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Sum rule for the spectra of x^{2m} potentials

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Abstract. An expression for $\mathrm{Tr}\,\hat{H}_m^{-1}$, where $\hat{H}_m = \frac{\hat{p}^2}{2} + \frac{x^{2m}}{2}$ is presented.

Anharmonic oscillators, or more generally, one-dimensional quantum-mechanical systems described by Hamiltonians with polynomial potentials have received considerable attention. This is due to the simplicity of these systems and the fact that the Schrödinger equation for the stationary states of these models is in general not exactly soluble.

Studying anharmonic oscillators has allowed us to obtain a deeper understanding of the perturbation theory (Bender and Wu 1968, 1969). It also contributed considerably to the development of various approximation techniques in quantum mechanics. Pade approximants, Hill determinants, Riccati–Hill method, series expansion method, variational calculations and many other methods have been used for solving the Schrödinger equation for anharmonic oscillators. Due to a lack of space we refer only to a few papers: Killingbeck (1980), Arteca *et al* (1984), Weniger *et al* (1993) where more references to the works devoted to this subject can be found.

In the present paper we consider a particular case of an anharmonic oscillator, namely the system described by the following one-dimensional Hamiltonian

$$\hat{H}_m = \frac{\hat{p}^2}{2} + \frac{\beta}{2} x^{2m} \tag{1}$$

where m is an integer positive number. With the help of the scaling transformation $x \to \beta^{-\frac{1}{2m+2}} x$ the Schrödinger equation corresponding to the Hamiltonian (1) can be reduced to an analogous equation with the parameter $\beta = 1$. Therefore we shall assume that in equation (1) the parameter $\beta = 1$.

The energy spectrum of the Hamiltonians $\hat{H}_m$ can be found analytically in two cases: $m = 1$ (harmonic oscillator) and $m = \infty$ (square well potential). The eigenvalues of $\hat{H}_m$ with $1 < m < \infty$ have to be determined numerically.

Although the exact spectrum of $\hat{H}_m$ with $1 < m < \infty$ is unknown, one can obtain in a simple way the relation which the exact eigenvalues of $\hat{H}_m$ are to satisfy. To obtain this relation we shall use a well known formula

$$\mathrm{Tr}\,\hat{H}_m^{-1} = \sum_{n=1}^{\infty} \frac{1}{E_n^{(m)}} = -2\int_{-\infty}^{\infty} G(x, x, E = 0)\,\mathrm{d}x \tag{2}$$

where $G(x, x', E = 0)$ is the Green's function of the problem

$$\frac{\mathrm{d}^2 y(x)}{\mathrm{d}x^2} - x^{2m} y(x) = 0 \tag{3}$$

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where $y(x)$ satisfies the boundary conditions $\lim_{x\to\pm\infty} y(x) = 0$.

The Green's function of problem (3) can be constructed according to the well known prescription (Kamke 1961)

$$G(x_1, x_2, E = 0) = \frac{\phi_1(x_<)\phi_2(x_>)}{W(x_1)} \tag{4}$$

where $\phi_1(x)$ and $\phi_2(x)$ are solutions of equation (3) satisfying conditions $\lim_{x\to-\infty} \phi_1(x) = 0$ and $\lim_{x\to+\infty} \phi_2(x) = 0$; $W(x) = \phi_1(x)\phi_2'(x) - \phi_1'(x)\phi_2(x)$, $x_<$ and $x_>$ are the lesser and the greater, respectively, of x_1 and x_2. The solutions $\phi_1(x)$, $\phi_2(x)$ are given by the following formulae (Kamke 1961)

$$\phi_2(x) = \sqrt{x} K_{\frac{1}{2m+2}}\left(\frac{x^{m+1}}{m+1}\right) \tag{5a}$$

$$\phi_1(x) = \phi_2(-x) = \sqrt{-x} K_{\frac{1}{2m+2}}\left(\frac{(-x)^{m+1}}{m+1}\right) \tag{5b}$$

where $K_\nu(z)$ is a modified Bessel function (Abramovitz and Stegun 1964). Both $\phi_1(x)$ and $\phi_2(x)$ are entire functions of x. With the help of the known formulae of an analytic continuation of modified Bessel functions (Abramovitz and Stegun 1964) formula (5*b*) can be rewritten more conveniently as

$$\phi_1(x) = \sqrt{x}\left(K_{\frac{1}{2m+2}}\left(\frac{x^{m+1}}{m+1}\right) + \frac{\pi}{\sin\left(\frac{\pi}{2m+2}\right)} I_{\frac{1}{2m+2}}\left(\frac{x^{m+1}}{m+1}\right)\right) \tag{6}$$

where $K_\nu(z)$, $I_\nu(z)$ are modified Bessel functions.

