Anal.Math.Phys.
DOI 10.1007/s13324-015-0106-4

Estimate from below for the $x^2 y^4$ potential and closely related potentials

Brice Camus[1]

Received: 20 April 2015 / Revised: 3 June 2015 / Accepted: 9 June 2015

Abstract We give a lower bound on the ground-state energy for the 2-dimensional Schrödinger operator with non-confining potential $x^2 y^4$ on $\mathbb{R}^2$. A method for potentials in dimension $n > 2$ with similar scaling properties is given.

Keywords Ground-state energy · Schrödinger operators · Spectral estimates

1 Introduction and main results

In a very nice article [9], Simon considers Schrödinger operators $-\Delta + V$ with non-confining potentials on $\mathbb{R}^2$ of the special form $V(x, y) = |x|^\alpha |y|^\beta$, $\beta \geq \alpha > 0$, leading to the challenging problem of estimating precisely the counting function of eigenvalues $N(E)$ as $E \to +\infty$. By an easy argument, constructing 'hard walls' by taking powers of the potential V, his result can be applied to the Dirichlet-Laplacian on unbounded domains

$$\Omega_\gamma := \{(x, y) \in \mathbb{R}^2 : |x|^\gamma |y| < 1\}, \quad \gamma > 0.$$

The reader can observe that these 'billards' cannot be governed by usual Weyl-type asymptotics since the Lebesgue volume of Ω_γ is infinite. A similar phenomena holds for the underlying Schrödinger operators of symbols $p(x, y, \xi, \eta) = \xi^2 + \eta^2 + x^\alpha y^\beta$ since the classically allowed areas $\{p \leq E\} \subset \mathbb{R}^4$ are of infinite volume for any positive values of α, β and E. For this reason the precise spectral analysis of p leads

✉ Brice Camus
brice.camus@uni-due.de

1 Mathematisches Institut, Ludwig Maximilians Universität München, Theresienstr. 39, 80803 Munich, Germany

Published online: 17 June 2015

to difficulties and standard methods (e.g. micro-local analysis) cannot be applied. A set of rigorous mathematical methods, strongly based on the Feynman–Kac path integral, is given in [10].

Several generalizations of this, somehow difficult, problem to estimate the number of high energy eigenvalues when the classical volume is infinite are given in [1,5,8,11]. See also our contribution [4] in higher dimension and [7] for some abstract bound on some more general Schrödinger operators with polynomial potentials and magnetic field. Working with 'operator valued trace formulae' or 'operator valued potentials' was also successfully used by A. Laptev and T. Weidl to estimate eigenvalues of Schrödinger operators. See [6] for a description of these results with applications to Lieb–Thirring inequalities.

For example, in physics these 2-dimensional product potential $|x|^\alpha |y|^\beta$ are interesting for 'quantum point contacts' and conductance of materials. See [2] for applications and several references in physics.

In the present work we give an explicit lower bound for the ground state energy of the 2-dimensional Schrödinger operator $H = -\Delta + x^2 y^4$ on $L^2(\mathbb{R}^2)$. By theorem 1.2 of [10] we have the asymptotics:

$$\mathrm{Tr}(e^{-tH}) \sim \omega \frac{\Gamma(5/2)}{\sqrt{\pi}} t^{-2}, \text{ as } t \to 0^+,$$
$$\omega = \mathrm{Tr}\left(\left(-\frac{d^2}{dz^2} + |z|^4\right)^{-3/2}\right) < \infty.$$

This result implies that the spectrum of H is discrete (we recall an easy proof of this fact below). Also by a Tauberian argument, this gives a reliable formula for the counting function of eigenvalues less than E: the large E behavior of $N_H(E)$ and the small t behavior of $\mathrm{Tr}(e^{-tH})$ differ only by a factor Γ.[1]

Our main result concerns the smallest eigenvalue of H:

$$\lambda_0 = \inf\{\lambda,\ \lambda \in \sigma(H)\},$$

the so called ground-state energy of H. In general it is easy to get an upper-bound on λ_0 (e.g. by mini-max) but to get a lower bound is more complicated. Clearly $\lambda_0 \geq 0$ but we can improve:

Theorem 1 *For each $t > 0$, set:*

$$\mathcal{Z}_{SB}(t) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{1}{\sinh(t\sqrt{2k+1})},$$
$$\mathcal{E}(t) = \frac{1}{2}\left(\frac{1}{\sinh(t)} + \frac{1}{t^2}\int_t^{\infty} \frac{z\,dz}{\sinh(z)}\right),$$

[1] The point is that Γ is the Mellin-transform of $t \mapsto e^{-t}$ on the multiplicative group $\mathbb{R}_+$.

then

$$\lambda_0 \geq -\max\left(\frac{1}{t}\mathrm{Log}(\mathcal{Z}_{SB}(t)\right) \geq -\max\left(\frac{1}{t}\mathrm{Log}(\mathcal{E}(t)\right) \geq C > 0.$$

This maximum can be estimated from below with $C \sim 1$.

