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MAGIC SUM RULES FOR CONFINEMENT POTENTIALS

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A B S T R A C T

It is shown that there exists a hierarchy of sum rules for the inverse power sums of bound state energies which can be exactly calculated for confinement potentials of the form $V(r) = gr^p$, $p > 0$, $g > 0$. The sum rules offer a new method for the calculation of low-lying energy levels. A few illustrative examples of possible applications are given.

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The discovery of the J/ψ and T particles has stimulated much interest in potential models within the framework of non-relativistic quantum mechanics. The potentials which have been phenomenologically successful in describing the charmonium and upsiion spectrum increase for large quark-antiquark separation and thus have built in the confinement of quarks. [For recent reviews, see 1) and 2).] However, up to now, the Schrödinger equation could not be solved analytically for the relevant potentials (with the exception of the S-waves in a linear potential, the harmonic oscillator and the infinite square well). It is therefore highly desirable to have other methods at hand to get information on bound state energies and other physical quantities of interest.

In this letter I shall show that an hitherto unknown class of sum rules for the inverse power sums of bound state energies can be exactly calculated for power-law potentials. Among many interesting applications of these sum rules there is a novel method to calculate the lowest energy eigenvalues by means of an embracing relation (lower and upper bounds which exponentially converge to the exact eigenvalues). The crucial point in the derivation of the new sum rules is the observation³⁾ that the Green function G_ℓ of the radial Schrödinger operator H_ℓ can be exactly calculated for power-law potentials of the form $V(r) = gr^p$, $p > -2$.

In Ref. 3), I derived from a general transformation formula for Green functions⁴⁾ the following expression for the exact Green function for power-law potentials ($p > -2$, $r' > r$)

$$G_\ell(r, r') \equiv \sum_{n=0}^{\infty} \frac{u_{n\ell}(r) u_{n\ell}(r')}{E_{n\ell}}$$

$$= \frac{4m}{\hbar^2} \frac{\sqrt{rr'}}{p+2} K_L(\vartheta') I_L(\vartheta)$$

$$\vartheta = \frac{2}{p+2} \sqrt{\frac{2mg}{\hbar^2}} r^{\frac{p+2}{2}}, \quad \vartheta' = \frac{2}{p+2} \sqrt{\frac{2mg}{\hbar^2}} r'^{\frac{p+2}{2}}, \quad L = \frac{2\ell+1}{p+2}. \quad (1)$$

Here n and ℓ denote the radial quantum number and angular momentum, respectively, and $u_{n\ell}(r)$ are the reduced (normalized) radial wave functions with energy $E_{n\ell}$ (only the discrete spectrum will be considered). K_L and I_L are the modified Bessel functions. The Green function (1) has been explicitly checked in Ref. 3) and 4) for the Coulomb potential ($p=-1$), the harmonic oscillator ($p=2$) and the infinite square well of radius R ($g=R^{-p}$, $p \rightarrow \infty$).

Since the Green function (1) in general does not allow a direct determination of the bound state energies, we propose to work with the following (weighted) energy moments

$$M_{\ell}^{(N,k)} \equiv \text{Tr} (r^k G_{\ell}^{(N)}) = \sum_{n=0}^{\infty} \frac{\langle r^k \rangle_{n\ell}}{E_{n\ell}^N}. \quad (2)$$

Here $G_{\ell}^{(N)}$ is a kind of generalized Green function defined by the recursion relation ($G_{\ell}^{(0)} \equiv \delta(r-r')$, $G_{\ell}^{(1)} \equiv G_{\ell}$)

$$\begin{aligned} G_{\ell}^{(N)}(r, r') &\equiv \int_0^{\infty} dr'' G_{\ell}(r, r'') G_{\ell}^{(N-1)}(r'', r') \\ &= \sum_{n=0}^{\infty} \frac{u_{n\ell}(r) u_{n\ell}(r')}{E_{n\ell}^N}, \end{aligned} \quad (3)$$

and $\langle r^k \rangle_{n\ell}$ is the k^{th} moment of the spatial probability distribution in the state $|n, \ell\rangle$ ($k > -3-2\ell$)

$$\langle r^k \rangle_{n\ell} = \int_0^{\infty} dr r^k [u_{n\ell}(r)]^2. \quad (4)$$

Since for power-law potentials the exact G_{ℓ} is explicitly given by (1), the $G_{\ell}^{(N)}$'s can be exactly calculated by means of (3).

