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# Geometric spectral inversion

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**Abstract.** We suppose that the trajectory function  $F(v)$ , which describes how the lowest eigenvalue of the Schrödinger Hamiltonian operator  $H = -\Delta + vf(x)$  depends on the coupling parameter  $v$ , is known, and from this we reconstruct the *shape*  $f(x)$  of the potential. If  $f$  is symmetric and non-decreasing for  $x > 0$ , then  $f(0)$  can be determined from  $F$ ; in the case of bounded potentials with area, the area can also be determined. If  $F$  is a possible trajectory, then the inverse  $\Lambda^{-1}(F) = f$  is proved to be unique. Square wells and separable potentials are immediately invertible, and square wells  $f^\square$  are also extremal: they bound the range of  $\Lambda$  by the general inequality  $F^\square < F$ . With the help of the kinetic-potential formalism, approximate inversion formulae are derived by a variational method and also by envelope representations.

## 1. Introduction

Geometrical considerations of the type we shall consider in this paper become a quantum-mechanical spectral problem when the Hamiltonian operator  $H$ , which generates the spectrum, depends smoothly on certain parameters. Spectral objects such as eigenvalues depend in turn on these parameters and in so doing they generate curves or surfaces in a Euclidean space. In this paper we investigate the following elementary question: if we know how the lowest eigenvalue of a Schrödinger operator depends on the coupling parameter, is this sufficient to reconstruct the shape of the potential? In an earlier paper [1] we showed that the specific question whether or not a symmetric potential had a flat (horizontal) patch at its centre could be answered unambiguously by studying the dependence  $F(v)$  of the lowest eigenvalue on the coupling parameter; moreover, by studying  $F(v)$  a lower bound could be established on the size of this patch. In this paper we carry this analysis further.

We consider Schrödinger Hamiltonian operators of the form  $H = -\Delta + vf(x)$ , where  $f(x)$  is the shape of a non-constant symmetric potential in  $\mathbb{R}$  which is bounded below and is non-decreasing on  $[0, \infty)$ . By a simple variational argument we can show that for all  $v > 0$  the Hamiltonian  $H$  has a discrete eigenvalue  $F(v)$  at the bottom of its spectrum; we shall refer to  $F$ , or its graph  $(v, F(v))v > 0$ , as the *energy trajectory* of  $f(x)$ . We therefore have

$$-\psi_{xx}(x, v) + vf(x)\psi(x, v) = F(v)\psi(x, v) \quad v > 0. \quad (1.1)$$

Familiar examples are the sech-squared potential [2]

$$-\operatorname{sech}^2(x) = f(x) \longrightarrow F(v) = -\left[\left(v + \frac{1}{4}\right)^{1/2} - \frac{1}{2}\right]^2 \quad (1.2)$$

and the harmonic oscillator

$$x^2 = f(x) \longrightarrow F(v) = v^{1/2}. \quad (1.3)$$

The purpose of this paper is to study 'geometric spectral inversion', that is to say the inverse transformation:  $F \rightarrow f$ .

When it is more fully developed, it is expected that geometric spectral inversion will enjoy practical scientific application. The problem of screened-Coulomb potentials in atomic physics is one possibility. In the context of a one-particle model such a potential is experienced by an outer electron or, say, a 'visiting' pion. Here atomic spectral data would be available corresponding to a set of values of the coupling parameter of the model. Similarly, with other  $N$ -body problems, one might have ground-state spectral data for various values of  $N$ . In nuclear physics, for example, the masses of a sequence of nuclei immediately give the corresponding binding energies. If the particles are identical, or can be considered approximately identical within an isotopic-spin model, then quantum-mechanical non-individuality induces [3], via permutation symmetry, a relation between the  $N$ -body problem and a scaled two-body problem having an overall factor of  $N - 1$  and a coupling parameter enhanced by the factor  $N/2$ . Within such an approximation the nuclear masses determine the ground-state energies of a one-particle problem for a sequence of values of the coupling parameter. Such sparse spectral information might seem rather far from having the whole of the trajectory  $F$ : but given the known concavity property of trajectories, even a few isolated values of  $F(v)$  would enable the reconstruction of a smooth approximation for  $F(v)$  from which, by geometric spectral inversion, an approximation could be obtained in turn for the underlying pair-potential shape  $f$ .

