Envelope theory in spectral geometry

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It is shown that the discrete spectrum of Schrödinger Hamiltonians of the form $H = -\Delta + vf$ may be represented by the semiclassical expression $E_{nl} = \min_{r>0} \{K_{nl}^{(f)}(r) + vf(r)\}$. The K functions are found to be invariant with respect to coupling and shifts: $K^{(Af+B)} = K^{(f)}$. For pure power laws, $f(r) = \mathrm{sgn}(q)r^q$, and the log potential, they are also invariant with respect to scale, and have the simple forms $(P_{nl}(q)/r)^2$ and $(L_{nl}/r)^2$, respectively. K functions are also derived for sech-squared and Hulthén potentials. If $f = g(h)$, where g is a smooth transformation, then the envelope approximation is expressed in terms of K by the relation $K^{(f)} \simeq K^{(h)}$. When the transformation g has definite convexity, then the approximation immediately yields eigenvalue bounds for all n and l. The theory is used to prove the log-power theorem $L_{nl} = P_{nl}(0)$, which, in turn, generates a simple eigenvalue formula for the log potential.

I. INTRODUCTION

We study Schrödinger Hamiltonians of the form

$$H = -\Delta + vf(r), \tag{1.1}$$

where f is the shape of a central potential in $\mathbb{R}^N$, and v is a positive coupling parameter. We consider attractive potentials with the property that, for v sufficiently large, the Hamiltonian H has some discrete eigenvalues $E_n = F_n(v)$. The eigenvalues are ordered so that $E_n \leqslant E_m$ for $m > n$, $n = 1,2,3,...$, where the index n labels the eigenvalues corresponding to the states in a given angular-momentum subspace. For definiteness, we shall now adopt a notation suitable for $\mathbb{R}^3$, in which $l \geqslant 0$ denotes the usual orbital angular-momentum quantum number.

The term *spectral geometry*[1] refers to the study of the geometrical relationship between the potential shape f and the set $\{F_{nl}\}$ of energy trajectories generated by f. If the potential has more than one parameter, then, instead of curves, one might have to work with more general energy hypersurfaces. The central-field eigenvalue problem

$$\left[-\frac{\hbar^2}{2m} \Delta_{r'} + V_0 f\left(\frac{r'}{a}\right) \right] \Psi(\mathbf{r}') = \mathscr{E}\Psi(\mathbf{r}'), \tag{1.2}$$

which has the three physical parameters, m, V_0, and a, may be reduced to the dimensionless form $H\psi = E\psi$ by means of the scale changes

$$\mathbf{r} = \frac{\mathbf{r}'}{a}, \quad \psi(\mathbf{r}) = \Psi(\mathbf{r}'), \quad v = \frac{2mV_0 a^2}{\hbar^2}, \quad E = \frac{2m\mathscr{E}a^2}{\hbar^2}. \tag{1.3}$$

Therefore, to this level of generality, it is sufficient to develop our geometrical theory in terms of the dimensionless one-parameter Hamiltonian H given by Eq. (1.1).

An essential feature of our approach to spectral geometry is the reformulation of the standard min–max characterization[2-5] of discrete Schrödinger eigenvalues by means of *kinetic potentials*.[6,7] We shall summarize this theory briefly in Sec. II. The principal idea is that the

minimization of the Rayleigh quotient $(\psi, H\psi)/(\psi, \psi)$ is performed in two stages. The first stage involves only the *shape f* of the potential and leads to a family $\{\bar{f}_{nl}\}$ of kinetic potentials $\bar{f}_{nl}(s)$. The second stage begins with a kinetic potential $\bar{f}_{nl}(s)$ and yields the corresponding eigenvalue E_{nl} as the outcome of the semiclassical optimization

$$E_{nl}=F_{nl}(v)=\min_{s>0}\{s+v\bar{f}_{nl}(s)\}, \tag{1.4}$$

in which the variable $s>0$ represents the kinetic energy. The point of all this is that the kinetic potentials behave very nicely under both smooth transformations and sums. The present paper concerns developments in the transformational aspect of the theory.

