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Microlocal Scattering Theory for Discrete Schrödinger Operators and Related Topics

By

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Abstract

We discuss several recent results on spectral and scattering theory for a model which generalizes discrete and continuous Schrödinger operators with short-range and long-range perturbations. Many of these were inspired by old papers by Isozaki and Kitada of 1980's.

§ 1. Model

We first consider the discrete Schrödinger operator on $\mathbb{Z}^d$, $d \geq 1$:

$$Hu[n] = -\frac{1}{2} \sum_{|m-n|=1} u[m] + V[n]u[n], \quad u[\cdot] \in \ell^2(\mathbb{Z}^d),$$

where $V[\cdot]$ is a real-valued function on $\mathbb{Z}^d$. If $V[\cdot]$ is bounded, which we assume, then H is a bounded self-adjoint operator on $\ell^2(\mathbb{Z}^d)$. This is also called **Anderson tight-binding model**, and widely used in solid state physics to describe electrons and phonons in crystals. We denote the discrete Fourier transform (or the inverse Fourier series expansion) by

$$Fu(\xi) = (2\pi)^{-d/2} \sum_{n\in\mathbb{Z}^d} u[n]e^{-in\cdot\xi}, \quad \xi \in \mathbb{T}^d = (\mathbb{R}/2\pi\mathbb{Z})^d,$$

for $u \in \ell^1(\mathbb{Z}^d)$. Note F is a unitary operator from $\ell^2(\mathbb{Z}^d)$ to $L^2(\mathbb{T}^d)$. Formally, we can write

$$\hat{H} = FHF^* = -\sum_{j=1}^{d} \cos(\xi_j) + V[-D_\xi], \quad \text{on } L^2(\mathbb{T}^d),$$

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where $V[-D_\xi]$ is considered as a Fourier multiplier on $\mathbb{T}^d$, defined as $V[-D_\xi] = FV[\cdot]F^*$.
We wish to consider $V[-D_\xi]$ as a **pseudodifferential operator** on $\mathbb{T}$.
We denote the difference operator by $\tilde{\partial}$:

$$\tilde{\partial}_j\varphi[n] = \varphi[n+e_j] - \varphi[n], \quad n \in \mathbb{Z}^d, j = 1, \dots, d,$$

where $\{e_j\}$ is the standard basis on $\mathbb{R}^d$.
Let $\mu \in \mathbb{R}$. If $V[\cdot]$ satisfies

$$\left|\tilde{\partial}^\alpha V[n]\right| \leq C_\alpha \langle n\rangle^{\mu-|\alpha|}, \quad n \in \mathbb{Z}^d,$$

for any multi-index $\alpha \in \mathbb{Z}_+^d$ with some $C_\alpha > 0$, then we can show that there is $\tilde{V}(x) \in C^\infty(\mathbb{R}^d)$ such that

$$\left|\partial_x^\alpha \tilde{V}(x)\right| \leq C'_\alpha \langle x\rangle^{\mu-|\alpha|}, \quad x \in \mathbb{R}^d$$

for any $\alpha \in \mathbb{Z}_+^d$ with some $C'_\alpha > 0$, and

$$\tilde{V}(n) = V[n] \quad \text{for } n \in \mathbb{Z}^d.$$

$\tilde{V}(x)$ may be quantized using pseudodifferential operator calculus: For $\varphi \in C_0^\infty(\mathbb{T}^d)$ with the support in a local coordinate $K_\varepsilon = (-\pi+\varepsilon, \pi-\varepsilon)^d \Subset (-\pi,\pi)^d \subset \mathbb{T}^d$. Let $\chi \in C_0^\infty((-\pi,\pi)^d)$ such that $\chi(\xi) = 1$ on K_ε. Then we set

$$\tilde{V}(-D_\xi)\varphi(\xi) = (2\pi)^{-d} \iint e^{-i(\xi-\eta)\cdot x}\chi(\eta)\tilde{V}(x)\varphi(\eta)d\eta dx, \quad \xi \in (-\pi,\pi)^d \subset \mathbb{T}^d.$$

