PHYSICAL REVIEW A VOLUME 50, NUMBER 4 OCTOBER 1994

Spectral inheritance of potentials with flat bottoms

Richard L. Hall
Department of Mathematics and Statistics, Concordia University, 1455 de Maisonneuve Boulevard West, Montréal, Québec, Canada H3G 1M8
(Received 23 May 1994)

A particle moves in one spatial dimension in an attractive symmetric potential $vf(x)$ and obeys nonrelativistic quantum mechanics. It is supposed that the trajectory function $F(v)$, which tells us how the ground-state energy depends on the coupling parameter v, is known. We determine the minimum $f(0)$ of the potential and the mean kinetic energy $s(v)$ from $F(v)$, and we prove that the potential shape $f(x)$ has the constant value $f(0)$ on an interval $[-a,a]$ if and only if s is bounded for all $v>0$. Moreover, if $s<K$, then $a>(\pi/2)[\hbar/(2mK)]^{1/2}$. These are partial results towards *geometric spectral inversion,* the determination of the potential shape f from the corresponding ground-state energy trajectory F.

PACS number(s): 03.65.Ge, 02.40.Hw

I. INTRODUCTION

In this paper we present some specific constructive results concerning an interesting inversion problem in quantum mechanics: if we know how the lowest eigenvalue of a Schrödinger Hamiltonian depends on the potential coupling parameter, are these data sufficient to reconstruct the shape of the potential? We shall call this problem "geometric spectral inversion" to distinguish it from standard inverse scattering theory. In a nutshell our main result is the following: from the ground-state energy against the coupling curve $F(v)$, we can determine whether or not the potential has a flat (horizontal) patch at its center and if it does we can provide a lower bound to the size of this patch.

We consider a single particle of mass m which moves in one spatial dimension in a potential $V(x)$ and obeys nonrelativistic quantum mechanics. We suppose that the potential is attractive and symmetric and has the form $V(x)=V_0 f(x/b)$, where V_0 and b are coupling and range parameters, and f is the shape of the potential. By an elementary scaling argument in which $x/b=x'\to x$ Schrödinger's equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi+V_0 f(x/b)\Psi=\mathcal{E}\Psi \tag{1.1}$$

may be written as

$$-\psi_{xx}(x,v)+vf(x)\psi(x,v)=F(v)\psi(x,v)\ , \quad v>0\ , \tag{1.2}$$

where the dimensionless coupling and energy parameter are given by

$$v=\frac{2mV_0 b^2}{\hbar^2} \text{ and } F(v)=\frac{2mb^2\mathcal{E}}{\hbar^2}\ . \tag{1.3}$$

In this form the Hamiltonian $H=-\Delta+vf(x)$ has only one parameter, the coupling v. The function $F(v)$ which tells us how the energy depends on the coupling is called the "energy trajectory" corresponding to the potential shape f. We usually find $F(v)$ from $f(x)$ by solving Schrödinger's equation (1.2) for the ground-state energy for each value of $v>0$. For attractive potentials in one dimension, a simple variational argument shows that a discrete eigenvalue $F(v)$ exists for every positive value of v.

For example, in the case of the sech-squared potential [1], we have

$$\begin{aligned} f(x)=-\mathrm{sech}^2(x)\to F_n(v) \\ =-[(v+\tfrac{1}{4})^{1/2}-(n+\tfrac{1}{2})]^2\ , \end{aligned} \tag{1.4}$$

where $n=0,1,2,\ldots$. In Fig. 1 we exhibit graphs of some of these energy trajectories. Inverse scattering theory [2–6] allows us to reconstruct the potential $vf(x)$ from various subsets of the spectral and scattering data. The inverse problem in the coupling constant (fixed energy) is well understood and is discussed in detail by Chadan and Sabatier [2]. The spectral data in this problem correspond to the intersection of a horizontal line $E=c$ with