If a potential f is a smooth transformation g of a soluble potential h, so that $f(r)=g(h(r))$, then the corresponding kinetic potentials $\{\bar{f}_{nl}\}$, which are ordered like the eigenvalues, transform approximately in the same way as the potentials. That is to say, we have the envelope approximation

$$\bar{f}_{nl}(s)\simeq g(\bar{h}_{nl}(s)), \tag{1.5}$$

where, if g is convex, we get lower bounds ($\simeq\,=\,>$) for *all* n and l, and if g is concave we get upper bounds ($\simeq\,=\,<$) for *all* n and l. This result has[6] a very interesting geometrical interpretation in terms of envelopes: If we think of $f=g(h)$ as a function of h, then each tangent line to the graph of g is a shifted h-potential which is soluble and has a known energy trajectory; the *envelope* of this family of trajectories is precisely the trajectory we get when the right side of Eq. (1.5) is substituted in Eq. (1.4). Because of this geometrical interpretation we sometimes refer to these results collectively as 'the method of potential envelopes' or 'the envelope approximation.'

Our first principal new result, which we derive in Sec. III, is that there exist changes of variable $s\rightarrow r$ defined by the equations $\bar{f}_{nl}(s)=f(r)$ so that the minimization (1.4), which yields the eigenvalues, can be expressed in the form

$$E_{nl}=F_{nl}(v)=\min_{r>0}\{K_{nl}^{(f)}(r)+vf(r)\}. \tag{1.6}$$

There are a number of advantages to this new formulation. The K functions are invariant with respect to the coupling and shifts of the potential: thus $K^{(Af+B)}=K^{(f)}$. For pure power-law potentials $f(r)=\text{sgn}(q)\,r^q$, they are also invariant under scale changes: the K functions in this case have the simple form $K_{nl}^{(f)}(r)=(P_{nl}(q)/r)^2$, where the $P_{nl}(q)$ are precisely the functions (of q) which emerged naturally in our earlier study[1] of the spectral geometry of the power-law potentials. We also derive some explicit K functions for the log, the sech-squared, and the Hulthén potentials. For the log potential, we obtain $K_{nl}^{(\log)}(r)=(L_{nl}/r)^2$, where the L_{nl} are constants.

Another, interesting invariance property of the K functions is to do specifically with the envelope approximation. If $f=g(h)$, then, in terms of the new formulation, the envelope approximation (1.5) becomes simply

$$K^{(f)}\simeq K^{(h)}, \tag{1.7}$$

and the corresponding expression for the eigenvalues is therefore given by

$$E_{nl}=F_{nl}(v)\simeq\min_{r>0}\{K_{nl}^{(h)}(r)+vf(r)\}. \tag{1.8}$$

If the transformation g has definite convexity, then the approximation (1.8) immediately yields energy *bounds* for all the eigenvalues.[7]

This new formulation of envelope theory enables us to prove the log-power theorem which states that $L_{nl} = P_{nl}(0)$. This result reveals the intimate relationship which exists between the spectra generated by the power-law potentials and the log potential. Consequently, we are able to characterize completely the complicated behavior of the power-law eigenvalues $E_{nl}^{(q)}$ near $q=0$. Conversely, the approximate formula we obtained in Ref. 1 for $P_{nl}(q)$ can now be used to provide a simple expression for the eigenvalues associated with the log potential.

