + \frac{1}{2i}\{a_0, b_0\}\Big) \in h^2\, S(MM').$$

Function spaces $M^{\mathrm{W}}(x, hD)$ is invertible for $h > 0$ sufficiently small (see below). This allows us to define $\mathscr{H}(M; h) = \{u \in \mathscr{S}'(\mathbb{R}^d) \mid M(x, hD_x) u \in L^2(\mathbb{R}^d)\}$. The Schwartz space $\mathscr{S}(\mathbb{R}^d)$ is dense in $\mathscr{H}(M; h)$.

Continuity $\|a^{\mathrm{W}}(x, hD_x; h)\|_{L^2 \to L^2} = O(1)$ uniformly in $h \in (0, h_0]$ if $a \in S(1)$. More generally, one has that $\|a^{\mathrm{W}}(x, hD_x; h)\|_{\mathscr{H}(MM'; h) \to \mathscr{H}(M; h)} = O(1)$ uniformly in $h \in (0, h_0]$ if $a \in S(M)$.

Gårding inequality $\langle a^{\mathrm{W}}(x, hD_x; h) u, u\rangle \geq -C\, h \|u\|^2$ uniformly in $h \in (0, h_0]$ if $a \in S(1)$, $a \geq 0$.

Ellipticity and parametrices $a \in S^{\mathrm{reg}}(M)$ is elliptic if $|a_0(x, \xi)| \geq C\, M(x, \xi)^{-1}$. In this case, there exists a $b \in S^{\mathrm{reg}}(1/M)$ such that $a \sharp b = 1 + r$, $b \sharp a = 1 + s$, where $r, s \in \bigcap_{N \in \mathbb{N}_0} h^N S(1)$. b^{W} is called a parametrix of a^{W}. In the elliptic case, $a^{\mathrm{W}}(x, hD; h)$ is invertible for $h > 0$ sufficiently small.

3 Functional calculus and spectral theory

Essential selfadjointness Let $P = p^{\mathrm{W}}(x, hD_x; h)$, where $p \in S^{\mathrm{reg}}(M)$. Suppose that p is real-valued, $p_0 \geq 0$, and $M = 1 + p_0$. Then $P(h)$ as an unbounded operator in $L^2(\mathbb{R}^d)$ is essentially selfadjoint with domain $\mathscr{S}(\mathbb{R}^d)$ and selfadjoint with domain $\mathscr{H}(M; h)$ for $h > 0$ sufficiently small. In the sequel, we shall understand by $P(h)$ its selfadjoint realization. Let $\{E(B; h)\}_{B \in \mathscr{B}(\mathbb{R})}$ denote its spectral measure.

Counting function Let $\alpha < \beta$ and suppose that $\liminf_{|x|+|\xi| \to \infty} \operatorname{dist}\big(p_0(x, \xi), [\alpha, \beta]\big) > 0$. Then the spectrum of P in a neighborhood of $[\alpha, \beta]$ is discrete and

$$\begin{aligned}(2\pi h)^d\, \sharp\{\text{eigenvalues of } P(h) \text{ in } [\alpha, \beta]\} &= (2\pi h)^d \operatorname{tr} E([\alpha, \beta]; h) \\ &= \operatorname{vol}\{(x, \xi) \mid p_0(x, \xi) \in [\alpha, \beta]\} + O(h) \quad \text{as } h \to 0.\end{aligned}$$

Helffer-Sjöstrand formula Let $f \in \mathscr{C}^\infty_{\mathrm{comp}}(\mathbb{R})$ and $\tilde{f}$ be an almost analytic extension[1]. Then

$$f(P) = \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar z} \tilde{f}(z)\, (P - z)^{-1}\, dx\, dy,$$

where $z = x + iy$.

[1] That is, $\tilde{f} \in \mathscr{C}^\infty_{\mathrm{comp}}(\mathbb{C})$, $\partial_{\bar z} \tilde{f}(z) = O(|\Im z|^N)$ for any $N > 0$, and $\tilde{f}\big|_{\mathbb{R}} = f$.

