PASTURFEST HAGEN
The density of surface states as the total time delay

Hermann Schulz-Baldes

Erlangen

Basic model for quantum surface states

Hilbert space $\ell^2(\mathbb{Z}^d) = \ell^2(\mathbb{Z}^{d_1}) \otimes \ell^2(\mathbb{Z}^{d_2})$ with $d = d_1 + d_2$

Hamiltonian $H = H_0 + \lambda V$ with coupling constant $\lambda > 0$

H_0 translation invariant with $\sigma(H_0) = [E_-, E_+]$
band function analytic with no further local extrema

V supported by $\mathbb{Z}^{d_1} \times \{0\}$, short range and $\mathbb{Z}^{d_1}$-covariant
(or *metrically transitive* or *homogeneous*, *e.g.* periodic, random)

Fact: surface states outside of $\sigma(H_0)$ and on top of it

sound or elastic surface waves: Rayleigh ($\sim$1900)
electromagnetic surface waves: Sommerfeld school ($\sim$1905)
solid state systems: Tamm (1932) and Shockley (1939)
quantum Hall systems (1980's), topological insulators (2000's)
Davies-Simon (1978), Englisch, Kirsch, Schröder, Simon (1990)
Pastur (1995), Jaksic-Molchanov-Pastur (1998)

Main Result

Theorem (Schulz-Baldes 2013) $d \geq 3$ and $\lambda > 0$ small. Then

$$\begin{aligned} \mathcal{T}_1 \mathrm{Tr}_2(P_{\mathrm{sur}}) &= -\frac{1}{2\pi\imath} \int_{E_-}^{E_+} dE \ \mathcal{T}_1(S_E^* \partial_E S_E) \\ \text{surface state density} &= -\,\text{total time delay density} \end{aligned}$$

Here:

P_{sur} projection in $\ell^2(\mathbb{Z}^d)$ onto all surface states, covariant

$\mathcal{T}_1$ trace per unit volume on $\mathbb{Z}^{d_1}$, Tr_2 trace on $\mathbb{Z}^{d_2}$

$$\mathcal{T}_1 \mathrm{Tr}_2(P_{\mathrm{sur}}) = \mathbf{E} \sum_{n_2 \in \mathbb{Z}^{d_2}} \langle 0, n_2 | P_{\mathrm{sur}} | 0, n_2 \rangle$$

S_E on shell scattering matrix

S_E covariant unitary operator on $\ell^2(\mathbb{Z}^{d_1})$, differentiable in E

Analogy with Levinson's Theorem

V compactly supported, no smallness assumption on λ

$$\#\text{ eigenvalues of } H \;=\; -\frac{1}{2\pi\imath}\int_{E_-}^{E_+} dE\ \mathrm{Tr}(S_E^*\partial_E S_E)$$

Corrections for half-bound states (non-generic), not embedded eig.

Well-known: for $H_0 = -\Delta$ on $L^2(\mathbb{R}^3)$ and V spherically symmetric

Then $L^2(\mathbb{R}^3) \cong L^2(\mathbb{R}_>, dE) \otimes L^2(\mathbb{S}^2)$ and

S_E unitary on-shell S-matrix on $L^2(\mathbb{S}^2)$ given by $\mathbf{1} +$ compact

No symmetry assumption: Newton (1990)

Index Theorem approach: Kellendonk-Richard+coll. (since 2006)

For tight-binding operators $d \geq 3$: Bellissard-Schulz-Baldes (2012)
also Kohmoto, Koma, Nakamura (2013)

Known results on spectral and scattering theory

halfspace, V random i.i.d. surface potential with a.c. distribution

Jaksic-Molchanov (1999), also Grinshpun (1995):
$d = 2$ or λ large or small $\Longrightarrow$ Anderson localization on $\mathbb{R} \setminus \sigma(H_0)$

Jaksic-Last (2000): almost surely spectrum of H a.c. on $\sigma(H_0)$

Here: small λ $\Longrightarrow$ only a.c. spectrum

Existence wave op.: Chahrour-Shabani (2000) Jaksic-Last (2000)

$$W_\pm \;=\; \mathrm{s}\text{-}\lim_{t\to\pm\infty} \; e^{\imath Ht}\, e^{-\imath H_0 t}$$

Jaksic-Last (2001) With Π projection on surface $\ell^2(\mathbb{Z}^{d_1})$

$$\mathrm{Ran}(W_\pm) \;=\; \left\{ \psi \in \ell^2(\mathbb{Z}^d) \;\middle|\; \int_0^\infty dt\; \|\Pi\, e^{-\imath tH}\,\psi\|^2 \;<\; \infty \right\}^{\mathrm{cl}}$$

Plan for more technical part of talk

In the theorem above: $P_{\mathrm{sur}} = \mathbf{1} - W_\pm W_\pm^*$

Link to spectral shift? Kostrykin-Schrader (2000), Chahrour (2000)

Belief: main formula holds without hypothesis λ small and $d \geq 3$

Main points to be discussed in this talk:

1) construction of a unbounded conjugate operator A with

$$\imath[A, H_0] \;=\; F(H_0) \geq 0$$

2) rescaled energy and interaction representation (REI)

3) explicit formula for the wave operators

4) exact sequence

Conjugate operator = generator of energy flow

Fourier transform $\mathcal{F} H_0 \mathcal{F}^* = \text{mult}(\mathcal{E})$ with $\mathcal{E} : \mathbb{T}^d \to \mathbb{R}$ real analytic

Slowed down Morse vector field on $\mathbb{T}^d$

$$\widehat{X} \;=\; F \circ \mathcal{E}\, \frac{\nabla \mathcal{E}}{\|\nabla \mathcal{E}\|^2} \qquad F(E) \;=\; 2\, \frac{(E - E_-)(E_+ - E)}{E_+ - E_-}$$

Classical energy flow θ_b (infinitely fast near critical points)

$$(e^{\imath b A}\, \phi)(k) \;=\; \det(\theta_b'(k))^{\frac{1}{2}}\, \phi(\theta_b(k)) \qquad \phi \in C_0^\infty(\mathbb{T}^d \setminus \mathcal{S})$$

Theorem A selfadjoint with $\imath[A, H_0] = F(H_0) \geq 0$ and

$$A \;=\; \frac{1}{2} \sum_{j=1}^{d} (X_j\, Q_j + Q_j\, X_j)$$

Rescaled energy $B = f(H_0)$ with $f = \int_{E_r} \frac{de}{F(e)}$ satisfies $\imath[A, B] = \mathbf{1}$

REF representation

$\Sigma = \Sigma_{E_r}$ reference Fermi surface at E_r with Riemannian volume ν

With Coarea formula and identification of level surfaces:

$$\int_{\mathbb{T}^d} dk\, \phi(k) \;=\; \int_{\mathbb{R}} db \int_{\Sigma} \nu(d\sigma)\; \left|\det(\theta_b'|_{T_\sigma \Sigma})\right| \; \left|\widehat{X}(\theta_b(\sigma))\right| \; \phi(\theta_b(\sigma))$$

Hence unitary $\mathcal{U} : L^2(\mathbb{T}^d) \to L^2(\mathbb{R}_b) \otimes L^2(\Sigma, \nu)$ defined by

$$(\mathcal{U}\phi)_b(\sigma) \;=\; \left|\det(\theta_b'|_{T_\sigma \Sigma})\right|^{\frac{1}{2}} \; \left|\widehat{X}(\theta_b(\sigma))\right|^{\frac{1}{2}} \; \phi(\theta_b(\sigma))$$

Rescaled energy + Fermi surface (REF) representation, *e.g.* of $W_\pm$

$$\mathcal{U}\mathcal{F}W_\pm\mathcal{F}^*\mathcal{U}^* \;:\; L^2(\mathbb{R}_b) \otimes L^2(\Sigma, \nu) \to L^2(\mathbb{R}_b) \otimes L^2(\Sigma, \nu)$$

Then $\mathcal{U}\mathcal{F}A\mathcal{F}^*\mathcal{U}^* = \imath\partial_b$, REF in Bellissard-Schulz-Baldes (2012)

local version away from critical points in Birman-Yafaev (1992)

REI representation

Define $\psi_{n_1,b}(\sigma) = (\mathcal{U}\mathcal{F}|n_1,0\rangle)_b(\sigma)$ vectors in $L^2(\Sigma,\nu)$ and

$$\mathcal{D}_b = \mathrm{span}\left\{\psi_{n_1,b}\,\middle|\, n_1 \in \mathbb{Z}^{d_1}\right\}^{\mathrm{cl}} \subset L^2(\Sigma,\nu)$$

$$\mathcal{F}_b = \mathrm{Ran}\Big(\sum_{n_1\in\mathbb{Z}^{d_1}} |n_1\rangle\langle\psi_{n_1,b}|\Big) \subset \ell^2(\mathbb{Z}^{d_1})$$

Key fact: $\mathcal{F}_b = \mathrm{Ran}\,\Im m\,\Pi(E-\imath 0-H_0)^{-1}\Pi^*$ with $b = f(E)$

Partial isometries

$$\Pi_b \,:\, \mathcal{F}_b \subset \ell^2(\mathbb{Z}^{d_1}) \to \mathcal{D}_b \subset L^2(\Sigma,\nu)$$

$$\Pi_B = \int^{\oplus} db\,\Pi_b \,:\, L^2(\mathbb{R}_b)\otimes\ell^2(\mathbb{Z}^{d_1}) \to L^2(\mathbb{R}_b)\oplus L^2(\Sigma,\nu)$$

Definition Operator O on $L^2(\mathbb{R}_b)\oplus L^2(\Sigma,\nu)$ REI representable iff

$$O = \Pi_B\,\Pi_B^*\,O\,\Pi_B\,\Pi_B^*$$

Then $\Pi_B^*\,O\,\Pi_B$ is its REI representation on $L^2(\mathbb{R}_b)\otimes\ell^2(\mathbb{Z}^{d_1})$