The energy moments (2) provide a new method for the calculation of bound state energies. To demonstrate this, let us consider the case $k = 0$ in (2), i.e., the inverse power sums of the energy eigenvalues, $M_{\ell}^{(N)} \equiv M_{\ell}^{(N,0)} = \sum_{n=0}^{\infty} E_{n\ell}^{-N}$. If we assume that the energies are ordered ($p > 0$, $g > 0$), $0 < E_{0\ell} < E_{1\ell} < \dots$, the N^{th} and $(N+1)^{\text{th}}$ moment give for the lowest energy $E_{0\ell}$ (for a given angular momentum ℓ) the following embracing relation

$$L_{\ell}^{(N)} \equiv \left(\frac{1}{M_{\ell}^{(N)}} \right)^{\frac{1}{N}} < E_{0\ell} < \frac{M_{\ell}^{(N)}}{M_{\ell}^{(N+1)}} \equiv R_{\ell}^{(N)}. \quad (5)$$

In contrast to many other methods for the calculation of energy levels, relation (5) simultaneously gives an upper and lower bound. Thus we can define the N^{th} approximant $[E_{0\ell}]_N$ to the energy $E_{0\ell}$ together with its error $[\Delta_{0\ell}]_N$ by ^{*)}

*) The method can be repeated for the next excited level.

$$[E_{0\ell}]_N \equiv \frac{1}{2} (R_\ell^{(N)} + L_\ell^{(N)})$$

$$[\Delta_{0\ell}]_N \equiv \frac{1}{2} (R_\ell^{(N)} - L_\ell^{(N)}). \quad (6)$$

It is easy to see that both L and R converge for $N \rightarrow \infty$ exponentially to the true eigenvalue

$$R_\ell^{(N)} \sim E_{0\ell} [1 + e^{-N \ln(E_{1\ell}/E_{0\ell})}]$$

$$L_\ell^{(N)} \sim E_{0\ell} [1 - \frac{1}{N} e^{-N \ln(E_{1\ell}/E_{0\ell})}]. \quad (7)$$

To demonstrate that the moment method as described above really works, we have checked it for several cases. The results for the infinite square well of radius R will be presented here. By means of a recursion formula, we have calculated the first six moments ($p=\infty$)

$$\varepsilon M_\ell^{(1)} = \frac{1}{2(2\ell+3)}, \quad \varepsilon = \frac{\hbar^2}{2mR^2}$$

$$\varepsilon^2 M_\ell^{(2)} = \frac{1}{2(2\ell+3)^2(2\ell+5)}$$

$$\varepsilon^3 M_\ell^{(3)} = \frac{1}{(2\ell+3)^3(2\ell+5)(2\ell+7)}$$

$$\varepsilon^4 M_\ell^{(4)} = \frac{10\ell+27}{2(2\ell+3)^4(2\ell+5)^2(2\ell+7)(2\ell+9)}$$

$$\varepsilon^5 M_\ell^{(5)} = \frac{14\ell+45}{(2\ell+3)^5(2\ell+5)^2(2\ell+7)(2\ell+9)(2\ell+11)}$$

$$\varepsilon^6 M_\ell^{(6)} = \frac{168\ell^3 + 1700\ell^2 + 5678\ell + 6219}{(2\ell+3)^6(2\ell+5)^3(2\ell+7)^2(2\ell+9)(2\ell+11)(2\ell+13)} \quad (8)$$

As is well known, the energies for the infinite square well are given by $E_{n\ell} = \varepsilon [j_{n+1}(\ell + \frac{1}{2})]^2$, where $j_m(\lambda)$ denotes the m^{th} positive zero of the Bessel function $J_\lambda(x)$ [with $j_m(\frac{1}{2}) = m\pi$, $m=1,2,\dots$]. Hence the moments (8) are equivalent to the

following sum rules for the zeros of Bessel functions^{*)}

$$\sum_{n=0}^{\infty} \frac{1}{[j_{n+1}(\ell+1/2)]^{2N}} = \varepsilon^N M_{\ell}^{(N)}. \quad (9)$$

The magic sum rules (9) nicely illustrate the point we would like to make in this paper: although there exists no closed expression for the individual zeros of Bessel functions ($\lambda \neq \frac{1}{2}$), their inverse power sums can be exactly calculated and are given by the simple expression (8). In what follows we shall show that the same holds true for the inverse power sums of the bound state energies for power-law potentials.

