Influence of Curvature on Impurity Spectrum in Quantum Dot

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Model of quantum dot

- We take the two-dimensional Laplace-Beltrami operator and we choose the harmonic oscillator potential to take the confinement into the account.
- The impurity si modelled by a point potential (δ-interaction).
- The point potential is introduced with the help of the self-adjoint extension method which yields a boundary condition.

Problem

- At first we consider the flat case (Euclidian plane) and an arbitrary position of the impurity.
- Next we deal with a non-zero curvature (Lobachevsky plane), but we restrict ourselves to the case when the impurity is localized in the center of the potential. This problem still remains open.
- In both cases we find an explicit formula for the Green function of the total hamiltonian.
- Moreover we try to analyze the spectrum in dependence of the problem parameters.

Quantum dot with impurity in Eucledian plane-model

Two-dimensional isotropic harmonic oscillator:

$$H = -\Delta + \frac{1}{4}\omega^2 x^2, \quad \text{where } \omega \geq 0$$

$$Dom(H) = span\left\{ x_1^{n_1} x_2^{n_2} \mathrm{e}^{-\frac{\omega x^2}{4}} \,\middle|\, n_1, n_2 \in \mathbb{N}_0 \right\}$$

Perturbed hamiltonian $H_\alpha(q)$, $\alpha \in \mathbb{R}$, is a selfadjoint extension of the following symmetric operator:

$$Dom(H(q)) := \{f \in Dom(H) |\, f(q) = 0\}, \quad H(q) := H \restriction_{Dom(H(q))}$$

Spectrum

Krein formula:

$$\mathcal{G}_z^{\alpha,q}(x,y) = \mathcal{G}_z^{\mathrm{ho}}(x,y) - [Q(z,q)-\alpha]^{-1}\mathcal{G}_z^{\mathrm{ho}}(x,q)\mathcal{G}_z^{\mathrm{ho}}(q,y),$$

where $Q(z,q) = \mathcal{G}_{z,\mathrm{reg}}^{\mathrm{ho}}(q,q)$ is the regularized Green function of H evaluated in $x = y = q$ (so-called Krein Q-function).

- An eigenvalue λ_n of H of the multiplicity k_n is an eigenvalue of H_α of the multiplicity $k_n + 1$, k_n or $k_n - 1$.
- Additional eigenvalues different from λ_n are solutions to the equation

$$Q(z,q) = \alpha.$$

Green function of two-dimensional isotropic harmonic oscillator

- In the polar coordinates:

$$\mathcal{G}_z^{\mathrm{ho}}(r\hat{\varphi}, r'\hat{\varphi}') = \frac{1}{2\pi} \sum_{n=-\infty}^{\infty} \mathcal{G}_n^z(r, r')\mathrm{e}^{in(\varphi-\varphi')}$$

$$\mathcal{G}_n^z(r, r') = \frac{\Gamma\left(\frac{1}{2}(|n| + 1 - \frac{z}{\omega})\right)}{\omega\Gamma(|n| + 1)} \frac{1}{rr'} M_{\frac{z}{2\omega}, \frac{|n|}{2}} \left(\frac{\omega}{2} r_<^2\right) W_{\frac{z}{2\omega}, \frac{|n|}{2}} \left(\frac{\omega}{2} r_>^2\right)$$

$$(H - z)\mathcal{G}_z^{\mathrm{ho}}(x, y) = \delta(x - y), \quad \text{for } z \in \mathbb{C} \setminus \sigma(H),$$

where $M_{a,b}$ and $W_{a,b}$ denote the Whittaker functions and $r_<, r_>$ are the smaller and the greater of r and r', respectively.

- The divergent part: $-\frac{1}{2\pi} \ln |x - y|$

Comparing the following expressions for the free hamiltonian Green function $\mathcal{G}_z(x-y) = \frac{i}{4} H_0^{(1)}(\sqrt{z}|x-y|)$ we obtain a series for the divergent part $(z<0)$:

- $\mathcal{G}_z(x-y) \overset{|x-y|\to 0}{\sim} -\frac{1}{2\pi}\left(\ln|x-y| + \ln\frac{\sqrt{-z}}{2} - \Psi(1)\right)$
- $\mathcal{G}_z(x-y) = \frac{i}{4} \sum_{n=-\infty}^{\infty} H_n^{(1)}(i\sqrt{-z}r_>) J_n(i\sqrt{-z}r_<) \cos[n(\varphi-\varphi')]$