For the last 40 years there has been intense interest in inverse problems related to quantum mechanics. Many fundamental results concerning inverse scattering theory and the relation between Schrödinger operators and nonlinear waves are now available in monographs [4–8]. The so-called 'inverse problem in the coupling constant' (for example Chadan and Sabatier [4, p 406]) must be distinguished from the problem introduced in this paper. In the former problem, expressed partly here in our notation, one has in addition to the normalization constants for scattering states, spectral data in the form of the set  $\{v_i\}$  of values of  $v$  such that  $F^{(i)}(v_i) = E$  has a fixed value, where  $F^{(i)}$  is the trajectory function for the  $i$ th eigenvalue of  $H$ . That is to say, for fixed energy one has a set of characteristic values of the coupling parameter  $v$ . In our problem we have, corresponding to an unknown potential shape  $f$ , a function  $F$  which describes how the lowest eigenvalue of  $H = -\Delta + v f(x)$  depends on the coupling parameter  $v$ . The 'transform', which we earlier [9] called  $\Lambda$ , satisfies  $F = \Lambda(f)$ : in this paper we turn our attention principally to the inverse  $\Lambda^{-1}$ .

Since the spectrum of  $H$  is invariant under translation along the  $x$ -axis, we shall regard the 'horizontal' shifts of  $f$  to be equivalent. We shall prove in section 2 that  $F$  determines the minimum of  $f$ . It is natural therefore to shift  $f$  so that, without loss of generality, its minimum occurs at  $x = 0$ . Vertical shifts of  $f$ , by  $b$  say, simply change  $F(v)$  to  $F(v) + bv$ . Consequently, we are able to show, without loss of generality, that the frame for  $f$  can be fixed by the imposition of conditions such as  $f(0) = -1$ , or alternatively for potentials not bounded above,  $f(0) = 0$ . In fact we shall derive a prescription for the 'normalization' of a given trajectory  $F$  so that it would correspond to a potential shape  $f$  obeying such a condition. For potential shapes  $f$  which have area  $2A = \int_{-\infty}^{\infty} |f(x)| dx$  we shall show that the trajectory  $F$  determines  $A$ ; for such potentials it is convenient to tighten the normalization so that  $A = 1$ .

Square wells occupy a potentially important place in this study. If it is known that  $f$  is square, then up to the trivial shifts discussed above and under standard normalization,  $F$  determines  $f$  uniquely for  $f(0) = -1$  and  $A = 1$  and therefore  $f$  is determined. In addition to the square wells being immediately invertible, they have another interesting

feature: amongst the bounded symmetric semi-monotone potentials, the square wells are extremal; they have the lowest of all possible trajectories  $F$ . Consider, for example, the 'suspect' trajectory  $F^*(v) = -v^2/(1+v)$ . If  $F^*$  were a trajectory for some potential shape  $f^*$ , we can prove that  $f^*$  would have to satisfy  $A = 1$  and  $f^*(0) = -1$ . However, no inverse exists for  $F^*$  because it lies beneath the normalized square-well trajectory  $F^\square$ . In order to prove results like this we use a refinement [10] of the usual comparison theorem of quantum mechanics which is discussed in section 3.

In section 4 we briefly recall some results from kinetic-potential theory and use these to generate approximate inversion formulae by a variational method and also by the use of envelope representations in the form given in [11]. In section 5 we derive inversion results for separable potentials. Finally, in section 6 we discuss the general question of uniqueness: we are able to prove for symmetric potentials which are monotone for  $x > 0$  that if the trajectory  $F$  exists then the inverse  $f$  is unique.

## 2. The normalization of trajectories

The main results of this section presuppose that the unknown potential shape  $f$  is symmetric, semi-monotone, and bounded below. Then, from the given trajectory function  $F$ , we can determine whether the unknown potential shape  $f$  is bounded above and also whether it has area: in these cases the bounds and the area can be determined from  $F$ . Once these parameters are found, the potential and the trajectory function can be conveniently scaled to a standard normal form.