Comments

- Such an inequality is valid in higher dimension, when $x \in \mathbb{R}^p$ and $y \in \mathbb{R}^q$ for $V(x) = ||x||^2||y||^4$. Here the double bar indicates an Euclidean norm.
- An explicit generalization to operators with a special scaling like $V(x, y, z) = x^2y^4z^8$, and so on, is possible. See Sect. 2 for details.
- The series $\mathcal{Z}_{SB}$ is a theta-Jacobi sum for the Harmonic oscillator. The asymptotics of $\mathcal{Z}_{SB}(t)$ or $\mathcal{E}(t)$ as $t \to 0^+$ are useful to bound from above the number of eigenvalues of H below a given high-energy level E. See [10] or [4] for details.
- We get a numerical value for C by estimating the integral defining $\mathcal{E}$.

Proof of Theorem 1 For all basic questions on spectral theory I will refer to the classical textbook [3]. First, recall that for a Schrödinger operator with a positively homogeneous potential of degree $c \neq -2$, i.e. $V(tx) = |t|^c V(x)$ for all x, we have the following scaling relations for all $\mu > 0$:

$$\sigma(-\Delta + \mu V) = \mu^{\frac{2}{c+2}}\sigma(-\Delta + V), \tag{1}$$

$$\sigma(-\mu\Delta + V) = \mu^{\frac{c}{c+2}}\sigma(-\Delta + V). \tag{2}$$

These equalities are between sets (the respective spectra) and these scaling relations are independent of the dimension n. For example, the semi-classical Hamiltonian $-\hbar^2\Delta + x^2y^4$ is unitarily-equivalent to $\hbar^{\frac{3}{2}}(-\Delta + x^2y^4)$.

For $t > 0$ the quantum partition function is

$$\mathcal{Z}_Q(t) = \mathrm{Tr}\,(e^{-tH}) := \sum_{j=0}^{\infty} e^{-t\lambda_j},$$

and when this makes sense we have $e^{-\lambda_0 t} \leq \mathcal{Z}_Q(t)$. Since for almost all operators we cannot determine the eigenvalues λ_j of H, to get a good lower bound on λ_0 it is pertinent to try to get a good upper bound on $\mathcal{Z}_Q(t)$. Usually, in statistical physics or quantum-chemistry, the method is to approximate $\mathcal{Z}_Q(t)$ by a classical quantum function $\mathcal{Z}_{cl}(t)$. But, when it works, it is perhaps not very good since the classical approximation has only a rational or polynomial decay w.r.t. t but $\mathcal{Z}_Q$ is usually of exponential decay if $H > 0$.

For the operator $H = -\Delta + x^2y^4$ on $L^2(\mathbb{R}^2)$ this 'trick' to estimate the quantum partition function by a classical integral fails. Indeed if we define:

$$\mathcal{Z}_{cl}(t) = \frac{1}{(2\pi)^2}\int_{T^*\mathbb{R}^2} e^{-t(\xi^2+\eta^2+x^2y^4)}dxdyd\xi d\eta,$$

we obtain:

$$(2\pi)^2 \mathcal{Z}_{cl}(t) = \left(\frac{\pi}{t}\right) \int\limits_{\mathbb{R}^2} e^{-tx^2y^4} dxdy = 2\left(\frac{\pi}{t}\right)^{\frac{3}{2}} \int\limits_0^\infty \frac{dy}{y^2} = +\infty.$$

Hence the (Golden–Thompson) inequality $\mathcal{Z}_Q(t) \leq \mathcal{Z}_{cl}(t)$ is of no use here.

