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# Eigenvalue bounds for polynomial central potentials in $d$ dimensions

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## Abstract

If a single particle obeys non-relativistic QM in  $\mathbf{R}^d$  and has the Hamiltonian  $H = -\Delta + f(r)$ , where  $f(r) = \sum_{i=1}^k a_i r^{q_i}$ ,  $2 \leq q_i < q_{i+1}$ ,  $a_i \geq 0$ , then the eigenvalues  $E = E_{n\ell}^{(d)}(\lambda)$  are given approximately by the semi-classical expression  $E = \min_{r>0} \left\{ \frac{1}{r^2} + \sum_{i=1}^k a_i (P_i r)^{q_i} \right\}$ . It is proved that this formula yields a lower bound if  $P_i = P_{n\ell}^{(d)}(q_1)$ , an upper bound if  $P_i = P_{n\ell}^{(d)}(q_k)$  and a general approximation formula if  $P_i = P_{n\ell}^{(d)}(q_i)$ . For the quantum anharmonic oscillator  $f(r) = r^2 + \lambda r^{2m}$ ,  $m = 2, 3, \dots$  in  $d$  dimension, for example,  $E = E_{n\ell}^{(d)}(\lambda)$  is determined by the algebraic expression  $\lambda = \frac{1}{\beta} \left( \frac{2\alpha(m-1)}{mE-\delta} \right)^m \left( \frac{4\alpha}{(mE-\delta)} - \frac{E}{(m-1)} \right)$ , where  $\delta = \sqrt{E^2 m^2 - 4\alpha(m^2 - 1)}$  and  $\alpha, \beta$  are constants. An improved lower bound to the lowest eigenvalue in each angular-momentum subspace is also provided. A comparison with the recent results of Bhattacharya *et al* (1998 *Phys. Lett. A* **244** 9) and Dasgupta *et al* (2007 *J. Phys. A: Math. Theor.* **40** 773) is discussed.

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## 1. Introduction and main results

The purpose of the present work is to establish a global bound formula for the discrete spectrum  $\{E_{n\ell}^{(d)}\}$ ,  $n = 1, 2, \dots$ ,  $l = 0, 1, 2, \dots$  of the  $d$ -dimension Schrödinger equation with polynomial potentials given by

$$\bar{H}\psi = \left( -\Delta + \sum_{i=1}^k a_i r^{q_i} \right) \psi = E\psi, \quad 2 \leq q_i < q_{i+1}, \quad (1)$$

where  $\Delta$  is the  $d$ -dimensional Laplacian operator,  $r = \|\mathbf{r}\|$ ,  $\mathbf{r} \in \mathbf{R}^d$ , and the coefficients  $a_i \geq 0$ , are not all zero. The key motivation for our present study lies in the well-known fact that the majority of quantitative predictions of Schrödinger's equation with a polynomial potential (1) in nuclear, atomic, molecular, and condensed matter physics must usually rely on numerical estimates [1–5]. Thus, a simple global eigenvalue formula can serve as a basis for exploration and also for checking different approximate methods in quantum mechanics [6]. Another important motivation for the present work is a recent contribution by Dasgupta *et al* [7] regarding a general simple scheme for evaluating the ground state as well the excited-state energies for  $\lambda r^{2m}$  quantum anharmonic oscillators in one dimension, see also [6]. We provide in the present work a more general scheme sufficient to generate all energy levels in arbitrary dimension, not only of  $r^{2m}$  quantum anharmonic oscillators, but also for any polynomial potential of the form  $\sum_{i=1}^k a_i r^{q_i}$  with a sufficient degree of accuracy to be interesting. The purpose is not merely to obtain accurate energy eigenvalues for different polynomial potentials for which a large number of methods exist in the literature. Rather, we propose a simple approach which provides energy bounds as well as an approximate energy formula with a reasonable accuracy and with a minimum amount of effort. Consider, as an example, the celebrated quantum anharmonic oscillator [8–23] Hamiltonian  $-\Delta + r^2 + \lambda r^{2m}$ ,  $m = 2, 3, \dots$  in  $d$  dimensions: we show that for any state  $n = 1, 2, \dots$ , the eigenenergy  $E = E_{n\ell}^{(d)}(\lambda)$  is determined approximately by the expression

$$\lambda = \frac{1}{\beta} \left( \frac{2\alpha(m-1)}{mE - \delta} \right)^m \left( \frac{4\alpha}{(mE - \delta)} - \frac{E}{(m-1)} \right), \quad (2)$$

where  $\delta = \sqrt{E^2 m^2 - 4\alpha(m^2 - 1)}$  and  $\alpha$  and  $\beta$  are constants. Further, we show that upper or lower bounds for the energy eigenvalues (2) for a given state are expressed in terms of a single constant for any value of  $\lambda$ . The dependence of  $\alpha$  and  $\beta$  on  $m$  and  $d$  will be discussed in a subsequent section. We obtain our global eigenvalue formula for (1) by using the so-called  $P$ -representation [24] for the Schrödinger spectra generated by the pure power-law potential ( $q > 0$ ). In this representation, a discrete eigenvalue  $\epsilon$  is written as the minimum of a function of one variable  $r$  and a parameter  $P$ : this induces a one–one relation between  $\epsilon$  and  $P$ . More specifically, we write

