Localization of Eigenvalues by a Modification of Müller's Variational Principle in Some Exactly Solvable Cases

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Upper and lower bounds on the eigenvalues of Schrödinger operators with simple one and a simple three dimensional potential (well of finite depth, spherical δ-potential) are given by means of a modification of Müller's variational principle. The estimates, comparing them with the exact eigenvalues, show a localization of the eigenvalues even in a rough approximation for the trial operator.

1. Introduction

Recently, based on the work of Müller [1, 2, 3] and Sölter et al. [4], a variational principle for obtaining both upper and lower bounds for eigenvalues of Schrödinger operators has been given [5, 6, 7]. It is the purpose of this note to exhibit the numerical implementability of this procedure in the case of two simple exactly solvable problems:

The Schrödinger operator H with rectangular potential well of finite depth in one dimension is treated in chapter two. We review the basic inequality on the dimension of eigenspaces of H in the one dimensional case. We optimize the bound by using a Ritz ansatz for the trial operator. This reduces the problem to the calculation of the traces of the first powers of the Rollnik operator

$$W_\varkappa = |V|^{1/2}(-\varkappa^2 - T)^{-1} V^{1/2}.$$

It requires an elementary but tedious integration to calculate these traces. This is done in the appendix. Using these traces the localization of eigenvalues is demonstrated. In the limit of small width and great depth of the well (δ-potential) the resulting bounds are shown to converge to the exact eigenvalue.

In Chapt. 3 we treat the Schrödinger operator with potential concentrated on the surface of a sphere centered around the origin, $V(\boldsymbol{r}) = -d\delta(r-a)$. Using a simplified version (spherical symmetry) of the variational principle given in [7], we show the eigenvalues of the corresponding Schrödinger operator to be exactly localized.

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2. The One Dimensional Potential Well

2.1. Upper Bound on the Dimension of Eigenspaces

Let $H = T + V(x)$ be a Schrödinger operator with potential V such that the Rollnik operator

$$W_\varkappa = |V|^{1/2}(-\varkappa^2 - T)^{-1} V^{1/2} \tag{1}$$

is in some trace ideal $\mathfrak{T}_{2p}(L^2(\mathbb{R}))$, $p = 1, 2, 3, \ldots$, i.e. $\mathrm{tr}(|W_\varkappa|^{2p}) < \infty$. ($|V|^{1/2}(x) = |V(x)|^{1/2}$, $V^{1/2}(x) = \mathrm{sgn}\, V(x)\, |V|^{1/2}(x)$). Then the following inequality (modification of Müller's variational principle) holds [5, 6]:

$$\begin{aligned} &\mathrm{tr}(|[(W_\varkappa - 1)B + W_\varkappa]^\mathrm{P}|^2) \\ &\geq \dim\{\varphi \mid H\varphi = -\varkappa^2\varphi,\ \varphi \in D_\mathrm{H}\} = \mathrm{d}(H, -\varkappa^2) \end{aligned} \tag{2}$$

for every operator $B \in \mathfrak{T}_{2p}$, where H is defined in the quadratic form sense and $\varkappa$ is positive.

In one dimension the free resolvent has the kernel

$$(-\varkappa^2 - T)^{-1}(x, y) = -1/(2\varkappa) \cdot \exp(-\varkappa|x-y|). \tag{3}$$

Therefore, the Rollnik kernel is

$$W_\varkappa(y, x) = -1/(2\varkappa) \cdot |V|^{1/2}(y)\, e^{-\varkappa|x-y|}\, V^{1/2}(x).$$

Thus, given the kernel of B the left hand side of (2) is explicitly given as an integral.

2.2. Optimization of the Bound on the Dimension of Eigenspaces

As known from [5, 6] the optimal bound, i.e. equality in (2), holds for

$$B_{\mathrm{opt}} = -1 - (W_\varkappa - 1)^{-1}, \tag{4}$$

where $(W_\varkappa - 1)^{-1}$ is defined to be the inverse of $W_\varkappa - 1$ restricted to the space orthogonal to

Ker $(W_\varkappa - 1)$ and null on the space orthogonal to $(W_\varkappa - 1)(L^2(\mathbb{R}))$. Motivated by the Fredholm theory, which, if $-\varkappa^2$ is not an eigenvalue of H, yields a convergent series for B_{opt} in the powers of $W_\varkappa$ (see e.g. Simon [8])

$$B_{opt} = \sum_{m=1}^{\infty} a_n W_\varkappa^n, \qquad (5)$$

where the coefficients a_n are functions of the traces of $W_\varkappa^1$, $W_\varkappa^2$, ..., we make the Ritz ansatz

