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Coulomb plus power-law potentials in quantum mechanics

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Abstract

We study the discrete spectrum of the Hamiltonian $H = -\Delta + V(r)$ for the Coulomb plus power-law potential $V(r) = -1/r + \beta\,\mathrm{sgn}(q)r^q$, where $\beta > 0, q > -2$ and $q \neq 0$. We show by envelope theory that the discrete eigenvalues $E_{n\ell}$ of H may be approximated by the semiclassical expression $E_{n\ell}(q) \approx \min_{r>0}\{1/r^2 - 1/(\mu r) + \mathrm{sgn}(q)\beta(\nu r)^q\}$. Values of μ and ν are prescribed which yield upper and lower bounds. Accurate upper bounds are also obtained by use of a trial function of the form, $\psi(r) = r^{\ell+1}\,\mathrm{e}^{-(xr)^d}$. We give detailed results for $V(r) = -1/r + \beta r^q$, $q = 0.5, 1, 2$ for $n = 1$, $\ell = 0, 1, 2$, along with comparison eigenvalues found by direct numerical methods.

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1. Introduction

In this paper we derive upper and lower bound formulae for the spectrum of a single particle in three dimensions that obeys non-relativistic quantum mechanics and has Hamiltonian

$$H = -\omega\Delta - A/r + B\,\mathrm{sgn}(q)r^q \qquad \omega, A, B > 0 \quad \text{and} \quad q \neq 0, q > -2. \tag{1.1}$$

The Coulomb plus power-law potential is of interest in particle physics where it serves as a non-relativistic model for the principal part of the quark–quark interaction. This class of potentials has been well studied and much work has been done to approximate the eigenvalues, with or without the Coulomb term necessitated by QCD [1–14]. Our goal in this paper is to provide simple formulae for upper and lower energy bounds for this class of potentials. Firstly, we use the 'envelope method' [15, 16] to obtain upper and lower bound formulae for all the discrete eigenvalues. We also use a Gaussian trial function and the 'sum approximation' [17, 18] to improve the bounds for the bottom of each angular-momentum subspace. The

energy bounds discussed so far may all be expressed in terms of the following semiclassical energy formula:

$$\mathcal{E} \approx \min_{r>0} \left\{ \omega \frac{1}{r^2} - \frac{A}{\mu r} + B \operatorname{sgn}(q)(\nu r)^q \right\} \tag{1.2}$$

for suitable choices of the parameters $\mu > 0$ and $\nu > 0$. We also apply a variational method used earlier [19] which is based on the exact Coulomb wavefunction and yields accurate upper bounds for the bottom of each angular momentum subspace. We compare all these results with 'exact' eigenvalues computed by direct numerical integration.

For the class of potentials studied some exactly solvable cases exist for suitable values of the couplings ω, A, B, and the power q. For example, for the well-known hydrogenic atom and the harmonic oscillator potentials we have explicitly for $n = 1, 2, 3, \ldots$

$$q = -1 \quad \Rightarrow \quad E_{n\ell} = -\frac{A^2}{4\omega(n+\ell)^2} \tag{1.3}$$

and

$$q = 2 \quad \Rightarrow \quad E_{n\ell} = (\omega B)^{\frac{1}{2}}(4n + 2\ell - 1). \tag{1.4}$$

For $\ell = 0$, exact solutions are also available for the linear potential $q = 1$. We can simplify the coupling problem in general by the use of scaling arguments. If, for each fixed q, we denote the eigenvalues of $H = -\omega\Delta - A/r + Br^q$ by $\mathcal{E}(\omega, A, B)$, and consider a scale change of the form $s = r/\sigma$, and choose the scale $\sigma = \omega/A$, then it is straightforward to show that

$$\mathcal{E}(\omega, A, B) = \left(\frac{A^2}{\omega}\right) \mathcal{E}(1, 1, \beta) \qquad \beta = \left(\frac{B}{\omega}\right)\left(\frac{\omega}{A}\right)^{q+2}. \tag{1.5}$$