We can define $\tilde{V}(-D_\xi)$ for functions supported in other local coordinates similarly, and we can define $\tilde{V}(-D_\xi)$ globally using a partition of unity.
The extension $\tilde{V}(x)$ is not uniquely determined by $V[n]$, and hence $\tilde{V}(-D_\xi)$ is not unique either. We also note that it is not necessarily the same operator as $V[-D_\xi]$. But we can show

$$V[-D_\xi] - \tilde{V}(-D_\xi) = R, \text{ a smoothing operator on } \mathbb{T}^d,$$

under the above conditions on V and $\tilde{V}$. Thus we learn $\hat{H}$ is equivalent to the operator:

$$p(-D_\xi,\xi)\varphi(\xi) = (2\pi)^{-d} \iint e^{-i(\xi-\eta)\cdot x} p(x,\eta)\varphi(\eta)d\eta dx$$

for $\varphi \in C_0^\infty(\mathbb{T}^d)$ supported in such a local coordinate modulo smoothing operators, where

$$p(x,\xi) = -\sum_{j=1}^d \cos(\xi_j) + \tilde{V}(x).$$

This observation leads us to the following general model:

General Model: Let M be a d-dimensional complete Riemannian manifold with a positive density m, and let $\mathcal{H} = L^2(M, m)$. Let

$$H = H_0 + V$$

be a self-adjoint operator on $\mathcal{H}$.

Assumption A. We suppose $H_0 = p_0(\xi)\cdot$ is a multiplication operator by a real-valued smooth function $p_0(\xi)$, and V is a pseudodifferential operator with a symbol $V(x,\xi) \in S^{-\mu}_{1,0}$, i.e., $V(x,\xi)$ satisfies for any $\alpha, \beta \in \mathbb{Z}^d_+$,

$$\left|\partial_x^\alpha \partial_\xi^\beta V(x,\xi)\right| \leq C_{\alpha\beta} \langle x \rangle^{-\mu-|\alpha|}, \quad \xi \in M, x \in T^*_\xi M,$$

with some $C_{\alpha\beta} > 0$, where $\mu \in \mathbb{R}$. The quantization of $V(x,\xi)$ is given by

$$Vu(\xi) = V(-D_\xi, \xi)u(\xi) = (2\pi)^{-d} \iint e^{-i(\xi-\eta)\cdot x} V(x,\eta)u(\eta) d\eta dx$$

in a local coordinate of M as above.

We call V is **short-range type** if $\mu > 1$, and **long-range type** if $\mu \in (0,1]$.

Example I. (1) If we set $M = \mathbb{T}^d$, $p_0(\xi) = \sum \cos(\xi_j)$ and $V = V(x)$ be a smooth extension of $V[n]$, then we have the above discrete Schrödinger operator (under additional assumptions), and this model contains many models in solid state physics, e.g., the triangle lattice, etc., using different $p_0(\xi)$. We note, however, the hexagonal lattice, or the graphene, needs a system of operators, and it will be addressed later.
(2) If we set $M = \mathbb{R}^d$, and $V(x) \in C^\infty(\mathbb{R}^d)$, then we have the usual Schrödinger operators on Euclidean spaces. This model also includes higher order constant coefficient PDOs with long-range perturbations, or fractional power operators (with small generalizations).

§ 2. Spectral properties

We consider an energy interval I satisfying the following condition:

Assumption B. We suppose V is a long-range type perturbation (i.e., $\mu > 0$ in Assumption A), and consider the spectral properties of H in $I \Subset \mathbb{R}$ such that

$$v(\xi) \equiv dp_0(\xi) \neq 0, \quad \text{if } p_0(\xi) \in I.$$

Example II.

1. For the continuous Schrödinger operator case, 0 is the unique critical value of $p_0 = \frac{1}{2}|\xi|^2$.

2. For the square lattice, $\sigma(H_0) = [-d, d]$, and $v(\xi) = 0$ only if $p_0(\xi) \in \{-d, -d+2, \dots, d\}$. $-d$ and d are unique minimal/maximal value of p_0, and other critical values are saddle points.

3. For the 2D triangular lattice, $\sigma(H_0) = [0, 9/2]$ (with a suitable definition), and $v(\xi) = 0$ only if $p_0(\xi) \in \{0, 4, 9/2\}$. (4 is a saddle point of p_0, and the maximal value 9/2 has two maximal points. 0 is the unique minimum.)

Theorem 2.1. *The point spectrum in I: $\sigma_p(H) \cap I$ is a finite set with finite multiplicity, and the spectrum of H in I is absolutely continuous away from the point spectrum. Moreover,*

$$(H - \lambda \mp i0)^{-1} = \lim_{\varepsilon \to +0} (H - \lambda \mp i\varepsilon)^{-1}, \quad \lambda \in I \setminus \sigma_p(H),$$

exist as operators from $H^s(M)$ to $H^{-s}(M)$ with $s > 1/2$, where $H^p(M)$ denotes the Sobolev space of order $p \in \mathbb{R}$ on M.