$$B = \alpha W_\varkappa + \beta W_\varkappa^2 + ..., \qquad (6)$$

$\alpha, \beta, ...$ real parameters*. In the simplest case we choose $\beta = ... = 0$. Using this ansatz and assuming $W_\varkappa$ to be Hilbert-Schmidt, i.e. $p = 1$, and self adjoint we get

$$\text{tr} ((\alpha (W_\varkappa - 1) W_\varkappa + W_\varkappa)^2) = \alpha^2 \, \text{tr} (((W_\varkappa - 1) W_\varkappa)^2)$$
$$+ 2 \alpha \, \text{tr} ((W_\varkappa - 1) W_\varkappa^2) + \text{tr} (W_\varkappa^2), \qquad (7)$$

which has its minimum as function of α for

$$\alpha = - \, \text{tr} [(W_\varkappa - 1) W_\varkappa^2]/\text{tr}[((W_\varkappa - 1) W_\varkappa)^2]. \quad (8)$$

Inserting (8) into (7) and using inequality (2) yields

$$g(\varkappa) = [- (\text{tr} \, W_\varkappa^3)^2 + \text{tr} \, W_\varkappa^2 \cdot \text{tr} \, W_\varkappa^4] \qquad (9)$$
$$\cdot /[\text{tr} \, W_\varkappa^4 - 2 \, \text{tr} \, W_\varkappa^3 + \text{tr} \, W_\varkappa^2] \geqq d(H, -\varkappa^2).$$

2.3. Localization of Eigenvalues

For the sake of simplicity we choose V to be a well potential

$$V(x) = \begin{cases} 0 & \text{if } |x| > a, \\ - U & \text{if } |x| \leqq a, \end{cases} \qquad (10)$$

where the parameters a and U are adjusted such that the Schrödinger operator has exactly one eigenvalue. The Rollnik operator $W_\varkappa$ corresponding to the potential (10) is Hilbert-Schmidt and self adjoint.

Now, using the explicit expressions for the traces of $W_\varkappa^2$, $W_\varkappa^3$, and $W_\varkappa^4$ from the appendix we get an explicit expression for $g(\varkappa)$, which is plotted in figure one and two for $a = 1$ cm, $U = 1$ cm^{-1} and $a = 0.1$ cm, $U = 10$ cm^{-1} respectively:

Comparing the figure one and two with the exact eigenvalues given by the solution of the transcendent

* The Fredholm series can be renormalized in order to be applicable to operators in higher trace ideals, too. See e.g. Simon [8].
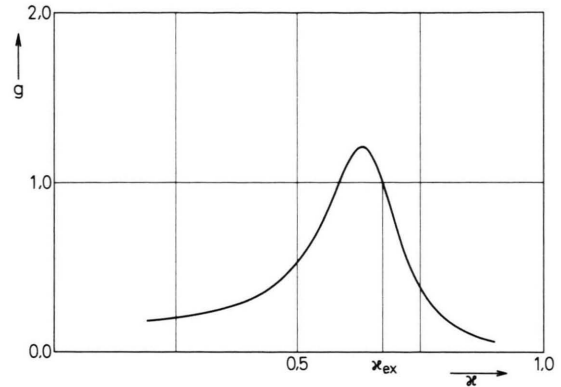

Fig. 1. Localization of the eigenvalue of a Schrödinger operator with well potential ($a = 1$ cm, $U = 1$ cm^{-1}). The exact eigenvalue is $\varkappa = 0.67361 ...$
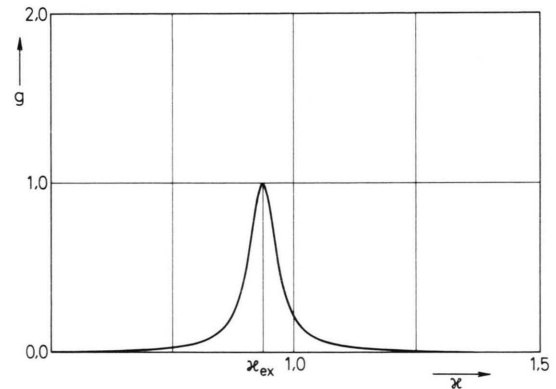

Fig. 2. Localization of the eigenvalue of a Schrödinger operator with narrow well potential ($a = 0.1$ cm, $U = 1$ cm^{-1}). The exact eigenvalue is $\varkappa = 0.94032 ...$ The bound on the dimension of eigenspaces is smaller than one for $\varkappa < 0.93515$ and $\varkappa > 0.94036$.

equation (Flügge [9])

$$\varkappa = (U - \varkappa^2)^{1/2} \, \text{tg} [(U - \varkappa^2)^{1/2} a] \qquad (11)$$

we see them bounded in between the points where $g(\varkappa)$ drops below one as expected by the general theory.

