Quantum evolution in the conduction band for a model of resonant heterostructure with artificial interface conditions in 1D.

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Motivation

A modified 1D Laplacian (*Faraj, Nier, M. 2011*)

$$\begin{cases} D(\Delta_\theta) = \left\{ u \in H^2(\mathbb{R}\setminus \{a,b\}) : \left[\begin{array}{l} e^{-\frac{\theta}{2}} u(b^+) = u(b^-);\ e^{-\frac{3}{2}\theta} u'(b^+) = u'(b^-) \\ e^{-\frac{\theta}{2}} u(a^-) = u(a^+);\ e^{-\frac{3}{2}\theta} u'(a^-) = u'(a^+) \end{array} \right. \right\} \\ \\ \Delta_\theta u(x) = u''(x) \quad \text{for } x \in \mathbb{R}\setminus \{a,b\} \ . \end{cases}$$

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Exterior complex dilation: $\quad -i\Delta_\theta \longrightarrow -ie^{-2\theta\,1_{\mathbb{R}\setminus(a,b)}(x)}\Delta_{2\theta}$

Lemma *Let* $\theta = i\tau$, $\tau > 0$. *Then:* $-ie^{-2\theta\,1_{\mathbb{R}\setminus(a,b)}(x)}\Delta_{2\theta}$ *is maximal accretive*.

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Lemma *Let* $\theta = i\tau$, $\tau > 0$. *Then:* $-ie^{-2\theta\, 1_{\mathbb{R}\setminus(a,b)}(x)}\Delta_{2\theta}$ *is maximal accretive.*

$$\mathcal{H}_\theta(\mathcal{V},\theta) = -e^{-2\theta\, 1_{\mathbb{R}\setminus(a,b)}(x)}\Delta_{2\theta} + \mathcal{V}\ , \quad \text{supp}\mathcal{V} = (a,b)$$

generates a dynamical system of contractions

$\Downarrow$

Adiabatic theory of resonances for $\mathcal{H}_\theta(\mathcal{V}) = -\Delta_\theta + \mathcal{V}$

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• Question: Are the quantum systems arising from Δ_θ *'close'* to the corresponding physical models ?

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Theorem (*M. 2012***)** *Let* $|\theta| < \delta$*, with* δ *small,* $\mathcal{V} \in L^2(\mathbb{R}, \mathbb{R})$*:* supp $\mathcal{V} = [a,b]$ *and* $\langle u, \mathcal{V}u \rangle > 0\ \forall u \in L^2((a,b))$, $\|u\|_2 = 1$. *For* $\mathcal{H}_\theta(\mathcal{V}) = -\Delta_\theta + \mathcal{V}$, $i\mathcal{H}_\theta(\mathcal{V})$ *generates a strongly continuous group of bounded operators on* $L^2(\mathbb{R})$, $e^{-it\mathcal{H}_\theta(\mathcal{V})}$, *which is holomorphic w.r.t.* θ *and allows the expansion*

$$e^{-it\mathcal{H}_\theta(\mathcal{V})} = e^{-it\mathcal{H}_0(\mathcal{V})} + \mathcal{R}(t,\theta) \ , \quad \sup_{t\in\mathbb{R}} \|\mathcal{R}(t,\theta)\| = \mathcal{O}(\theta) \ .$$

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- Question: Does there exist a scattering theory for the couple $\{\mathcal{H}_\theta(\mathcal{V}), \mathcal{H}_0(\mathcal{V})\}$?

- Strategy: we look for a small-θ expansion of the waves operators

$$\mathcal{W}_\theta = 1 + \mathcal{O}(\theta)$$

Non-mixed interface conditions

Assume: $\{\theta_1, \theta_2\} \in \mathbb{C}^2$, $\mathcal{V} \in L^2(\mathbb{R}, \mathbb{R})$ with: supp $\mathcal{V} = [a, b]$

$$D\left(Q_{\theta_1,\theta_2}(\mathcal{V})\right) = H^2\left(\mathbb{R}\backslash\{a,b\}\right) + \begin{cases} e^{-\frac{\theta_1}{2}}u(b^+) = u(b^-)\,, & e^{-\frac{\theta_2}{2}}u'(b^+) = u'(b^-)\,, \\ e^{-\frac{\theta_1}{2}}u(a^-) = u(a^+)\,, & e^{-\frac{\theta_2}{2}}u'(a^-) = u(a^+)\,, \end{cases}$$

$$\left(Q_{\theta_1,\theta_2}(\mathcal{V})\,u\right)(x) = -u''(x) + \mathcal{V}(x)\,u(x)\,, \qquad x \in \mathbb{R}\backslash\{a,b\}\ .$$