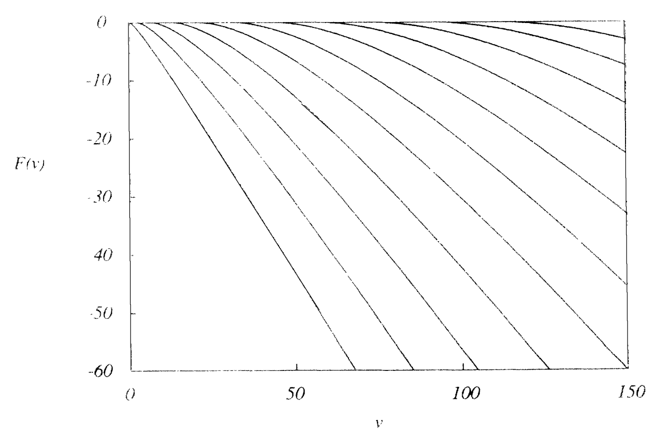

FIG. 1. Energy trajectories (1.4) for the sech-squared potential. Inverse scattering theory uses spectral data in the form of either (i) the energies on a vertical line $v=c$ or (ii) the couplings on a horizontal line $E=c$. Geometric spectral inversion claims that knowledge of the lowest trajectory $F(v)$ alone is sufficient to reconstruct an attractive symmetric potential shape $f(x)$.

 ©1994 The American Physical Society

all the trajectories. This must be distinguished from "geometric spectral inversion" which would claim to reconstruct a symmetric potential shape $f(x)$ from the ground-state energy trajectory $F(v)$ alone. For symmetric potentials, much less data are required by inverse scattering theory than in the more general case. In fact, if a symmetric potential increases to infinity (with x), then the energies alone are sufficient. An analysis of this phenomenon for Sturm-Liouville problems on a finite domain may be found in Ref. [7] and a discussion of the corresponding problem in quantum mechanics is given, for example, in Ref. [4].

However, in the present paper we do not solve the geometric spectral inversion problem completely. We offer instead some partial results. First of all, we shall show in Sec. II that the limit of the ratio $F(v)/v$ as $v \to \infty$ yields the minimum value of $f(x)$. Meanwhile, we find that the mean kinetic energy s is given in terms of the (ground-state) trajectory function $F(v)$ by the expression

$$\langle -\Delta \rangle = s = F(v) - vF'(v) \ . \tag{1.5}$$

Our most interesting results, which are established in Sec. III, may then be stated quite simply as follows: the potential has a flat bottom if and only if the kinetic energy s is *bounded* for all $v > 0$. Moreover, in the case that the potential has a flat bottom, we can estimate the size of the flat part of the potential by the following inequality ($\hbar = 2m = 1$):

$$s \le K \Longrightarrow f(x) = f(0) \ , \quad |x| < a, \text{ and } a > \frac{\pi}{2} K^{-1/2} \ . \tag{1.6}$$

Intuitively we may understand this in terms of the Rayleigh-Ritz (min-max) variational characterization [8–10] of the energy spectrum. If the potential strictly increases for $x > 0$ near $x = 0$, then, as the coupling v is increased, the variational principle forces the wave function to be progressively more concentrated near the origin; this, in turn, increases the average curvature; hence the kinetic energy increases without limit. If, on the other hand, the potential is flat on an interval $[-a,a]$, then, as v is increased, the wave function is concentrated on the whole of this interval and, in the limit $v \to \infty$, the situation is asymptotically like that of a square well of width $2a$. The main purpose of the present paper is to put this heuristic argument on a sound footing so that (1.6) becomes a step in the constructive theory of geometric spectral inversion.

The following subjective remark may be of some interest. We initially noticed the boundedness property of the kinetic energy for square wells and we supposed that it has to do with the fact that square wells are "cut off," that they vanish when $|x| > a$. Only after looking in this wrong direction for some considerable time did we manage to establish generally that flatness of the potential is the correct feature which is characterized unambiguously by bounded kinetic energies.

