Bounds on Schrödinger Eigenvalues

for Polynomial Potentials

in N Dimensions

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Abstract

If a single particle obeys non-relativistic QM in \mathbb{R}^N and has the Hamiltonian $H = -\Delta + \sum_{q>0} a(q)r^q$, $a(q) \ge 0$, then the lowest eigenvalue E is given approximately by the semi-classical expression $E = \min_{r>0} \left\{ \frac{1}{r^2} + \sum_{q>0} a(q)(P(q,N)r)^q \right\}$. It is proved that this formula yields a lower bound when $P(q,N) = \left(\frac{Ne}{2}\right)^{\frac{1}{2}} \left(\frac{N}{qe}\right)^{\frac{1}{q}} \left[\frac{\Gamma(1+\frac{N}{2})}{\Gamma(1+\frac{N}{q})}\right]^{\frac{1}{N}}$ and an upper bound when $P(q,N) = \left(\frac{Ne}{2}\right)^{\frac{1}{2}} \left(\frac{N}{qe}\right)^{\frac{1}{q}} \left[\frac{\Gamma(1+\frac{N}{2})}{\Gamma(1+\frac{N}{q})}\right]^{\frac{1}{N}}$ and an upper bound when N > 1. The general formula is applied to the examples $V(r) = r + r^2 + r^3$ and $V(r) = r^2 + r^4 + r^6$ in dimensions 1 to 10, and the results are compared to accurate eigenvalues obtained numerically.

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I Introduction and main result

In 1976 Barnes, Brascamp, and Lieb [1] employed a sharp form of Young's inequality to provide a general lower-bound formula for the lowest eigenvalue of the Schrödinger operator $H = -\Delta + V(r)$ in $N \ge 1$ spatial dimensions, where $r = ||\mathbf{r}||$, $\mathbf{r} \in \mathbb{R}^{N}$. The restriction on the potential V(r) is that

$$I(a) = \int e^{-aV(r)} d^N \mathbf{r} < \infty$$
(1.1)

for all a > 0. As an application they studied the pure power potentials

$$V(r) = v r^{q}, \quad v > 0, \quad q > 0,$$
 (1.2)

and they obtained the lower bound

$$E \ge Nv^{\frac{2}{q+2}} \left(\frac{2+q}{2q}\right) \left[\frac{\Gamma(1+\frac{N}{2})}{\Gamma(1+\frac{N}{q})}\right]^{\frac{2}{N(q+2)}} e^{\frac{q-2}{q+2}}.$$
(1.3)

Meanwhile a Gaussian 'trial function' provided the upper bound

$$E \le Nv^{\frac{2}{q+2}} \left(\frac{2+q}{2q}\right) \left[\frac{q\Gamma\left(\frac{N+q}{2}\right)}{N\Gamma\left(\frac{N}{2}\right)}\right]^{\frac{2}{q+2}}.$$
(1.4)

The purpose of this paper is to extend the pure power-law bounds (1.3) and (1.4) to the case of potentials which are positive combinations of positive powers. Thus the Hamiltonian we consider is given by

$$H = -\Delta + v \sum_{q>0} a(q)r^q, \quad va(q) \ge 0.$$

$$(1.5)$$

Our principal result is that the lowest eigenvalue of H is approximated by the semiclassical formula

$$E = \min_{r>0} \left\{ \frac{1}{r^2} + v \sum_{q>0} a(q) (P(q, N)r)^q \right\}$$
(1.6)

in which, for a lower bound, the numbers P(q, N) are given by

$$P = P_L(q, N) = \left(\frac{Ne}{2}\right)^{\frac{1}{2}} \left(\frac{N}{qe}\right)^{\frac{1}{q}} \left[\frac{\Gamma(1+\frac{N}{2})}{\Gamma(1+\frac{N}{q})}\right]^{\frac{1}{N}},$$
(1.7)

and for an upper bound by the formula

$$P = P_U(q, N) = \left(\frac{N}{2}\right)^{\frac{1}{2}} \left[\frac{\Gamma(\frac{N+q}{2})}{\Gamma(\frac{N}{2})}\right]^{\frac{1}{q}}.$$
(1.8)