In the Table we present a numerical evaluation of the embracing relation (5) for the infinite square well using the moments (8). The Table clearly demonstrates that the proposed moment method works well and that the degree to which the approximant (6) coincides with the true energy values even for small N is striking. For S-waves already the first approximant deviates from the exact energy only by 6%, and for $N = 5$ the discrepancy is only 2.75×10^{-4} !

Having demonstrated that the moment method based on the moments (2) and the embracing relation (5) works well in the case $p = \infty$, we would like to show that the moments can be exactly calculated in the general case $p < \infty$. Actually, the integrations to be carried out in (3) are rather tedious (for general p) and lead already for $N = 2$ to rather lengthy expressions in terms of Bessel and Lommel functions⁶⁾. Thus in this letter we content ourselves with the simplest case $N = 1$ ($p < \infty$).

Inserting (1) in (2) we obtain [$g > 0$, $p > 0$, $-2 < k < (p-2)/2$]

$$M_{\ell}^{(1,k)}(p) = \left(\frac{2m}{\hbar^2}\right)^{\frac{p-k}{p+2}} g^{-\frac{2+k}{p+2}} C_{(p)}^{(1,k)} S_{\ell}^{(1,k)}(p). \quad (10)$$

Expression (10) is the exact result for the first (weighted) energy moment for power-law potentials. The dependence on the angular momentum ℓ is completely determined by the function

*) After having derived the moments (8), we learned from Ref. 5) that the lowest sum rules of the type (9) have already been used by Euler in 1781 to determine the three smallest zeros of the Bessel function $J_0(2\sqrt{x})$. Thus we could justly call the moment method proposed in this letter a generalization of "Euler's method". The first five moments in (8) have been calculated first by Rayleigh⁵⁾.

$$S_{\ell}^{(1,k)}(p) = \frac{\Gamma\left(\frac{u+3+k}{p+2}\right)}{\Gamma\left(\frac{u+p+1-k}{p+2}\right)} \quad (11)$$

and C denotes a normalization which depends only on p and k

$$C^{(1,k)}(p) = 2^{-\frac{4+2k}{p+2}} (p+2)^{\frac{2k-2p}{p+2}} B\left(\frac{p-2-2k}{2p+4}, \frac{2+k}{p+2}\right). \quad (12)$$

[$B(x,y)$ is the beta function]. Carrying out the limit $p \rightarrow \infty$ in Eq. (10) (with $g = R^{-p}$) the result agrees with the first energy moment for the infinite square well given in (8).

For $k = 0$ we read off from (10) [by using the definition (2)]

$$E_{n\ell} = \left(\frac{\hbar^2}{2m}\right)^{\frac{p}{p+2}} g^{\frac{2}{p+2}} 2^{\frac{4}{p+2}} (p+2)^{\frac{2p}{p+2}} \varepsilon_{n\ell} \quad (13)$$

with dimensionless energies $\varepsilon_{n\ell}$. Equation (13) reveals the correct scaling behaviour in $\hbar$, m and g for power-law potentials⁷⁾. Using (13) we infer from (10) and (2) the general form of the k^{th} moment of the spatial probability distribution

$$\langle r^k \rangle_{n\ell} = \left(\frac{\hbar^2}{2mg}\right)^{\frac{k}{p+2}} \left(1 + \frac{p}{2}\right)^{\frac{2k}{p+2}} \rho_{n\ell}^{(k)}, \quad (14)$$

where the dimensionless moments $\rho_{n\ell}^{(k)}$ ($\rho_{n\ell}^{(0)}=1$) are independent of $\hbar$, m and g and satisfy the sum rule ($p>0$, $-2 < k < (p-2)/2$)

$$\sum_{n=0}^{\infty} \frac{\rho_{n\ell}^{(k)}}{\varepsilon_{n\ell}} = B\left(\frac{p-2-2k}{2p+4}, \frac{2+k}{p+2}\right) \frac{\Gamma\left(\frac{u+3+k}{p+2}\right)}{\Gamma\left(\frac{u+p+1-k}{p+2}\right)} \quad (15)$$

It is interesting to compare the general results (13) and (14) with the WKB prediction⁸⁾ ($p>0$, $k>-1$)

$$E_{n\ell}^{\text{WKB}} = \left(\frac{\hbar^2}{2m}\right)^{\frac{p}{p+2}} g^{\frac{2}{p+2}} \left[A(p) \left(n + \frac{u+3}{4}\right) \right]^{\frac{2p}{p+2}} \quad (16a)$$

$$A(p) = 2p\sqrt{\pi} \Gamma\left(\frac{3}{2} + \frac{1}{p}\right) / \Gamma\left(\frac{1}{p}\right)$$

$$\langle r^k \rangle_{n_0}^{\text{WKB}} = \left(\frac{E_{n_0}^{\text{WKB}}}{g} \right)^{\frac{k}{p}} \frac{B\left(\frac{k+1}{p}, \frac{1}{2}\right)}{B\left(\frac{1}{p}, \frac{1}{2}\right)} \quad (16b)$$

which shows, of course, the same scaling behaviour in $\hbar$, m and g .