More specifically, we suppose that the potential  $f$  is bounded below and that it is symmetric about its minimum point  $\hat{x}$ . Since the Laplacian is invariant under spatial translations it follows that we can replace  $x$  by  $x - \hat{x}$  everywhere in (1.1); that is to say, the spectrum of  $H$ , and in particular  $F(v)$ , is invariant under spatial translations. Consequently, without loss of generality, we henceforth assume that  $\hat{x} = 0$ . If in (1.1) we suppose that  $\|\psi\| = 1$ , then after an integration by parts we obtain the inequality

$$(\psi, H\psi) = F(v) = \|\psi_x\|^2 + v(\psi, f\psi) \geq v(\psi, f\psi) \geq vf(0). \quad (2.1)$$

By using (2.1) and a variational upper bound it is possible to establish a first constructive step towards the inverse  $F \rightarrow f$ , namely the following theorem which is proved in [1].

*Theorem 2.1.*

- (i)  $f$  is symmetric;
- (ii)  $f(x) \geq f(0)$ ;
- (iii)  $f$  is non-decreasing on  $[0, \infty)$ ;

$$\Rightarrow f(0) = \lim_{v \rightarrow \infty} \frac{F(v)}{v}. \quad (2.2)$$

For bounded potentials we are also able to prove the following theorem.

*Theorem 2.2.*

- (i)  $f$  is symmetric;
- (ii)  $f(x) \geq f(0)$ ;
- (iii)  $f$  is non-decreasing on  $[0, \infty)$ ;

$$(iv) \lim_{x \rightarrow \infty} \{f(x)\} = 0;$$

$$\Rightarrow \int_{-\infty}^{\infty} |f(x)| dx = 2A \iff A^2 = -\lim_{v \rightarrow 0} \frac{F(v)}{v^2}. \quad (2.3)$$

*Proof of theorem 2.2.* Firstly we suppose that the potential has area  $2A$ . If we replace  $x$  by  $x/a$  in Schrödinger's equation (1.1), define  $\Psi(x, v) = a^{-1/2} \psi(x/a, v)$ , and divide by  $a^2$ , then we obtain

$$-\Psi_{xx}(x, v) + va \frac{1}{a} f\left(\frac{x}{a}\right) \Psi(x, v) = \frac{1}{a^2} F((va)a) \Psi(x, v) \quad v > 0. \quad (2.4)$$

We now let  $a \rightarrow 0$ , keeping the product  $va$  constant at  $va = 1$ . In this limit the potential  $\frac{1}{a} f(\frac{x}{a})$  approaches the Dirac delta  $-2A\delta(x)$  and consequently the eigenvalue  $\frac{1}{a^2} F(va)$  approaches  $-A^2$ , the bottom of the spectrum of the well known one-dimensional Schrödinger Hamiltonian  $-\Delta - 2A\delta(x)$ .

Now we suppose that the limit on the right-hand side of (2.3) exists but that the potential-area integral diverges. We then construct a new potential  $f_c$  which agrees with  $f$  for  $|x| < c$  and is otherwise zero. The point  $c$  is chosen so that, for example,  $\int_{-\infty}^{\infty} |f_c(x)| dx = 4A$ . By the Rayleigh-Ritz (min-max) characterization of the spectrum [12-14], we conclude that

$$f(x) < f_c(x) \Rightarrow F(v) < F_c(v) \Rightarrow |F(v)| > |F_c(v)|.$$

This in turn implies that the corresponding limit for  $F_c$  on the right-hand side of (2.3) would yield a value  $A_c^2 < A^2$ . But  $A_c = 2A$ . Hence, the potential-area integral must converge and be equal to  $A$ .  $\square$

The first part of this proof could perhaps be made more formal by the use of a lower bound provided by the theorem of Spruch [15, p 200], and an upper bound provided by the (improper) trial function  $\phi(x) = N \exp(-\alpha|x|)$ .

For symmetric semi-monotone potentials which are bounded below we now try to extract from our knowledge of  $F$  some key features of the unknown potential shape  $f$ . We have to make assumptions about both  $f$  and  $F$ . For clarity our results are expressed in terms of the following theorem.