***f*(*P*) as semiclassical operator** $f(P(h)) = q^{\mathrm{W}}(x, hD; h)$, where $q \in S^{\mathrm{reg}}(\langle x,\xi\rangle^{-N})$ for any $N > 0$ and

$$q_0 = f(p_0), \quad q_1 = p_1 f'(p_0), \quad q_j = \sum_{l=1}^{2j-1} \Delta_{jl} f^{(l)}(p_0), \quad \forall j \ge 2,$$

where Δ_{jl} is a certain (universal) polynomial of $\partial_x^\alpha \partial_\xi^\beta p_m$ for $|\alpha| + |\beta| + m \le j$.

By integration,

$$(2\pi h)^d \operatorname{tr} f(P(h)) = \int_{\mathbb{R}^d} f(p_0(x,\xi))\, dx d\xi + h \int_{\mathbb{R}^d} p_1(x,\xi) f'(p_0(x,\xi))\, dx d\xi + O(h^2) \quad \text{as } h \to 0.$$

4 Perturbed periodic media

4.1 The model

The operator

$$\boxed{P_{A,\varphi} = \sum_{j=1}^{d} (D_{y_j} + A_j(hy))^2 + V(y) + \varphi(hy), \quad y \in \mathbb{R}^d,}$$

where $h > 0$ is small, describes the *motion of an electron in a periodic crystal with slowly varying exterior electric and magnetic fields*. For the potentials V, A, φ, we shall assume that

– $V \in \mathscr{C}^\infty(\mathbb{R}^d; \mathbb{R})$ is periodic with respect to a lattice $\Gamma \subset \mathbb{R}^d$,

– $\nabla A \in \mathscr{C}_b^\infty(\mathbb{R}^d; \mathbb{R}^{d\times d})$ (this allows a linear growth of A as it is the case, e.g., for a constant magnetic field),

– $\varphi \in \mathscr{C}_b^\infty(\mathbb{R}^d; \mathbb{R})$, $\lim_{|x|\to\infty} \varphi(x) = 0$.

Let $\lambda_1(\xi) \le \lambda_2(\xi) \le \lambda_3(\xi) \le \dots$ for $\xi \in \mathbb{R}^d$ be the Floquet eigenvalues of the operator $-\Delta + V(y)$. Taking the effective Hamiltonian in solid-state physics is to replace, for $h > 0$ small, the operator $P_{A,\varphi}$ by the collection of semiclassical operators

$$\boxed{\lambda_l(hD_x + D_y + A(x)) + \varphi(x), \quad \forall l \in \mathbb{N}.}$$

Here, we shall see a justification for this replacement when computing the number of eigenvalues of $P_{A,\varphi}$ in a spectral gap of $-\Delta + V(y)$ in the limit $h \to 0$.

We closely follow the references [1, Chap. 13], [2].

4.2 Semiclassical reduction

In $P_{A,\varphi} = p^{\mathrm{W}}(hy, y, D_y + A(x))$, where $p(x,y,\eta) = |\eta|^2 + V(y) + \varphi(x)$, $h > 0$ does not happen to be a semiclassical parameter. Along with this operator, therefore, we shall also consider the operator $P = p^{\mathrm{W}}(x, y, hD_x + D_y + A(x))$ acting in $L^2(\mathbb{R}^{2d}_{x,y})$.

In a first part, in place of $p(x,y,\eta) = |\eta|^2 + V(y) + \varphi(x)$, we will consider more general symbols $p(x,y,\eta) = \sum_{|\alpha|\le m} a_\alpha(x,y)\eta^\alpha$ satisfying the following assumptions:

– (real-valuedness) $p \in \mathscr{C}^\infty(\mathbb{R}^{3d})$ is real-valued,

– (periodicity) $p(x, y+\gamma, \eta) = p(x,y,\eta)$ for all $\gamma \in \Gamma$,

– (strong ellipticity) $\sum_{|\alpha|=m} a_\alpha(x,y)\eta^\alpha \ge C|\eta|^m$ for some $C > 0$ (in particular, m has to be even).

The operator $P = p^{\mathrm{W}}(x, y, hD_x + D_y + A(x))$ acting in $L^2(\mathbb{R}^{2d})$ is selfadjoint with domain $\{u \in L^2(\mathbb{R}^{2d}) \mid (hD_x + D_y + A(x))^\alpha u \in L^2(\mathbb{R}^{2d})\ \forall \alpha \in \mathbb{N}_0^{2d}, |\alpha| \le m\}$.