From (16) we can evaluate the N^{th} sum rule for S-waves in the WKB approximation ($-1 < k < [(2N-1)p-2]/2$)

$$\left[\sum_{n=0}^{\infty} \frac{g_{n_0}^{(k)}}{E_{n_0}^N} \right]^{\text{WKB}} = 2^{\frac{4N+2k}{p+2}} \left[\frac{p+2}{A(p)} \right]^{\frac{2pN-2k}{p+2}} \frac{B\left(\frac{k+1}{p}, \frac{1}{2}\right)}{B\left(\frac{1}{p}, \frac{1}{2}\right)} \cdot \zeta\left(\frac{2pN-2k}{p+2}, \frac{3}{4}\right). \quad (17)$$

[$\zeta(z, \alpha)$ is the generalized zeta function⁹⁾]. The breakdown of the WKB approximation at $k = -1$ comes from the pole of the beta function in (16b). Of course, the exact r -moments (4) are regular at $k = -1$. The pole in the approximation (16b) is a reflection of the fact that the simple power-law behaviour, $\langle r^k \rangle_{n_0}^{\text{WKB}} \sim n^{2k/(p+2)}$, breaks down at $k = -1$. Indeed, for e.g. the harmonic oscillator one obtains after a lengthy calculation⁶⁾

$$\begin{aligned} \left\langle \frac{1}{r} \right\rangle_{n_0}^{\text{OSC}} &= \left(\frac{2mg}{\hbar^2} \right)^{1/4} \frac{1}{\pi} \frac{\Gamma(n+1)}{\Gamma(n+3/2)} \left[\psi(n+3/2) + \gamma + 4 \ln 2 + O\left(\frac{1}{n}\right) \right] \\ &\simeq \frac{2}{\pi} \left(\frac{E_{n_0}^{\text{OSC}}}{g} \right)^{-1/2} \ln\left(n + \frac{3}{2}\right), \end{aligned} \quad (18)$$

where $\psi(x)$ is the logarithmic derivative of the gamma function and γ denotes Euler's constant. Since we found a similar logarithmic violation of the WKB formula (16b) in the case of the infinite square well we are led to the conjecture ($a, b, c = \text{const.}$, n large)

$$\left\langle \frac{1}{r} \right\rangle_{n_0} = a \left(\frac{E_{n_0}}{g} \right)^{-1/p} \left[\ln(b+n) + c \right] \quad (19)$$

for all power-law potentials with $0 < p < \infty$.

Since the moments (4) are finite for $k > -3-2l$ one may wonder why the sum rule (15) has a pole already at $k = -2$. If one investigates the moments (4) for

$k < -2$ one discovers that they show an unexpected behaviour as a function of n . The simplest example is again the harmonic oscillator where the Feynman-Hellmann theorem [see Eq. (22)] gives $\langle r^{-2} \rangle_{nl}^{OSC} = 2(2mg/\hbar^2)^{1/2}/(2l+1)$ which is independent of n ! Thus the moments (10) do not exist for $p = 2$, $k = -2$ in agreement with our restriction $k > -2$.

As an illustration, we have evaluated the sum rules (15) and (17) for the quartic potential in the case of S-waves. From the WKB approximation (17) we obtained for $k = 0$, $N = 1$, the value $13.267^{(*)}$ which agrees remarkably well with the exact number 13.211 derived from (15). The WKB result is somewhat too large in agreement with the empirical fact that the WKB energies approximate the exact energies from below.