$$(-\Delta + r^q)\psi_{n\ell}^{(d)} = \epsilon_{n\ell}^{(d)}(q)\psi_{n\ell}^{(d)} \Rightarrow \epsilon_{n\ell}^{(d)}(q) = \min_{r>0} \left[ \frac{1}{r^2} + (P_{n\ell}^{(d)}(q)r)^q \right], \quad (3)$$

where

$$P_{n\ell}^{(d)}(q) = [\epsilon_{n\ell}^{(d)}(q)]^{(2+q)/2q} \left[ \frac{2}{2+q} \right]^{1/q} \left[ \frac{q}{2+q} \right]^{1/2}. \quad (4)$$

This may seem at first sight rather inconvenient since the computation of  $P$  requires the knowledge of  $\epsilon$ . An important advantage of (4), however, is that the computation of  $P$  is independent of the potential parameters. In other words, the computation of  $P$  for  $H = -\Delta + r^q$  is sufficient to yield the discrete spectrum of the Hamiltonian  $H_v = -\Delta + vr^q$  with eigenvalues given by

$$E_{n\ell}^{(d)}(q) = \min_{r>0} \left[ \frac{1}{r^2} + v(P_{n\ell}^{(d)}(q)r)^q \right] \quad (5)$$

for arbitrary  $v > 0$ . This may seem unnecessary for a Hamiltonian of the form  $H_v$  because a simple scaling argument shows  $E_{n\ell}^{(d)}(q; v) = v^{2/(q+2)} E_{n\ell}^{(d)}(q)$ ; but for polynomial potentials, as in (1), where  $a_i > 0$ ,  $i = 1, 2, \dots, k$ , equations (3)–(4) play an important role in establishing

some of the general energy formulas [25] through the decomposition of the Hamiltonian (1) by means of

$$H = -\Delta + \sum_{i=1}^k a_i r^{q_i} = \sum_{i=1}^k \omega_i H^{(i)}, \tag{6}$$

where

$$H^{(i)} = -\Delta + \frac{a_i}{\omega_i} r^{q_i}, \tag{7}$$

and  $\{\omega_i\}_{i=1}^k$  is an arbitrary set of positive weights with sum equal to 1. Further, it is worth mentioning that this dependence can be resolved for certain special values of  $q$ , for example if  $q = 2$ , we know that [26]

$$P_{n\ell}^d(2) \Rightarrow \begin{cases} P_{n\ell}^d(2) = (2n + l + \frac{d}{2} - 2) & \text{if } d \geq 2 \\ P_n(2) = (n - \frac{1}{2}) & \text{if } d = 1. \end{cases} \tag{8}$$

The main results of the present work may be summarized by the following two theorems in which  $\ell$  is to be ignored when  $d = 1$ .

**Theorem A.** Eigenvalue bounds for the spectrum  $\{E_{n\ell}^{(d)}\}$  of the Hamiltonian (1) are given by

$$\mathcal{E} \equiv \min_{r>0} \left[ \frac{1}{r^2} + \sum_{i=1}^k a_i (P_i r)^{q_i} \right], \tag{9}$$

where

- (i) if  $P_i = P_{n\ell}^{(d)}(q_i)$ , then  $\mathcal{E} \leq E_{n\ell}^{(d)}$
- (ii) if  $P_i = P_{n\ell}^{(d)}(q_k)$  then  $\mathcal{E} \geq E_{n\ell}^{(d)}$ .

Here the numbers  $P_{n\ell}^{(d)}(q_i)$  are given by (4).

**Theorem B.** The eigenvalues of the Hamiltonian (1) are given approximately by the semiclassical formula

$$\mathcal{E} \equiv \min_{r>0} \left[ \frac{1}{r^2} + \sum_{i=1}^k a_i (P_i r)^{q_i} \right], \tag{10}$$

where, for the lowest eigenvalue in each angular-momentum subspace, and  $d \geq 1$ , we have the followings.

- (i) For  $n = 1$  and  $P_i = P_{1\ell}^{(d)}(q_i)$ ,  $i = 1, \dots, k$ , then  $\mathcal{E} \leq E_{1\ell}^{(d)}$  for all  $d \geq 1$  and  $l = 0, 1, 2, \dots$ .
- (ii) For  $n \geq 2$  and  $P_i = P_{n\ell}^{(d)}(q_i)$ ,  $i = 1, \dots, k$ ,  $\mathcal{E} \approx E_{n\ell}^{(d)}$ .  
Further, for the lowest eigenvalue in  $d \geq 1$ , we have
- (iii)  $\mathcal{E} \leq E_{10}^{(d)}$  if the numbers  $P_i$  are replaced by the explicit lower approximations for  $P_{10}^{(d)}(q_i)$  given by

$$P_i = \left(\frac{de}{2}\right)^{\frac{1}{2}} \left(\frac{d}{q_i e}\right)^{\frac{1}{q_i}} \left[ \frac{\Gamma(1 + \frac{d}{2})}{\Gamma(1 + \frac{d}{q_i})} \right]^{\frac{1}{d}}, \quad e = \exp(1). \tag{11}$$