Comparing figure one and figure two with each other shows, that the localization of the eigenvalue is better in the case, where the potential is localized (Fig. 2), than in the case, where the potential is spread out (Fig. 1). This is a manifestation of a general feature which we shall discuss in the next section.

2.4. Limit of the δ-potential

The transcendent equation (11) for the eigenvalues becomes explicitly solvable in the case $c = 2 a U = \text{const}$, $a \to 0$, i.e. for $V(x) = -c\,\delta(x)$:

$$\varkappa = c/2. \tag{12}$$

The traces of the powers of $W_\varkappa$ become

$$\operatorname{tr}(W_\varkappa^n) = (c/2\varkappa)^n \tag{13}$$

in this case. Inserting (13) into (9) yields

$$g(\varkappa) = \frac{-\left(\dfrac{c}{2\varkappa}\right)^6 + \left(\dfrac{c}{2\varkappa}\right)^2\left(\dfrac{c}{2\varkappa}\right)^4}{\left(\dfrac{c}{2\varkappa}\right)^4 - 2\left(\dfrac{c}{2\varkappa}\right)^3 + \left(\dfrac{c}{2\varkappa}\right)^2}, \tag{14}$$

which vanishes except for $\varkappa = c/2$, where the denominator also vanishes. Thus, in this limit case our rough approximation to the optimal trial operator B_{opt} yields the exact eigenvalue. (We remark, that the Fredholm series (5) for B_{opt} contains only the $W_\varkappa^1$-term in the case of the δ-potential. Our Ritz ansatz reproduces this "series".)

3. The Potential $V(r) = -c\,\delta(r - a)$

For Schrödinger operators H with three dimensional spherical symmetric potentials holds the following bound on the dimension of eigenspaces corresponding to given angular momentum quantum number l, m [5, 7]:

$$\operatorname{tr}(\,(W_\varkappa^{l,m} - 1)\,B + |W_\varkappa^{l,m}|^2) \tag{15}$$
$$\geq \dim\{\psi \in D_H \mid H\psi = -\varkappa^2\psi,\ \psi(\mathbf{r}) = \varphi(r)\,Y_{l,m}(\Omega)\};$$

$B \in \mathfrak{T}_2(L^2(\mathbb{R}_+, dr))$, $\varkappa > 0$, $Y_{l,m}$ are spherical harmonics, and

$$W_\varkappa^{l,m}(r, r') = -|V|^{1/2}(r)\,K_{l+1/2}(\varkappa r_>) \tag{16}$$
$$\cdot I_{l+1/2}(\varkappa r_<)\,(r'\,r)^{1/2}\,V^{1/2}(r')$$

$(r_> = \max(r, r')$, $r_< = \min(r, r')$, $K_{l+1/2}$ and $I_{l+1/2}$ modified spherical Bessel functions.

Though obvious, the exact solution of the eigenvalue equation for $H = -\Delta - c\,\delta(r - a)$ seems to be unknown in the literature: Defining $f(z) = \varphi(z/\varkappa)$ one gets the radial equation

$$f''(z) + \frac{2}{z} f'(z)$$
$$+ (-1 - l(l+1)/z^2 - V(z/\varkappa)/\varkappa^2)\,f(z) = 0. \tag{17}$$

Requiring the continuity of the logarithmic derivative yields

$$f(\varkappa a + 0) = f(\varkappa a - 0), \tag{18}$$
$$f'(\varkappa a + 0) - f'(\varkappa a - 0) = -(c/\varkappa)\,f(\varkappa a).$$

For $z \neq \varkappa a$ (17) is Bessel's differential equation. Thus, in order to get a normalizable function with finite kinetic energy f has to have the form

$$f(z) = \begin{cases} A\,(\pi/(2z))^{1/2}\,I_{l+1/2}(z) & \text{if } z < \varkappa a, \\ B\,(\pi/(2z))^{1/2}\,K_{l+1/2}(z) & \text{if } z \geq \varkappa a. \end{cases} \tag{19}$$

Now, using the continuity conditions (17) and (18) and the formula for the Wronskian of $I_{l+1/2}$ and $K_{l+1/2}$ (Abramowitz and Stegun [10]) one ends up with the eigenvalue equation

$$h(\varkappa) = I_{l+1/2}(\varkappa a)\,K_{l+1/2}(\varkappa a)\,c\,a = 1. \tag{20}$$

Analogously to chapter two we shall reproduce this result by the modification of Müller's variational principle for the three dimensional spherical symmetric case. Formally we only have to replace in the formulae (7), (8), and (9) $W_\varkappa$ by $W_\varkappa^{l,m}$. The traces of the powers of $W_\varkappa^{l,m}$ are

$$\operatorname{tr}(W_\varkappa^{l,m})^n = (a\,c\,K_{l+1/2}(\varkappa a)\,I_{l+1/2}(\varkappa a))^n. \tag{21}$$

Thus the left hand side of (15) as a function of $\varkappa$ becomes

$$(-h^6(\varkappa) + h^6(\varkappa))/(h^4(\varkappa) - 2h^3(\varkappa) + h^2(\varkappa)) \tag{22}$$

which vanishes except for $h(\varkappa) = 1$.