Since numerical estimates of such eigenvalues are readily available today, the main point of this result is its generality and simplicity. All the parametric dependence of the eigenvalue is captured by the energy-bound formulas. Thus, for example, the minimization in (1.5) can easily be performed exactly to yield parametric formulas (v(r), E(r)) for the dependency of the eigenvalue E on the overall coupling parameter v. For N > 1, it is possible to use the same formula (1.6) even when the Coulomb term $-a(-1)r^{-1}$ is also added: in this case $P(-1, N) = \frac{1}{2}(N-1)$ must be used for the lower bound. For the upper bound (1.8) continues to be valid, although alternative Pnumbers derived from an exponential trial function, and presented in Section III, may be useful if the Coulomb coefficient is sufficiently large. The addition of the Coulomb term does not depend on Young's inequality and the *overall* potential is not restricted by the inequality (1.1).

The derivation of the lower bound given in Section II below uses the lower bound (1.3) for pure powers and the 'sum approximation' [2,3], which is outlined briefly so as to make the present paper more self-contained. The pure-power lower bounds are used in lieu of exact values, which, of course, would be preferred. For q = -1 and q = 2 these bounds are in fact exact. The upper bound is obtained by a straightforward application of a trial function and a minimization with respect to scale. It is perhaps interesting that both general bounds may be expressed by the same semi-classical formula: one simply has to insert the appropriate P numbers. In Section III we present some numerical results for the two examples $V(r) = r + r^2 + r^3$ and $V(r) = r^2 + r^4 + r^6$ in dimensions 1 to 10.

II Energy bounds

The derivation of the lower bound is based on two elements: a variational representation for Schrödinger eigenvalues; and a variational argument that applies to sums of potential terms. For dimensions 1 and 3 this approach has been developed earlier [2,3]. We now present the essence of the idea, specialized for our present application to discrete sums of pure powers. For some of the technical details we shall have to refer to the earlier papers.

First, suppose that E(q) represents the lowest eigenvalue of the Hamiltonian $H = -\Delta + \operatorname{sgn}(q)r^{q}$, then E(q) has the representation

$$E(q) = \min_{r>0} \left[\frac{P(q)^2}{r^2} + \operatorname{sgn}(q) r^q \right]$$
(2.1*a*)

$$= \min_{r>0} \left[\frac{1}{r^2} + \operatorname{sgn}(\mathbf{q}) (\mathbf{P}(\mathbf{q})\mathbf{r})^{\mathbf{q}} \right]$$
(2.1*b*)

$$= \operatorname{sgn}(q) \left(1 + \frac{q}{2} \right) \left(\frac{2}{|q|} \right)^{\frac{q}{2+q}} P(q)^{\frac{2q}{2+q}}, \quad q \neq 0.$$
 (2.1c)

The step from (2.1a) to (2.1b) invloves a scale change in the 'dummy' variable r. Thus for each power q, (2.1c) establishes a monotonic functional relationship between E(q)and P(q). The dependence of P(q) on q is much smoother than that of E(q), which has an infinite derivative at q = 0. It has been proved [3], for example, that P(q) is a monotonic increasing function and that the limit $q \to 0$ yields the eigenvalues of the Log potential.