*Theorem 2.3.*

- (i)  $f$  is symmetric;
- (ii)  $f(x) \geq f(0)$ ;
- (iii)  $f$  is non-decreasing on  $[0, \infty)$ ;
- (iv)  $F(v)/v \rightarrow b$  as  $v \rightarrow \infty$ ;
- (v)  $F(v)/v \rightarrow B$  as  $v \rightarrow 0$ ;
- (vi)  $F(v) - Bv/v^2 \rightarrow -A^2$  as  $v \rightarrow 0$ ;

$\Rightarrow$

- (1)  $f(0) = b$
- (2)  $f(x) \rightarrow B$  as  $x \rightarrow \infty$
- (3)  $\int_{-\infty}^{\infty} |f(x)| dx = 2A$ .

It follows immediately from theorem 2.3 that we can define in terms of  $F$  and  $f$  a 'normalized' trajectory function  $\tilde{F}$  and corresponding scaled potential  $\tilde{f}$  by

$$\tilde{F}(v) = \left(\frac{A}{B-b}\right)^2 F\left(\frac{(B-b)v}{A^2}\right) - \frac{Bv}{B-b} \tag{2.5}$$

and

$$\tilde{f}(x) = (B-b)^{-1} \left( f\left(\frac{Ax}{B-b}\right) - B \right) \tag{2.6}$$

where, from the claims of the theorem, we see that the normalized potential shape  $\tilde{f}$  has the properties:

$$\tilde{f}(0) = -1 \quad \lim_{x \rightarrow \infty} \tilde{f}(x) = 0 \quad \int_{-\infty}^{\infty} |\tilde{f}(x)| dx = 2. \tag{2.7}$$

Thus for any symmetric semi-monotone potential with a trajectory function  $F$  satisfying the three limits given as hypotheses in theorem 2.3, we may, without loss of generality, adopt the convenient normalized forms given by (2.5) and (2.6).

*Proof of theorem 2.3.* By adding  $\beta v\Psi$  to both sides of equation (2.4) we arrive at the following general correspondence:

$$\alpha v f\left(\frac{x}{a}\right) + \beta v \longleftrightarrow a^{-2} F(\alpha v a^2) + \beta v \tag{2.8}$$

where  $a > 0$ ,  $\alpha > 0$  and  $\beta$  are constants. If we choose the special case  $a = (B-b)/A$ ,  $\alpha = (B-b)^{-1}$  and  $\beta = -B/(B-b)$ , then we obtain, on the left and right of (2.8) respectively, the normalized potential shape  $\tilde{f}$  and trajectory function  $\tilde{F}$ . The hypotheses (iv)–(vi) then imply that  $\tilde{F}$  satisfies the 'normalized' limits:

- (a)  $\tilde{F}(v)/v \rightarrow -1$  as  $v \rightarrow \infty$
- (b)  $\tilde{F}(v)/v \rightarrow 0$  as  $v \rightarrow 0$
- (c)  $\tilde{F}(v)/v^2 \rightarrow -1$  as  $v \rightarrow 0$ .

We now apply theorems 2.1 and 2.2 to  $\tilde{f}$  and  $\tilde{F}$  and deduce  $\tilde{f}(0) = -1$  and  $\int_{-\infty}^{\infty} |\tilde{f}(x)| dx = 2$ . The finiteness of the potential-area integral for  $\tilde{f}$  implies  $\lim_{x \rightarrow \infty} \tilde{f}(x) = 0$ . These three results establish (2.7) and the definition (2.6) yields the three claims of the theorem. □

### 3. Comparison theorems

The standard comparison theorem of quantum mechanics is an immediate consequence of the Rayleigh–Ritz (variational or min–max) characterization of the spectrum of the Schrödinger operator  $H = -\Delta + vf$  (see for example [13, p 75] or [14, p 152]). The expression of this theorem in the present context is simply

$$f^{(1)} < f^{(2)} \Rightarrow F^{(1)} < F^{(2)}. \tag{3.1}$$

However, this result is not strong enough for our purposes. The right-hand side of (3.1) can be implied under weaker ordering conditions, which allow the graphs of  $f^{(1)}$  and  $f^{(2)}$  to cross over [10]. For each normalized potential shape  $f$  we define a corresponding area function  $f_1$  defined by

$$f_1(x) = \int_0^x f(t) dt \quad x \geq 0. \tag{3.2}$$

With this definition, we restate from [10] the following theorem.