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· The set $\left\{Q_{\theta_1,\theta_2}(\mathcal{V})\,,\ (\theta_1,\theta_2) \in \mathbb{C}^2\right\}$ is closed w.r.t. the adjoint operation

$$\left(Q_{\theta_1,\theta_2}(\mathcal{V})\right)^* = Q_{-\theta_2^*,-\theta_1^*}(\mathcal{V})$$

· The subset of selfadjoint operators is defined by:

$$\theta_j = \rho_j e^{i\varphi_j}, \qquad \begin{cases} \varphi_1 + \varphi_2 = \pi + 2\pi k\,, & k \in \mathbb{Z} \\ \rho_1 = \rho_2 \end{cases}$$

· $\mathcal{H}_\theta(\mathcal{V}) = Q_{\theta,3\theta}(\mathcal{V})$

We consider $\mathcal{V}^h = V + W^h, \quad h \in (0, h_0]$ s.t.:

$$\text{supp } V = [a, b] \ , \quad \text{supp } W^h = \{x \in (a, b) \ , \ d(x, U) \leq h\} \subset (a, b) \ ,$$

$$1_{[a,b]} V > c \, , \quad \sup \left\{ \|V\|_{L^\infty(\mathbb{R})} \, , \left\| W^h \right\|_{L^\infty(\mathbb{R})} \right\} \leq \frac{1}{c} \, .$$

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Let: $Q_D^h(\mathcal{V}^h) = -h^2 \Delta_{[a,b]}^D + \mathcal{V}^h$

Assumption1: There exists a real λ^0 and a cluster $\left\{\lambda_j^h\right\}_{j=1}^{\ell} \subset \sigma\left(Q_D^h(\mathcal{V}^h)\right)$ s.t.

$i)$ $c \leq \lambda^0 \leq \inf_{[a,b]} V - c \leq \|V\|_{L^\infty(\mathbb{R})} \leq \frac{1}{c}$,

$ii)$ $d\left(\lambda^0, \sigma\left(Q_D^h(\mathcal{V}^h)\right) \setminus \left\{\lambda_j^h\right\}_{j=1}^{\ell}\right) \geq c$, $\qquad iii)$ $\max_{1 \leq j \leq \ell} \left|\lambda_j^h - \lambda^0\right| \leq \frac{c}{h}$.

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Assumption 2: Let z_j^h denote the resonance associated to λ_j^h. Then: $\left|\text{Im } z_j^h\right| \gtrsim e^{-\frac{2S_0}{h}}$, where $S_0 = d_{Ag}\left(\{a,b\}, U, V, \lambda^0\right)$

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Define:

$$D\left(Q^h_{\theta_1,\theta_2}(\mathcal{V}^h)\right) = H^2\left(\mathbb{R} \backslash \{a,b\}\right) + \begin{cases} e^{-\frac{\theta_1}{2}} u(b^+) = u(b^-) \, , & e^{-\frac{\theta_2}{2}} u'(b^+) = u'(b^-) \, , \\ e^{-\frac{\theta_1}{2}} u(a^-) = u(a^+) \, , & e^{-\frac{\theta_2}{2}} u'(a^-) = u(a^+) \, , \end{cases}$$

$$\left(Q^h_{\theta_1,\theta_2}(\mathcal{V}^h) \, u\right)(x) = -h^2 u''(x) + \mathcal{V}^h(x) \, u(x) \, , \qquad x \in \mathbb{R} \backslash \{a,b\} \ .$$

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Question: Are $e^{-itQ^h_{\theta_1,\theta_2}(\mathcal{V}^h)}$ and $e^{-itQ^h_{0,0}(\mathcal{V}^h)}$ close uniformly in time for $h \in (0, h_0]$?