Using Floquet-Bloch transformation (with respect to y), the complexity of the problem can be reduced. Namely, the unitary map

$$\Phi = e^{i\langle\theta, x/h-y\rangle}\mathscr{U} : L^2(\mathbb{R}^{2d}_{x,y}) \to \{v \in L^2_{\mathrm{loc}}(\mathbb{R}^{3d}) \mid v(x,y+\gamma,\theta) = v(x,y,\theta)\ \forall\gamma\in\Gamma,$$
$$v(x,y,\theta+\gamma^*) = e^{i\langle\gamma^*, x/h-y\rangle}v(x,y,\theta)\ \forall\gamma^*\in\Gamma^*,\ (2\pi)^{-d}\iiint_{\mathbb{R}^d_x\times W_y\times B_\theta}|v(x,y,\theta)|^2\,dx\,dy\,d\theta < \infty\}$$

has the property that (recall that $|W| = 1$, $|B| = (2\pi)^d$)

$$\Phi P\Phi^* = \int_B^{\oplus} P\,\frac{d\theta}{(2\pi)^d},$$

where the fiber operators are independent of $\theta\in B$ and act as $P = p^{\mathrm{W}}(x,y,hD_x+D_y+A(x))$ in $\mathscr{H}^0 = \{v \in L^2_{\mathrm{loc}}(\mathbb{R}^{2d}) \mid v(x,y+\gamma) = v(x,y)\ \forall\gamma\in\Gamma,\ \iint_{\mathbb{R}^d_x\times W_y}|v(x,y)|^2\,dx\,dy<\infty\}$ with domain $\mathscr{H}^m = \{v\in\mathscr{H}^0 \mid (hD_x+D_y+A(x))^\alpha v\in\mathscr{H}^0\ \forall\alpha\in\mathbb{N}_0^{2d},\ |\alpha|\le m\}$.

In particular, the spectrum of P acting in $L^2(\mathbb{R}^{2d})$ agrees with the spectrum of P acting in $\mathscr{H}^0$ (as subsets of $\mathbb{R}$).

4.3 The Grushin problem

Now, the operator P acting in $\mathscr{H}^0$ will be regarded a semiclassical operator (with respect to the x variables) taking values in the operators on the torus $\mathbb{R}^d/\Gamma$ (with respect to the y variables).

We fix a compact interval $I\subset\mathbb{R}$. Then there are an $N\in\mathbb{N}$, a complex neighborhood $\mathscr{V}\subseteq\mathbb{C}$ of I, and functions[2] $\psi_j(x,y,\xi)\in\mathscr{C}^\infty(\mathbb{R}^{3d})\cap\mathscr{C}^\infty(\mathbb{R}^{2d}_{x,\xi};K^m_\xi)$ for $1\le j\le N$, where $K^0 = \{u\in L^2_{\mathrm{loc}}(\mathbb{R}^d)\mid u(y+\gamma) = u(y)\ \forall\gamma\in\Gamma\}$, $K^m_\xi = \{u\in K^0 \mid (D_y+\xi)^\alpha u\in K^0\ \forall\alpha\in\mathbb{N}_0^d,\ |\alpha|\le m\}$, with the properties

- $\psi_j(x,y,\xi+\gamma^*) = e^{-i\langle\gamma^*,y\rangle}\psi_j(x,y,\xi)$ for all $\gamma^*\in\Gamma^*$,
- $\|\partial_x^\alpha\partial_\xi^\beta\psi_j(x,y,\xi)\|_{K^m_\xi}\le C_{\alpha\beta}$ for all $\alpha,\beta\in\mathbb{N}_0^d$,

such that, for $(x,\xi,\lambda)\in\mathbb{R}^{2d}\times\mathscr{V}$, the operator-valued symbol

$$\underline{p}(x,\xi,\lambda) = \begin{pmatrix} p^{\mathrm{W}}(x,y,D_y+\xi)-\lambda & R_-(x,\xi)\\ R_+(x,\xi) & 0\end{pmatrix} : \begin{matrix}K^m_\xi\\ \oplus\\ \mathbb{C}^N\end{matrix} \to \begin{matrix}K^0\\ \oplus\\ \mathbb{C}^N\end{matrix},$$

where $R_+(x,\xi)u = \{\langle u,\psi_j(x,\cdot,\xi)\rangle_{K^0}\}_{j=1}^N$, $R_-(x,\xi)\alpha = \sum_{j=1}^N\alpha_j\psi_j(x,\cdot,\xi)$, is pointwise invertible. Moreover, its pointwise inverse

$$\mathscr{E}_0(x,\xi,\lambda) = \begin{pmatrix} E_0(x,\xi,\lambda) & E_{0,+}(x,\xi,\lambda)\\ E_{0,-}(x,\xi,\lambda) & E_{0,-+}(x,\xi,\lambda)\end{pmatrix} : \begin{matrix}K^0\\ \oplus\\ \mathbb{C}^N\end{matrix} \to \begin{matrix}K^m_\xi\\ \oplus\\ \mathbb{C}^N\end{matrix}$$

is uniformly bounded in (x,ξ,λ) together with all its derivatives.