II. SPECTRAL GEOMETRY AND KINETIC POTENTIALS

For definiteness, we present this brief summary of spectral geometry for $N=3$ spatial dimensions; it will be clear from this special case how to obtain the corresponding results for other values of N. In the abstract theory[2-5] of Schrödinger operators $H = \hat{K} + V$ one thinks of the potential $V = vf$ as a perturbation of the positive–definite kinetic energy operator $\hat{K} = -\Delta$. If $\mathscr{D}_n$ is an n-dimensional subspace of $L^2(\mathbb{R}^3)$ contained in the domain of H and contained in the angular-momentum subspace labeled by the spherical harmonic Y_l^m then, we can define the nth eigenvalue E_{nl} ($n=1,2,...$) by the min–max expression:

$$E_{nl} = \inf_{\mathscr{D}_n} \ \sup_{\substack{\psi \in \mathscr{D}_n \\ \|\psi\|=1}} (\psi, H\psi). \tag{2.1}$$

Kinetic potentials arise when one effects this minimization in two stages. At the first stage, we scale the linear space $\mathscr{D}_n$ so that we can fix the value of the mean kinetic energy $(\psi, K\psi) = s$, then we minimize over all scales, that is to say, over all values of $s > 0$. Thus if $\mathscr{D}_n = \mathrm{Span}\{\phi_i\}_{i=1}^n$, and $\hat{\sigma}\phi_i(x) = \phi_i(\sigma x)$, $\sigma > 0$, then we define

$$\hat{\sigma}\mathscr{D}_n = \mathrm{Span}\{\hat{\sigma}\phi_i\}_{i=1}^n \tag{2.2}$$

and

$$\mathscr{D}_n = \bigcup_{\sigma > 0} \hat{\sigma}\mathscr{D}_n. \tag{2.3}$$

Of course, this union of scaled linear spaces is not itself a linear space. Now we are in a position to define kinetic potentials by the expression:

$$\bar{f}_{nl}(s) = \inf_{\mathscr{D}_n} \ \sup_{\substack{\psi \in \mathscr{D}_n \\ \|\psi\|=1 \\ (\psi, K\psi)=s}} (\psi, f\psi). \tag{2.4}$$

A kinetic potential (a contraction of the term *minimum mean isokinetic potential*) represents the result of min–max applied to the potential *shape f*: the coupling parameter v is not included. Only in the final stage of minimization do we recover the eigenvalue in terms of v, thus

$$E_{nl} = F_{nl}(v) = \min_{s>0}\{s + v\bar{f}_{nl}(s)\}. \tag{2.5}$$

It is not difficult to show[6,7] that the kinetic potentials are *convex*, that they are ordered like the eigenvalues, that is to say, $F > G \Rightarrow \bar{f} > \bar{g}$, and that they obey the scaling rule:

$$Af(r/b) + B \rightarrow A\bar{f}(sb^2) + B, \quad A, b > 0. \tag{2.6}$$

We can use calculus to invert Eq. (2.5) and express kinetic potentials in terms of the trajectory functions. Thus from Eq. (2.5) we have the transformation pairs:

$$s = F_{nl}(v) - vF'_{nl}(v), \quad \bar{f}_{nl}(s) = F'_{nl}(v), \tag{2.7}$$

and

$$v^{-1} = -\bar{f}'_{nl}(s), \quad v^{-1}F_{nl}(v) = \bar{f}_{nl}(s) - s\bar{f}'_{nl}(s). \tag{2.8}$$

Fortunately, because of Eq. (2.7), we do not have to use the abstract definition (2.4) in order to construct component kinetic potentials from known trajectory functions. Meanwhile, the transformation (2.8) allows us to reconstruct the energy spectrum from the kinetic potentials.

In the case of power-law potentials with shapes

$$f(r) = \text{sgn}(q)r^q, \quad q \geqslant -1, \quad q \neq 0, \tag{2.9}$$

elementary scaling arguments[1] tell us that the energy trajectories are given by

$$F_{nl}^{(q)}(v) = E_{nl}^{(q)} v^{2/(q+2)}, \tag{2.10}$$

where $E_{nl}^{(q)} = F_{nl}^{(q)}(1)$. It follows from Eq. (2.7) that the corresponding kinetic potentials are given by

$$\bar{f}_{nl}(s) = (2/q)|qE_{nl}^{(q)}/(2+q)|^{(q+2)/2}s^{-q/2}. \tag{2.11}$$

The formulas for the well-known examples of the Coulomb potential and the harmonic oscillator are therefore given, respectively, by

$$f(r) = -r^{-1} \to F_{nl}^{(-1)}(v) = -\frac{v^2}{4(n+l)^2} \to \bar{f}_{nl}(s) = -\frac{s^{1/2}}{(n+l)} \tag{2.12}$$

and

$$f(r) = r^2 \to F_{nl}^{(2)}(v) = (4n+2l-1)v^{1/2} \to \bar{f}_{nl}(s) = (2n+l-1/2)^2 s^{-1}. \tag{2.13}$$