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Let $[\Lambda_1, \Lambda_2]$ fulfill (uniformly w.r.t. $h \in (0, h_0]$)

$$0 \leq \Lambda_1 < \Lambda_2 \leq \inf_{[a,b]} V - c \, , \quad \sigma\left(Q_D^h(\mathcal{V}^h)\right) \cap [\Lambda_1, \Lambda_2] = \left\{\lambda_j^h\right\}_{j=1}^{\ell} \, ,$$

$\Pi\left([\Lambda_1, \Lambda_2]\right) =$ spectral projector over $[\Lambda_1, \Lambda_2]$ associated with $Q_{0,0}^h(\mathcal{V}^h)$.

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Work in progress. *In the Assumptions 1 and 2,* $-iQ_{\theta_1,\theta_2}^h(\mathcal{V}^h)$ *generates a strongly continuous group:* $\Pi\left([\Lambda_1, \Lambda_2]\right) L^2(\mathbb{R}) \to L^2(\mathbb{R})$*, analytic w.r.t.* θ_j *and s.t.*

$$\sup_{t \in \mathbb{R}} \left\| \left(e^{-itQ_{\theta_1,\theta_2}^h(\mathcal{V}^h)} - e^{-itQ_{0,0}^h(\mathcal{V}^h)} \right) \Pi\left([\Lambda_1, \Lambda_2]\right) \right\|_{\mathcal{L}(L^2(\mathbb{R}))} = \sum_{j=1,2} \mathcal{O}\left(\theta_j h^{-N_0}\right) \, .$$

Resolvent analysis

Krein's like formulas (*boundary value triples technique*):

Let: $D(Q^h(\mathcal{V})) = H^2(\mathbb{R}\backslash\{a,b\})$, $Q^h(\mathcal{V})\,u = -h^2 u''(x) + \mathcal{V}u$ for $x \neq a, b$.

$$\Gamma : D(Q^h(\mathcal{V})) \to \mathbb{C}^4 \qquad \Gamma_0^h u = h^2 \begin{pmatrix} u'(b^-) - u'(b^+) \\ u(b^+) - u(b^-) \\ u'(a^-) - u'(a^+) \\ u(a^+) - u(a^-) \end{pmatrix}, \qquad \Gamma_1 u = \frac{1}{2} \begin{pmatrix} u(b^+) + u(b^-) \\ u'(b^+) + u'(b^-) \\ u(a^+) + u(a^-) \\ u'(a^+) + u'(a^-) \end{pmatrix}.$$

$$Q^h_{\theta_1,\theta_2}(\mathcal{V}) \subset Q^h(\mathcal{V}) : u \in D\left(Q^h_{\theta_1,\theta_2}(\mathcal{V})\right) \Rightarrow A^h_{\theta_1,\theta_2}\Gamma_0^h u = B_{\theta_1,\theta_2}\Gamma_1 u$$

$$A^h_{\theta_1,\theta_2} = \frac{1}{h^2}\begin{pmatrix} a(\theta_1,\theta_2) & \\ & a(-\theta_1,-\theta_2) \end{pmatrix}, \qquad B_{\theta_1,\theta_2} = \begin{pmatrix} b(\theta_1,\theta_2) & \\ & b(-\theta_1,-\theta_2) \end{pmatrix},$$

$$a(\theta_1,\theta_2) = \begin{pmatrix} 1 + e^{\frac{\theta_2}{2}} & 0 \\ 0 & 1 + e^{\frac{\theta_1}{2}} \end{pmatrix}, \qquad b(\theta_1,\theta_2) = 2\begin{pmatrix} 0 & 1 - e^{\frac{\theta_2}{2}} \\ e^{\frac{\theta_1}{2}} - 1 & 0 \end{pmatrix}.$$

In particular $Q^h_{0,0}(\mathcal{V})$ *is the 'reference' restriction:* $u \in D\left(Q^h_{0,0}(\mathcal{V})\right) \Rightarrow \Gamma_0^h u = 0$.