4.4 The effective Hamiltonian

Quantizing the symbol $\mathscr{E}_0(x,\xi,\lambda)$ (where ξ becomes $hD_x+A(x)$) and applying the symbol calculus yields, for $\lambda\in\mathscr{V}$ and $h>0$ sufficiently small, an inverse

$$\mathscr{E}^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) = \begin{pmatrix} E^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) & E_+^{\mathrm{W}}(x,hD_x+A(x),\lambda;h)\\ E_-^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) & E_{-+}^{\mathrm{W}}(x,hD_x+A(x),\lambda;h)\end{pmatrix} : \begin{matrix}\mathscr{H}^0\\ \oplus\\ L^2(\mathbb{R}^d;\mathbb{C}^N)\end{matrix} \to \begin{matrix}\mathscr{H}^m\\ \oplus\\ L^2(\mathbb{R}^d;\mathbb{C}^N)\end{matrix}$$

[2] The functions $\psi_j(x,y,\xi)$ are something like the Bloch functions, except that we want them independent of $\lambda\in\mathscr{V}$.

of

$$\underline{p}^{\mathrm{W}}(x,hD_x+A(x),\lambda)=\begin{pmatrix} P-\lambda & R_-^{\mathrm{W}}(x,hD_x+A(x)) \\ R_+^{\mathrm{W}}(x,hD_x+A(x)) & 0 \end{pmatrix}: \begin{matrix}\mathscr{K}^m \\ \oplus \\ L^2(\mathbb{R}^d;\mathbb{C}^N)\end{matrix} \to \begin{matrix}\mathscr{K}^0 \\ \oplus \\ L^2(\mathbb{R}^d;\mathbb{C}^N)\end{matrix}.$$

Furthermore, $\mathscr{E}(x,\xi,\lambda;h)\sim\sum_{j\geq 0}h^j\mathscr{E}_j(x,\xi,\lambda)$ possesses a full asymptotic expansion. The entry of $\mathscr{E}^{\mathrm{W}}(x,hD_x+A(x),\lambda)$ in the lower-right corner, $\boxed{E_{-+}^{\mathrm{W}}(x,hD_x+A(x),\lambda;h),}$ is called the effective Hamiltonian.

4.5 The operator P_0

It is readily seen that the operator $P_0=p^{\mathrm{W}}(hy,y,D_y+A(hy))$ acting in $L^2(\mathbb{R}^d)$ with domain $\{v\in L^2(\mathbb{R}^d)\mid (D_y+A(hy))^\alpha v\in L^2(\mathbb{R}^d)\ \forall\alpha\in\mathbb{N}_0^d,|\alpha|\leq m\}$ is unitarily equivalent to the operator P acting in $L^0=\{\sum_{\gamma\in\Gamma}v(x)\delta(x-hy+h\gamma)\mid v\in h^{d/2}L^2(\mathbb{R}^d)\}$ with domain $L^m=\{u\in L^0\mid (hD_x+D_y+A(x))^\alpha u\in L^0\ \forall\alpha\in\mathbb{N}_0^d,|\alpha|\leq m\}$ (upon making use of the altered Floquet-Bloch transformation Φ a second time).