4. Conclusions

The Chapt. 2 and 3 demonstrate the numerical implementability of Müller's variational principle in two simple cases. Amazingly enough even a rough approximation for the optimal trial operator B_{opt} is able to localize an eigenvalue of a well potential. Moreover, if the potential is localized (δ-potential), the methods yields exactly the eigenvalue.

Finally let us mention the following: We do not claim that there always occurs an eigenvalue of the Schrödinger operator, if $g(\varkappa)$ is bigger or equal to one; but we do claim that eigenvalues cannot occur, if $g(\varkappa)$ is less than one. In this sense our method is complementary to the Weinstein procedure (Weinstein [11]). For a more complete discussion of this point see [6].

Appendix

Traces of Iterated Rollnik Kernels of One Particle in a Potential Well

The traces can be expressed by integrals as follows:

$$\mathrm{tr}\,(W_\varkappa^k) = (U/(2\varkappa))^k \int_{-a}^{a} \mathrm{d}x_1 \dots \int_{-a}^{a} \mathrm{d}x_k$$
$$\cdot\, e^{-\varkappa(|x_1-x_2|+\dots+|x_k-x_1|)}\,. \tag{1}$$

a) $k = 2$:

$$\mathrm{tr}\,(W_\varkappa^2) = \left(\frac{U}{2\varkappa}\right)^2 \int_{-a}^{a} \mathrm{d}x_1 \int_{-a}^{a} \mathrm{d}x_2\, e^{-2\varkappa|x_1-x_2|}$$

$$= \left(\frac{U}{2\varkappa}\right)^2 \int_{-a}^{a} \mathrm{d}x_1 \left(\int_{-a}^{x_1} \mathrm{d}x_2\, e^{-2\varkappa(x_1-x_2)}\right. \tag{2}$$

$$\left. + \int_{x_1}^{a} \mathrm{d}x_2\, e^{-2\varkappa(x_2-x_1)}\right)$$

$$= \frac{U^2}{8\varkappa^4}\,(4\varkappa a - 1 + e^{-4\varkappa a})\,.$$

b) $k = 3$:

$$\mathrm{tr}\,(W_\varkappa^3) = \left(\frac{U}{2\varkappa}\right)^3 \int_{-a}^{a} \mathrm{d}x_1 \int_{-a}^{a} \mathrm{d}x_2 \int_{-a}^{a} \mathrm{d}x_3$$
$$\cdot\, e^{-\varkappa(|x_1-x_2|+|x_2-x_3|+|x_3-x_1|)}$$

$$= \left(\frac{U}{2\varkappa}\right)^3 \int_{-a}^{a} \mathrm{d}x_1 \int_{-a}^{a} \mathrm{d}x_2 \int_{-a}^{a} \mathrm{d}x_3$$
$$\cdot\, \{e^{-\varkappa(|x_1-x_2|+|x_2-x_3|+|x_3-x_1|)}$$
$$\cdot\, (\theta(x_1-x_2) + \theta(x_2-x_1))$$
$$\cdot\, (\theta(x_2-x_3) + \theta(x_3-x_2))$$
$$\cdot\, (\theta(x_3-x_1) + \theta(x_1-x_3))\}$$

$$\tag{3}$$
$$= \dots = \frac{3}{16}\,\frac{U^3}{\varkappa^6}\,[e^{-4\varkappa a} + 2a\varkappa(e^{-4\varkappa a}+1) - 1]\,,$$

where we have introduced the Heaviside functions to get rid of the absolute values in the exponentials. The same applies for $k > 3$.

c) $k = 4$:

$$\mathrm{tr}\,(W_\varkappa^4) = \left(\frac{U}{2\varkappa}\right)^4 \int_{-a}^{a} \mathrm{d}x_1 \dots \int_{-a}^{a} \mathrm{d}x_4$$
$$\cdot\, e^{-\varkappa(|x_1-x_2|+|x_2-x_3|+|x_3-x_4|+|x_4-x_1|)}$$

$$= \dots = \frac{U^4}{128\,\varkappa^8}\,(40\varkappa a + 80\varkappa a\, e^{-4\varkappa a}$$
$$+ 64\varkappa^2 a^2\, e^{-4\varkappa a} + 28\, e^{-4\varkappa a} + e^{-8\varkappa a} - 29)\,.$$

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