We note that, for the harmonic oscillator and the sech-squared potential (discussed below), we obtain the corresponding eigenvalue formulas for the case of *one* spatial dimension if we set $l=0$ and replace $2n$ by n.

The S states of the sech-squared[8] and Hulthén[9] potentials have the following respective eigenvalues, and corresponding kinetic potentials given by Eq. (2.7):

$$f(r) = -\text{sech}^2(r) \to F_{n0}(v) = -[(v+1/4)^{1/2} - (2n+1/2)]^2, \tag{2.14}$$

$$\to \bar{f}_{n0}(s) = \frac{-2s}{[(s+v)^2+s]^{1/2}+s+v}, \quad v = 2n(2n-1); \tag{2.15}$$

and

$$f(r) = -\frac{1}{e^r-1} \to F_{n0}(v) = \frac{(v-n^2)^2}{4n^2}, \tag{2.16}$$

$$\to \bar{f}_{n0}(s) = -\frac{1}{2}\left[\left[\frac{4s}{n^2}+1\right]^{1/2} - 1\right]. \tag{2.17}$$

Another potential of interest is the log potential. In this case we have[6] for the eigenvalues of the Hamiltonian $H = -\Delta + v \ln(r)$:

$$f(r) = \ln(r) \rightarrow F_{nl}(v) = -\tfrac{1}{2} v \ln(v/v_{nl}), \tag{2.18}$$

$$\rightarrow \bar{f}_{nl}(s) = E_{nl}^L - \tfrac{1}{2} \ln(2es), \tag{2.19}$$

where

$$v_{nl} = e^{2E_{nl}^L} \quad \text{and} \quad E_{nl}^L = F_{nl}(1). \tag{2.20}$$

These expressions look very different from the power-law results which we found above. However, we shall see below, in the new formulation of the theory, the log potential takes its natural place 'between' the Coulomb and linear potentials.

III. SPECTRAL GEOMETRY AND K FUNCTIONS

The relationship between the trajectory functions F and the kinetic potentials $\bar{f}$, expressed either by the minimization (2.5) or by the differential transformation pairs (2.7) and (2.8), is essentially a Legendre transformation.[10] This aspect of the relationship is most transparent if, instead of $F(v)$, we use $G(u) = uF(1/u)$, as we did in Ref. 6.

However, we now explore a different idea. At the expense of some complication of the expression for the kinetic energy in the semiclassical form (2.5), we try to replace the kinetic potential $\bar{f}$ by the potential f itself. This is possible in general because we know from Eq. (2.8) that $\bar{f}$ is monotone decreasing, and consequently invertible. We can therefore parametrize $\bar{f}_{nl}(s)$ in terms of the variable r by the relation

$$\bar{f}_{nl}(s) = f(r), \tag{3.1}$$

and invert this to give what we call the K function $K_{nl}^{(f)}$ (relative to f), that is to say

$$s = (\bar{f}_{nl}^{-1} \circ f)(r) \equiv K_{nl}^{(f)}(r). \tag{3.2}$$

It follows from this definition and Eq. (2.6) that the K functions obey the the rule:

$$f(r) \rightarrow K(r) \Rightarrow Af(r/b) + B \rightarrow (1/b^2)K(r/b), \quad A,b > 0. \tag{3.3}$$