Let $V^0=\{\sum_{\gamma\in\Gamma}v_\gamma\delta(x-h\gamma)\mid\{v_\gamma\}\in l^2(\Gamma)\}$. Checking continuity[3] of all the operators involved between the corresponding spaces, one gets from the previous results that, for $\lambda\in\mathscr{V}$ and $h>0$ sufficiently small,

$$\underline{p}^{\mathrm{W}}(x,hD_x+A(x),\lambda)=\begin{pmatrix} P-\lambda & R_-^{\mathrm{W}}(x,hD_x+A(x)) \\ R_+^{\mathrm{W}}(x,hD_x+A(x)) & 0 \end{pmatrix}: \begin{matrix}L^m \\ \oplus \\ (V^0)^N\end{matrix} \to \begin{matrix}L^0 \\ \oplus \\ (V^0)^N\end{matrix}$$

with inverse

$$\mathscr{E}^{\mathrm{W}}(x,hD_x+A(x),\lambda;h)=\begin{pmatrix} E^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) & E_+^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) \\ E_-^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) & E_{-+}^{\mathrm{W}}(x,hD_x+A(x),\lambda;h) \end{pmatrix}: \begin{matrix}L^0 \\ \oplus \\ (V^0)^N\end{matrix} \to \begin{matrix}L^m \\ \oplus \\ (V^0)^N\end{matrix}.$$

One of the main features is that, for $\lambda\in\mathscr{V}$ and $h>0$ sufficiently small,

$$\boxed{\lambda\in\sigma(P_0)\ \text{ iff }\ 0\in\sigma(E^{\mathrm{W}}(x,hD_x+A(x),\lambda;h)),}$$

where in the right-hand side $E^{\mathrm{W}}(x,hD_x+A(x),\lambda;h)$ acts as bounded operator in $(V^0)^N$.

4.6 The Schrödinger operator

Eventually, we take $p(x,y,\eta)=|\eta|^2+V(y)+\varphi(x)$ (see above). Recall that $\lambda_1(\xi)\leq\lambda_2(\xi)\leq\lambda_3(\xi)\leq\ldots$ for $\xi\in\mathbb{R}^d$ are the Floquet eigenvalues of $-\Delta+V(y)$. Then, for $\lambda\in\mathscr{V}$,

$$\det E_{0,-+}(x,\xi;\lambda)=0\ \text{ iff }\ \lambda=\lambda_l(\xi)+\varphi(x)\text{ for some }l\geq 1.$$

4.7 Eigenvalues in a spectral gap

Suppose that $I\subset\mathbb{R}$ is a compact interval such that $\sigma(-\Delta+V(y))\cap I=\emptyset$. Then the spectrum of $P_{A,\varphi}(h)$ can be shown to be discrete in I. Moreover, for any $f\in\mathscr{C}_{\mathrm{comp}}^\infty(I)$, one has

$$\boxed{\operatorname{tr}f(P_{A,\varphi})\sim(2\pi h)^{-d}\sum_{j\geq 0}a_jh^j\quad\text{as }h\to 0,}$$

[3]For instance, $b\in S(1)$ with $b(x,\xi+\gamma^*;h)=b(x,\xi;h)$ for all $\gamma^*\in\Gamma^*$ implies $b^{\mathrm{W}}(x,hD_x+A(x))\in\mathscr{L}(V^0)$ uniformly in $h\in(0,h_0]$. We shall also need the fact that $b^{\mathrm{W}}(x,hD_x+A(x))$ is of trace class and $\operatorname{tr}b^{\mathrm{W}}(x,hD_x+A(x)=(2\pi h)^{-d}\iint_{\mathbb{R}^d\times B}b(x,\xi)\,dx\,d\xi+O(h^\infty)$ as $h\to 0$ provided that b has compact support in x.

where the coefficients $a_j \in \mathbb{C}$ are (in principle) computable. Especially,

$$\boxed{a_0 = \iint_{\mathbb{R}^d_x \times B_\xi} \sum_{l\geq 1} f(\lambda_l(\xi) + \varphi(x))\, dx d\xi.}$$

(Note that the sum under the integral is finite as $\lambda_l(\xi) \to \infty$ as $l \to \infty$ uniformly in $\xi \in B$ and $\varphi(x) \to 0$ as $|x| \to \infty$. By the same reason, integration with respect to x is effectively only over a finite region.)

Proof. Choose a function[4] $\widetilde{\varphi} \in \mathscr{C}^\infty_b(\mathbb{R}^d)$ such that $\big(\sigma(-\Delta + V(y)) + \widetilde{\varphi}(\mathbb{R})\big) \cap I = \emptyset$ and $\widetilde{\varphi}(x) = \varphi(x)$ for large $|x|$. Then $E_{-+} - \widetilde{E}_{-+}$ is of trace class, where $\widetilde{E}_{-+}$ is E_{-+}, but constructed for $\widetilde{\varphi}$ in place of φ.