Krein's like formulas (*boundary value triples technique*):

Setting: $\mathcal{N}_{z,h} = Ker(Q^h(\mathcal{V}) - z)$; $\gamma_{z,h}(\mathcal{V}) = \left(\Gamma_0^h \big|_{\mathcal{N}_{z,h}} \right)^{-1}$; $q(z,\mathcal{V},h) = \Gamma_2 \circ \gamma_{z,h}(\mathcal{V})$

$$\left(Q^h_{\theta_1,\theta_2}(\mathcal{V}) - z\right)^{-1} - \left(Q^h_{0,0}(\mathcal{V}) - z\right)^{-1} =$$

$$- \sum_{i,j=1}^4 \left[\left(B_{\theta_1,\theta_2}\, q(z,\mathcal{V},h) - A^h_{\theta_1,\theta_2} \right)^{-1} B_{\theta_1,\theta_2} \right]_{ij} \left\langle \gamma_{\bar{z},h}(e_j,\mathcal{V}), \cdot \right\rangle_{L^2(\mathbb{R})} \gamma_{z,h}(e_i,\mathcal{V}) \,,$$

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A corresponding formula for eigenfunctions

$$\psi^h_{\theta_1,\theta_2}(x,k,\mathcal{V}) - \psi^h_{0,0}(x,k,\mathcal{V}) =$$
$$-\sum_{i,j=1}^4 \left[\left(\mathcal{M}^h\left(|k|,\theta_1,\theta_2,\mathcal{V}\right)\right)^{-1} B_{\theta_1,\theta_2}\right]_{ij} \left[\Gamma_1 \psi^h_{0,0}(\cdot,k,\mathcal{V})\right]_j g_{|k|,h}(e_i,\mathcal{V}),$$

$$\mathcal{M}^h\left(k,\theta_1,\theta_2,\mathcal{V}\right) = \lim_{z\to k^2 \pm i0} B_{\theta_1,\theta_2}\, q(z,\mathcal{V},h) - A^h_{\theta_1,\theta_2},$$
$$g_{k,h}(e_j,\mathcal{V}) = \lim_{z\to k^2 \pm i0} \gamma_{z,h}(e_j,\mathcal{V}).$$

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The explicit form of the coefficients depends on the choice of the basis in $\mathcal{N}_{z,h}$.

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A possible choice: $\mathcal{N}_{z,h} = l.c.\left\{\mathcal{G}^{z,h}(x,b),\ \mathcal{H}^{z,h}(x,b),\ \mathcal{G}^{z,h}(x,a),\ \mathcal{H}^{z,h}(x,a)\right\}$

Definition: $\left(Q^h_{0,0}(\mathcal{V}) - z\right) \mathcal{G}^z(\cdot,y) = \delta(\cdot - y)$, $\quad \mathcal{H}^z(\cdot,y) = \partial_2 \mathcal{G}^z(x,y)$.

Resolvent analysis

Krein's like formulas (*boundary value triples technique*):

$$\mathcal{M}^h\left(k,\theta_1,\theta_2,\mathcal{V}^h\right) = B_{\theta_1,\theta_2}\, q(k,h) - A^h_{\theta_1,\theta_2}$$

$$A^h_{\theta_1,\theta_2} = diag\left(\frac{2}{h^2} + \mathcal{O}\left(\theta_1\right) + \mathcal{O}\left(\theta_2\right)\right)\,, \qquad B_{\theta_1,\theta_2} = \mathcal{O}\left(\theta_1\right) + \mathcal{O}\left(\theta_2\right)$$

$$q(k,h) \sim \begin{pmatrix} G^{k,h}(b,b) & -\left(H^{k,h}\left(b^-,b\right)\right) & G^{k,h}(b,a) & -H^{k,h}(b,a) \\ H^{k,h}\left(b^-,b\right) & -\partial_1 H^{k,h}(b,b) & H^{k,h}(a,b) & -\partial_1 H^{k,h}(b,a) \\ G^{k,h}(a,b) & -H^{k,h}(a,b) & G^{k,h}(a,a) & -\left(H^{k,h}\left(a^+,a\right)\right) \\ H^{k,h}(b,a) & -\partial_1 H^{k,h}(a,b) & H^{k,h}\left(a^+,a\right) & -\partial_1 H^{k,h}(a,a) \end{pmatrix}$$