II. ENERGY TRAJECTORIES AND KINETIC POTENTIALS

In the abstract theory [9,10] of Schrödinger operators, the potential $vf(x)$ in our problem would be regarded as a perturbation of the positive-definite Laplacian operator $-\Delta$. The idea behind "kinetic potentials" is an analytical realization of this abstract notion; it was introduced in Ref. [11] and was extended to excited states in Ref. [12] and has been used recently to analyze power-law potentials [13]. For the bottom of the spectrum, the case that concerns us principally in this paper, one sets $\langle -\Delta \rangle = s$. Then the kinetic potential (minimum mean isokinetic potential) $\bar{f}(s)$ is that function of s satisfying $\langle f \rangle = \bar{f}(s)$. The advantage of this is that kinetic potentials allow us to represent conveniently the way in which parametric dependencies of the operator flow via the variational characterization through to the corresponding spectrum: this is the main concern of what we call "spectral geometry."

We now present a short self-contained introduction to kinetic potentials. We suppose that $H = -\Delta + vf$ is bounded below and self-adjoint, and throughout this section ψ represents the exact normalized ground state for coupling v, as shown in (1.2). We have, therefore,

$$F(v) = (\psi, H\psi) = (\psi, -\Delta\psi) + v(\psi, f\psi) \ . \tag{2.1}$$

Hence

$$F'(v) = 2(\psi_v, H\psi) + (\psi, f\psi) = 2F(v)(\psi_v, \psi) + (\psi, f\psi) \ .$$

The normalization of ψ implies that $(\psi_v, \psi) = 0$. Consequently

$$F'(v) = (\psi, f\psi) \ . \tag{2.2}$$

This result may also be obtained by an application of the Hellmann-Feynman theorem [14–17]. If we change the coupling to u in the Hamiltonian but *not* in the wave function, we have by the variational characterization

$$f(u) \le [\psi, (-\Delta + uf)\psi] = F(v) + (u - v)(\psi, f\psi) \ . \tag{2.3}$$

Hence, by using (2.2) we find

$$F(u) \le F(v) + (u - v)F'(v) \ . \tag{2.4}$$

That is to say, the trajectory function $F(v)$ lies beneath its tangents and is *concave*. We are now in a position to define the kinetic potential $\bar{f}$ associated with F by the following parametric relations in terms of v:

$$\begin{aligned} s &= \|\psi_x\|^2 = F(v) - vF'(v) \ , \\ \bar{f}(s) &= (\psi, f\psi) = F'(v) \ . \end{aligned} \tag{2.5}$$

We may regard the correspondence $\bar{f} \leftrightarrow F$ as a *transformation* provided we can invert $\bar{f}$. This is always possible because $\bar{f}$ is monotone *decreasing*. From (2.5) we conclude

$$\frac{ds}{dv} = -vF''(v) > 0 \Longrightarrow \bar{f}\,'(s) = -\frac{1}{v} < 0 \ . \tag{2.6}$$

Furthermore, we can show that $\bar{f}(s)$ is *convex* for

$$\bar{f}''(s)=\frac{1}{v^2}\frac{dv}{ds}=-\frac{1}{v^3F''(v)}>0\ . \tag{2.7}$$

We note that monotonicity of the *potential* f itself is *not* required for these results. Apart from the sign, the relation between $\bar{f}$ and F is that of a *Legendre transformation* [18] for we have

$$\bar{f}''(s)F''(v)=-\frac{1}{v^3}<0\ . \tag{2.8}$$

Because of the convexity of $\bar{f}$ we can express the eigenvalue $F(v)$ in the form

$$F(v)=\min_{s>0}\{s+v\bar{f}(s)\}\ , \tag{2.9}$$

that is to say, the inverse transformation $\bar{f}\to F$ is given by

$$\begin{aligned} v^{-1}&=-\bar{f}'(s)\ ,\\ F(v)&=[s+v\bar{f}(s)]\ . \end{aligned} \tag{2.10}$$

The idea is that we perform the variational procedure in two stages: for each value of $\langle -\Delta\rangle=s$ we find the minimum mean potential shape $\langle f\rangle=\bar{f}(s)$, and then we recover the energy eigenvalue, for each value of v, by minimizing over the kinetic energy s.

