Density of states for periodic Schrödinger operators

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Periodic operators. Density of states

The Schrödinger operator in $L^2(\mathbb{R}^d), d \geq 2$:

$$H = -\Delta + V, \quad V = V(\mathbf{x}), \mathbf{x} \in \mathbb{R}^d;$$

V is a real-valued function, periodic w.r.t. to a lattice Γ, i.e.

$$V(\mathbf{x}) = V(\mathbf{x} + \gamma), \quad \gamma \in \Gamma.$$

Usually assume for simplicity: $\Gamma = (2\pi\mathbb{Z})^d$.

Dual lattice: $\Gamma^\dagger$.
Standard fundamental domains: $\mathcal{O}, \mathcal{O}^\dagger$.
For $\Gamma = (2\pi\mathbb{Z})^d$: $\mathcal{O} = [0, 2\pi)^d$, $\mathcal{O}^\dagger = [0, 1)^d$.

Density of states:

$$\boxed{D(\lambda) = D(\lambda; H) = \lim_{L\to\infty} \frac{N(\lambda; H_D^L)}{L^d}.}$$

H_D^L is H restricted to $(0, L)^d$ with the Dirichlet b.c.

Alternative definition via the

Floquet decomposition

Let $H(\mathbf{k}) = (\mathbf{D}+\mathbf{k})^2 + V$, $\mathbf{D} = -i\nabla$, on $\mathbb{T}^d = \mathbb{R}^d/\Gamma$. Spectrum of $H(\mathbf{k})$ is discrete:

$$\lambda_1(\mathbf{k}) \le \lambda_2(\mathbf{k}) \le \cdots \le \lambda_j(\mathbf{k}) \le \dots$$

Each $\lambda_j(\ \cdot\ )$ is continuous in $\mathbf{k}$ and $\mathbb{Z}^d$-periodic. Counting function:

$$N(\lambda; \mathbf{k}) = \#\{j : \lambda_j(\mathbf{k}) \le \lambda\}.$$

Then

$$\boxed{D(\lambda) = \frac{1}{(2\pi)^d} \int_{\mathcal{O}^\dagger} N(\lambda; \mathbf{k}) d\mathbf{k}.}$$

Density of states for PDO's. Let $a_0(\boldsymbol{\xi}) \to \infty$ as $|\boldsymbol{\xi}| \to \infty$. Then

$$D(\lambda, A_0) = \frac{1}{(2\pi)^d} |\{\boldsymbol{\xi} : a_0(\boldsymbol{\xi}) \le \lambda\}|.$$

Thus

$$D_0(\lambda) = D(\lambda; H_0) = \frac{\mathrm{w}_d}{(2\pi)^d} \lambda^{\frac{d}{2}}, \ \lambda \ge 0.$$

Asymptotics as $\lambda \to \infty$:

$$N(\lambda, \mathbf{k}) = \frac{\mathsf{w}_d}{(2\pi)^d} \lambda^{\frac{d}{2}} + O(\lambda^{\frac{d-1}{2}}),$$

$$D(\lambda) = \frac{\mathsf{w}_d}{(2\pi)^d} \lambda^{\frac{d}{2}} + O(\lambda^{\frac{d-2}{2}}).$$

Conjecture:

$$D(\lambda) = D_0(\lambda)\left[1+\sum_{j=1}^{N} b_j\lambda^{-j}+o(\lambda^{-N})\right], \ \lambda \to \infty, \ \forall N.$$

Proved for $d = 1$, D. Schenk, M. Shubin (1987).

For $d > 1$???

M. Shubin(1976, 79), $d \geq 1$:

$$D(\lambda) = D_0(\lambda)\Big(1 + O(\lambda^{-1})\Big).$$

B. Helffer, A. Mohamed (1998), $d \geq 2$:

$$D(\lambda) = D_0(\lambda)\Big[1 + b_1\lambda^{-1} + O(\lambda^{-\frac{3}{2}+\epsilon})\Big], \ \forall\epsilon > 0,$$

$$b_1 = -\frac{d}{2|\mathcal{O}|}\int_{\mathcal{O}} V(\mathbf{x})d\mathbf{x}.$$

Yu. Karpeshina (2000), $d \geq 2$: $\lambda^{\epsilon} \to \ln\lambda$.