For Krein Q-function, we conclude:

$$Q(z,q) = \begin{cases} \sum_{n=1}^{\infty} \left(\frac{1}{\pi}\mathcal{G}_n^z(q,q) + \frac{1}{2} Y_n(\sqrt{z}q) J_n(\sqrt{z}q)\right) + \frac{1}{2\pi}\mathcal{G}_0^z(q,q) \\ + \frac{1}{4} Y_0(\sqrt{z}q) J_0(\sqrt{z}q) - \frac{1}{2\pi}\left(\ln\frac{\sqrt{z}}{2} - \Psi(1)\right) \quad \text{for } z>0 \\ \\ \sum_{n=1}^{\infty} \left(\frac{1}{\pi}\mathcal{G}_n^z(q,q) - \frac{i}{2} H_n^{(1)}(i\sqrt{-z}q) J_n(i\sqrt{-z}q)\right) \\ + \frac{1}{2\pi}\mathcal{G}_0^z(q,q) - \frac{i}{4} H_0^{(1)}(i\sqrt{-z}q) J_0(i\sqrt{-z}q) \\ - \frac{1}{2\pi}\left(\ln\frac{\sqrt{-z}}{2} - \Psi(1)\right) \quad \text{for } z<0. \end{cases}$$

Figure: Krein Q-function for several values of q

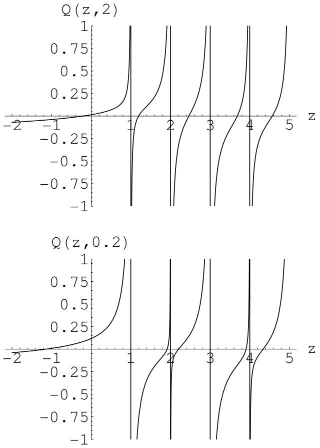
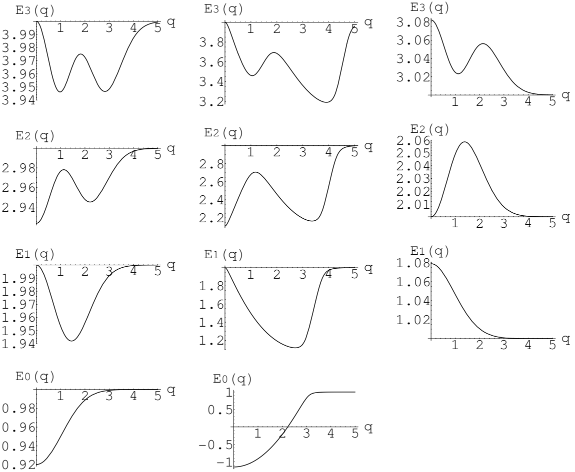


Figure: Energy levels E_n for $\alpha = 2, \ \alpha = 0, \ \alpha = -2$



Quantum dot with impurity in Lobachevsky plane-model

Lobachevsky plane $\mathbb{L}_a^2$ in polar coordinates

$$ds^2 = d\varrho^2 + a^2 \sinh^2 \frac{\varrho}{a} d\theta^2,$$

where $0 > const. = R = -\frac{2}{a^2}$ is scalar curvature

Hamiltonian of the two-dimensional isotropic harmonic oscillator with the central point interaction in the Lobachevsky plane is a s.a. extension of:

$$H = -\frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} \sqrt{g} g^{ij} \frac{\partial}{\partial x^j} - \frac{1}{4a^2} + \frac{1}{4} a^2 \omega^2 \sinh^2 \left(\frac{\varrho}{a}\right)$$

$$Dom(H) = C_0^\infty(\mathbb{L}_a^2 \setminus \{0\})$$

Partial wave decomposition

- Substitution $\xi = \cosh\frac{\varrho}{a}$ yields

$$H=\frac{1}{a^2}\left[(1-\xi^2)\frac{\partial^2}{\partial\xi^2}-2\xi\frac{\partial}{\partial\xi}+(1-\xi^2)^{-1}\frac{\partial^2}{\partial\theta^2}+\frac{a^4\omega^2}{2}(\xi^2-1)-\frac{1}{4}\right]=:\frac{1}{a^2}\tilde{H}.$$

- $\tilde{H}$ may be decomposed in the following way

$$\tilde{H}=\bigoplus_{n=-\infty}^{\infty}\tilde{H}_n$$

$$\tilde{H}_n=(1-\xi^2)\frac{\partial^2}{\partial\xi^2}-2\xi\frac{\partial}{\partial\xi}-n^2(1-\xi^2)^{-1}+\frac{a^4\omega^2}{2}(\xi^2-1)-\frac{1}{4},\quad Dom(\tilde{H}_n)=C_0^\infty(1,\infty)$$

- We conclude
  - $\tilde{H}_n$ is e.s.a. for $n\neq 0$
  - $\tilde{H}_0$ has deficiency indices (1,1)