We now consider the spectrum of a Hamiltonian whose potential is the sum of terms each of which could alone support a bound state for any positive value of the coupling parameter. Since the potentials we shall use in this paper are mixtures of attractive powers, this assumption is satisfied. To fix ideas we consider the case of just two such terms:

$$H = -\Delta + ar^{p} + br^{q} = \omega \left(-\Delta + \frac{a}{\omega} r^{p} \right) + (1 - \omega) \left(-\Delta + \frac{b}{(1 - \omega)} r^{q} \right), \quad 0 < \omega < 1.$$
(2.2)

The functions $F_p(v) = E(p)v^{\frac{2}{2+p}}$ and $F_q(v) = E(q)v^{\frac{2}{2+q}}$ describe how the lowest eigenvalues of $H_p = -\Delta + vr^p$ and $H_q = -\Delta + vr^q$ depend on the coupling parameter v. By employing the (unknown) exact ground state Ψ as a 'trial function' in the identity (2.2) we see that the lowest eigenvalue E of H is bounded below by the expression

$$E > \max_{\omega \in (0,1)} \left[\omega F_p\left(\frac{a}{\omega}\right) + (1-\omega)F_q\left(\frac{b}{(1-\omega)}\right) \right].$$
(2.3)

This could be described as an optimized Weyl lower bound [4-6].

We have proved [2] that, in terms of the P numbers, the optimized lower bound (2.3) may be recast into the semi-classical form

$$E > \min_{r>0} \left[\frac{1}{r^2} + a(P(p)r)^p + b(P(q)r)^q \right].$$
(2.4)

The maximization in (2.3) has not been converted into the minimization of (2.4). The general derivation is given in Ref. [2]: by setting up the so-called 'kinetic-potential' formalism it is possible to show that any discrete Schrödinger eigenvalue can be expressed in a semi-classical form, including a minimization; then it is proved that the optimal lower bound, corresponding in our application to (2.3), is expressed in this formalism by replacing the unknown kinetic potential for the sum by the sum of

the kinetic potentials of the components; for pure powers, these components are the potential terms themselves, with the P numbers inserted. In the semi-classical form (2.4) we note that the mean kinetic energy $\langle -\Delta \rangle$ has been replaced by $1/r^2$ and the mean potential energy is obtained from the potential function itself my the insertion of the appropriate P numbers in each term. Thus, by an immediate generalization, we obtain the general form (1.6) for the lower bound. Since we have the *lower bounds* (1.3) for the single-power eigenvalues E(N,q) at our disposal, we obtain the corresponding P_L (1.7) by applying the monotonic correspondence (2.1c). A sharpending of the bounds could be obtained by using known *exact* single-power eigenvalues, say, for q = 1. However, our main purpose is to establish simple and general eigenvalue formulas. As an indication of the extensibility of the results, we point out that the addition of a Coulomb term for $N \geq 2$ is obtained by using the same formula (1.6) with the additional (exact) P value

$$E(N, -1) = -\frac{1}{(N-1)^2} \implies P = P_L = \frac{1}{2}(N-1), \quad N \ge 2.$$
 (2.5)

We now turn to the upper bounds. Whenever we apply a trial function Φ to the Hamiltonian and we minimize with respect to a scale parameter σ ($r \rightarrow r' = \sigma r$), the result can be expressed in the semi-classical form (1.6). We can see this by the following general dimensional (or scaling) argument: the mean kinetic energy necessarily has the form

$$<-\Delta> = (\Phi, -\Delta\Phi)/||\Phi||^2 = K/\sigma^2,$$
 (2.6)

and the mean powers have the form

$$\langle \operatorname{sgn}(q)r^{q} \rangle = \operatorname{sgn}(q)(Q\sigma)^{q},$$
(2.7)

for suitable K and Q. By writing $K/\sigma^2 = 1/r^2$, and defining $P = Q/K^{\frac{1}{2}}$, and minimizing over the scale (expressed now in terms of r) we see that (1.6) is indeed the general form of the result. All we need to do is to compute the $P = P_U$ numbers for each 'shape' of trial function. For Gaussian and exponential trial functions we obtain respectively

$$P = P_U(q, N) = P_g(q, N) = \left(\frac{N}{2}\right)^{\frac{1}{2}} \left[\frac{\Gamma(\frac{N+q}{2})}{\Gamma(\frac{N}{2})}\right]^{\frac{1}{q}}$$
(2.8)

and

$$P = P_U(q, N) = P_e(q, N) = \frac{1}{2} \left[\frac{\Gamma(N+q)}{\Gamma(N)} \right]^{\frac{1}{q}}.$$
(2.9)

The exponential result may be useful if the Coulomb term is included (for $N \ge 2$) since, for example, a Gaussian wave function produces an 8% error in the pure Coulomb case when N = 3.