- (iv)  $\mathcal{E} \geq E_{10}^{(d)}$  if the numbers  $P_i$  are replaced by the explicit upper approximations to  $P_{10}^{(d)}(q_i)$  given by

$$P_i = \left(\frac{d}{2}\right)^{\frac{1}{2}} \left[ \frac{\Gamma(\frac{d+q_i}{2})}{\Gamma(\frac{d}{2})} \right]^{\frac{1}{q_i}}. \tag{12}$$

The difference between the two parts of theorem B is that, in the first part (i)–(ii), the  $P$  numbers are to be computed from the pure-power energies by use of (4), whereas, in the second part (iii)–(iv), the  $P$  numbers are given explicitly in terms of the Gamma function. We use the term ‘semiclassical’ in the following sense: once the component kinetic potentials have been fixed by the  $P$  numbers, what remains is a minimization over a real function; in the approximation, this expresses the trade-off between the kinetic and potential energies; the final picture is semiclassical since the kinetic energy is reduced to  $1/r^2$  and a wave equation is no longer involved.

In the following section, we discuss the proof of these two theorems. Applications to anharmonic oscillators are presented in sections (3) and (4), and a summary is given in section (5).

## 2. Proof of theorems A and B

### 2.1. Proof of theorem A

The proof of theorem A depends on the application of envelope theory and kinetic potentials technique developed earlier by Hall [27–29] and used successfully since then. We shall outline here a brief summary of the theory to provide us with sufficient details to prove the theorem, and we refer the interested reader to [27–29] for more details. For simplicity, we present this brief summary for the case of  $d = 3$  spatial dimensions: for arbitrary  $d$ , the extension is straightforward. Consider the Schrödinger operators of the form

$$H = -\Delta + v f(r), \quad (13)$$

where  $f$  is the shape of a central potential in  $\mathbf{R}^3$  and  $v > 0$  is the coupling parameter. The principal idea of envelope theory [27, 28] is that the minimization of the Rayleigh quotient  $(\psi, H\psi)/(\psi, \psi)$  is performed in two stages. The first stage, with  $(\psi, -\Delta\psi) = s$  fixed, involves only the shape of the potential  $f$  and leads to a family  $\{\bar{f}_{n\ell}\}$  of kinetic potentials  $\bar{f}_{n\ell}(s)$ . Here  $s$  is a positive constraint variable: it only becomes the mean kinetic energy when the minimization of the sum of the kinetic and potential energies has been effected. We have

$$E_{n\ell} = \min_{s>0} \{s + v \bar{f}_{n\ell}(s)\}, \quad (14)$$

in which the critical value of  $s = (\psi, -\Delta\psi) > 0$  is the mean kinetic energy. The kinetic potentials [25], which represent the result of min–max theory applied to the potential shape  $f$  for fixed  $s$ , are given as a Legendre transformation  $\{s = E(v) - vE'(v), \bar{f}(s) = E'(v)\}$  of the function  $E(v)$ , which describes how the eigenvalue depends on the coupling  $v$ . They may also be defined by the following general formula:

$$\bar{f}_{n\ell}(s) = \inf_{\mathcal{D}_{n\ell}} \sup_{\substack{\psi \in \mathcal{D}_{n\ell} \\ \|\psi\|=1}} \int \psi(r) f([(\psi, -\Delta\psi)/s]^{1/2} r) \psi(r) d^3r, \quad (15)$$

where  $\mathcal{D}_{n\ell}$  is the span of a set of  $n$  linearly independent functions. It is interesting to note that the kinetic potential  $\bar{f}_{n\ell}$  can be replaced by the potential  $f(r)$  itself through the parameterization of  $\bar{f}_{n\ell}(s)$  in terms of the variable  $r$  (used here as a new parameter to replace  $s$ ), that is to say  $\bar{f}_{n\ell}(s) = f(r)$ . We now invert this monotone function to give the  $K$  functions [29]

$$s = (\bar{f}_{n\ell}^{-1} \circ f)(r) = K_{n\ell}^{(f)}(r). \quad (16)$$

It is easy to show that the  $K$  functions obey the scaling property

$$A f\left(\frac{r}{b}\right) + B \rightarrow \left(\frac{1}{b^2}\right) K\left(\frac{r}{b}\right), \quad (17)$$

and in general they are independent of coupling and potential shifts [29]. The eigenvalues are recovered from the  $K$  functions by the expression

$$E_{n\ell} = F_{n\ell}(v) = \min_{r>0} \{ K_{n\ell}^{(f)}(r) + vf(r) \}. \tag{18}$$

For the power-law potentials  $f(r) = r^q$ , it is known by means of simple scaling argument that the spectrum of the pure-power Hamiltonian satisfies

$$-\Delta + vr^q \rightarrow F_{n\ell}^{(q)}(v) = E_{n\ell}^{(q)}(1)v^{2/(q+2)}. \tag{19}$$