Krein's like formulas (*boundary value triples technique*):

$$\mathcal{M}^h\left(k,\theta_1,\theta_2,\mathcal{V}^h\right)=B_{\theta_1,\theta_2}\,q(k,h)-A^h_{\theta_1,\theta_2}$$

$$A^h_{\theta_1,\theta_2}=diag\left(\frac{2}{h^2}+\mathcal{O}(\theta_1)+\mathcal{O}(\theta_2)\right)\,,\qquad B_{\theta_1,\theta_2}=\mathcal{O}(\theta_1)+\mathcal{O}(\theta_2)$$

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Proposition *Let* $u\left(\cdot,y'\right)=\left\{G^{k,h}\left(\cdot,y'\right),\partial_1^J H^{k,h}\left(\cdot,y'\right),\psi^h_{0,0}(\cdot)\right\}$, *with* $k^2\in[\Lambda_1,\Lambda_2]$. *In the Assumption 1, we have*

$$\sup_{y,y'=a,b}\left|1_{[a,b]}u\left(y,y'\right)\right|\leq C_{a,b,c}\left(h^{-N}+h^{-(N+1)}e^{-\frac{2S_0}{h}}\left(\sup_{j\leq\ell}\left|\operatorname{Im} z^h_j\right|^{-1}\right)\right)\,.$$

Krein's like formulas (*boundary value triples technique*):

$$\mathcal{M}^h\left(k,\theta_1,\theta_2,\mathcal{V}^h\right) = B_{\theta_1,\theta_2}\, q(k,h) - A^h_{\theta_1,\theta_2}$$

$$A^h_{\theta_1,\theta_2} = diag\left(\frac{2}{h^2} + \mathcal{O}\left(\theta_1\right) + \mathcal{O}\left(\theta_2\right)\right)\,, \qquad B_{\theta_1,\theta_2} = \mathcal{O}\left(\theta_1\right) + \mathcal{O}\left(\theta_2\right)$$

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Proposition *Let* $k^2 \in [\Lambda_1,\Lambda_2]$ *and* $\left|\theta_{j=1,2}\right| \lesssim h^{N_0}$, *with* N_0 *large.*
In the Assumptions 1 and 2, we have

$$\psi^h_{\theta_1,\theta_2}(\cdot,k,\mathcal{V}^h) - \psi^h_{0,0}(\cdot,k,\mathcal{V}^h) =$$
$$\mathcal{O}\left(\theta_2\right) G^{|k|,h}(\cdot,b) + \mathcal{O}\left(\theta_1\right) H^{|k|,h}(\cdot,b) + \mathcal{O}\left(\theta_2\right) G^{|k|,h}(\cdot,a) + \mathcal{O}\left(\theta_1\right) H^{|k|,h}(\cdot,a)$$

Wave operators

A stationary definition:

$$\mathcal{W}^h_{\theta_1,\theta_2}(x,y) = \int_{\mathbb{R}} \frac{dk}{2\pi h}\, 1_{[\Lambda_1,\Lambda_2]}\left(k^2\right) \psi^h_{\theta_1,\theta_2}(x,k,\mathcal{V}^h) \left(\psi^h_{0,0}(y,k,\mathcal{V}^h)\right)^* .$$

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$$Q^h_{\theta_1,\theta_2}(\mathcal{V}^h)\mathcal{W}^h_{\theta_1,\theta_2} = Q^h_{0,0}(\mathcal{V}^h)\mathcal{W}^h_{\theta_1,\theta_2}$$

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Generalized Fourier transform associated to $Q^h_{0,0}(\mathcal{V}^h)$

$$\left(\mathcal{F}^h_{\mathcal{V}^h}\varphi\right)(k) = \int_{\mathbb{R}} \frac{dx}{(2\pi h)^{1/2}} \left(\psi^h_{0,0}\left(x,k,\mathcal{V}^h\right)\right)^* \varphi(x)\,, \qquad \varphi \in L^2(\mathbb{R})\,.$$