Lemma 1 *The spectrum of $H = -\Delta + x^2y^4$ is discrete.*

Proof of Lemma 1 Each of the 1-dimensional operators:

$$-\Delta_x + |x|^2 \geq \nu_2, \; -\Delta_y + |y|^4 \geq \nu_4$$

has a strictly positive lowest eigenvalue (here resp. ν_2 and ν_4). Via Eq. (1) for all $a \in (0, 1)$ we have in terms of quadratic forms on $H^1(\mathbb{R}^2)$:

$$H{=}a(-\Delta{+}x^2y^4){+}(1{-}a)(-\Delta{+}x^2y^4) \geq a\nu_4(-\Delta_x{+}|x|^{\frac{2}{3}}){+}(1{-}a)\nu_2(-\Delta_y{+}|y|^2).$$

Each of the operators appearing in the r.h.s. is a 1-dimensional Schrödinger operator with confining potential. A fortiori H has compact resolvent. □

Remark 1 Of course $\nu_2 = 1$ (ground-state energy of an harmonic oscillator) and the proof of the Lemma also gives an easy bound from below for H in term of the $|x|^{\frac{2}{3}}$ potential.

We can write an operator $A = -\Delta + V(x, y)$, $(x, y) \in \mathbb{R}^p \times \mathbb{R}^q = \mathbb{R}^{p+q}$ on $L^2(\mathbb{R}^{p+q})$, with $V(x, y)$ continuous and bounded from below as a sum:

$$A = -\Delta_x + A_x, \; A_x = -\Delta_y + V(x, y),$$

where A_x is viewed as an operator on $L^2(\mathbb{R}^q)$, i.e. x is a parameter. When A_x has compact resolvent, let $\lambda_k(x)$ be its increasing sequence of eigenvalues (repeated according to their multiplicities as usual). Define:

$$\mathcal{Z}_{SB}(t) := \mathrm{Tr}_{L^2(\mathbb{R}^q)}(\mathrm{Tr}_{L^2(\mathbb{R}^p)} e^{-tH}) = \sum_k \mathrm{Tr}_{L^2(\mathbb{R}^p)}(e^{-t(\Delta_x + \lambda_k(x))}),$$

$$\mathcal{Z}_{cl}(t) = \int\limits_{T^*\mathbb{R}^{p+q}} \frac{e^{-t(||\xi||^2 + V(x,y))}}{(2\pi)^{p+q}} d^{p+q}\xi d^p x d^q y.$$

Here SB stands for ‘sliced bread’, a terminology introduced by B. Simon. The reader should be warned that there is a second way to slice an operator in the form:

$$\mathcal{Z}^*_{SB}(t) := \mathrm{Tr}_{L^2(\mathbb{R}^p)}(\mathrm{Tr}_{L^2(\mathbb{R}^q)} e^{-tH}) = \sum_k \mathrm{Tr}_{L^2(\mathbb{R}^q)}(e^{-t(\Delta_y + \nu_k(y))}),$$

where the $\nu_k(y)$ are now the eigenvalues of $A_y = -\Delta_x + V(x, y)$. Also in general it is easy to check that:

$$\mathcal{Z}^*_{SB}(t) \neq \mathcal{Z}_{SB}(t).$$

These 'sliced-traces' $\mathcal{Z}_{SB}$ and $\mathcal{Z}^*_{SB}$ give a better description of the true quantum partition function $\mathcal{Z}_Q$ since we always have (see Theorem 2.1 of [10]):

$$\mathcal{Z}_Q(t) \leq \mathcal{Z}_{SB}(t) \leq \mathcal{Z}_{cl}(t),$$
$$\mathcal{Z}_Q(t) \leq \mathcal{Z}^*_{SB}(t) \leq \mathcal{Z}_{cl}(t).$$

Now for our potential $V(x, y) = x^2 y^4$, using Eq. (1) the eigenvalues of $-\Delta_x + x^2 y^4$ are $\nu_k(y) = y^2(2k + 1)$, $k \in \mathbb{N}$. It follows that for our specific operator H we have:

$$\mathcal{Z}_Q(t) \leq \mathcal{Z}_{SB}(t) = \sum_{k=0}^{\infty} \mathrm{Tr}_{L^2(\mathbb{R})} \left(e^{-t(-\frac{d^2}{dy^2} + (2k+1)y^2)} \right).$$

By Eq. (1), the spectrum of each of these operator is $\sqrt{2k+1}(2m + 1)$ for $m \in \mathbb{N}$. Since everything is positive, we have obtained:

$$\mathcal{Z}_{SB}(t) = \sum_{m=0}^{\infty} \sum_{l=0}^{\infty} e^{-t(\sqrt{2l+1}(2m+1)} = \frac{1}{2} \sum_{l=0}^{\infty} \frac{1}{\sinh(t\sqrt{2l+1})}$$

Using that:

$$\lambda_0 \geq -\frac{1}{t} \log(\mathcal{Z}_Q(t)) \geq -\frac{1}{t} \log(\mathcal{E}(t)),$$

we can take the sup w.r.t. $t > 0$ in the r.h.s. for both quantities. The inequality for $\mathcal{E}$ follows by monotony w.r.t. l in our series (see Sect. 2 for details). □