For the Wronsky determinant $W(x)$ one has

$$W(x) = \phi_1(x)\phi_2'(x) - \phi_1'(x)\phi_2(x) = -\frac{(m+1)\pi}{\sin\left(\frac{\pi}{2m+2}\right)}. \tag{7}$$

Substituting expressions (4)–(7) into formula (2) and performing integrations with the help of known formulae (Gradshtein and Ryzhik 1965) one obtains

$$\begin{aligned}\operatorname{Tr} \hat{H}_m^{-1} = {} & \frac{8\sin\left(\frac{\pi}{2m+2}\right)}{(2m+2)\pi}\left(\frac{1}{m+1}\right)^{\frac{m-1}{m+1}} \Gamma\left(\frac{3}{2m+2}\right)\Gamma\left(\frac{1}{m+1}\right)2^{-\frac{2m}{m+1}} \\ & \times \left\{\frac{\Gamma\left(\frac{1}{m+1}\right)\Gamma\left(\frac{1}{2m+2}\right)}{2\Gamma\left(\frac{2}{m+1}\right)} + \frac{\pi}{\sin\left(\frac{\pi}{2m+2}\right)}\frac{\Gamma\left(\frac{2m-2}{2m+2}\right)}{\Gamma\left(\frac{2m}{2m+2}\right)\Gamma\left(\frac{2m+1}{2m+2}\right)}\right\}.\end{aligned} \tag{8}$$

In the limit $m \to \infty$ formula (8) yields $\operatorname{Tr} \hat{H}_\infty^{-1} = \frac{4}{3}$. One could expect this result since in the limit $m \to \infty$ the potential x^{2m} becomes a square well potential: $U(x) = 0$ if $|x| \leqslant 1$, $U(x) = +\infty$ if $|x| > 1$, with the spectrum $E_n = (\pi^2 n^2)/8$ (Landau and Lifshitz 1975) for which, as simple calculation shows, $\sum_{n=1}^{\infty} \frac{1}{E_n^{(\infty)}} = \frac{4}{3}$.

To summarize, a simple analytical expression for the trace of $\hat{H}_m^{-1}$, where $\hat{H}_m$ is the Hamiltonian (1) with $m > 1$, is obtained.

This expression can be used to check the accuracy of the calculations of the spectrum of $\hat{H}_m$. One should note that because of the rather slow convergence of a series $1/(E_n^{(m)})$ (semiclassical estimation suggests that $E_n^{(m)} \sim n^{\frac{2m}{m+1}}$ when $n \to \infty$) the direct calculation of the sum in (2) is inefficient. However, for excited states the semiclassical formulae provide reliable estimations for energy levels. Therefore, the contribution of the levels with large n to the sum (2) can be calculated analytically.

Knowledge of Green's function (4) allows us, in principle, to calculate the expressions $\mathrm{Tr}\,\hat{H}_m^{-2}$, $\mathrm{Tr}\,\hat{H}_m^{-3}\ldots$, i.e. to calculate the coefficients of the following series in powers of E

$$\mathrm{Tr}(\hat{H}_m - E)^{-1} = \sum_{n=0}^{\infty} E^n\,\mathrm{Tr}\,\hat{H}_m^{-n-1}. \tag{9}$$

The function on the left-hand side of equation (9) is a meromorphic function of E having poles at the points $E = E_n^{(m)}$—the energy levels of $\hat{H}_m$. A meromorphic function can be reconstructed (for example with the help of the Pade approximants method) if sufficiently many coefficients of its Tailor series are known.

Numerical results for the coefficients of the series (9) and Pade analysis of the series (9) will be presented elsewhere.

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References

Abramovitz M and Stegun I 1964 *Handbook of Mathematical Functions* (New York: Dover)
Arteca G A, Fernandez F M and Castro E A 1984 *J. Math. Phys.* **25** 932
Bender C M and Wu T T 1968 *Phys. Rev. Lett.* **21** 406
Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
Gradshtein I S and Ryzhik I M 1965 *Tables of Integrals, Series and Products* (New York: Academic)
Kamke E 1961 *Ordinary Differential Equations* (Moscow: Fizmatgiz)
Killingbeck J 1980 *J. Phys. A: Math. Gen.* **13** 49
Landau L D and Lifshitz E M 1975 *Quantum Mechanics* (Oxford: Pergamon)
Weniger E J, Čížek J and Vinette F 1993 *J. Math. Phys.* **34** 571