Hence, the full problem is now reduced to the simpler one-parameter problem

$$H = -\Delta - 1/r + \beta \operatorname{sgn}(q) r^q \qquad E = E(\beta) = \mathcal{E}(1, 1, \beta) \qquad \beta > 0. \tag{1.6}$$

2. Energy bounds by the envelope method and the sum approximation

The comparison theorem tells us that an ordering between potentials implies an ordering between the corresponding eigenvalues. The 'envelope method' [15, 16] is based on this theorem and establishes upper and lower bound formulae for a wide class of attractive spherically-symmetric potentials. We need a solvable model $-\Delta + h(r)$ which provides an 'envelope basis' for the study of the problems of the form $-\Delta + g(h(r))$, where the transformation function g is monotone increasing and of definite convexity: when g is convex, we obtain lower bounds; when g is concave, the theory yields upper bounds. The natural basis in this context is a single power-law potential. The spectrum of a Hamiltonian of the form

$$H = -\Delta + \operatorname{sgn}(q) r^q \qquad \text{where} \quad q > -2 \quad \text{and} \quad q \neq 0 \tag{2.1}$$

may be represented *exactly* by the following semiclassical expression [11, 16]:

$$E_{n\ell} = \min_{r>0} \left\{ \frac{1}{r^2} + \operatorname{sgn}(q)(P_{n\ell}(q) r)^q \right\} \tag{2.2a}$$

$$= \operatorname{sgn}(q) \left(1 + \frac{q}{2}\right) \left(\frac{2P_{n\ell}(q)^2}{|q|}\right)^{\frac{q}{2+q}}. \tag{2.2b}$$

The function $P = P_{n\ell}(q)$ is known as the P-representation, for the Schrödinger spectra generated by the power-law potentials. It is convenient to use the P function to study and

Table 1. The 'input' values $P_{n\ell}(\frac{1}{2})$ and $P_{n\ell}(1)$ to be used in the general formula (2.5) for the energies corresponding to the potential $V(r) = -1/r + \beta\,\mathrm{sgn}(q)r^q$. These P-values yield upper bounds when $q \leqslant \frac{1}{2}$, or $q \leqslant 1$, respectively.

n	ℓ	$P_{n\ell}(\frac{1}{2})$	$P_{n\ell}(1)$
1	0	1.302 66	1.376 08
2	0	2.973 87	3.181 31
3	0	4.654 40	4.992 55
4	0	6.337 42	6.805 14
5	0	8.021 49	8.618 23
1	1	2.297 47	2.371 92
2	1	3.939 66	4.155 01
3	1	5.601 54	5.953 00
4	1	7.271 94	7.757 01
5	1	8.946 79	9.564 08
1	2	3.295 35	3.370 18
2	2	4.922 61	5.141 35
3	2	6.570 89	6.929 11
4	2	8.230 22	8.725 15
5	2	9.896 19	10.525 96
1	3	4.294 24	4.369 23
2	3	5.912 40	6.132 98
3	3	7.550 77	7.913 04
4	3	9.201 18	9.702 36
5	3	10.859 29	11.497 48
1	4	5.293 52	5.368 63
2	4	6.905 60	7.127 32
3	4	8.536 58	8.901 48
4	4	10.179 64	10.685 21
5	4	11.831 10	12.475 32

analyse the spectra of these problems mainly because it is known [11] that $P_{n\ell}(q)$ is monotone in q and it is also smoother than $E_{n\ell}$ as a function of q; the case $q = 0$ corresponds exactly to the log potential. From (1.3) and (1.4) we find, in particular, that

$$P_{n\ell}(-1) = n + \ell \tag{2.3}$$

and

$$P_{n\ell}(2) = 2n + \ell + 1/2. \tag{2.4}$$

In table 1 we exhibit some numerical values for $P_{n\ell}\left(\frac{1}{2}\right)$ and $P_{n\ell}(1)$. We have found the exact eigenvalues for the linear potential in terms of the zeros of the Airy function, but those for $q = \frac{1}{2}$ have to be computed numerically: this use of some isolated numerical input is justified since, for each $\{n, \ell\}$ pair, the resulting approximation formulae include all the potential parameters but depend only on a single 'numerical input'. Envelope theory [12, 17] shows that the eigenvalues of the Coulomb plus power-law potential may be approximated by the following semiclassical expression:

$$\mathcal{E} \approx \min_{r>0}\left\{\frac{1}{r^2} - \frac{1}{\mu r} + \beta\,\mathrm{sgn}(q)(\nu r)^q\right\} \qquad \text{where} \quad \mu, \nu > 0. \tag{2.5}$$