**Theorem 3.1.**

- (i)  $f$  is symmetric;
- (ii)  $f(x) \geq f(0)$ ;
- (iii)  $f$  is non-decreasing on  $[0, \infty)$ ;
- (iv)  $f_1^{(1)} < f_1^{(2)}$ ;

$$\Rightarrow F^{(1)} < F^{(2)}. \tag{3.3}$$

An immediate consequence of this theorem is that the square-well trajectory is extremal. If  $f$  is a normalized potential and  $f^\square$  is a normalized square well, then necessarily  $f_1^\square < f_1$ . Thus for normalized potentials we always have the following theorem.

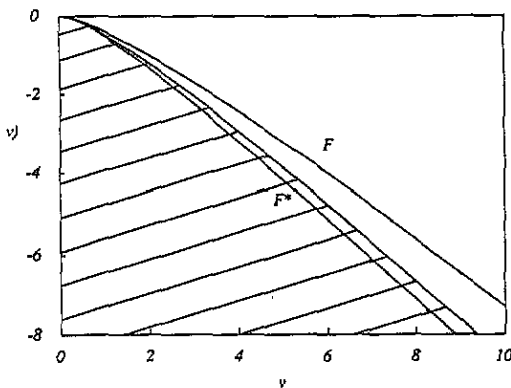
**Theorem 3.2.**

$$F^\square < F. \tag{3.4}$$

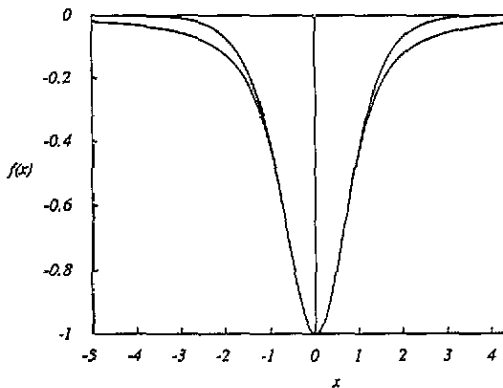
As an example we consider the suspect trajectory

$$F^*(v) = -\frac{v^2}{(1+v)}. \tag{3.5}$$

It follows from theorem 2.3 that  $A = 1, B = 0$  and  $b = -1$  so that the corresponding potential  $f^*$ , if it exists, is normalized. However, as figure 1 illustrates, it turns out that  $F^* < F^\square$ . Hence  $F^*$  cannot be a trajectory and  $f^*$  does not exist. Since we are interested in  $\Lambda^{-1}$  it is obviously very important to know as much as possible about the range of  $\Lambda$ ; normalized functions of  $v$  with plots in the shaded region in figure 1 are not in this range.



**Figure 1.** The 'forbidden' shaded region is bounded by the extremal energy trajectory  $F^\square(v)$  of the normalized square-well potential. The suspect trajectory  $F^*(v) = -v^2/(1+v)$  'appears' to be the spectral image of a potential  $f^*(x)$  which has area two, vanishes as  $x \rightarrow \infty$ , and satisfies  $f^*(0) = -1$ . However, since  $F^*(v)$  lies below  $F^\square(v)$  no such potential  $f^*(x)$  exists.  $F(v)$  is the known trajectory equation (1.2) for the normalized sech-squared potential.



**Figure 2.** The sech-squared potential  $f$  and the approximate inverse  $f^{(A)}$  (the lower curve) reconstructed from  $\bar{f}$  by the Gaussian inversion formula (4.8).

#### 4. Two approximate inversion formulae

We now derive two approximate inversion formulae. Our derivations depend on the kinetic-potential formalism the elements of which we shall recall only very briefly here. In the abstract theory [12–14] 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 first introduced in [9] and was extended to excited states in [16]. For the bottom of the spectrum, which is the case that concerns us principally in this paper, one sets  $\langle -\Delta \rangle = s$ . Then the kinetic potential (minimum mean-iso-kinetic potential)  $\bar{f}(s)$  is that function of  $s$  satisfying  $\langle f \rangle = \bar{f}(s)$ . The advantage of this is that the kinetic potentials allow us to conveniently represent the way in which parametric dependences of the operator flow via the Rayleigh–Ritz (min–max) principle through to the corresponding spectrum: this is the main concern of what we call ‘spectral geometry’. A very concise independent derivation of the elements of the theory may be found in [1].