We now assume that the potential is bounded below and symmetric about its minimum point $\hat{x}$ and nondecreasing for $x>\hat{x}$. Since the energy spectrum is invariant under shifts along the x axis, we assume henceforth, without any loss of generality, that the minimum value of $f(x)$ occurs at $x=\hat{x}=0$. The first general result which we shall need is

$$f(0)=\lim_{v\to\infty}\frac{F(v)}{v}\ . \tag{2.11}$$

We establish this limit in the following way. If in (1.2) we suppose that $\|\psi\|=1$, then, after an integration by parts, we have

$$\begin{aligned}(\psi,H\psi)&=F(v)\\ &=\|\psi_x\|^2+v(\psi,f\psi)\geq v(\psi,f\psi)\geq vf(0)\ . \end{aligned}\tag{2.12}$$

If we now employ, for example, the normalized trial function

$$\phi(x)=(v/\pi^2)^{1/8}\exp(-v^{1/2}x^2/2)\ , \tag{2.13}$$

then the variational upper estimate $(\phi,H\phi)$ leads to the inequality

$$\frac{F(v)}{v}<\frac{1}{2v^{1/2}}+(\phi,f\phi)\ . \tag{2.14}$$

In the limit $v\to\infty$, $(\phi,f\phi)\to f(0)$. Hence from (2.12) and (2.14) we have

$$\frac{F(v)}{v}\geq f(0)\ \text{and}\ \lim_{v\to\infty}\frac{F(v)}{v}\not> f(0)\ .$$

From these two relations we conclude (2.11). Thus we are able to deduce from $F(v)$ the minimum value $f(0)$ of the potential. This is our first constructive step towards the inverse $F\to f$.

An important additional tool which we shall need is the following.

Concentration lemma.

$$q(v)=\int_{-a}^{a}\psi^2(x,v)dx>\frac{f(a)-F'(v)}{f(a)-f(0)}\to 1\ ,\quad v\to\infty\ , \tag{2.15}$$

which makes more precise the intuitive notion mentioned in the Introduction that the wave function becomes more concentrated near the origin as v increases. We prove this lemma by the following argument. Since $f(x)$ has minimum value $f(0)$, we know from (2.2) that

$$F'(v)=\bar{f}(s)=(\psi,f\psi)\geq f(0)\ . \tag{2.16}$$

Because of the limit (2.11) and l'Hôpital's rule we deduce that the lower bound $f(0)$ is achieved in the large v limit. Meanwhile, we know that $F'(v)$ decreases monotonically to $f(0)$ because we showed above that $F''(v)<0$. Thus, for each $v>0$, there exists a number $a(v)>0$ such that $f(a)=F'(v)$ and $f(a)>F'(u)$, for all $u>v$. We now define $q(v)$ to be the probability mass in the interval $[-a,a]$, thus

$$q(v)=\int_{-a}^{a}\psi^2(x,v)dx\ . \tag{2.17}$$

From (2.2), we have

$$F'(v)=(\psi,f\psi)=\int_{|x|\leq a}\psi^2 f dx+\int_{|x|\geq a}\psi^2 f\,dx\ . \tag{2.18}$$

We obtain a lower estimate to the right-hand side of (2.18) if only the smallest value of $f(x)$ is used in each of the two regions . That is to say, we obtain the inequality

$$F'(v)\geq qf(0)+(1-q)f(a)\ . \tag{2.19}$$

Hence, for each a such that $f(a)>f(0)$ and for all v sufficiently large, we conclude the concentration lemma (2.15).