Radial part of Green function $\mathcal{G}_z$ $(\mathrm{d}\theta = 0)$

- To find the Krein Q-function, we may restrict ourselves to the radial part of the Green function since

$$Q(z)=\mathcal{G}_{z,reg}(1,0;1,0) \text{ and } \mathcal{G}_z(\xi,\theta;1,0)=\mathcal{G}_z(\xi),$$

- and hence $(\tilde{H}-z)\mathcal{G}_z(\xi)=(\tilde{H}_0-z)\mathcal{G}_z(\xi)=0 \quad \text{for } \xi\in(1,\infty).$

$$(\tilde{H}_0-z)\mathcal{G}_z=\left[(1-\xi^2)\frac{\partial^2}{\partial\xi^2}-2\xi\frac{\partial}{\partial\xi}-c^2\xi^2+\lambda_\nu(c)\right]\mathcal{G}_z=0$$

$$\text{where } c^2=-\frac{a^4\omega^2}{2}, \quad \lambda_\nu(c)=-z-\frac{a^4\omega^2}{2}-\frac{1}{4}$$

The only solution which is in $L^2((1,\infty),a^2\mathrm{d}\xi)$ near infinity is the following combination of radial spheroidal functions:

$$R_\nu^{0(3)}=R_\nu^{0(1)}+iR_\nu^{0(2)}$$

Asymptotic expansion for $R_\nu^{0(3)}$ as $\xi \to 1+$

- We make use of the relation

$$R_\nu^{0(3)} = [i\cos(\nu\pi)]^{-1}\left[R_{-\nu-1}^{0(1)} - \mathrm{e}^{-i\pi(\nu+1/2)} R_\nu^{0(1)}\right].$$

- Then we convert radial spheroidal functions to angular spheroidal functions with the help of so-called joining factor

$$R_\nu^{0(1)}(c,\xi) = \kappa_\nu^{0(1)}(c)\,\frac{\mathrm{e}^{-i\pi\nu}}{\pi}\,\frac{(c\xi)^\nu}{(c)^\nu(\xi)^\nu}\left[\frac{\pi}{2}\left(2\cos(\nu\pi) - \frac{\sqrt{-\xi-1}}{\sqrt{\xi+1}}\sin(\nu\pi)\right)S_\nu^{0(1)}(c,\xi) - \sin(\nu\pi)S_\nu^{0(2)}(c,\xi)\right]$$

- Angular spheroidal functions may be written in infinite series of Legendre functions

$$S_\nu^{0(2)}(c,\xi) = \sum_{k=-\infty}^{\infty} d_k^{0\nu}(c)\,Q_{\nu+2k}^0(\xi)$$

- Using the asymptotic expansion

$$Q_\nu^0(\xi) \overset{\xi\to 1}{\sim} -\frac{1}{2}\ln\left(\frac{\xi-1}{2}\right) + \Psi(1) - \Psi(\nu+1) - i\frac{\pi}{2} + O((\xi-1)\ln(\xi-1))$$

we conclude that

$$R_\nu^{0(3)}(c,z) \overset{\xi\to 1}{\sim} \alpha\ln(\xi-1) + \beta + O((\xi-1)\ln(\xi-1)).$$

The ratio $\frac{\beta}{\alpha}$ is propotional to the Krein Q-function and holds

$$Q(\lambda_\nu(c)) \propto \frac{\beta}{\alpha} = -\ln(2) - 2\Psi(1) + \frac{2}{A_\nu(c)}\Psi s_\nu(c) - \frac{2\pi}{\tan(\nu\pi)}\left(\frac{\kappa_{-\nu-1}^{0(1)}(c)}{\kappa_\nu^{0(1)}(c)}e^{i\pi(3\nu+3/2)} - 1\right)$$

where $A_\nu(c) = \sum_{k=-\infty}^{\infty} d_k^{0\nu}(c)$, $\quad \Psi s_\nu(c) = \sum_{k=-\infty}^{\infty} d_k^{0\nu}(c)\Psi(\nu+2k+1)$

Theorem

Let $d(x,y)$ denotes the geodesic distance between the points x, y of a two-dimensional manifold X of bounded geometry. Let $U \in \mathcal{P}(X) := \left\{ U \mid U_+ := \max(U,0) \in L^{p_0}_{loc}(X),\ U_- := \max(-U,0) \in \sum_{i=1}^{n} L^{p_i}(X) \right\}$ *for an arbitrary $n \in \mathbb{N}$ and $2 \le p_i \le \infty$ and $A \in (C^\infty(X))^2$. Then the Green function $\mathcal{G}_{A,U}$ of the Schrödinger operator $H_{A,U} = -\Delta_A + U$ has the same on-diagonal singularity as that for the Laplace-Beltrami operator, i.e.,*

$$\mathcal{G}_{A,U}(x,y;\zeta) = \frac{1}{2\pi} \ln \frac{1}{d(x,y)} + \mathcal{G}^{reg}_{A,U}(x,y;\zeta),$$

where $\mathcal{G}^{reg}_{A,U}$ is continuous on $X \times X$. [BGP]

