SPECTRAL SUM RULES FOR CONFINEMENT POTENTIALS^{*)}

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A B S T R A C T

We outline the "sum rule method" recently proposed by the author for estimating low-lying energy levels. As an example, the method is applied to one- and three-dimensional confinement potentials. The estimates obtained for the ground state energies are accurate within an error of about 10^{-4} per cent.

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Consider the motion of a particle with mass m in the spherically symmetric confinement potential $V(r) = gr^p$, $g > 0$, $p > 0$. The corresponding radial Schrödinger operator H_ℓ (with angular momentum ℓ) has only a discrete spectrum, $0 < E_{0\ell} < E_{1\ell} < \dots$. Define the energy moments ($N \in \mathbb{N}$ with $N > (p+2)/2p$)

$$M_\ell^{(N)} \equiv \sum_{n=0}^{\infty} \frac{1}{E_{n\ell}^N} \quad (1)$$

("Zeta function" of the hermitian operator H_ℓ evaluated at $S = N$). We then derive the following embracing relation¹ for the lowest energy $E_{0\ell}$

$$[M_\ell^{(N)}]^{-\frac{1}{N}} \equiv L_\ell^{(N)} < L_\ell^{(N+1)} < \dots < E_{0\ell} < \dots < R_\ell^{(N+1)} < R_\ell^{(N)} \equiv \frac{M_\ell^{(N)}}{M_\ell^{(N+1)}} \quad (2)$$

where the lower (L) and upper (R) bounds converge for $N \rightarrow \infty$ exponentially to the exact energy.

To make practical use of (2), one needs a general method for computing the moments (1). This is provided by the closed integral expression¹

$$M_\ell^{(N)} = \text{Tr } H_\ell^{-N} = \int \prod_{k=1}^N dr_k G_\ell(r_1, r_2) G_\ell(r_2, r_3) \dots G_\ell(r_N, r_1) \quad (3)$$

where G_ℓ denotes the Green's function of H_ℓ . Equations (1) and (3) yield a hierarchy of spectral sum rules for the negative power sums of bound state energies. In conjunction with (2), the sum rules provide the basis of a new and extremely accurate method for estimating low-lying energy levels.

From a general transformation formula² for non-Gaussian path integrals we obtain³ the following Green's function for the above potential $V(r)$ ($r' > r$)

$$G_\ell(r, r') = \frac{4\pi}{r^2} \frac{\sqrt{rr'}}{p+2} K_L\left(\frac{2}{p+2} \sqrt{\frac{2mg}{r^2}} r'^{\frac{p+2}{2}}\right) I_L\left(\frac{2}{p+2} \sqrt{\frac{2mg}{r^2}} r^{\frac{p+2}{2}}\right) \quad (4)$$

K_L , I_L are the modified Bessel functions, $L = (2\ell+1)/(p+2)$. From (4) and (3) we derive the $N = 1$ sum rule ($p > 2$)¹

$$M_\ell^{(1)} = \left(\frac{2m}{r^2(p+2)^2}\right)^{\frac{p}{p+2}} (4g)^{-\frac{2}{p+2}} B\left(\frac{p-2}{2p+4}, \frac{2}{p+2}\right) \frac{\Gamma\left(\frac{p+3}{p+2}\right)}{\Gamma\left(\frac{p+1}{p+2}\right)} \quad (5)$$

$B(x, y)$ is the beta function. The $N = 2$ sum rule has been presented at the workshop, but will not be given here. Let us consider, instead, an infinite square well of radius R ($g = R^{-p}, p > \infty$). As an example, we give the sum rules for $N = 1, 2$ and 6 ($\varepsilon = \pi^2/2mR^2$)¹

$$\varepsilon M_{\ell}^{(1)} = [2(2\ell+3)]^{-1}, \quad \varepsilon^2 M_{\ell}^{(2)} = [2(2\ell+3)^2(2\ell+5)]^{-1}$$

$$\varepsilon^6 M_{\ell}^{(6)} = \frac{168\ell^3 + 1700\ell^2 + 5678\ell + 6219}{(2\ell+3)^6(2\ell+5)^3(2\ell+7)^2(2\ell+9)(2\ell+11)(2\ell+13)} \quad (6)$$

For $\ell = 0$, $\varepsilon M_0^{(N)} = \zeta(2N)/\pi^{2N}$, where $\zeta(s)$ is the zeta function of Riemann.

A numerical computation shows that the embracing relation (2) converges extremely fast (see Table 1 in ¹). From the sum rules for $N = 5, 6$ we obtain the following estimates for the lowest and first excited state: $E_{00} = 1.000\ 000\ 74$, $E_{10} = 0.995\ 731$. (Here and in the following, all values are normalized to the exact energies.) Obviously, the method works very well and leads to high precision estimates for the energies.

It should be clear that our "sum rule method" is not restricted to the radial Schrödinger equation. To give another example, we consider the one-dimensional quartic ($p=4$) and sextic ($p=6$) oscillators. Using the moments given in ⁴ we obtain the following estimates for the two lowest states: $E_0 = 1.000\ 003$, $E_1 = 0.990\ 911$ ($p=4$) and $E_0 = 1.000\ 002$, $E_1 = 0.993\ 611$ ($p=6$).

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