III. THE SPECTRAL CHARACTERIZATION OF POTENTIALS WITH FLAT BOTTOMS

We first show that the kinetic energy is bounded if the potential has a flat bottom. Suppose that the flat region is of length $2a$, that is to say, for $a>0$

$$f(x)=f(0)\ ,\quad |x|\leq a\ . \tag{3.1}$$

Then it is clear that $f(x)$ lies below an infinite square well. More specifically, we have

$$f(x)\leq w(x)=\begin{cases} f(0)\ , & |x|<a\\ \infty\ , & |x|\geq a\ . \end{cases} \tag{3.2}$$

The bottom of the spectrum of $-\Delta+vw(x)$ is $vf(0)+(\pi/2a)^2$; meanwhile, $f(0)<(\psi,f\psi)=\bar{f}(s)$. Consequently, in terms of the kinetic-potential formalism, we deduce the inequalities

$$s+vf(0)\leq F(v)=s+v\bar{f}(s)\leq vf(0)+\left[\frac{\pi}{2a}\right]^2\ , \tag{3.3}$$

where s stands for the critical value in (2.9), *after* minimization. Hence we conclude that the kinetic energy is bounded above by

$$s \le \left[\frac{\pi}{2a} \right]^2 . \tag{3.4}$$

We now use the concentration lemma and calculus of variations to establish a lower bound to the kinetic energy s. We choose $a>0$ sufficiently large that $f(a)>f(0)$ and keep a fixed. We then consider v sufficiently large that $f(a)>F'(v)$; this allows us to employ the concentration lemma. With these assumptions we write

$$\begin{aligned} s &= \int_{-\infty}^{\infty} \psi_x^2(x,v)dx \ge \int_{|x|\le a} \psi_x^2(x,v)dx \\ &= q(v)\int_{|x|\le a} \phi_x^2(x,v)dx , \end{aligned} \tag{3.5}$$

where ϕ is the normalized restriction of ψ to $[-a,a]$ given by

$$\phi(x,v)= \begin{cases} \psi(x,v)q^{-1/2}(v) , & |x| \le a \\ 0 , & |x|>a . \end{cases} \tag{3.6}$$

For each fixed v, finding the minimum possible value of the integral on the right-hand side of (3.5) is a problem in the calculus of variations. Namely, we have to solve

$$\int_{-a}^{a} [\phi'(x)]^2 dx \longrightarrow \text{minimum subject to } \int_{-a}^{a} \phi^2(x)dx = 1 \tag{3.7}$$

in which we have temporarily dropped the dependence of ϕ on v. Except for the boundary conditions, this is exactly the elementary quantum-mechanical problem of a particle in a box. Indeed, if we could assume $\phi(-a)=\phi(a)=0$, then the lower bound for this integral would be precisely the lowest energy of a particle in a box (with $\hbar=2m=1$), that is to say $(\pi/2a)^2$. We have proved earlier [19] that for symmetric potentials which are nondecreasing for $x>0$ the ground-state wave function monotonically decreases for $x>0$. This fact together with the concentration lemma implies that $\psi(a,v)$, and therefore also $\phi(a,v)$, tends to zero as $v \longrightarrow \infty$. Hence, the vanishing boundary condition is met in the large-v limit. Meanwhile $q(v) \longrightarrow 1$. Hence, from (3.5) we see that, for each a such that $f(a)>f(0)$ we have established the limit

$$\lim_{v\uparrow\infty}(s) \ge \left[\frac{\pi}{2a} \right]^2 . \tag{3.8}$$

This result is the key to our problem. If $f(x)$ is strictly increasing from $x=0$, then $f(a)>f(0)$ for every $a>0$, however small; hence, as v increases, we deduce that the kinetic energy increases without bound. If, on the other hand, we find from $F(v)$ that $s \le K$, then (3.8) puts a lower limit to the size of a. That is to say, we have proved the claim made in the Introduction

$$s \le K \Longrightarrow f(x)=f(0) , \quad |x|<a , \quad \text{and } a > \frac{\pi}{2}K^{-1/2} . \tag{3.9}$$

IV. CONCLUSION

By looking at the ground-state energy trajectory F alone we can determine some basic features of the symmetric attractive potential f which generates the trajectory. The specific results we report concern the shape of f near $x=0$ and we have shown how these features may be deduced unambiguously from the properties of $F(v)$ for large values of v. Since some of the essential monotone properties which we have used are also present in the first excited state [19], our partial inverse results can be extended to problems in three dimensions, provided the coupling is large enough to support a bound state.