In order to compute the kinetic potentials  $\bar{f}_{n\ell}(s)$ , we note from the minimization process of (14) that  $\bar{f}'_{n\ell}(s) = -v^{-1}$ , and consequently we have

$$s = F_{n\ell}^{(q)}(v) - v\bar{f}_{n\ell}(s) \Rightarrow \bar{f}_{n\ell}(s) = \frac{d}{dv} F_{n\ell}^{(q)}(v), \tag{20}$$

which implies using (19) that

$$\bar{f}_{n\ell}(s) = \frac{2}{q+2} v^{-\frac{q}{q+2}} E_{n\ell}^{(q)}(1). \tag{21}$$

On the other hand, we have from the lhs of (20) that

$$v^{-1} F_{n\ell}^{(q)}(v) = \bar{f}_{n\ell}(s) - s\bar{f}'_{n\ell}(s), \tag{22}$$

which implies using (21) that

$$\bar{f}_{n\ell}(s) = \frac{2}{q} \left( \frac{q E_{n\ell}^{(q)}}{q+2} \right)^{(q+2)/2} s^{-q/2}. \tag{23}$$

The  $K$  functions are then computed by means of (16) and (20)–(23) to yield

$$K_{n\ell}^{(f)}(r) = \left( \frac{2}{q} \right)^{2/q} \left( \frac{q E_{n\ell}^{(q)}}{q+2} \right)^{(q+2)/q} \frac{1}{r^2} = \left( \frac{P_{n\ell}(q)}{r} \right)^2, \tag{24}$$

where we have defined

$$P_{n\ell}(q) = (E_{n\ell}^{(q)})^{(2+q)/2q} \left[ \frac{2}{2+q} \right]^{1/q} \left[ \frac{q}{2+q} \right]^{1/2}. \tag{25}$$

The eigenvalues are then recovered by (18) as

$$E_{n\ell} = \min_{r>0} \left\{ \left( \frac{P_{n\ell}(q)}{r} \right)^2 + vr^q \right\}. \tag{26}$$

In order to obtain a definite bound, Hall [27] used interesting geometric interpretation in terms of envelopes. If the potential shape  $f(r) = g(h(r))$  is a smooth transformation  $g$  of a soluble potential  $h$ , then the kinetic potentials associated with  $f(r)$  are given by

$$f(r) = g(h(r)) \Rightarrow \bar{f}_{n\ell}(s) \approx g(\bar{h}_{n\ell}(s)), \tag{27}$$

and the corresponding  $K$  functions satisfies

$$K_{n\ell}^{(f)} = (g \circ \bar{h}_{n\ell})^{-1} \circ (g \circ h) \approx \bar{h}_{n\ell}^{-1} \circ h = K_{n\ell}^{(h)}. \tag{28}$$

Therefore

$$f = g(h) \Rightarrow K^{(f)} \cong K^{(h)}, \tag{29}$$

and the eigenvalue approximations are given by

$$E_{n\ell} \approx \min_{r>0} \{ K_{n\ell}^{(h)}(r) + vf(r) \} \tag{30}$$

in which  $g$  no longer appears. This expression yields upper or lower bounds depending, respectively, whether  $g$  is concave or convex [25, 26]. For  $f(r) = g(r^q) = \sum_{i=1}^k a_i r^{q_i}$ , since  $q_i < q_{i+1}$ , clearly  $g$  is convex if  $q = q_1$  (lower bound) and concave if  $q = q_k$  (upper bound). We therefore have, by using (30) with  $h(r) = r^q$ ,

$$E_{n\ell} = \min_{r>0} \left\{ \left( \frac{P_{n\ell}(q)}{r} \right)^2 + v \sum_{i=1}^k a_i r^{q_i} \right\}. \quad (31)$$

Or, equivalently, and by a change in the minimization variable,

$$E_{n\ell} = \min_{r>0} \left\{ \frac{1}{r^2} + v \sum_{i=1}^k a_i (P_{n\ell}(q)r)^{q_i} \right\}. \quad (32)$$

With  $v = 1$ , this equation yields (9) and we obtain a lower bound if  $q = q_1$  and an upper bound if  $q = q_k$ . This completes the proof of the theorem.

## 2.2. Proof of theorem B

The first part of theorem B was introduced [25] to improve the lower bounds for the ground state energy obtained in theorem A. The second part is based on the Barnes *et al*'s [30] general lower bound formula for the lowest eigenvalue of the Schrödinger operator  $H = -\Delta + V(r)$  in  $d \geq 1$  spatial dimensions. The extension to the potential sums, such as that of (1), was introduced in [31], where a detailed proof of theorem B can be found.