Formulas for wave and scattering operators

Theorem For $d \geq 3$ and λ small, wave operator REI representable and with $G_0(z) = \Pi^*(z - H_0)^{-1}\Pi$ and $b = f(E)$

$$\Pi_B^*(\mathcal{U}\,\mathcal{F}\,W_\pm\,\mathcal{F}^*\,\mathcal{U}^* - \mathbf{1})\Pi_B \;=$$

$$\imath\big|\Im m\, G_0(E)\big)\big|^{\frac{1}{2}}\,\big(\pm\mathbf{1} + \tanh\big(\tfrac{\pi}{2}A\big)\big)\big(\lambda^{-1} - V\,G_0(E\mp\imath 0)\big)^{-1}V\big|\Im m\, G_0(E)\big|^{\frac{1}{2}}$$

Comments

RHS continuous function of A and B and covariant on $\ell^2(\mathbb{Z}^{d_1})$

λ small: easy way to insure existence of inverse (not necessary)

Similar formulas: Kellendonk-Richard(2006), Richard-Tiedra(2012)

$S = W_+^* W_- = \lim_t e^{\imath t H_0} e^{-\imath t H} W_- = \lim_t e^{\imath t B} W_- e^{-\imath t B}$ boost in A

Corollary Scattering operator energy fibered and REI representable

$$S_E \;=\; \mathbf{1} - 2\imath\big|\Im m\, G_0(E)\big)\big|^{\frac{1}{2}}\,\big(\lambda^{-1} - V\,G_0(E\mp\imath 0)\big)^{-1}V\big|\Im m\, G_0(E)\big|^{\frac{1}{2}}$$

Exact sequence for surface scattering

$$0 \;\to\; C_0(\mathbb{R}) \hookrightarrow\; C_\infty(\mathbb{R}) \cong C([0,1]) \;\overset{\text{ev}}{\to}\; \mathbb{C}\oplus\mathbb{C} \;\to\; 0$$

$$0 \;\to\; C_0(\mathbb{R}^2) \;\hookrightarrow\; C_\infty(\mathbb{R}^2) \cong C(\overline{\mathbb{D}}) \;\overset{\text{ev}}{\to}\; C(\mathbb{S}^1) \cong C(\square) \;\to\; 0$$

$$0 \;\to\; C_0^*(A,B) \cong \mathcal{K} \;\hookrightarrow\; C_\infty^*(A,B) \;\overset{\text{ev}}{\to}\; C(\square) \;\to\; 0$$

$$0 \;\to\; C_0^*(A,B)\otimes\mathcal{A} \;\hookrightarrow\; C_\infty^*(A,B)\otimes\mathcal{A} \;\overset{\text{ev}}{\to}\; C(\square)\otimes\mathcal{A} \;\to\; 0$$

where $\mathcal{A} = C(\Omega) \rtimes \mathbb{Z}^{d_1}$ algebra of covariant operators on $\ell^2(\mathbb{Z}^{d_1})$

$\mathbf{1}\otimes\mathbf{1}\otimes\mathbf{1}\otimes S \in C(\square)\otimes\mathcal{A}$ as $S = \int^{\oplus} db\, S_b$

$P_{\rm sur} \in C_0^*(A,B)\otimes\mathcal{A}$

$W_- \in C_\infty^*(A,B)\otimes\mathcal{A}$ and $\mathrm{Lift}(\mathbf{1}\otimes\mathbf{1}\otimes\mathbf{1}\otimes S) = W_-$

$$\mathrm{Ind}\big([S]_1\big) \;=\; [\mathbf{1}-(W_-)^*W_-]_0 \;-\; [\mathbf{1}-W_-(W_-)^*]_0 \;=\; -[P_{\rm sur}]_0$$

$$\frac{1}{2\pi\imath}\int_{-\infty}^{\infty} db\, \mathcal{T}_1\big((S_b)^*\,\partial_b S_b\big) \;=\; -\,\mathcal{T}_1\,\mathrm{Tr}_{L^2(\mathbb{R})}\big(P_{\rm sur}\big)$$

Resumé

1) natural construction of conjugate operator
2) REI representation leads to covariant wave and scattering ops
3) index theorem shows a Levinson-like formula

References

V. Jaksic, S. Molchanov, L. Pastur, *On the Propagation Properties of Surface Waves*, IMA Vol. Math. Appl. **96** (1998).

V. Jaksic, Y. Last, *Corrugated surfaces and the a.c. spectrum*, Rev. Math. Phys. **12**, 1465 (2000).

J. Kellendonk, S. Richard, *Levinson's theorem for Schrödinger operators with point interaction*, J. Phys. **A 39**, 14397 (2006).

J. Bellissard, H. Schulz-Baldes, *Scattering theory for lattice operators in dimension* $d \geq 3$, Rev. Math. Phys. **24**, (2012).

H. Schulz-Baldes, *The density of surface states as the total time delay*, `arXiv 1305.2187`