Since $V(r) = g(h(r))$ is at once a convex function of $h(r) = -1/r$ and a concave function of $h(r) = \mathrm{sgn}(q)r^q$, the spectral representation $P_{n\ell}(q)$ allows us to specify upper and lower

bound formulae as follows. If $\mu = \nu = P_{n\ell}(-1)$, then $\mathcal{E}$ is a lower bound for $E_{n\ell}$, and if $\mu = \nu = P_{n\ell}(q)$, then $\mathcal{E}$ is an upper bound. We may improve the lower bound for the bottom of each angular momentum subspace by using the sum approximation [17, 18], which is equivalent to the choice $\mu = P_{1\ell}(-1) = (\ell + 1)$ and $\nu = P_{1\ell}(q)$. For the bottom of the spectrum we can also improve the upper bound by using a Gaussian trial function and minimizing over scale: this is equivalent [12] to using the parameter values

$$\mu = \nu = P_{10}^{U} = \left(\frac{3}{2}\right)^{\frac{1}{2}} \left[\frac{2\Gamma((3+q)/2)}{\sqrt{\pi}}\right]^{\frac{1}{q}}. \tag{2.6}$$

We note that the *same* parameters μ and ν which guarantee that (2.5) yields various energy bounds may also be used in the 'full' semiclassical formula (1.2), including all the original Hamiltonian parameters $\{\omega, A, B\}$. In section 3 we apply (2.5) to the explicit cases $V(r) = -1/r + \beta r^q$ for $\ell = 0, 1, 2$, where $q = 1, 2$ and 0.5.

3. Variational method

The second approach in this paper is to use a trial function explored in previous work [19] to obtain accurate upper bounds for the bottom of each angular momentum subspace. We start with Schrödinger's equation

$$H\psi(r) = \left(-\Delta - \frac{1}{r} + \beta\,\mathrm{sgn}(q) r^q\right)\psi(r) = E_{n\ell}(\beta)\psi(r) \qquad q \neq 0 \quad q > -2. \tag{3.1}$$

This problem is solvable if $\beta = 0$, and the corresponding wavefunction $\psi(r)$ is given by

$$\psi(r) = r^{\ell+1}\,\mathrm{e}^{-xr} L_n^{2\ell+1}(2xr). \tag{3.2}$$

In order to obtain an upper bound for the bottom of each angular momentum subspace $E_{1\ell}$ for fixed power q we choose $\psi(r)$ to be of the following form

$$\psi(r) = r^{\ell+1}\,\mathrm{e}^{-(xr)^d} \tag{3.3}$$

and define $\mathcal{E}$ by $\mathcal{E}(\beta, x, d) = \frac{(\psi, H\psi)}{(\psi,\psi)}$, where x and d are variational parameters. Now, we minimize $\mathcal{E}$ with respect to x and d. The necessary conditions for a critical point are $\frac{\partial \mathcal{E}}{\partial x} = 0$ and $\frac{\partial \mathcal{E}}{\partial d} = 0$. Consequentially, using (3.1) and (3.3), we obtain the following upper bound formula for the eigenvalues $E_{1\ell}$

$$\mathcal{E}_{1\ell}(\beta, d, x) = a_1 x^2 - a_2 x + a_3 x^{-q} \tag{3.4}$$

where a_1, a_2 and a_3 are as given below

$$a_1 = 2^{\frac{2-2d}{d}} \frac{(2\ell+1)(2\ell+d+1)\Gamma\left(\frac{2\ell+1}{d}\right)}{\Gamma\left(\frac{2\ell+3}{d}\right)}$$

$$a_2 = 2^{\frac{1}{d}} \frac{\Gamma\left(\frac{2\ell+2}{d}\right)}{\Gamma\left(\frac{2\ell+3}{d}\right)}$$

$$a_3 = \mathrm{sgn}(q)\beta 2^{\frac{-q}{d}} \frac{\Gamma\left(\frac{2\ell+q+3}{d}\right)}{\Gamma\left(\frac{2\ell+3}{d}\right)}.$$