Thus K functions are generally independent of coupling and potential shifts. The eigenvalues are recovered from the K functions by the expression

$$E_{nl} = F_{nl}(v) = \min_{r>0} \{K_{nl}^{(f)}(r) + vf(r)\}. \tag{3.4}$$

If f is monotone we can change variables and rewrite Eq. (3.4) as

$$E_{nl} = F_{nl}(v) = \min_{f} \{\bar{f}_{nl}^{-1}(f) + vf\}. \tag{3.5}$$

With the optimization in this form, the reason for the *minimum* becomes clear: $\bar{f}_{nl}^{-1}(f)$ is a *convex* function of f. We can see this by the following argument. Let $p = \bar{f}^{-1}$. Then $p(\bar{f}(s)) = s$, and $p'(\bar{f}(s))\bar{f}'(s) = 1$: therefore p', like $\bar{f}'$, is negative. Differentiating again, we find

$$p''(\bar{f}(s))(\bar{f}'(s))^2 + p'(\bar{f}(s))\bar{f}''(s) = 0. \tag{3.6}$$

Hence $p = \bar{f}^{-1}$, like $\bar{f}$, is convex.

IV. POWER-LAW POTENTIALS

From Eqs. (2.11) and (3.2) we find that, for the power-law potentials $f(r) = \mathrm{sgn}(q)\, r^q$, the K functions all have the same form, namely,

$$K_{nl}^{(f)}(r) = (P_{nl}(q)/r)^2. \tag{4.1}$$

From the general transformation properties (3.3), or from the fact that, for power-law potentials, scale and coupling are interchangeable, it follows that this particular family of K functions are scale invariant: that is to say, $f(r)$ and $f(r/b)$ both have identical K functions. A simple computation yields the following general expression for the constants,

$$P_{nl}(q) = |E_{nl}^{(q)}|^{(2+q)/2q}\left[\frac{2}{2+q}\right]^{1/q}\left[\frac{|q|}{2+q}\right]^{1/2}, \quad q \neq 0. \tag{4.2}$$

It is convenient to force continuity at $q=0$ by defining

$$P_{nl}(0) \equiv \lim_{q \to 0} P_{nl}(q). \tag{4.3}$$

This definition is possible because, as we shall shortly see, the right side of Eq. (4.3) exists and equals L_{nl}, the corresponding constant for the log potential. For $q \neq 0$, this is not the first time that we have met these P coefficients. In fact, by serendipitous coincidence the $P_{nl}(q)$ are precisely the functions (of q) which emerged naturally in our earlier study[1] of the spectral geometry of the power-law potentials. There, we represented one power as a transformation of another, and, from a differential analysis of this relationship, we proved that the functions $P(q)$, unlike the energies $E(q)$ themselves, were smooth and monotone (increasing) in q. The P functions have now emerged again as the coefficients in the power-law special case of a general geometric theory of the Schrödinger spectrum.

For later reference we note that for the Coulomb potential ($q = -1$) and the harmonic oscillator ($q=2$), we have, respectively,

$$P_{nl}(-1) = (n+l), \quad P_{nl}(2) = (2n+l-1/2). \tag{4.4}$$

A simple but accurate interpolation formula which is exact for $q = -1$ and $q=2$ and all n and l is given[1] by

$$P_{nl}(q) \simeq \left\{(n+l)^\alpha + \frac{(q+1)}{3}\left[\left(2n+l-\frac{1}{2}\right)^\alpha - (n+l)^\alpha\right]\right\}^{1/\alpha}, \tag{4.5}$$

where $\alpha = 3.239\,692$ has been chosen to fit precisely one more value, namely, $P_{10}(1)$.

V. THE LOG POTENTIAL

In the present formulation of the theory, the log potential assumes its 'natural' place in the same category as the power-law potentials. We find, from Eqs. (2.19) and (3.2),

$$f(r) = \ln(r) \to K_{nl}^{(f)}(r) = (L_{nl}/r)^2, \tag{5.1}$$

where the constants L_{nl} are given in terms of the log-potential eigenvalues E_{nl}^L by

$$L_{nl} = \left(\frac{1}{2e}\right)^{1/2} e^{E_{nl}^L}. \tag{5.2}$$

TABLE I. The first 30 eigenvalues E_{nl}^L of $H = -\Delta + v\ln(r)$, with $v=1$, provided by the simple formula (5.5), along with accurate values (in parentheses) found by direct numerical integration. For $v \neq 1$, we have $E_{nl} = \frac{1}{2}v\ln(v/v_{nl})$, where $v_{nl} = e^{2E_{nl}^L}$.