## 3. Fractional anharmonic oscillator

Before we study specific problems in quantum mechanics, we first consider the application of theorems A and B to the class of arbitrary fractionally anharmonic oscillator Hamiltonians [32]:

$$H = -\Delta + \sum_{\delta \in Z} g_\delta r^\delta, \quad (33)$$

where  $Z$  is an arbitrary finite set of the integer or rational numbers and the coupling  $g_\delta$ ,  $\delta \in Z$  are chosen so that the Hamiltonian supports the existence of a discrete spectrum. It is known [32–35] that this class of Hamiltonian possesses elementary solutions for certain particular cases of the coupling  $g_\delta$ . For consistency, we assume  $\delta \geq 2$ , although the conclusions of theorems A and B are perfectly applicable for all  $\delta \geq -1$ , where, for example, the  $P$  number in the case  $\delta = -1$  is  $P_{n\ell}^{d \geq 2}(-1) = (n + l + d/2 - 3/2)$ . This class of Hamiltonian is a generalization of the Hamiltonian

$$H = -\Delta + Cr^\alpha + Dr^\beta, \quad \beta > \alpha > 0, \quad (34)$$

which has been used in the theory of heavy quarkonia [36, 37]. Denote  $q = \min_{\delta \in Z} \{\delta\}$  and  $Q = \max_{\delta \in Z} \{\delta\}$ . By using theorem A, we immediately find analytic expressions for lower bounds  $\epsilon_{n\ell}^d$  and upper bounds  $E_{n\ell}^d$  for the eigenvalues of the Hamiltonian (33): these can be written explicitly as

$$\epsilon_{n\ell}^d(\delta) = \min_{r>0} \left[ \frac{1}{r^2} + \sum_{\substack{\delta \in Z \\ q = \min\{\delta\} \\ \delta \in Z}} g_\delta (P(q)r)^\delta \right], \quad (35)$$

and

$$E_{n\ell}^d(\delta) = \min_{r>0} \left[ \frac{1}{r^2} + \sum_{\substack{\delta \in Z \\ Q = \max_{\delta \in Z} \{\delta\}}} g_\delta (P(Q)r)^\delta \right]. \tag{36}$$

Here the numbers  $P(q)$  and  $P(Q)$  are computed numerically by means of equation (3) for rational  $q, Q \neq -1, 2$  by the use of direct numerical integration of the corresponding Schrödinger equations  $(-\Delta + r^q)\psi = E_q\psi$  and  $(-\Delta + r^Q)\psi = E_Q\psi$ . An interesting improvement for the eigenvalues  $\epsilon_{1\ell}^d(\delta)$  and  $E_{1\ell}^d(\delta)$  can be obtained through the application of theorem B. The cost, however, is that the exact eigenvalues of the rational power-law potentials  $V(r) = r^\delta$  for each  $\delta \in Z$  must be computed numerically. Less accurate bounds can be obtained directly using the explicit  $P$  numbers (11) and (12). An important class [32] of the fractional anharmonic oscillator Hamiltonians (33) that have found many applications [32] in quantum field theory [33] is given by

$$H = -\Delta + V(r) = -\Delta + \sum_{j=1}^{2q+1} g_j r^{2j}, \quad g_{2q+1} = a^2 > 0. \tag{37}$$

This class of Hamiltonians has found many applications not only in quantum mechanics, where  $V(r)$  represents [32] an arbitrary potential not only in the limit  $q \rightarrow \infty$ , but also, for example, in the Reggeon field theorem on the lattice [38]. Theorem A gives immediate lower and upper bounds to the eigenvalues of (37) as

$$\epsilon_{n\ell}^d(\delta) = \min_{r>0} \left[ \frac{1}{r^2} + \sum_{j=1}^{2q+1} g_j (P_{n\ell}^d(2)r)^{2j} \right]. \tag{38}$$

and

$$E_{n\ell}^d(\delta) = \min_{r>0} \left[ \frac{1}{r^2} + \sum_{j=1}^{2q+1} g_j (P_{n\ell}^d(4q+2)r)^{2j} \right], \tag{39}$$

where  $P_{n\ell}^d(2)$  is given by equation (8) and  $P_{n\ell}^d(4q+2)$  is given by (3), respectively.

#### 4. Quantum anharmonic oscillator

In this section, we consider the Schrödinger equation

$$(-\omega\Delta + ar^2 + br^{2m})\psi = E(\omega, a, b)\psi, \quad m = 2, 3, 4, \dots, \tag{40}$$

where  $\omega, a$  and  $b$  are positive parameters and the potential in (33) is a single-well potential which describes for  $m = 2, 3, 4, 5, \dots$  the quartic, sextic, octic and decadic oscillators, and so on. It is easy to check that for the energy in (40), the following scaling relation holds:

$$E(\omega, a, b) = (a\omega)^{1/2} E\left(1, 1, \frac{b\omega^{(m-1)/2}}{a^{(m+1)/2}}\right), \tag{41}$$

$$\psi(r; \omega, a, b) = \psi\left(\left(\frac{a}{\omega}\right)^{\frac{1}{4}} r; 1, 1, \frac{b\omega^{(m-1)/2}}{a^{(m+1)/2}}\right).$$