Such results for discrete Schrödinger operators goes back at least to Boutet de Monvel-Sahbani [3] and Isozaki-Korotyaev [6].
The proof uses the standard Mourre theory, and we take the conjugate operator (formally) as

$$A = \frac{1}{2}(iA_0 - iA_0^*), \ A_0 = \chi(p_0(\xi)) \sum_{j,k} g^{jk}(\xi) \frac{\partial p_0}{\partial \xi_k}(\xi) \frac{\partial}{\partial \xi_j},$$

where $\chi \in C_0^\infty(\mathbb{R})$ such that $\mathrm{Supp}[\chi] \subset I$, and it is 1 on $I' \Subset I$, $\lambda \in I'$, $g^{ij}(\xi)$ is the (co)metric on $T_\xi^* M$.

§ 3. Short-range scattering theory

If V is short-range type, i.e., $\mu > 1$, then we can construct the time-dependent scattering theory following the very standard procedure:

Theorem 3.1. *The wave operators:*

$$W_\pm^I = \operatorname*{s-lim}_{t \to \pm\infty} e^{itH} e^{-itH_0} E_I(H_0)$$

exists and are compete: $\mathrm{Ran}[W_\pm^I] = E_I(H)\mathcal{H}_{ac}(H)$.

These imply the so-called **asymptotically free propagation** for the initial states in the continuous spectrum: If $u_0 \in E_I(H)\mathcal{H}_c(H)$, then there are $u_\pm \in E_I(H_0)\mathcal{H}$ such that

$$\left\| e^{-itH} u_0 - e^{-itH_0} u_\pm \right\| \to 0 \quad \text{as } t \to \pm\infty.$$

The proof of the existence uses the Cook-Kuroda method. We note we can use the non-stationary phase by the assumption: $v(\xi) = dp_0(\xi) \neq 0$ if $p_0(\xi) \in I$. The completeness follows from the limiting absorption priniciple, i.e., Theorem 2.1.
For more recent, general results on scattering theory, see, e.g., Ando-Isozaki-Morioka [1], Bellissard-Shulz-Baldes [2], etc.

§ 4. Long-range scattering theory

If V is long-range type, i.e., Assumption A with $\mu \in (0, 1]$, then the usual wave operators do not exist in general, and we need to introduce **modified** wave operators, which is constructed in terms of classical mechanics generated by the Hamiltonian $p(x, \xi) = p_0(\xi) + V(x, \xi)$ on T^*M. We refer, fore example, Yafaev [13] Chapter 10 for the case of Schrödinger operators.
For the moment, we have results for the square lattice case, i.e., $M = \mathbb{T}^d$, $V = V(x)$ (potential perturbation), and we need additional assumptions on $p_0(\xi)$. We are currently working on the general case.

Theorem 4.1 ([9]). *There are solutions to the Hamilton-Jacobi equation:*

$$\partial_t \Phi_\pm(t, \xi) = p(\partial_\xi \Phi_\pm(t, \xi), \xi) \quad \text{for } \xi\text{: } p_0(\xi) \in I \ \pm t \geq 0,$$

such that the modified wave operators

$$W_\pm^I = \operatorname*{s-lim}_{t \to \pm\infty} e^{itH} e^{-i\Phi_\pm(t,\xi)} E_I(H_0)$$

exist.

For the proof of Theorem 3, we analyze long-time behaviors of solutions to the Hamilton equation:

$$\frac{\partial}{\partial t} x(t) = \frac{\partial p}{\partial \xi}(x(t), \xi(t)), \quad \frac{\partial}{\partial t} \xi(t) = -\frac{\partial p}{\partial x}(x(t), \xi(t))$$

for $(x(t), \xi(t)) \in T^*M$, i.e., $\xi(t) \in M$ and $x(t) \in T^*_{\xi(t)}M$, then construct global solutions to the Hamilton-Jacobi equation.

For the completeness, Tadano recently proved it for the time-independent modifiers:

Theorem 4.2 (Tadano [12]). *One can construct Fourier integral operators $J_\pm^I$ such that $\|J_\pm^I e^{-itH_0} E_I(H_0)u\| \to \|E_I(H_0)u\|$ as $t \to \pm\infty$, and*

$$\tilde{W}_\pm^I = \operatorname*{s-lim}_{t \to \pm\infty} e^{itH} J_\pm^I e^{-itH_0} E_I(H_0)$$

exist and are complete: $\mathrm{Ran}[\tilde{W}_\pm^I] = E_I(H)\mathcal{H}_{ac}(H)$.