l	$n=1$	$n=2$	$n=3$	$n=4$	$n=5$
0	1.046 (1.044)	1.847 (1.847)	2.289 (2.290)	2.594 (2.596)	2.828 (2.830)
1	1.633 (1.641)	2.144 (2.151)	2.486 (2.491)	2.742 (2.746)	2.946 (2.949)
2	2.006 (2.013)	2.378 (2.387)	2.655 (2.663)	2.874 (2.880)	3.054 (3.059)
3	2.277 (2.284)	2.570 (2.580)	2.802 (2.810)	2.992 (2.999)	3.152 (3.159)
4	2.491 (2.497)	2.732 (2.742)	2.930 (2.940)	3.098 (3.107)	3.243 (3.251)
5	2.667 (2.673)	2.872 (2.881)	3.045 (3.055)	3.195 (3.205)	3.327 (3.335)

As with the power-law potentials, it follows from Eq. (3.3) that, in addition to the general invariance with respect to coupling and potential shifts, the K functions for the log potential are also invariant with respect to spatial scaling. The notion that the log potential lies 'between' the Coulomb and the linear potential can now immediately be illustrated by the inequalities:

$$P_{10}(-1) = 1 < L_{10} = 1.218 < P_{10}(1) = 1.376, \qquad (5.3)$$

in which the eigenvalues for the log and linear potential have been taken from the tables of Ref. 7. Since we know[1] that the coefficients $P_{nl}(q)$ are *monotone* increasing in q, it is clear from Eq. (5.3) that $P_{10}(q) = L_{10}$ for some $q \in [-1, 1]$. We now know that such an intimate relationship between the log and the power-law Schrödinger spectra is generally true. Indeed in Sec. VIII we use spectral geometry to prove the following.

Log-Power Theorem:

$$P_{nl}(0) = L_{nl}. \qquad (5.4)$$

By substituting our interpolation formula (4.5) for $P_{nl}(q)$ in Eq. (5.4) we immediately obtain from Eq. (5.2) the following approximate formula for the log-potential eigenvalues:

$$E_{nl}^L \simeq \frac{1}{2}(1+\ln(2)) + \frac{1}{\alpha}\ln\left(\frac{1}{3}\left[2(n+l)^\alpha + (2n+l-1/2)^\alpha\right]\right), \qquad (5.5)$$

in which $\alpha = 3.239\,692$. This simple formula gives the the first 30 eigenvalues, $n \leqslant 5$, $l \leqslant 5$, with error less than 1%, as is shown in Table I.

VI. THE HULTHÉN AND SECH-SQUARED POTENTIALS

For the S states of the Hulthén potential we have from Eqs. (2.17) and (3.2)

$$f(r) = -\frac{1}{e^r - 1} \rightarrow K_{n0}^{(f)}(r) = \frac{n^2 e^r}{(e^r - 1)^2}. \qquad (6.1)$$

For small r, this K function approaches n^2/r^2, in agreement with the Coulomb result, (4.1) and (4.4), for $l=0$.

Meanwhile, in one spatial dimension we have, for the harmonic oscillator

$$f(x) = x^2 \rightarrow K_n^{(f)}(x) = (n-1/2)^2/x^2. \qquad (6.2)$$

For the sech-squared potential we obtain from Eqs. (2.15) and (3.2)

$$f(x) = -\operatorname{sech}^2(x) \rightarrow K_n^{(f)}(x) = \frac{1}{\sinh^2 2x} + \frac{n(n-1)}{\sinh^2 x}, \qquad (6.3)$$

where $n=1,2,3,\dots$. Since the sech-squared shape is like a (shifted) harmonic oscillator for small x, it is not surprising that the formula for $K_n^{(f)}(x)$ approaches the expression on the right side of Eq. (6.2), as $x \rightarrow 0$. We note that we obtain the corresponding formulas for the S states ($l=0$) in three spatial dimensions if we replace n by $2n$ in Eqs. (6.2) and (6.3).