Thus the original problem (40) is essentially a single-parameter problem which we now write as

$$H^{(m)}\psi = (-\Delta + r^2 + \lambda r^{2m})\psi = E(\lambda)\psi, \quad m = 2, 3, 4, \dots, \tag{42}$$



where  $E(\lambda) = E(1, 1, \lambda)$  and  $\lambda = \frac{b\omega^{(m-1)/2}}{a^{(m+1)/2}}$ . The Schrödinger equation with the quantum anharmonic oscillators (42) are among the most widely studied models in quantum mechanics. In spite of their simplicity, they give rise to interesting problems, both computationally and conceptually [23]. A rigorous analysis of the mathematical properties of the anharmonic oscillator Hamiltonians  $H^{(2)}$  was made by Simon [8] and by the seminal work of Bender and Wu [9]. The aim in the discussion we present below is to derive simple upper and lower bound formulas based on theorems A and B. For the anharmonic oscillator potentials

$$f(r) = r^2 + \lambda r^{2m}, \quad m = 2, 3, \dots \tag{43}$$

Theorem A implies that

$$\mathcal{E}(\lambda) \approx \min_{r>0} \left[ \frac{1}{r^2} + \alpha r^2 + \lambda \beta r^{2m} \right], \tag{44}$$

where

- $\mathcal{E}(\lambda) \leq E(\lambda)$  is a lower bound, if  $\alpha = (P_{n\ell}(2))^2$  and  $\beta = (P_{n\ell}(2))^{2m}$ .
- $\mathcal{E}(\lambda) \geq E(\lambda)$  is an upper bound, if  $\alpha = (P_{n\ell}(2m))^2$  and  $\beta = (P_{n\ell}(2m))^{2m}$ .

Furthermore, theorem B implies that if  $\alpha = (P_{n\ell}(2))^2$  and  $\beta = (P_{n\ell}(2m))^{2m}$ , then  $\mathcal{E}(\lambda) \leq E(\lambda)$  for  $n = 1$ , and  $\mathcal{E}(\lambda) \approx E(\lambda)$  for all  $n \geq 2$ . Let  $x = r^2$ , we note that the minimization of (44) occurs at  $-\frac{1}{x^2} + \alpha + m\lambda\beta x^{m-1} = 0$ . Multiplying through by  $x$  and solving for  $\lambda\beta x^m$ , we can easily show that the minimization of (44) occurs at

$$r^2 = \frac{mE - \sqrt{E^2 m^2 - 4\alpha(m^2 - 1)}}{2\alpha(m - 1)}, \tag{45}$$

and consequently we have

$$\lambda = \frac{1}{\beta} \left( \frac{2\alpha(m - 1)}{mE - \delta} \right)^m \left( \frac{4\alpha}{(mE - \delta)} - \frac{E}{(m - 1)} \right), \tag{46}$$

where  $\delta = \sqrt{E^2 m^2 - 4\alpha(m^2 - 1)}$ . Thus for finding the energy eigenvalues of anharmonic-oscillator Hamiltonians  $H^{(m)}$  in (42) one has to solve equation (46) for the given  $\lambda$ . It is clear that at  $\lambda = 0$ , equation (46) implies  $E = 2\sqrt{\alpha}$ , with  $\alpha = (P_{n\ell}^{(d)}(2))^2 = (2n + l + \frac{d}{2} - 2)^2$ , as given by (8). Consequently,  $E = 4n + 2l + d - 4$ , the result for the  $d$ -dimensional harmonic oscillator [39]. When equation (46) is used to determine the lower or the upper bounds to the exact eigenvalues of the  $\lambda r^{2m}$  oscillator, it is clear that the formula is expressed in terms of a single constant for any value of  $\lambda$ . This follows from the fact that, for lower or upper bounds,  $\alpha^m = \beta$  and equation (46) reduces to

$$\lambda = \frac{2^m(m - 1)^{(m-1)}}{(m + 1)} \frac{(-E + \sqrt{m^2 E^2 - 4\alpha(m^2 - 1)})}{(mE - \sqrt{m^2 E^2 - 4\alpha(m^2 - 1)})^m}. \tag{47}$$

This is a remarkable simple formula that gives a global lower and upper bounds to the exact eigenvalues for a given  $\lambda$  for all  $n = 1, 2, \dots$  and  $l = 0, 1, 2, \dots$  in  $d$  dimensions, accordingly as  $\alpha = (2n + l + \frac{d}{2} - 2)^2$  and  $\alpha = (P_{n\ell}^{(d)}(2m))^2$ , respectively. In particular, a global formula that gives a lower bound for all  $n = 1, 2, \dots, m = 2, 3, \dots$  is

$$\lambda = \frac{2^m(m - 1)^{(m-1)}}{(m + 1)} \frac{(-E + \sqrt{m^2 E^2 - 4(2n + l + \frac{d}{2} - 2)^2(m^2 - 1)})}{(mE - \sqrt{m^2 E^2 - 4(2n + l + \frac{d}{2} - 2)^2(m^2 - 1)})^m}. \tag{48}$$

Note in the case of  $d = 1$ , we should set either  $l = -1$  or  $l = 0$  to obtain a lower bound to even or odd (exact) eigenvalues, respectively. Despite the generality of (47), we should like