2 Generalizations and application

(a) *Increasing the dimension of variables*

Now for $(x, y) \in \mathbb{R}^p \times \mathbb{R}^q$ we consider $V(x, y) = ||x||^2||y||^4$. That the spectrum of $-\Delta + V$ is discrete is established in [1] following the ideas of [10]. For $A_x = -\Delta_x + V(x, y)$ the eigenvalues are:

$$\lambda_k(y) = ||y||^2((2k_1 + 1) + \cdots + (2k_p + 1)), \quad k = (k_1, \ldots, k_p) \in \mathbb{N}^p.$$

It follows that the eigenvalues of $-\Delta_y + \lambda_k(y)$ are:

$$\nu_{k,l} = \sqrt{(2k_1 + 1) + \cdots + (2k_p + 1)}((2l_1 + 1) + \cdots (2l_q + 1)),$$
$$k = (k_1, \ldots, k_p) \in \mathbb{N}^p,\ l = (l_1, \ldots, l_q) \in \mathbb{N}^q.$$

And we get a pleasant upper bound (with exponential decay) given by:

$$\mathcal{Z}_{sb}(t) = \sum_{(k,l)\in\mathbb{N}^{p+q}} e^{-t\nu_{k,l}}.$$

Performing the summation w.r.t. the last index l_q and then comparing the resulting series with some multiple integrals it is not difficult to get the lower bound $\lambda_0 \geq 1$ (for the sliced operator there is a gap between the first eigenvalue 1 and the second one $\sqrt{3}$ that is of finite multiplicity p).

(b) *Increasing the number of variables*

That the spectrum of $-\Delta + |x_1|^{\alpha_1} \dots |x_n|^{\alpha_n}$, $\alpha \in \mathbb{R}^n_+$, is discrete on $L^2(\mathbb{R}^n)$ is established in [4] following the ideas of [10]. As announced the potential $x^2y^4z^8$ on $\mathbb{R}^3$ has also a pleasant scaling. Indeed, via Eq. (1) the spectrum of $-\Delta_x + V(x, y, z)$ is $(2j+1)y^2z^4$, $j \in \mathbb{N}$. By two successive applications of the sliced bread inequality we can use:

$$\begin{aligned}\mathcal{Z}_Q(t) \leq \tilde{\mathcal{E}}(t) &= \sum_{(j,k,l)\in\mathbb{N}^3} e^{-t(2j+1)^{\frac{1}{4}}(2k+1)^{\frac{1}{2}}(2l+1)} \\ &= \frac{1}{2}\sum_{(j,k)\in\mathbb{N}^2} \frac{1}{\sinh\left(t(2j+1)^{\frac{1}{4}}(2k+1)^{\frac{1}{2}}\right)}.\end{aligned}$$

The last expression is now a modified Tetha-Jacobi function for the operator $H = -\Delta + x^2y^4$ on $L^2(\mathbb{R}^2)$ sliced in the x-direction. By induction it is easy to increase the number of exponents and to link the dimension n to the dimension $(n-1)$. Aslo, observe that we can combine (a) and (b) to get explicit bounds for potentials $||x||^2||y||^4||z||^8$ in higher dimensions.

(c) *Semi-classics*

Because of the obvious scaling properties some similar results hold for a Hamiltonian depending on a small positive parameter h:

$$\begin{aligned}H_1 &= -h^2\Delta_{x,y} + ||x||^2||y||^4, \\ H_2 &= -h^2\Delta_x - \Delta_y + ||x||^2||y||^4, \\ H_3 &= -\Delta_x - h^2\Delta_y + ||x||^2||y||^4\end{aligned}$$

For example, the two last operators are useful to describe a system with a massive and a light or non-massive particle (one particle is tagged with h). Observe that all the respective ground-state energies are different since by Eq. (2) these are given by $\lambda_{0,1} = h^{\frac{3}{2}}\lambda_0$, $\lambda_{0,2} = h\lambda_0$ and $\lambda_{0,3} = h^{\frac{4}{3}}\lambda_0$.