By using (3.4) we derive the following equation for x:

$$x^{q+2} - \frac{a_2}{2a_1} x^{q+1} - \frac{q a_3}{2a_1} = 0. \tag{3.5}$$

After solving (3.5) to obtain x from the numerical solution of $\frac{\partial \varepsilon}{\partial d} = 0$ we find d for $n = 1$ and $\ell = 0$ and then we use the same d value for all ℓ.

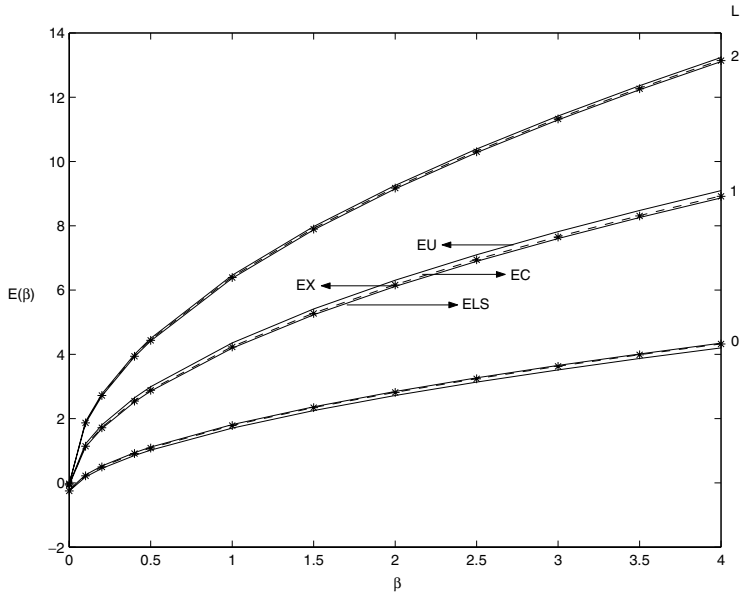

Figure 1. The eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r^2$ for $N = 3$, $n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(2)$, for $\ell = 1, 2$ and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(2)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(2)$ and $\mu = P^U_{1\ell}(-1)$ in formula (2.5). The dashed curve EC represents the upper bound by formula (3.4). The stars EX represent accurate numerical data.

4. Results and conclusion

We have found general semiclassical energy formulae (1.2) and (2.5) for the eigenvalues generated by the Coulomb plus power-law potentials. Specific values for the parameters μ and ν are given which guarantee that the formulae yield bounds for all the discrete energies. By using a more finely tuned wavefunction, we have also derived an improved upper bound (3.4) valid for the bottom of each angular momentum subspace. We may rewrite (2.5) in the form of a pair of parametric equations for the curve $\{\beta, E(\beta)\}$. For fixed $q > -1$ we obtain

$$\beta = \frac{1}{|q|(\nu r)^q}\left(\frac{2}{r^2} - \frac{1}{\mu r}\right) \qquad E(\beta) = \frac{1+2/q}{r^2} - \frac{1+1/q}{\mu r}. \tag{4.1}$$

By envelope theory, we know that these parametric equations yield a lower bound if $\mu = \nu = P_{n\ell}(-1) = (n + \ell)$, and an upper bound when $\mu = \nu = P_{n\ell}(q)$. For the bottom of each angular momentum subspace the prescription $\mu = P_{1\ell}(-1) = (\ell + 1)$, $\nu = P_{1\ell}(q)$ yields an improved lower bound. An improved upper bound for the bottom of the spectrum is given by using the 'Gaussian' P-numbers (2.6). In figures 1–3, we plot the function $E(\beta)$ for $n = 1$, $\ell = 0, 1, 2$ for the Coulomb plus harmonic oscillator ($q = 2$), Coulomb plus linear ($q = 1$) and Coulomb plus $r^{0.5}$ potentials, along with the corresponding accurate variational bounds using (3.4) (dashed line), and some comparison numerical values represented as stars. The advantage of the semiclassical formulae is that they describe in approximate analytical form how the eigenvalues depend on all the parameters of the problem.