**Table 1.** Values of  $P_{10}^{(1)}(2m)$  and  $\beta = (P_{n\ell}^{(1)}(2m))^{2m}$  for different  $m$ .

$m$	$P_{10}^{(1)}(2m)$	$\beta$
2	0.648 283 101 647 7214	0.176 627 696 530 9679
3	0.752 213 287 729 7533	0.181 153 198 043 2237
4	0.830 692 879 447 4723	0.226 737 786 349 0461
5	0.892 746 975 167 7408	0.321 576 181 371 2828
6	0.943 407 187 840 8251	0.497 038 660 113 3180

to make two immediate remarks concerning the application of theorem A: (i) formula (47), in general, gives a loose bound; (ii) the upper bound  $\alpha = (P_{n\ell}^{(d)}(2m))^2$ ,  $m = 2, 3, \dots$  which is obtained by means of equation (4), requires the knowledge of the exact eigenvalues of the Schrödinger equation  $(-\Delta_d + r^{2m})\psi = \epsilon_{n\ell}^{(d)}(2m)\psi$ . In this paper, we have found the values of  $P_{n\ell}^{(d)}(2m)$  by the numerical integration of the Schrödinger equation just mentioned, and then we used equation (4) to find the corresponding  $P$  numbers. For immediate use of equations (47) and (48), we report in table 1 the values of  $P_{10}^{(1)}(2m)$  and  $\beta = (P_{n\ell}^{(1)}(2m))^{2m}$  for different values of  $m$ .

In order to illustrate the above discussion, we consider the case of finding the eigenvalues of the anharmonic oscillator Hamiltonian  $-\frac{d^2}{dr^2} + r^2 + 0.01r^4$ . Equation (48) gives a lower bound 1.002 48 and equation (47) with  $\alpha = (P_{10}^{(1)}(2m))^2$  gives an upper bound of 1.320 38. The exact eigenvalue in this case reads 1.007 37. In order to improve these bounds, we can make use of theorem B. For the ground state eigenvalues in  $d \geq 1$ , the first part of theorem B can be applied to obtain a more accurate lower bound formula. Further, the second part of theorem B can be used to obtain straightforward lower and upper bounds without the necessity of the numerical computation of  $P$  numbers, thanks to the explicit approximate values of  $P_{10}^{(d)}(2m)$  given by (11) and (12). In either case, equation (46) gives a simple general formula for the energy bound of  $E = E(\lambda)$  with reasonable accuracy

$$\frac{1}{2^m} \frac{(m-1)^{(m-1)}}{(m+1)} \frac{(-E + \sqrt{m^2(E^2 - d^2) + d^2})}{(mE - \sqrt{m^2(E^2 - d^2) + d^2})^m} = \beta\lambda, \tag{49}$$

for  $m = 2, 3, \dots$ , where now if  $\beta = (P_{10}^{(d)}(2m))^{2m}$  as given by table (1), equation (48) gives a lower bound for given  $\lambda$ . The results of this formula are illustrated in the last columns of tables 2 and 3. On the other hand, if  $\beta$  is a fixed number given by (11) and (12), then equation (49) gives lower and upper bounds, respectively. Note that theorem B still allows us to conclude that equation (49) yields a reasonable approximation to the excited-state energies for  $n \geq 2$ . However, in this case  $\beta = (P_{n0}^{(d)}(2m))^{2m}$  is strictly given by (4). In the case of  $d = 1$ , equation (48) reads ( $m = 2, 3, \dots$ )

$$\frac{1}{2^m} \frac{(m-1)^{(m-1)}}{(m+1)} \frac{(-E + \sqrt{m^2(E^2 - 1) + 1})}{(mE - \sqrt{m^2(E^2 - 1) + 1})^m} = \beta\lambda, \tag{50}$$

where  $\beta = (P_{10}^{(1)}(2m))^{2m}$  is given by (11) and (12) for a lower and an upper bounds respectively. Equation (50) can be compared with the recent formula introduced by Bhattacharya *et al* [6] for the approximate ground state energy of the Hamiltonian  $-\Delta + r^2 + \lambda r^{2m}$  in one dimension, namely

$$(E^{(m)})^{(m+1)} - (E^{(m)})^{(m-1)(1+2/(m+2+\lambda))} = (K_0^{(m)})^{(m+1)}\lambda, \tag{51}$$

**Table 2.** Calculated values of upper and lower bounds, using (43), to the ground state energy of the quartic anharmonic oscillator, along with exact values, for different values of  $\lambda$ . The comparison between the lower bound  $E_L$  given by equation (43) using the exact values of  $\beta$  by means of table 1, and the approximate eigenvalues  $E_b$  of Bhattacharya *et al* [6] using (44) are also shown.

