Spectral Density Calculations for Schrodinger Operators in 1 Dimension

We consider functions $P = P(x,\lambda)$, $Q = Q(x,\lambda)$, $R = R(x,\lambda)$, such that, for each solution $y = y(x,\lambda)$ of the differential equation

$$-\frac{d^2 y(x,\lambda)}{dx^2} + q(x)y(x,\lambda) = \lambda\, y(x,\lambda)$$
$$(x \in [0,\infty),\ \lambda \in \mathbb{R})$$

the quadratic form

$$Py^2 + Qyy' + Ry'^2 \text{ is independent of } x.$$

We require P, Q, R to satisfy

$$\left.\begin{aligned} \frac{dP}{dx} &= (\lambda - q)Q \\ \frac{dQ}{dx} &= -2P + 2(\lambda - q)R \\ \frac{dR}{dx} &= -Q \end{aligned}\right\} \beta = 4PR - Q^2 = \text{const.}$$

From the linear system for P, Q, R

we have

$$\frac{d^2R}{dx^2} = -\frac{dQ}{dx} = 2P - 2(\lambda - q)R.$$

Hence

$$\frac{d}{dx}\left\{ \frac{d^2R}{dx^2} + 2(\lambda - q)R \right\} = 2\frac{dP}{dx}$$

$$= 2(\lambda - q)Q = -2(\lambda - q)\frac{dR}{dx}.$$

Hence

$$[R'' + 2(\lambda - q)R]' + 2(\lambda - q)R'$$

$$= 0$$

Note that if y_1, y_2 both satisfy the Schrödinger equation (with same λ value) then a solution for (P, Q, R) is

$$(P, Q, R)$$

$$= (y_1' y_2' \, , \, -(y_1 y_2' + y_2 y_1'), \, y_1 y_2).$$

In particular, defining 2 solutions $u(x, \lambda)$, $v(x, \lambda)$ by

$$\left.\begin{array}{ll} u(0, \lambda) = 1 & v(0, \lambda) = 0 \\ u'(0, \lambda) = 0 & v'(0, \lambda) = 1 \end{array}\right\}$$

we find the general solution for $R(x, \lambda)$ is $R = au^2 + buv + cv^2$.

(a, b, c constants).

Moreover, β

$$= 2R \frac{d^2R}{dx^2} - \left(\frac{dR}{dx}\right)^2 + 4(\lambda - q) R^2$$

$$= 4ac - b^2.$$

Now consider a solution

$$R = au^2 + buv + cv^2 \quad \text{for } R(x, \lambda),$$

such that (i) $a > 0$

(ii) $\beta = 4ac - b^2 = 4$.

Define A, B by

$$\frac{1}{B} = a, \quad \frac{2A}{B} = b, \quad \frac{A^2 + B^2}{B} = c$$

Then $$R = \frac{(u + Av)^2 + B^2 v^2}{B}$$

$$= \frac{|u + Mv|^2}{\operatorname{Im} M}, \text{ where}$$

$$M = M(\lambda) = A + iB.$$

IF $M(\lambda) = m_+(\lambda)$ = boundary value of m-function, then

$$\text{Spectral density} = \frac{1}{\pi} \operatorname{Im} M(\lambda) = \frac{1}{\pi R(0, \lambda)}$$

$$= \frac{1}{\pi (P v^2 + Q v v' + R v'^2)}$$

Any solution $R(x, \lambda)$ for R, satisfying $\beta = 4$, will give rise to an expression for spectral density (Dirichlet operator)

$$= \frac{1}{\pi\,(Pv^2 + Qvv' + Rv'^2)}$$ provided either

(i) $R(x, \lambda) \to R(\lambda)$ as $x \to \infty$, or, more generally,

(ii) $R(x, \lambda) \sim F(x, \lambda)$ as $x \to \infty$, with $\dfrac{\partial F(x, \lambda)}{\partial x} \to 0$, or (less generally)

(iii) $Q(x, \lambda) \to 0$ as $x \to \infty$, or

(iv) $R(x, \lambda)$ is periodic in x.

Such conditions hold for

a) potentials $1/(1+x)^\beta$ for any $\beta > 0$.

b) potential $q(x) = -x^2$

c) potential $q(x) = \cos x$

Moreover, the same functions P, Q, R allow one to determine the spectral density for the Schrödinger operator $-\frac{d^2}{dx^2} + q(x)$ subject to a general boundary condition

$$(\cos\alpha) f(0) + \sin\alpha\, f'(0) = 0.$$

If, in that case, we define solution v_α of $-y'' + qy = \lambda y$, with

$$\left.\begin{aligned} v_\alpha(0,\lambda) &= -\sin\alpha \\ v_\alpha'(0,\lambda) &= \cos\alpha \end{aligned}\right\}$$

then the spectral density is

$$\frac{1}{\pi\left(P v_\alpha^2 + Q v_\alpha v_\alpha' + R v_\alpha'^2\right)}$$

Ideas of value distribution may be used to describe the asymptotics of solutions $y(x, \lambda)$ of the Schrödinger equation in the limit as $x \to \infty$.