We suppose that  $H = -\Delta + vf$  is bounded below and is self-adjoint and throughout this section  $\psi$  represents the exact normalized ground state for coupling  $v$ , as shown in (1.1). We have, therefore,

$$F(v) = (\psi, H\psi) = (\psi, -\Delta\psi) + v(\psi, f\psi). \tag{4.1}$$

From this starting point we are able to prove [1] that  $F'(v)$  is given by

$$F'(v) = (\psi, f\psi) \tag{4.2}$$

and that  $F(v)$  is concave, that is to say  $F''(v) < 0$ . The definition of the kinetic potential  $\bar{f}(s)$  associated with the potential shape  $f(x)$  is given by

$$\begin{aligned} \bar{f}(s) &= \inf_{\psi \in \mathcal{D}(H)} (\psi, f\psi) \\ \|\psi\| &= 1 \\ (\psi, -\Delta\psi) &= s \end{aligned} \tag{4.3}$$

where  $\mathcal{D}(H)$  is the domain of  $H$ . By considering finite-dimensional subspaces and scaling, to keep  $s$  constant, similar expressions can also be written for the excited states [16]. It follows [1] that kinetic potentials are monotone decreasing and convex; a kinetic potential and its corresponding energy trajectory are, in fact, related by a Legendre transformation [17]. More specifically, we have the following parametric relations in terms of the potential coupling  $v$ :

$$\begin{cases} s = \|\psi_x\|^2 = F(v) - vF'(v) \\ \bar{f}(s) = (\psi, f\psi) = F'(v). \end{cases} \tag{4.4}$$

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

$$F(v) = \min_{s>0} \{s + v\bar{f}(s)\}. \tag{4.5}$$

This formula is fundamental to this section of the paper. The idea is that we perform min–max 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  $s$ . The point of all this is that kinetic potentials are much easier to approximate than energy trajectories.

We are now in a position to derive the first approximation formula for the inverse of  $F$ . In view of the variational expression (4.3) we may use a 'trial' wavefunction  $\phi(x, s)$  satisfying  $\|\phi\| = 1$  and  $\|\phi_x\|^2 = s$  and obtain

$$\bar{f}(s) < \bar{f}_\phi(s) = (\phi, f\phi). \tag{4.6}$$

With respect to each specific choice of  $\phi$ , (4.6) generates an approximate inversion formula. Thus the Gaussian choice

$$\phi(x, s) = \left(\frac{2s}{\pi}\right)^{1/4} e^{-sx^2} \tag{4.7}$$

leads to the general 'Gaussian inversion' formula:

$$\bar{f}(s) < (\phi, f\phi) \Rightarrow \frac{f(\sqrt{t/2})}{\sqrt{\pi t}} \approx \mathcal{L}^{-1}\left(\frac{\bar{f}(s)}{\sqrt{s}}\right) \tag{4.8}$$

where  $\mathcal{L}$  is the usual Laplace transform. It is tempting to wish that  $\approx$  would also preserve the ordering  $>$ ; however, this desirable relation does not seem to follow immediately from the properties of the inverse Laplace transform [18]. As an example we shall apply (4.8) to  $\bar{f}$  for the ground state of the sech-squared potential [11] given by

$$f(x) = -\operatorname{sech}^2(x) \rightarrow \begin{cases} F(v) = -[(v + \frac{1}{4})^{1/2} - \frac{1}{2}]^2 \\ \bar{f}(s) = \frac{-2s}{[s^2 + s]^{1/2} + s}. \end{cases} \tag{4.9}$$

We obtain

$$\mathcal{L}^{-1}\left(\frac{\bar{f}(s)}{\sqrt{s}}\right) = \mathcal{L}^{-1}\left(-2\left[\sqrt{s+1} - \sqrt{s}\right]\right). \tag{4.10}$$

Thus

$$-\operatorname{sech}^2(x) = f(x) \approx f^{(A)}(x) = -\frac{\sinh(x^2)}{x^2} e^{-x^2}. \tag{4.11}$$

The approximate potential  $f^{(A)}(x)$  is a good approximation for small  $x$ . However, the Gaussian wavefunction is not (simply) exponential for large  $x$  (as is the exact wavefunction), so as the approximate potential has a  $1/x^2$  tail it gives a wrong approximation; the actual ordering  $f^{(A)} < f$  is, however, what we would expect. Plots of  $f(x)$  and  $f^{(A)}(x)$  are shown in figure 2. A variety of other inversion formulae may similarly be derived by choosing different shapes for the trial function  $\phi$ . We face the same sort of choice, of course, when we use variational methods in the 'forward' direction  $f \rightarrow F$ .