We note that the time-independent modifiers $J^I_\pm$ are constructed using suitable solutions to the eikonal equation: $p(\partial_\xi\Psi_\pm(x,\xi),\xi) = E \in I$. The asymptotic completeness implies the property: If $u_0 \in E_I(H)\mathcal{H}_c(H)$, then there are $u_\pm \in E_I(H_0)\mathcal{H}$ such that $\|e^{-itH}u_0 - J^I_\pm e^{-itH_0}u_\pm\| \to 0$ as $t \to \pm\infty$.

§ 5. Microlocal resolvent estimates

Resolvent estimates with direction-dependent cut-off's, or microlocal localizations, goes back to at least E. Mourre, and Isozaki and Kitada [IK1] proved a so-called microlocal resolvent estimates. Here we discuss a generalized and somewhat more precise version of them.

We suppose V is long-range type. As we discussed in Section 2, for $\lambda \in I \setminus \sigma_p(H)$, the boundary value of the resolvent $(H-\lambda \mp i0)^{-1}$ exist as operators from $H^s(M)$ to $H^{-s}(M)$, $s > 1/2$. Let $K_\pm(\lambda) \in \mathcal{S}'(M\times M)$ be their distribution kernels.

We write $\mathrm{WF}(T)$ be the wave front set of a distribution T. We recall a (semiclassical) definition of the wave front set. Let $T \in \mathcal{S}'(\mathbb{R}^N)$, and let $(x,\xi) \in T^*\mathbb{R}^N = \mathbb{R}^{2N}$, $\xi \neq 0$. Then $(x,\xi) \notin \mathrm{WF}(T)$ if there is $a \in C_0^\infty(\mathbb{R}^{2N})$ such that $a(x,\xi) \neq 0$ and

$$\|a(x,hD_x)T\|_{L^2} = O(h^\infty), \quad \text{as } h \to 0,$$

We now define $\Sigma_0, \Sigma_\pm(\lambda), \Sigma'_\pm(\lambda) \subset T^*(M\times M)$ as follows:

$$\begin{aligned}\Sigma_0 &= \big\{(x,\xi,-x,\xi) \bigm| (x,\xi) \in T^*M\big\},\\ \Sigma_\pm(\lambda) &= \big\{(x+tv(\xi),\xi,-x,\xi) \bigm| (x,\xi) \in T^*M, p_0(\xi)=\lambda, \pm t \geq 0\big\},\\ \Sigma'_\pm(\lambda) &= \big\{(tv(\xi),\xi) \bigm| p_0(\xi)=\lambda, \pm t\geq 0\big\} \times \big\{(-tv(\xi),\xi) \bigm| p_0(\xi)=\lambda, \mp t \geq 0\big\}\end{aligned}$$

Theorem 5.1 ([11]). *For $\lambda \in I \setminus \sigma_p(H)$, $\mathrm{WF}(K^\pm(\lambda)) \subset \Sigma_0 \cup \Sigma_\pm(\lambda) \cup \Sigma'_\pm(\lambda)$.*

Σ_0 corresponds to singularities of pseudodifferential operators, i.e., diagonal singularities.

$\Sigma_\pm(\lambda)$ describe the singularities generated by the free motion. In fact, we can easily show

$$\mathrm{WF}(\mathrm{Ker}[(H_0-\lambda\mp i0)^{-1}]) = \Sigma_0 \cup \Sigma_\pm(\lambda).$$

$\Sigma_\pm(\lambda)$ are the only singularities generated by the scattering phenomena. For the "+" case, $\Sigma_+(\lambda)$ corresponds to classical trajectories $(x(t),\xi(t))$ with the energy λ such that

$$x(t) \sim tv(\xi_+), \quad \xi(t) \to \xi_+ \quad \text{as } t \to +\infty.$$

Microlocal resolvent estimates of Isozaki-Kitada type follows easily from this result: Suppose $K \Subset I \setminus \sigma_p(H)$, and suppose $a_\pm(x,\xi) \in S^0_{1,0}$ such that

$$\mathrm{Supp}[a_\pm] \subset \left\{(x,\xi) \in T^*M \;\middle|\; \pm\frac{x\cdot v(\xi)}{|x|\,|v(\xi)|} \geq \pm\gamma_\pm, p_0(\xi) \in K\right\},$$

where $-1 < \gamma_- < \gamma_+ < 1$. We set

$$A_\pm = a_\pm(-D_\xi, \xi).$$

Theorem 5.2 (Two-sided microlocal resolvent estimates). *$A_\mp(H-\lambda\mp i0)^{-1}A_\pm^*$ are smoothing operators, i.e., they are bounded from $H^{-N}(M)$ to $H^N(M)$ with any N.*