For $d = 3$:

$$D(\lambda) = D_0(\lambda)\Big[1+b_1\lambda^{-1}+\widehat{D}\lambda^{-\frac{3}{2}}+O(\lambda^{-\frac{3}{2}-\delta})\Big], \ \delta > 0.$$

In fact $\widehat{D} = 0$!

Coefficients can be found from the asymptotics

$$\int_{\mathbb{R}} e^{-t\lambda} D(\lambda) d\lambda, \quad t \to 0.$$

Numerous works: Gilkey, Polterovich, Hitrik.

$$b_2 = \frac{d(d-2)}{8|\mathcal{O}|} \int_{\mathcal{O}} V(\mathbf{x})^2 d\mathbf{x}.$$

Known: for even d's one has $b_j = 0$, $j \geq d/2 + 1$. Korotyaev-Pushnitski (2002).

Theorem (Main result). *Let* $d = 2$, $\hat{V}(\mathbf{0}) = 0$. *Then*

$$D(\lambda) = D_0(\lambda)\Big(1 + O(\lambda^{-\frac{11}{5}+\epsilon})\Big), \ \forall \epsilon > 0.$$

Alternatively

$$D(\lambda) = D_0(\lambda)\Big(1 + b_1\lambda^{-1} + b_2\lambda^{-2} + O(\lambda^{-\frac{11}{5}+\epsilon})\Big).$$

Perturbation theory: "Resonant" and "non-resonant" eigenvalues

Proposition. *Let* A *and* $B = A + T$, $\|T\| < \infty$, *be self-adjoint op-s with discrete spectra. Suppose that for some* j

$$P_A T P_A = 0, \;\; P_A = P_A\Big(\lambda_j(A) - \mu, \lambda_j(A) + \mu\Big),$$

that is

$$T = \begin{bmatrix} 0 & T_{12} \\ T_{21} & T_{22} \end{bmatrix}.$$

Then

$$|\lambda_j(B) - \lambda_j(A)| \leq 4\|T\|^2 \mu^{-1}.$$

Unperturbed problem:

Egnvs: $(\mathbf{m}+\mathbf{k})^2,\ \mathbf{m}\in\mathbb{Z}^d,$
Egnfuncts: $e^{i\mathbf{m}\mathbf{x}}$.

Suppose $V(\mathbf{x}) = \cos\boldsymbol{\theta}\mathbf{x}$, $\boldsymbol{\theta}\in\mathbb{Z}^d$.

Denote $\rho = \sqrt{\lambda}$.

Non-resonant zone:

$$\Omega_{\boldsymbol{\theta}}(\rho) = \{\mathbf{m} : |\mathbf{m}+\mathbf{k}| \approx \rho,\ |(\mathbf{m}+\mathbf{k})\boldsymbol{\theta}| \gg 1\},$$

Resonant zone:

$$\begin{aligned}(\mathbf{m}+\mathbf{k})^2 &\approx (\mathbf{m}+\mathbf{k}\pm\boldsymbol{\theta})^2 \\ &= (\mathbf{m}+\mathbf{k})^2 \pm 2\boldsymbol{\theta}(\mathbf{m}+\mathbf{k}\pm\boldsymbol{\theta}/2),\end{aligned}$$

that is

$$\Lambda_{\boldsymbol{\theta}}(\rho) = \{\mathbf{m} : |\mathbf{m}+\mathbf{k}| \approx \rho,\ |(\mathbf{m}+\mathbf{k}\pm\boldsymbol{\theta}/2)\boldsymbol{\theta}| \approx 0\}.$$

E. Trubovitz, H. Knörrer ('90, '91),
M. Skriganov (80's),
Yu. Karpeshina (90's).

Idea: to reduce H to the operator with a symbol $a^o = a^o(\boldsymbol{\xi})$. G. Rosenblum '78.