III Two Examples

We now consider the examples

$$V_1(r) = r + r^2 + r^3 \tag{3.1}$$

and

$$V_2(r) = r^2 + r^4 + r^6. aga{3.2}$$

In Tables 1 and 2 we exhibit the results obtained by use of the eigenvalue formula (1.6) for these potentials in dimensions 1 to 10, along with some accurate values obtained by the direct numerical integration of Schrödinger's equation.

IV Conclusion

The simple and general result of Barnes, Brascamp, and Lieb [1] for bounds on Schrödinger eigenvalues corresponding to pure power potentials has been extended to sums of such powers. The more general bounds are obtained from the semi-classical formula (1.6) which involves a minimization over a single variable. This formula is extensible, as we have demonstrated with the addition of a Coulomb term. The formula can also be sharpened by the use of more accurate P numbers which could be obtained, for the lower bound, by more accurate single-power eigenvalues, and, for the upper bound, by the use of an improved wave function. In all of these results the dimension N is kept as a free parameter.

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References

- J. F. Barnes, H. J. Brascamp, and E. H. Lieb, In: Studies in Mathematical Physics: Essays in Honor of Valentine Bargmann (Edited by E. H. Lieb, B. Simon, and A. S. Wightman) (Princeton University Press, Princeton, 1976). p 83
- [2] R. L. Hall, J. Math. Phys. **33**, 1710 (1992).
- [3] R. L. Hall, J. Math. Phys. **34**, 2779 (1993).
- [4] H. Weyl, Math. Ann. **71**, 441 (1911).
- [5] Ky Fan, Proc. Nat. Acad. Sci. (U.S.) **35**, 652 (1949).
- [6] A. Weinstein and W. Stenger, Methods of Intermediate Problems for Eigenvalues (Academic, New York, 1972). Weyl's Theorem is given on p.163.

Table 1 Table of ground-state eigenvalues of $H = -\Delta + r + r^2 + r^3$ in N spatial dimensions. Lower and upper bounds, E_L and E_U , have been calculated with the general formula (1.6), and accurate values E have been obtained by direct numerical integration of Schrödinger's equation.

N	E_L	E	E_U
1	1.7987	1.8306	1.8309
2	3.5233	3.5644	3.5655
3	5.2608	5.3066	5.3087
4	7.0258	7.0746	7.0778
5	8.8210	8.8720	8.8762
6	10.6459	10.6987	10.7037
7	12.4991	12.5534	12.5593
8	14.3792	14.4348	14.4415
9	16.2848	16.3415	16.3489
10	18.2143	18.2720	18.2801

Table 2 Table of ground-state eigenvalues of $H = -\Delta + r^2 + r^4 + r^6$ in N spatial dimensions. Lower and upper bounds, E_L and E_U , have been calculated with the general formula (1.6), and accurate values E have been obtained by direct numerical integration of Schrödinger's equation.

N	E_L	E	E_U
1	1.5209	1.6149	1.6582
2	3.3367	3.5139	3.5979
3	5.4053	5.6564	5.7784
4	7.6976	8.0155	8.1727
5	10.1924	10.5713	10.7615
6	12.8734	13.3086	13.5298
7	15.7275	16.2151	16.4657
8	18.7440	19.2809	19.5593
9	21.9140	22.4974	22.8024
10	25.2300	25.8574	26.1878