Our second approximate formula is based on the inversion of the 'potential envelope method' [9]. Recently this method has been recast [11] into a form that allows us to consider the approximations for  $\Lambda^{-1}(F)$  which we now derive. The idea in the forward direction is that a potential  $f$  of interest is represented as a smooth monotone transformation  $g$  of a soluble potential  $h$ , that is to say

$$f(x) = g(h(x)) \quad \text{or} \quad f = g \circ h. \tag{4.12}$$

Each tangent to  $g$  is a shifted  $h$ -potential of the form  $\alpha + \beta h(x)$ . Since  $h$  is solvable the Schrödinger spectrum is known for each tangential potential. The envelope approximation then consists of a reconstruction in the spectral picture of the envelope of the family of 'tangential trajectories'. If the transformation function  $g$  has definite convexity, then one also obtains energy bounds. In terms of kinetic potentials the envelope method has the following simple expression [9]:

$$f = g \circ h \Rightarrow \bar{f} \approx g \circ \bar{h} \tag{4.13}$$

where  $\approx$  equals  $>$  if  $g$  is convex and  $\approx$  equals  $<$  if  $g$  is concave. As we have seen,  $F$  and  $\bar{f}$  are transforms of each other. Thus, in our inverse problem if we have reason to hope that the 'envelope basis'  $h$  provides a good representation for  $f$  in the sense that the transformation function  $g$  would not vary very strongly, then our search for  $f$  becomes a search for  $g$ , or an approximation for  $g$ .

Since  $h$  is solvable, the corresponding kinetic potential  $\bar{h}$  is known. The monotonicity of kinetic potentials allows us to solve for  $s$  in terms of  $\bar{h}$ . This simple argument immediately yields an approximate solution to the inversion problem  $\bar{f} \rightarrow f$ . We start with (4.13) and extract the following approximate formulae for the transformation function  $g$  and the potential  $f$ :

$$g \approx g^{(A)} = \bar{f} \circ \bar{h}^{-1} \Rightarrow f \approx f^{(A)} = g^{(A)} \circ h = \bar{f} \circ \bar{h}^{-1} \circ h. \tag{4.14}$$

The approximate transformation function  $g^{(A)}$  may or may not turn out to have definite convexity ( $\bar{f}$  is given and the envelope basis  $\bar{h}$  is chosen). If  $h$  is monotone on  $x > 0$  then the approximation  $f^{(A)}$  is monotone and the correspondence  $\bar{f} \rightarrow f^{(A)}$  is invertible. In fact we have in this case

$$\bar{f} = f^{(A)} \circ h^{-1} \circ \bar{h}. \tag{4.15}$$

However, without having stronger comparison theorems at our disposal we cannot extract any ordering relation between  $f^{(A)}$  and  $f$ . Let us suppose, for example, that  $h$  is semi-monotone and that  $g^{(A)}$  is convex. Then we know by (4.13) that the trajectory  $F$  is a lower bound to the exact trajectory  $F^{(A)}$  corresponding to the fictitious potential  $f^{(A)}$ . It is therefore consistent to expect, in terms of definition (3.2), that  $f_1 < f_1^{(A)}$ : but the most we can say with certainty at the moment is  $f_1 \neq f_1^{(A)}$ .

If as in [11] we define the  $K$ -function associated with a potential  $f$  by

$$\bar{f}(s) = f(x) \Rightarrow s = K^{(f)}(x) = (\bar{f}^{-1} \circ f)(x) \tag{4.16}$$

then our envelope approximation formula becomes

$$f(x) \approx f^{(A)}(x) = \bar{f}(K^{(h)}(x)). \tag{4.17}$$

Instead of a trial function we must choose a trial envelope basis  $h$ . As an illustration we suppose that we are given the ground-state energy trajectory  $F(v)$  (1.2) for the sech-squared potential and we choose a harmonic-oscillator envelope basis  $h(x) = x^2$ . For the ground state of the harmonic oscillator we have from [11]  $K^{(h)}(x) = (4x^2)^{-1}$ . From the given trajectory  $F(v)$  we use (4.4) to obtain the kinetic potential  $\bar{f}(s)$  as given in (4.9). Consequently, from (4.17), we obtain

$$-\operatorname{sech}^2(x) = f(x) \approx f^{(A)}(x) = \bar{f}\left(\frac{1}{4x^2}\right) = -\frac{2}{(1 + 4x^2)^2 + 1}. \tag{4.18}$$