Implementation: Find a unitary U such that $A = U^* H U \approx a^o(\mathbf{D})$.
Let $U(t) = e^{it\Psi}$ with $\Psi = \Psi^*$, $\Psi = \mathrm{Op}(\psi)$,
$A = U(-1)HU(1)$,
$\mathrm{ad}(A; B) = i[A, B]$, $\mathrm{ad}^n(A; B) = i[\mathrm{ad}^{n-1}(A; B), B]$.
Then

$$A = H + \int_0^1 U(-\tau)\,\mathrm{ad}(H; \Psi) U(\tau) d\tau.$$

By induction:

$$A = H + \sum_{j=1}^{M} \frac{1}{j!} \mathrm{ad}^j(H; \Psi) + R_{M+1},$$

$$R_{M+1} = \int_0^1 d\tau_1 \int_0^{\tau_1} d\tau_2 \dots \int_0^{\tau_M} U(-s)\,\mathrm{ad}^{M+1}(H; \Psi) U(s) ds.$$

Write this for $M = 1$:

$$A = H_0 + V + i[H_0, \Psi] + \dots$$

Want to find Ψ from

$$i[H_0, \Psi] + V = 0.$$

Let $\psi(\mathrm{x},\boldsymbol{\xi}) = (2\pi)^{-d/2}\sum_{\boldsymbol{\theta}} e^{i\boldsymbol{\theta}\mathrm{x}}\psi(\boldsymbol{\theta},\boldsymbol{\xi})$.

Commutator equation. Rewrite the equation for $\boldsymbol{\theta} \neq 0$:

$$i\Big(|\boldsymbol{\xi}+\boldsymbol{\theta}|^2 - |\boldsymbol{\xi}|^2\Big)\widehat{\psi}(\boldsymbol{\theta},\boldsymbol{\xi}) = -\widehat{V}(\boldsymbol{\theta}),$$

$$i2\boldsymbol{\theta}\Big(\boldsymbol{\xi}+\boldsymbol{\theta}/2)\widehat{\psi}(\boldsymbol{\theta},\boldsymbol{\xi}) = -\widehat{V}(\boldsymbol{\theta}). \qquad (1)$$

To avoid the resonance set introduce a cut-off, $\zeta_{\boldsymbol{\theta}} \in \mathrm{C}^\infty$:

$$\zeta_{\boldsymbol{\theta}}(\boldsymbol{\xi}) = \Upsilon\left(\frac{\boldsymbol{\theta}(\boldsymbol{\xi}+\boldsymbol{\theta}/2)}{|\boldsymbol{\theta}|L}\right), L > 0.$$

Define

$$V(\mathrm{x}) = V^\sharp(\mathrm{x},\boldsymbol{\xi}) + V^\flat(\mathrm{x},\boldsymbol{\xi});$$

$$V^\flat(\mathrm{x},\boldsymbol{\xi}) = (2\pi)^{-d/2}\sum_{\boldsymbol{\theta}}\widehat{V}(\boldsymbol{\theta})\zeta_{\boldsymbol{\theta}}(\boldsymbol{\xi})e^{i\boldsymbol{\theta}\mathrm{x}},$$

$$V^\sharp(\mathrm{x},\boldsymbol{\xi}) = (2\pi)^{-d/2}\sum_{\boldsymbol{\theta}}\widehat{V}(\boldsymbol{\theta})\varphi_{\boldsymbol{\theta}}(\boldsymbol{\xi})e^{i\boldsymbol{\theta}\mathrm{x}},\ \varphi_{\boldsymbol{\theta}} = 1-\zeta_{\boldsymbol{\theta}}.$$

Instead of (1) solve

$$i2\boldsymbol{\theta}\Big(\boldsymbol{\xi}+\boldsymbol{\theta}/2)\widehat{\psi}(\boldsymbol{\theta},\boldsymbol{\xi}) = -\widehat{V}(\boldsymbol{\theta})\varphi_{\boldsymbol{\theta}}(\boldsymbol{\xi}).$$

Then $A = H_0 + V^\flat + \dots$.