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$$\left(\mathcal{W}^h_{\theta_1,\theta_2} - \Pi\left([\Lambda_1,\Lambda_2]\right)\right)\varphi = \sum_{\alpha=a,b}\left[\phi^h_\alpha + \psi^h_\alpha\right],$$

$$\phi^h_\alpha(x) = \int_{\mathbb{R}} \frac{dk}{(2\pi h)^{1/2}} \mathcal{O}(\theta_2)\, 1_{\Omega_c(\mathcal{V})}\left(k^2\right) G^{|k|,h}\left(x,\alpha,\mathcal{V}^h\right)\left(\mathcal{F}^h_{\mathcal{V}^h}\varphi\right)(k), \quad \alpha \in \{a,b\},$$

$$\psi^h_\alpha(x) = \int_{\mathbb{R}} \frac{dk}{(2\pi h)^{1/2}} \mathcal{O}(\theta_1)\, 1_{\Omega_c(\mathcal{V})}\left(k^2\right) H^{|k|,h}(x,\alpha,\mathcal{V}^h)\left(\mathcal{F}^h_{\mathcal{V}^h}\varphi\right)(k), \quad \alpha \in \{a,b\}.$$

Wave operators

A stationary definition:

$$\mathcal{W}^h_{\theta_1,\theta_2}(x,y) = \int_{\mathbb{R}} \frac{dk}{2\pi h} 1_{[\Lambda_1,\Lambda_2]}\left(k^2\right) \psi^h_{\theta_1,\theta_2}(x,k,\mathcal{V}^h) \left(\psi^h_{0,0}(y,k,\mathcal{V}^h)\right)^* .$$

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Generalized Fourier transform associated to $Q^h_{0,0}(\mathcal{V}^h)$

$$\left(\mathcal{F}^h_{\mathcal{V}^h}\varphi\right)(k) = \int_{\mathbb{R}} \frac{dx}{(2\pi h)^{1/2}} \left(\psi^h_{0,0}\left(x,k,\mathcal{V}^h\right)\right)^* \varphi(x) , \qquad \varphi \in L^2(\mathbb{R}) .$$

$$\left(\mathcal{W}^h_{\theta_1,\theta_2} - \Pi\left([\Lambda_1,\Lambda_2]\right)\right)\varphi = \sum_{\alpha=a,b}\left[\phi^h_\alpha + \psi^h_\alpha\right] ,$$

$$\left\|\sum_{\alpha=a,b}\left[\phi^h_\alpha(x) + \psi^h_\alpha(x)\right]\right\|_{L^2(\mathbb{R})} \lesssim \left(\frac{|\theta_1|}{h^2} + \frac{|\theta_2|}{h^2}\right) \|\varphi\|_{L^2(\mathbb{R})} ,$$

Wave operators

A stationary definition:

$$\mathcal{W}^h_{\theta_1,\theta_2}(x,y) = \int_{\mathbb{R}} \frac{dk}{2\pi h} 1_{[\Lambda_1,\Lambda_2]}\left(k^2\right) \psi^h_{\theta_1,\theta_2}(x,k,\mathcal{V}^h) \left(\psi^h_{0,0}(y,k,\mathcal{V}^h)\right)^* .$$

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Generalized Fourier transform associated to $Q^h_{0,0}(\mathcal{V}^h)$

$$\left(\mathcal{F}^h_{\mathcal{V}^h}\varphi\right)(k) = \int_{\mathbb{R}} \frac{dx}{(2\pi h)^{1/2}} \left(\psi^h_{0,0}\left(x,k,\mathcal{V}^h\right)\right)^* \varphi(x), \qquad \varphi \in L^2(\mathbb{R}).$$

$$\left(\mathcal{W}^h_{\theta_1,\theta_2} - \Pi\left([\Lambda_1,\Lambda_2]\right)\right)\varphi = \sum_{\alpha=a,b}\left[\phi^h_\alpha + \psi^h_\alpha\right],$$

$$\left\|\sum_{\alpha=a,b}\left[\phi^h_\alpha(x) + \psi^h_\alpha(x)\right]\right\|_{L^2(\mathbb{R})} \lesssim \left(\frac{|\theta_1|}{h^2} + \frac{|\theta_2|}{h^2}\right)\|\varphi\|_{L^2(\mathbb{R})},$$

$$\Longrightarrow \left\|\mathcal{W}^h_{\theta_1,\theta_2} - \Pi\left([\Lambda_1,\Lambda_2]\right)\right\|_{\mathcal{L}(L^2(\mathbb{R}),L^2(\mathbb{R}))} = \mathcal{O}\left(\frac{\theta_1}{h^2}\right) + \mathcal{O}\left(\frac{\theta_2}{h^2}\right).$$