One considers the distribution of values of $y(x, \cdot)$ as a function of λ, for large x.

Starting from the identities that

$$u = R^{1/2} \left\{ B^{1/2} \cos \int_0^x \frac{1}{R(t)}\, dt - A B^{-1/2} \sin \int_0^x \frac{1}{R(t)}\, dt \right\}$$

$$v = R^{1/2} B^{-1/2} \sin \int_0^x \frac{1}{R(t)}\, dt ,$$

one may show that, asymptotically for large x,

$\theta(x, \lambda) = \int_0^x \frac{1}{R(t)}\, dt$ is uniformly distributed mod π, as a function of λ. For the matrix of u_α, v_α and their derivatives, we have

$$\begin{pmatrix} u_\alpha & v_\alpha \\ u_\alpha' & v_\alpha' \end{pmatrix} = \begin{pmatrix} F_\alpha (B_\alpha \cos\theta_\alpha - A_\alpha \sin\theta_\alpha) & F_\alpha \sin\theta_\alpha \\ B_\alpha G_\alpha \cos(\theta_\alpha + \beta) - A_\alpha G_\alpha \sin(\theta_\alpha + \beta) & G_\alpha \sin(\theta_\alpha + \beta) \end{pmatrix}$$

(x, λ) in general.

General solution for R is given in terms of particular solution R_0 (with $\beta = 4$) by

$$R = R_0 \left(A + B \cos \int_0^x \frac{2}{R_0(t)}\, dt + C \sin \int_0^x \frac{2}{R_0(t)}\, dt \right)$$

where to maintain $\beta = 4$ we require

$$A^2 - B^2 - C^2 = 1.$$

If $R_0 = a_0 u^2 + b_0 uv + c_0 v^2$, we have

$$\int_0^x \frac{1}{R_0(t)}\, dt = \cot^{-1}\left(\frac{u + A_0 v}{B_0 v} \right) + \pi N(x, \lambda)$$

($N(x,\lambda)$ = no. of zeroes of $v(x,\lambda)$ in interval $(0, x)$).

As $x \to \infty$, $\int_0^x \frac{2}{R_0(t)}\, dt$, if $M(\lambda) = m_+(\lambda)$, may be regarded as uniformly distributed (modulo 2π) as a function of λ.

Any other solution for $R(x,\lambda)$ has

$$\text{ave}\left\{ \frac{R(x,\lambda)}{R_0(x,\lambda)} \right\} > 1 \text{ in limit as } x \to \infty.$$

Example

Suppose $q' \in L^1(0,\infty)$ with $q \to 0$ as $x \to \infty$

Define P_0, Q_0, R_0 by

$$\left.\begin{aligned} P(x,\lambda) &= (\lambda - q(x))^{\alpha} P_0(x,\lambda) \\ Q &= (\lambda - q)^{\beta} Q_0 \\ R &= (\lambda - q)^{\gamma} R_0 \end{aligned}\right\} \begin{aligned} &\alpha - \beta \\ &= \beta - \gamma \\ &= \tfrac{1}{2}. \end{aligned}$$

Change variable from x to

$$s = \int^{x} (\lambda - q(t))^{1/2}\, dt$$

Then

$$\frac{d}{ds}\begin{pmatrix} P_0 \\ Q_0 \\ R_0 \end{pmatrix} = \mathbb{A}\begin{pmatrix} P_0 \\ Q_0 \\ R_0 \end{pmatrix} + \frac{q'}{(\lambda - q)^{3/2}}\begin{pmatrix} \alpha P_0 \\ \beta Q_0 \\ \gamma R_0 \end{pmatrix}$$

Here $\mathbb{A} = \begin{pmatrix} 0 & 1 & 0 \\ -2 & 0 & 2 \\ 0 & -1 & 0 \end{pmatrix}$ (eigenvalues $0, \pm 2i$)

Converts to integral equation

$$\underline{\mathbb{P}}_0(s) = \left\{ \begin{matrix} \text{eigenvector with} \\ \text{eigenvalue } 0 \end{matrix} \right\} - \int_s^{\infty} e^{\mathbb{A}(s-t)} \Phi(t) \underline{P}_0(t)\, d$$

Take eigenvector $= \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$, $\alpha = \frac{1}{2}$ $\beta = 0$, $\gamma = -\frac{1}{2}$