Classes of PDO's: $\mathbf{S}_\alpha(L), L > 0$. Represent:

$$b(\mathbf{x}, \boldsymbol{\xi}) = \frac{1}{(2\pi)^{\frac{d}{2}}} \sum_{\boldsymbol{\theta}} \hat{b}(\boldsymbol{\theta}, \boldsymbol{\xi}) e^{i\boldsymbol{\theta}\mathbf{x}}$$

$B = \mathrm{Op}(b)$ is symmetric if

$$\hat{b}(\boldsymbol{\theta}, \boldsymbol{\xi}) = \overline{\hat{b}(-\boldsymbol{\theta}, \boldsymbol{\xi} + \boldsymbol{\theta})}.$$

$b \in \mathbf{S}_\alpha(L)$ if

$$|\partial_{\boldsymbol{\xi}}^{\mathrm{s}} \hat{b}(\boldsymbol{\theta}, \boldsymbol{\xi})| \le C_{\mathrm{s},l} \langle \boldsymbol{\theta} \rangle^{-l} L^{\alpha - |\mathrm{s}|}.$$

Operations $\flat, \sharp, o$:

$$b^\flat(\mathbf{x}, \boldsymbol{\xi}) = (2\pi)^{-d/2} \sum_{\boldsymbol{\theta} \neq 0} \hat{b}(\boldsymbol{\theta}, \boldsymbol{\xi}) \zeta_{\boldsymbol{\theta}}(\boldsymbol{\xi}) e^{i\boldsymbol{\theta}\mathbf{x}},$$

$$b^\sharp(\mathbf{x}, \boldsymbol{\xi}) = (2\pi)^{-d/2} \sum_{\boldsymbol{\theta} \neq 0} \hat{b}(\boldsymbol{\theta}, \boldsymbol{\xi}) \varphi_{\boldsymbol{\theta}}(\boldsymbol{\xi}) e^{i\boldsymbol{\theta}\mathbf{x}},$$

$$b^o(\mathbf{x}, \boldsymbol{\xi}) = (2\pi)^{-d/2} \hat{b}(\mathbf{0}, \boldsymbol{\xi}).$$

Symmetry is preserved.

Taking $M = 2$ one gets:

Theorem 2. *$\exists$ a $\Psi \in \mathbf{S}_{-1}(L)$ such that*

$$A_1 = e^{-i\Psi} H e^{i\Psi} = A^o + V^\flat + V_2^\flat + T_2^\flat + O(L^{-4}),$$
$$A^o = H_0 + V_2^o + T_2^o,$$

with

$$V_2 = \mathrm{ad}(V; \Psi), \ T_2 = -\frac{1}{2}\mathrm{ad}(V^\sharp; \Psi).$$

Operators in the strips:

Model operators $A = \mathrm{Op}(a)$ in $\mathsf{L}^2(\mathbb{R}^d)$, $T = \mathrm{Op}(t)$ in $\mathsf{L}^2(\mathbb{R})$. Denote $\boldsymbol{\xi} = (\xi_1, \hat{\boldsymbol{\xi}})$:

$$a(\mathbf{x}, \boldsymbol{\xi}) = \hat{\boldsymbol{\xi}}^2 + t(x_1, \xi_1), \ t(x_1, \xi_1) = \xi_1^2 + b(x_1, \xi_1).$$

Then

$$D(\lambda, A) = \frac{\omega_{d-2}}{2(2\pi)^{d-1}} \int_{-\infty}^{\lambda} D(\mu, T)(\lambda - \mu)^{\frac{d-3}{2}} d\mu.$$

Case $d = 1$ studied in AS '02. It yields: $D(\lambda, A_1) = D(\lambda, A^o)$. Condition $d = 2$ is crucial!!!.

Operator A^o

Symbol a^o:

$$a^o(\boldsymbol{\xi}) \sim |\boldsymbol{\xi}|^2 + \frac{1}{(2\pi)^d} \sum_{\boldsymbol{\theta} \neq 0} \frac{|\boldsymbol{\theta}|^2 |\widehat{V}(\boldsymbol{\theta})|^2}{4|\boldsymbol{\theta}\boldsymbol{\xi}|^2 - |\boldsymbol{\theta}|^4}.$$

Theorem 3. *For large $\lambda > 0$ and $L = \lambda^{3/10}$:*

$$D(\lambda, A^o) \sim D_0(\lambda)\Big(1 + b_2\lambda^{-2} + O(\lambda^{-\frac{11}{5}+\epsilon})\Big), \forall \epsilon > 0.$$

Proof: find the volume of $\{\boldsymbol{\xi} : a_0(\boldsymbol{\xi}) \leq \lambda\}$.