Recently, Baumgartner, Grosse and Martin¹¹⁾ derived several interesting theorems on the order of levels in potential models. In addition they formulated some improved versions as conjectures. For the quartic potential the conjecture states that the $(n-1)^{th}$ level with angular momentum $l + \sqrt{6}$ lies above the n^{th} level with angular momentum l , i.e., $E_{n,l} < E_{n-1,l+\sqrt{6}}$. If the conjecture is true, the following inequality should hold for the first energy moment

$$M_{l+\sqrt{6}}^{(1)} < M_l^{(1)} - \frac{1}{E_{0l}}. \quad (20)$$

For $l = 0$ we compute from (10) for the left-hand side of (20) 0.4846 and for the right-hand side, 0.5026 ($\hbar=2m=g=1$)^{**)}. Clearly, the inequality (20) is satisfied, and we can conclude that the Baumgartner-Grosse-Martin conjecture is likely to be correct for $l = 0$ and, moreover, seems to be rather optimal in the sense that the inequality (20) is saturated within 3.7%.

Many other sum rules of the type discussed in this letter can be derived for the energy moments (2)⁶⁾. Here we add only the following ($p \geq 2$)

$$\sum_{n=0}^{\infty} \frac{\langle r^{-2} \rangle_{nl}}{E_{nl}^2} = \left(\frac{4m}{\hbar^2} \right) \frac{\psi\left(\frac{l+3}{p+2} + \frac{p-2}{p+2}\right) - \psi\left(\frac{l+3}{p+2}\right)}{(p+2)(l+1)} M_l^{(1,0)}(p). \quad (21)$$

*) The value for $\zeta(4/3, 3/4)$ has been taken from Ref. 10).

**) Here the value $E_{00} = 3.7997$ for the ground state energy has been used¹²⁾.

Equation (21) follows from (2) by taking the derivative with respect to ℓ (for $k=0$, $N=1$) and using the Feynman-Hellmann theorem in the form

$$\frac{\partial E_{n\ell}}{\partial \ell} = \left\langle \frac{\partial H_{\ell}}{\partial \ell} \right\rangle_{n\ell} = \frac{\hbar^2}{2m} (n+1) \left\langle \frac{1}{r^2} \right\rangle_{n\ell}. \quad (22)$$

In this note we have shown that the energy moments (2) can be exactly calculated and that they lead to magic sum rules for power-law potentials. We have given two illustrative examples of possible applications: a check of the accuracy of the WKB approximation and a test of the Baumgartner-Grosse-Martin conjecture on the order of levels. The moments themselves offer an interesting and novel method to calculate low-lying energy levels. This has been demonstrated for the infinite square well.

Finally, it may be worthwhile to point out that the moments introduced in this paper are different from the moments studied in 13), and which are the non-relativistic analogues of the moments used in the famous QCD sum rules¹⁴⁾. There exists, however, the following relation connecting the moments (2) and the moments used in 13) (which we denote by M_N^{QCD}) ($p>0$, $N=2,3,\dots$; $|E| < E_{00}$)

$$\begin{aligned} M_N^{\text{QCD}} &\equiv \sum_{n=0}^{\infty} \frac{4\pi |\psi_n(0)|^2}{(E_{n0} - E)^N} \\ &= \left(\frac{2m g}{\hbar^2} \right)^p \sum_{v=0}^{\infty} \frac{(N+v-1)!}{v! (N-1)!} M_0^{(N+v, p-1)}(p) (-E)^v. \quad (23) \end{aligned}$$

The question whether the moments (2) have a direct application in QCD will be studied elsewhere⁶⁾.

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NOTE ADDED IN PROOF

In the meantime I have checked that the conjecture stated in Eq. (19) is correct within the WKB approximation by following the lines indicated to me by A. Martin. It is a pleasure to thank A. Martin for explaining to me his proof of the conjecture.

	N	$L_{\lambda}^{(N)}$	$[E_{0\lambda}]_N$	$R_{\lambda}^{(N)}$
$\lambda = 0$	1	0.61	1.06	1.52
	2	0.961	1.01	1.064
	3	0.994	1.004	1.013
	4	0.998 983	1.001 032	1.003 080
	5	0.999 801	1.000 275	1.000 748
$\lambda = 5$	1	0.3	1.26	2.2
	2	0.81	1.04	1.26
	3	0.94	1.021	1.10
	4	0.979	1.012	1.044
	5	0.992	1.006	1.021

Table Evaluation of the embracing relation (5) for the infinite square well using the moments (8) for $\lambda = 0, 5$ and $N = 1$ to 5. Also shown is the N^{th} approximant $[E_{0\lambda}]_N$, Eq. (6). The values are normalized to the exact energies, $E_{00} = \epsilon\pi^2$ and $E_{05} = \epsilon 87.531\ 218$, respectively, where the first zero of the Bessel function of order $11/2$ has been taken from Ref. 15).

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