VII. ENVELOPE THEORY AND THE TRANSFORMATION INVARIANCE OF K

If the potential shape f is a transformation $g(h)$ of a monotone potential h, then, as we explained in the Introduction, we define the envelope approximation (relative to the basis h) to mean precisely

$$\bar{f}_{nl}(s) \simeq g(\bar{h}_{nl}(s)). \qquad (7.1)$$

The K function corresponding to the envelope approximation is very interesting. By substituting the right side of Eq. (7.1) in the definition (3.2) of the K functions we obtain

$$K_{nl}^{(f)} \simeq (g \circ \bar{h}_{nl})^{-1} \circ (g \circ h) = \bar{h}_{nl}^{-1} \circ h = K_{nl}^{(h)}. \qquad (7.2)$$

In terms of K functions, therefore, the envelope approximation may be expressed in the form,

$$f = g(h) \rightarrow K^{(f)} \simeq K^{(h)}. \qquad (7.3)$$

If we wish to be sure about energy *bounds*, then we must first study the transformation function g to determine its convexity. Once this analysis is completed, the function g can be ignored since the eigenvalue approximations are given by the expression

$$E_{nl} = F_{nl}(v) \simeq \min_{r>0} \{ K_{nl}^{(h)}(r) + v f(r) \}, \qquad (7.4)$$

in which g no longer appears. This expression yields upper or lower bounds depending, respectively, whether g is concave or convex. It is easy to remember this result because, for example, if g is concave, then the tangents to $f = g(h)$ lie above f, and we therefore obtain upper bounds; similarly it is clear that we get lower bounds in the convex case.

In order to analyze the nature of the optimization we can reparametrize in terms of h and obtain, instead of Eq. (7.4), the expression

$$E_{nl} = F_{nl}(v) \simeq \min_h \{ \bar{f}_{nl}^{-1}(h) + v g(h) \}. \qquad (7.5)$$

We know by the argument given in Sec. III that $\bar{f}_{nl}^{-1}(h)$ is convex. If g is also convex, then the critical point is indeed a minimum. If g is concave, there may be critical points of different types; however, in *this* case, we obtain an upper energy bound; consequently the minimum is again required because we would wish to choose the best such bound.

VIII. PROOF OF THE LOG-POWER THEOREM

We prove this theorem by using spectral geometry. We first represent the power-law potentials as smooth transformations of the log potential. Thus

$$\operatorname{sgn}(q) r^q = f(r) = g(h(r)), \quad h(r) = \ln(r), \quad r > 0. \qquad (8.1)$$

Consequently,

$$g(h) = \text{sgn}(q) e^{qh}. \tag{8.2}$$

Since $g'(h) = |q| e^{qh} > 0$, it follows that g is monotone increasing. A further differentiation yields

$$g''(h) = q|q| e^{qh}. \tag{8.3}$$

Thus, the transformation function g is convex (leading to lower energy bounds) if $q > 0$, and g is concave (leading to upper bounds) if $q < 0$.

We first consider the convex case $q > 0$. We have from Eqs. (4.1), (5.1), and (7.3)

$$(P_{nl}(q)/r)^2 = K_{nl}^{(f)}(r) \simeq K_{nl}^{(h)}(r) = (L_{nl}/r)^2. \tag{8.4}$$

The left side of Eq. (8.4) yields the exact energy, whereas, because g is convex, the right side yields a lower bound. Hence we have:

$$\min_{r>0}\left\{\frac{P_{nl}^2(q)}{r^2} + \text{sgn}(q) r^q\right\} = E_{nl}^{(q)} > \min_{r>0}\left\{\frac{L_{nl}^2}{r^2} + \text{sgn}(q) r^q\right\}. \tag{8.5}$$