This result may be considered as a long-time propagation estimate, and actually it is proved using an argument similar to the proof of the microlocal smoothing properties. This estimate is useful in the analysis of the scattering matrix.

We note that we may ask the strength of singularities of the resolvents. Namely, what are the Sobolev singularities of $\mathrm{WF}(K^\pm(\lambda))$ on $\Sigma_\pm(\lambda)$ and $\Sigma'_\pm(\lambda)$, respectively? They correspond to the strength of scattered waves, and it seems an interesting problem.

§ 6. Properties of scattering matrices

Here we suppose V is short-range type, and consider the scattering matrix. As we noted in Section 3, wave operators $W_\pm^I$ exist and complete, and hence the **scattering operator**:

$$S^I = (W_+^I)^* W_-^I\text{: a unitary on } E_I(H_0)\mathcal{H} = L^2(\{\xi\in M \,|\, p_0(\xi)\in I\}).$$

By the intertwining property: $HW_\pm^I = W_\pm^I H_0$, we also learn S^I commutes with H_0, i.e, $H_0S^I = S^IH_0$, and hence S^I is decomposed to a family of operators

$$S(\lambda)\in\mathcal{L}(L^2(\Lambda(\lambda))), \quad \lambda\in I, \quad \Lambda(\lambda) = \big\{\xi\in M \;\big|\; p_0(\xi)=\lambda\big\}.$$

$S(\lambda)$ is called the **scattering matrix**. The scattering matrix $S(\lambda)$ is a unitary operator on the energy surface $\Lambda(\lambda)$, $\lambda\in I$.

Under our assumption, we can show that $S(\lambda)$ is a pseudodifferential operator on $\Lambda(\lambda)$, and we can compute the leading term.

Theorem 6.1 ([10]). *For each $\lambda\in I\setminus\sigma_p(H)$, $S(\lambda)$ is a pseudodifferential operator with its symbol in $S^0_{1,0}(\Lambda(\lambda))$. Moreover,*

$$\mathrm{Sym}(S(\lambda)) = e^{-i\psi(x,\xi)} + R(x,\xi),$$

where $\mathrm{Sym}(A)$ *denotes the symbol of A,*

$$\psi(x,\xi) = \int_{-\infty}^{\infty} V(x+tv(\xi),\xi)dt \quad \text{for } \xi\in\Lambda(\lambda), x\in T_\xi^*\Lambda(\lambda), \tag{6.1}$$

and $R\in S^{-\mu}_{1,0}(\Lambda(\lambda))$.

We note $S(\lambda)$ is a pseudodifferential operator on a manifold $\Lambda(\lambda)$ with the symbol in $S^0_{1,0}$, and hence the symbol is well-defined modulo $S^{-1}_{1,0}$, in general. But in our case, we can easily show

$$\psi(x,\xi) \in S^{-\mu+1}_{1,0}(\Lambda(\lambda)), \quad \text{and hence} \quad e^{-i\psi(x,\xi)} - 1 \in S^{-\mu+1}_{1,0}(\Lambda(\lambda)).$$

Thus $S(\lambda) - 1$ has a symbol in $S^{-\mu+1}_{1,0}$, and the symbol is well-defined modulo $S^{-\mu}_{1,0}$. The main contribution $\psi(x,\xi)$ is a generalization of the Borm approximation in the classical quantum mechanics.

The proof of Theorem 7 employs an argument analogous to Isozaki-Kitada [IK2]. Namely,

- A construction of Isozaki-Kitada modifiers (which is, in fact, a parametrix of wave operators).
- Microlocal resolvent estimates.
- Representation formula of scattering operators (due to Lippmann-Schwinger, ..., Isozaki-Kitada, Yafaev, etc.).

Related results: It is known (under more general conditions) that $S(\lambda)$ is an FIO due to Melrose-Zworski [8], Ito-N [7], etc. Yafaev [14] used a similar technique to study high energy asymptotics of scattering matrix.

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