(d) *A numerical value for the potential x^2y^4*

Since we are dealing with a monotone function on $\mathbb{R}^+$ we have:

$$\mathcal{Z}_{SB}(t) = \frac{1}{2}\sum_{k=0}^{\infty} \frac{1}{\sinh(t\sqrt{2k+1})} \leq \frac{1}{2\sinh(t)} + \frac{1}{2}\int_0^{\infty} \frac{1}{\sinh(t\sqrt{2x+1})}dx.$$

By change of variable in this integral and scaling t out we get:

$$\mathcal{Z}_{SB}(t) \le \mathcal{E}(t) = \frac{1}{2\sinh(t)} + \frac{1}{2t^2}\int_t^\infty \frac{z dz}{\sinh(z)}.$$

Hence we always have:

$$\lambda_0 \ge -\max_{\{t>0\}} \frac{\log(\mathcal{E}(t))}{t}.$$

It is possible to write down $\mathcal{E}(t)$ in terms of Log and poly-Log functions, but a numerical simulation with mathematica delivers $\lambda_0 \ge C \sim 0,9999$ as lower bound. Both supremum for Z_{SB} and the integral approximation seems to be 1, indicating that the term $(2\sinh(t))^{-1}$ is good enough to obtain a realistic lower bound for λ_0.

Remarks

- Up to lower order terms, the small t behavior of $Z_{SB}(t) \sim \frac{\pi^2}{8t^2}$ is only an upper bound, bigger than the optimal one computed in [10] since we are using here the 'wrong' way to slice our potential x^2y^4. The way degree 4 then degree 2 gives a better bound for $\mathcal{Z}_Q$ in 0^+ but no explicit lower bound for λ_0.
- This coefficient $\frac{\pi^2}{8}$ is precisely related to the zeta-Riemann function and appears as the trace of a power of the resolvent:

$$\mathrm{Tr}((-\Delta + x^2)^{-2}) = \sum_{n=0}^{\infty} \frac{1}{(2n+1)^2} = \frac{\pi^2}{8}.$$

  Using, again, Eq. (1) it is easy to see that this phenomena (a zeta coefficient and an harmonic oscillator) appears for any operator $-\Delta + |x|^{\beta-2}|y|^{\beta}$, $\beta > 2$ on $L^2(\mathbb{R}^2)$. Indeed, the scaling w.r.t. $|x|$ gives a new family of potentials:

$$V_k(y) = \nu_k(|y|^{\beta})^{\frac{2}{2+\beta-2}} = \nu_k|y|^2,$$

  the numbers ν_k being the strictly increasing sequence of eigenvalues of $-\Delta + |x|^{\beta-2}$ on $L^2(\mathbb{R})$.

References

1. Aramaki, J., Nurmuhammad, A.: A note on non-classical eigenvalue asymptotics. Hokkaido Math. J. **30**, 307–325 (2001)
2. Bauer, F., Heyder, J., Schubert, E., Borowsky, D., Taubert, D., Bruognolo, B., Schuh, D., Wegscheider, W., von Delft, J., Ludwig, S.: Microscopic origin of the 0.7-anomaly in quantum point contacts. Nature **501**, 73–78 (2013)
3. Berezin, F.A., Shubin, M.A.: The Schrödinger equation. Springer, Netherlands (1991)
4. Camus B., Rautenberg, N.: Higer dimensional nonclassical eigenvalue asymptotics. J. Math. Phys. **56**, 021506 (2015). doi:10.1063/1.4908126
5. Exner P., Barseghyan, D.: Spectral estimates for a class of Schrödinger operators with infinite volume phase space and potential unbounded from below. J. Phys. A: Math. Theor. **45**, 075204 (2012). doi:10.1088/1751-8113/45/7/075204

6. Laptev, A., Weidl, T.: Recent results on Lieb–Thirring inequalities. Journes Equations aux Drives Partielles (2000) (Exp. No. XX, 14 pp., Univ. Nantes, Nantes, 2000)
7. Mohamed, A., Nourrigat, J.: Encadrement du $N(\lambda)$ pour un oprateur de Schrödinger avec des champs électrique et magnétiques. J. Math Pures et Appl. **70**(1), 87–99 (1991)
8. Robert, D.: Comportement asymptotique des valeurs propres d'opérateurs du type Schrödinger à potentiel "dégénéré". J. Math Pures Appl. **61**, 275–300 (1982)
9. Simon, B.: Some quantum operators with discrete spectrum but classically continuous spectrum. Ann. Phys. **146**, 209–220 (1983)
10. Simon, B.: Nonclassical eigenvalue asymptotics. J. Funct. Anal. **53**(1), 84–98 (1983)
11. Solomyak, M.Z.: Asymptotic behavior of the spectrum of the Schrödinger operator with nonregular homogeneous potential. Mat. Sb. (N.S.) **127**(169), 21–39 (1985) (no. 1)