Since the minima in Eq. (8.5) are also monotone (increasing) in the positive constants multiplying the kinetic-energy factor r^{-2}, we have proved the inequality

$$L_{nl} < P_{nl}(q), \quad q > 0. \tag{8.6}$$

An exactly similar argument for $q < 0$ leads to the complementary result

$$P_{nl}(q) < L_{nl}, \quad q < 0. \tag{8.7}$$

These two inequalities and the monotony of $P_{nl}(q)$, as a function of q, proved in Ref. 1, establish the *log-power theorem*

$$\lim_{q\to 0} P_{nl}(q) = L_{nl}. \tag{8.8}$$

$\square$

From the standpoint of the eigenvalues, this theorem, which relates the Schrödinger spectra generated by the log and the power-law potentials, appears deeply buried. Indeed, the eigenvalues $E_{nl}^{(q)}$ are discontinuous in q and approach ± 1 as q approaches zero, respectively, from the left or right. Meanwhile the eigenvalues E_{nl}^L start at E_{10}^L ($\simeq 1.044$) and increase with n and l without bound.

We can now describe how the power-law eigenvalues depend on q near $q = 0$. We find from Eqs. (4.2) and (8.8)

$$|E_{nl}^{(q)}| \simeq \frac{[L_{nl}]^q}{\gamma(q/2)}, \tag{8.9}$$

where the function γ is defined by $\gamma(x) = |x|^x$. This curious function has limit 1 as $x \to 0$. Consequently, as we expect, the right side of Eq. (8.9) approaches 1 as $q \to 0$. However, the derivative $\gamma'(x) = \gamma(x)\{1 + \ln|x|\}$ approaches $-\infty$ as $x \to 0$. Consequently, the entire family of graphs of $|E_{nl}^{(q)}|$ pass through the point $(q, |E|) = (0,1)$ with infinite slopes. Illustrations of the graphs of the absolute values $|E_{nl}^{(q)}|$, as functions of q, may be found in Ref. 1. The log-power theorem has enabled us to complete the characterization of the complicated behavior of these functions near $q = 0$.

IX. CONCLUSION

In this paper we have reformulated our theory of spectral geometry in terms of K functions. The new representation,

$$E_{nl} = F_{nl}(v) = \min_{r>0}\{K_{nl}^{(f)}(r) + vf(r)\}, \tag{9.1}$$

for the discrete Schrödinger spectrum has a number of advantages over the earlier expression (2.5) in terms of kinetic potentials. Now, the kinetic energy is represented by a positive K function with a pole at zero; meanwhile, the potential-energy function in the semiclassical expression is identical to the potential in Schrödinger's equation. The balance between kinetic and potential energies, which yields the spectrum, is perhaps easier to study when it is expressed in this way.

In principle, a new complication has now been introduced, namely, the dependence of the K functions on the potential. The invariance of K with respect to coupling, spatial translations, and additive shifts of the potential certainly reduces the impact of this shortcoming. However, a much more important and attractive aspect of the new formulation is the transformation invariance $K^{(g(h))} \simeq K^{(h)}$ of the envelope approximation. For a given fixed envelope basis h, this invariance frees the K function of any residual potential dependence and allows the semiclassical form to exhibit approximately how features of the potential shape f flow through to the Schrödinger spectrum it generates.

In Ref. 1 we sought to understand how the eigenvalues $E_{nl}^{(q)}$ corresponding to pure power-law potentials depended on the power q. The principal result of that article was the proof that $P_{nl}(q)$ is a monotone increasing function of q. The new formulation of envelope theory has made possible the discovery of the log-power theorem, $L_{nl} = P_{nl}(0)$. This result, relating two seemingly different quantum-mechanical problems, is certainly interesting in itself, and it allows us to characterize the complicated behavior of the eigenvalues $E_{nl}^{(q)}$ near $q=0$. Conversely, we can now use the interpolation for $P_{nl}(q)$, which we obtained in Ref. 1, to provide a simple eigenvalue formula for the log potential.

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