$\lambda$	Exact value	Lower bound using equation (43)	Upper bound using equation (43)	$E_b$ Reference [6]	$E_L$ using equation (43)
0.001	1.000 75	1.000 62	1.000 75	1.000 79	1.000 71
0.01	1.007 37	1.006 14	1.007 39	1.007 83	1.006 97
0.1	1.065 29	1.055 85	1.066 20	1.070 05	1.062 75
0.2	1.118 29	1.102 88	1.120 62	1.127 02	1.114 73
1.0	1.392 35	1.355 10	1.403 32	1.411 55	1.387 54
4.0	1.903 14	1.836 99	1.928 81	1.914 89	1.898 95
10.0	2.449 17	2.356 48	2.488 62	2.450 05	2.445 75
50.0	4.003 99	3.841 639	4.078 522	3.996 21	4.001 82
100.0	4.999 42	4.793 95	5.095 16	4.991 61	4.997 66
1000.0	10.639 79	10.194 49	10.851 51	10.635 21	10.638 96
2000.0	13.388 44	12.827 06	13.655 91	13.384 74	13.387 78

**Table 3.** Calculated values of upper and lower bounds to the ground state energies of the sextic anharmonic oscillator along with exact values for different values of  $\lambda$ . The comparison between the lower bound  $E_L$  given by equation (43) and the approximate eigenvalues  $E_b$  of Bhattacharya *et al* [6] using (44) are also shown.

$\lambda$	Exact value	Lower bound using equation (43)	Upper bound using equation (43)	$E_b$ Reference [6]	$E_L$ using equation (43)
0.001	1.001 85	1.000 932	1.001 859	1.001 43	1.001 44
0.01	1.016 74	1.008 994	1.017 387	1.013 74	1.013 66
0.1	1.109 08	1.070 681	1.119 935	1.105 65	1.099 20
0.2	1.173 89	1.119 782	1.192 805	1.175 13	1.162 61
1.0	1.436 53	1.334 560	1.484 050	1.448 70	1.424 00
4.0	1.830 44	1.675 050	1.916 177	1.831 93	1.820 58
10.0	2.205 72	2.004 582	2.322 916	2.192 35	2.197 34
50.0	3.159 02	2.850 163	3.348 809	3.134 71	3.153 04
100.0	3.716 98	3.347 427	3.946 987	3.693 48	3.711 87
1000.0	6.492 35	5.828 630	6.914 382	6.476 94	6.489 41
2000.0	7.701 74	6.911 387	8.205 757	7.688 61	7.699 25

where  $K_0^{(2)} = 1.060\,362\,09$ ,  $K_0^{(3)} = 1.144\,802\,45$ ,  $K_0^{(4)} = 1.225\,820\,11$  are the coefficients of the first terms in the respective strong-coupling expansion computed by Weniger [23]. In tables 2 and 3, we have compared our lower and upper bounds given by (49), for the quartic and sextic anharmonic oscillators, along with the exact eigenvalues obtained by the direct integration of the corresponding Schrödinger equation. We have also compared the best lower bound  $E_L$  obtained using (49), where  $\beta$ -values were given by table 1, with the approximate eigenvalues of the ground state energy  $E_b$  computed by Bhattacharya *et al* [6] using formula (50). Recently, Dasgupta *et al* [7] have extended the work of Bhattacharya *et al* [6] to evaluate the excited-state energies, still in the one-dimensional case. As in the case of the ground state (50), they found that the excited-state energies for the  $\lambda r^{2m}$  oscillator defined by the one-dimensional Hamiltonian operator  $H = -d^2/dr^2 + r^2 + \lambda r^{2m}$  are also a polynomial equation of the same degree and are given by

$$\left(\frac{E^{(m,n)}}{2n+1}\right)^{(m+1)} - \left(\frac{E^{(m,n)}}{2n+1}\right)^{(m-1)} = (K_0^{(m,n)})^{(m+1)}\lambda, \quad (52)$$

where  $E^{(m,n)}$  is the  $n^{\text{th}}$  excited-state energy of the  $\lambda r^{2m}$  oscillator and  $K_0^{(m,n)}$  are constants [7]. Our formulas (46) and (47) are more general and seem to yield more accurate results, even for large values of the coupling parameter  $\lambda$ .

## 5. Conclusion

The application of envelope theory and kinetic-potential techniques to polynomial potentials has yielded fairly general and good energy bounds for arbitrary values of the coupling constants. As the specific examples, the application of theorems A and B to the quantum anharmonic oscillators have produced a global energy formula sufficient to generate all energy levels in arbitrary dimension for  $r^{2m}$  anharmonic oscillators with a fair degree of accuracy. The main emphasis of this paper has been on energy formulas that are also bounds. However the energy formula of theorem B (ii), namely

$$E \approx \min_{r>0} \left[ \frac{1}{r^2} + \sum_{i=1}^k a_i (P_{n\ell}^{(d)}(q_i)r)^{q_i} \right],$$

which does indeed yield a lower bound for the bottom of spectrum ( $n = 1$ ) in each angular-momentum subspace, is a remarkably general and accurate approximation: it requires the input of the pure-power  $P$  numbers, and then predicts approximately, for all the eigenvalues in all dimensions, how the spectrum generated by the potential sum depends on the mixing parameters  $\{a_i\}$ ; it also has the attractive collocation property that it is exact whenever all but one of the potential coefficients are zero.

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