Krein Q-function

Using the previous theorem we conclude for the Krein Q-function

$$Q(\lambda_\nu(c)) = -\frac{1}{2\pi}\left(-\ln(2) - 2\Psi(1) + \frac{2}{A_\nu(c)}\Psi s_\nu(c)\right) + \frac{1}{\tan(\nu\pi)}\left(\frac{\kappa^{0(1)}_{-\nu-1}(c)}{\kappa^{0(1)}_{\nu}(c)} e^{i\pi(3\nu+3/2)} - 1\right)$$

- We may ask for which ν the spheroidal eigenvalue $\lambda_\nu(c)$, $c = i|c|$, is real.
- For those ν, the Krein Q-function should be real too.
- Knowing dependencies of $\lambda_\nu(c)$ and $Q(\lambda_\nu(c))$ on ν, we may find Q-function as a function of spectral parameter.
- For numerical computation we use a Mathematica package Spheroidal.m by Peter Falloon, which I have modified a bit, but it still gives wrong numbers for some values of parameters!

Figure: Dependence of $\lambda_\nu(l)$ on ν. It can be proved that $\lambda_\nu(c) \in \mathbb{R}$ for $\nu \in \mathbb{R}$. Note the axial symmetry with respect to $\nu = -1/2$.

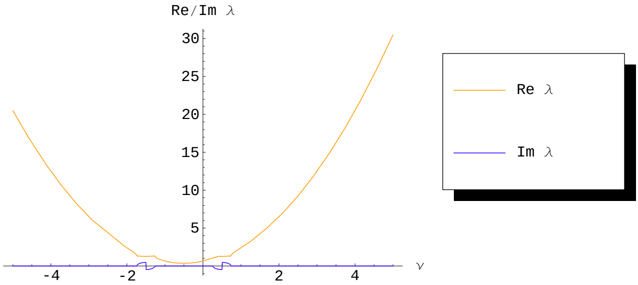


Figure: Dependence of $Q(\lambda_\nu(l))$ on ν.

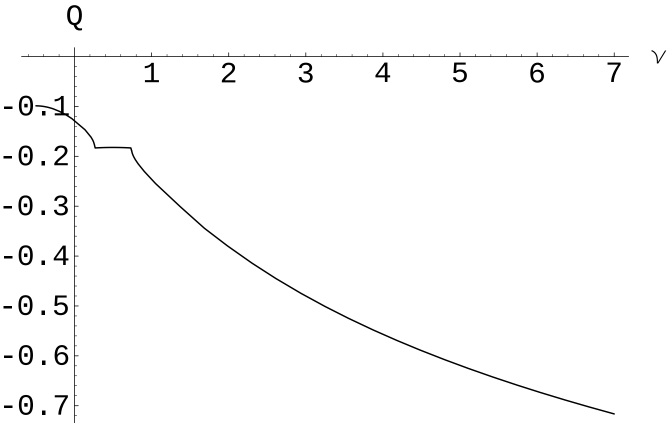
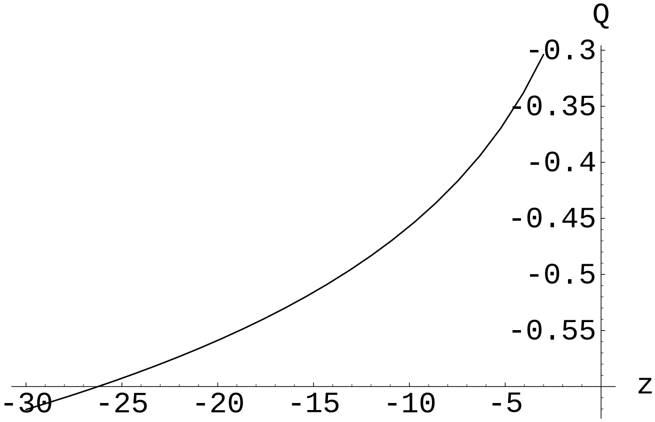


Figure: Krein Q-function as a function of the spectral parameter z. Unfortunately there are still 'white places'.



Fundamental references

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BGP J. Brüning, V. Geyler, and K. Pankrashkin. On-diagonal Singularities of the Green Functions for Schrödinger Operators. *Journal of Mathematical Physics*

AGG S. Albeverio, V. Geyler, and E.N. Grishanov. Point Perturbations in the Spaces of Constant Curvature *preprint*

Thank you for your attention!