Two areas of application immediately come to mind. In atomic physics screened Coulomb potentials [20–22] are used to model the spectrum generated by an outer electron. If the ground-state energies for a sequence of atoms are known, this is equivalent to knowing $F(v)$ for a sequence of values of v. However, as we have shown in Sec. II, the trajectory is concave so that isolated values of $F(v)$ could be joined by a smooth curve and from this curve an approximate picture of the potential f could in principle be reconstructed from the partial trajectory data. Similarly, for the many-body problem, the nonindividuality of identical particles induces a relationship [23] between the N-body energy and the energy of a specially constructed two-body problem having an overall factor of $N-1$ and a coupling enhanced by $N/2$. Here the ground-state energies for a sequence of values of N would again provide partial information concerning the energy trajectory of the reduced "two-body" problem. But first we must find out how to reconstruct *all* of the potential f from knowledge of the corresponding energy trajectory F.

ACKNOWLEDGMENT

Partial financial support of this work under Grant No. GP3438 from the Natural Sciences and Engineering Research Council of Canada is gratefully acknowledged.

[1] S. Flügge, *Practical Quantum Mechanics* (Springer, New York, 1974).
[2] K. Chadan and P. C. Sabatier, *Inverse Problems in Quantum Scattering Theory* (Springer, New York, 1989).
[3] R. G. Newton, *Scattering Theory of Waves and Particles* (Springer, New York, 1982).
[4] B. N. Zakhariev and A. A. Suzko, *Direct and Inverse Problems: Potentials in Quantum Scattering* Theory (Springer, Berlin, 1990).
[5] G. Eilenberger, *Solitons* (Springer, Berlin, 1983).
[6] M. Toda, *Nonlinear Waves and Solitons* (Kluwer, Dordrecht, 1989).
[7] V. Barcilon, J. Math. Phys. **15**, 429 (1974).
[8] E. Prugovecki. *Quantum Mechanics in Hilbert Space*

(Academic, New York, 1981).

[9] M. Reed and B. Simon, *Methods of Modern Mathematical Physics IV: Analysis of Operators* (Academic, New York, 1978).

[10] W. Thirring, *A Course in Mathematical Physics 3: Quantum Mechanics of Atoms and Molecules* (Springer, New York, 1981).

[11] R. L. Hall, J. Math. Phys. **24**, 324 (1983).

[12] R. L. Hall, J. Math. Phys. **25**, 2087 (1984).

[13] R. L. Hall, Phys. Rev. A **39**, 5500 (1989).

[14] H. Hellmann, Acta Physiochem. URSS I, **6**, 913 (1935); IV, **2**, 225 (1936); *Einführung in die Quantenchemie* (F. Denticke, Leipzig, 1937), p. 286.

[15] R. P. Feynman, Phys. Rev. **56**, 340 (1939).

[16] E. Merzbacher, *Quantum Mechanics, 2nd ed.* (Wiley, New York, 1970).

[17] C. Quigg and J. L. Rosner, Phys. Rep. **56**, 167 (1979).

[18] I. M. Gelfand and S. V. Fomin, Calculus of Variations (Prentice-Hall, Englewood Cliffs, NJ, 1963).

[19] R.L. Hall, J. Phys. A: Math. Gen. **25**, 4459 (1992).

[20] J. McKennan, L. Kissel, and R. H. Pratt, Phys. Rev. A **13**, 532 (1976).

[21] C. H. Mehta and S. H. Patil, Phys. Rev. A **17**, 34 (1978).

[22] R. L. Hall, Phys. Rev. A **32**, 14 (1985).

[23] R. L. Hall, Phys. Rev. A **45**, 7682 (1992).