Using the identities

$$\begin{aligned}(P-\lambda)^{-1} &= E - E_+ E_{-+}^{-1} E_-,\\ E_{-+}^{-1} &= \widetilde{E}_{-+}^{-1} - E_{-+}^{-1}\big(E_{-+} - \widetilde{E}_{-+}\big)\widetilde{E}_{-+}^{-1},\end{aligned}$$

which hold for $\lambda \in \mathscr{V} \setminus \mathbb{R}$ (and as identities for meromorphic operator functions also for $\lambda \in \mathscr{V}$), and the fact that E and $\widetilde{E}_{-+}^{-1}$ are holomorphic in $\mathscr{V}$ (the latter for $\mathscr{V}$ a sufficiently small neighborhood of I), the Helffer-Sjöstrand formula gives

$$\begin{aligned}f(P_{A,\varphi}) &= \frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda) E_+ E_{-+}^{-1}\big(E_{-+} - \widetilde{E}_{-+}\big)\widetilde{E}_{-+}^{-1} E_-\, L(d\lambda)\\ &= -\frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda) E_+ \big(E_{-+}^{-1} - \widetilde{E}_{-+}^{-1}\big) E_-\, L(d\lambda)\end{aligned}$$

where $\widetilde{f}$ is an almost analytic extension of f (supported in $\mathscr{V}$) and $L(d\lambda)$ is the Lebesgue measure in $\mathbb{C}$.

Further using the identity $\partial_\lambda E_{-+} = E_- E_+$ (which follows as the operators R_+^{W} and R_-^{W} are independent of λ), one obtains

$$\operatorname{tr} f(P_{A,\varphi}) = -\frac{1}{\pi}\operatorname{tr}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda)\big(E_{-+}^{-1} - \widetilde{E}_{-+}^{-1}\big)E_- E_+\, L(d\lambda) = -\frac{1}{\pi}\operatorname{tr}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda) E_{-+}^{-1}\partial_\lambda E_{-+}\, L(d\lambda),$$

But $r^{\mathrm{W}}(x, hD_x + A(x); h) = -\frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda) E_{-+}^{-1}\partial_\lambda E_{-+}\, L(d\lambda)$ for some $r(x,\xi;h) \in S(1; \mathscr{L}(\mathbb{C}^N))$ which is Γ^*-periodic in ξ and has a full asymptotic expansion $r(x,\xi;h) = \sum_{j\geq 0} h^j r_j(x,\xi)$ as $h \to 0$, where

$$r_0(x,\xi) = -\frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda) E_{0,-+}^{-1}\partial_\lambda E_{0,-+}\, L(d\lambda)$$

It follows that $\operatorname{tr} f(P_{A,\varphi}) \sim (2\pi h)^{-d}\sum_{j\geq 0} a_j h^j$ as $h \to 0$ for certain coefficients $a_j \in \mathbb{C}$. Further,[5]

$$a_0 = \iint_{\mathbb{R}^d \times B}\Big(-\frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar\lambda} f(\lambda)\frac{\partial_\lambda \det E_{0,-+}(x,\xi,\lambda)}{\det E_{0,-+}(x,\xi,\lambda)}\, L(d\lambda)\Big)\, dx d\xi = \iint_{\mathbb{R}^d \times B}\sum_{l\geq 1} f(\lambda_l(\xi + \varphi(x)))\, dx d\xi,$$

which completes the proof. □

[4]In particular, $\operatorname{tr} f(P_{A,\widetilde{\varphi}}) = O(h^\infty)$ as $h \to 0$ according to the above formula.

[5]Use the following two facts:

- (Liouville's formula) For analytic matrix functions, $\operatorname{tr}\big(A(\lambda)^{-1}\partial_\lambda A(\lambda)\big) = \dfrac{\partial_\lambda \det A(\lambda)}{\det A(\lambda)}$.
- For a function g analytic in a neighborhood of $\operatorname{supp}\widetilde{f}$, $-\frac{1}{\pi}\int_{\mathbb{C}} \partial_{\bar\lambda}\widetilde{f}(\lambda)\,\dfrac{\partial_\lambda g(\lambda)}{g(\lambda)}\, L(d\lambda) = \sum_l \widetilde{f}(\lambda_l)$, where the λ_l are the zeros of g in $\operatorname{supp}\widetilde{f}$.

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