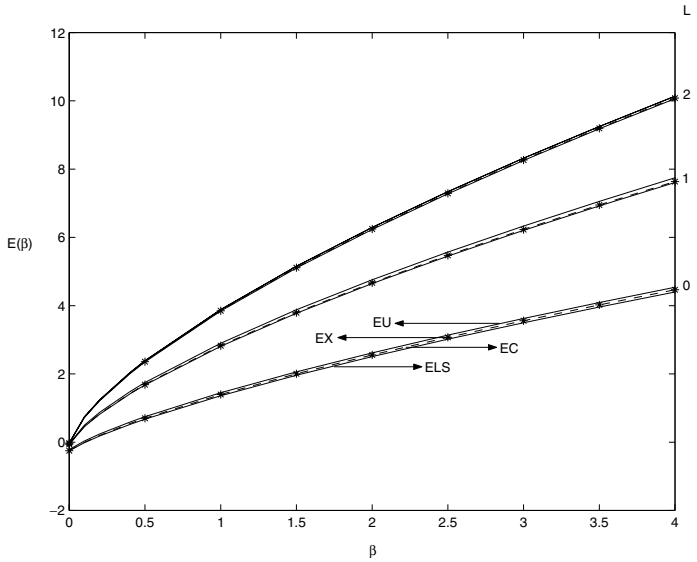

Figure 2. The eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r$ for $N = 3, n = 1$, and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(2)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(1)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(1)$ and $\mu = P^U_{1\ell}(-1)$ in formula (2.5). The dashed curve EC represents the upper bound by formula (3.4). The stars EX represent accurate numerical data.

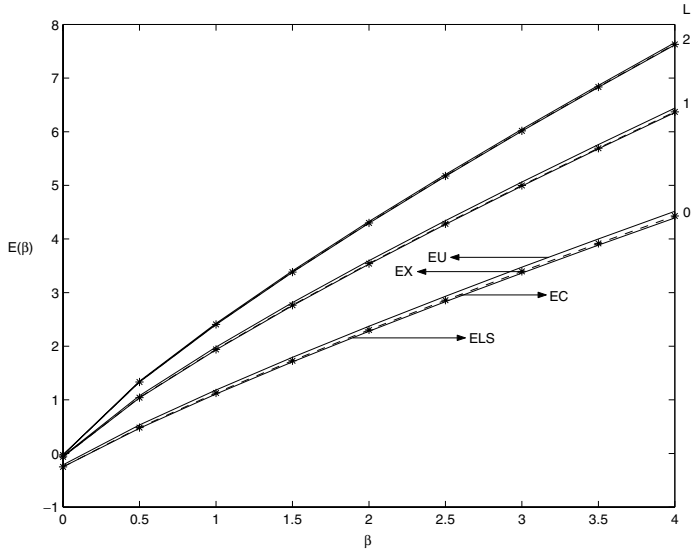

Figure 3. The eigenvalues $E(\beta)$ of the Hamiltonian $H = -\Delta - 1/r + \beta r^{0.5}$ for $N = 3, n = 1$ and $\ell = 0, 1, 2$. The continuous curves show the upper bound EU given by the envelope formula (2.5) with $\nu = \mu = P_{1\ell}(0.5)$, and the lower bound ELS by the sum approximation given by the same formula but with $\nu = P_{1\ell}(0.5)$ and $\mu = P_{1\ell}(-1)$. The upper bound for $\ell = 0$ is calculated using $\nu = P^U_{1\ell}(0.5)$ and $\mu = P^U_{1\ell}(-1)$ in formula (2.5). The dashed curve EC represents the upper bound by formula (3.4). The stars EX represent accurate numerical data.

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