This particular approximation turns out to be good for small  $x$ , but the tail is Coulombic instead of exponential. A more appropriate envelope basis would yield better results: the harmonic oscillator is hardly 'close' to the sech-squared potential.

### 5. Inversion for separable potentials

If we write the multiplicative potential  $vf(x)$  in Schrödinger's equation (1.1) in the form of the kernel of an integral operator, then we must adjoin a delta factor to obtain

$$\langle x|V|x'\rangle = vf(x)\delta(x-x'). \quad (5.1)$$

Such integral operators are therefore special. Another choice is the 'separable potentials' which have the distinct special form

$$\langle x|V|x'\rangle = -vf(x)f^*(x'). \quad (5.2)$$

In this section we shall speak of the 'shape'  $f$  of a potential in the sense of (5.2); we shall also assume that  $f$  is real, positive, symmetric, monotone increasing for  $x > 0$ , and vanishing at infinity. In this case Schrödinger's equation (1.1) becomes

$$-\psi_{xx}(x, v) + vf(x) \int f(x')\psi(x', v) dx' = F(v)\psi(x, v) \quad v > 0 \quad (5.3)$$

where the integral is over  $\mathbb{R}$ . As we shall see, the inverse spectral problem  $F \rightarrow f$  is soluble for such potentials.

It is convenient to convert to 'momentum space' for the discussion of separable potentials. We denote the symmetrized Fourier transform by a tilde and use  $k$  for the momentum variable, for example

$$\tilde{f}(k) = \int \langle k|x \rangle f(x) dx = \frac{1}{\sqrt{2\pi}} \int e^{-ikx} f(x) dx. \quad (5.4)$$

In momentum space (5.3) becomes

$$k^2\tilde{\psi}(k, v) - v\tilde{f}(k) \int \tilde{f}(k')\tilde{\psi}(k', v) dk' = F(v)\tilde{\psi}(k, v). \quad (5.5)$$

If we define  $c(v)$  and  $r(v)$  by the expressions

$$c(v) = \int \tilde{f}(k')\tilde{\psi}(k', v) dk' \quad \text{and} \quad r^2(v) = |F(v)| \quad (5.6)$$

then the (unique) solution of the 'forward' problem is given by

$$\tilde{\psi}(k, v) = \frac{vc(v)\tilde{f}(k)}{k^2 + r^2(v)} \quad (5.7)$$

and

$$\frac{1}{v} = \int \frac{\tilde{f}^2(k)}{k^2 + r^2(v)} dk. \quad (5.8)$$

These potentials support one and only one eigenvalue for all  $v > 0$ .

Equation (5.8) can be looked at in different ways. It gives a prescription for  $v^{-1} = u$  in terms of  $r$  and therefore of energy  $F$ ; since the right-hand side is monotone in  $r$  we can also solve uniquely for  $r$  (therefore energy) in terms of the reciprocal coupling  $u$ . Thus the

hypothesis of our inverse spectral problem could be expressed in the following way. We are given  $u$  as a function of  $r$  and we have to solve (5.8) for  $\tilde{f}$ ; more specifically, we have to invert the transformation  $\tilde{f} \rightarrow u$  given by

$$u(r) = \int \frac{\tilde{f}^2(k)}{k^2 + r^2} dk. \tag{5.9}$$

Widder [20, p 225] shows that the inverse of the ‘potential transform’  $\phi \rightarrow u$  defined by

$$u(r) = \frac{2}{\pi} \int_0^\infty \frac{k\phi(k)}{k^2 + r^2} dk \tag{5.10}$$

is given, at least formally, by the attractive expression

$$\phi(k) = \sin(\pi\theta/2)u(k) \quad \theta[u(k)] = -ku'(k). \tag{5.11}$$

Thus, by choosing

$$\phi(k) = \frac{\pi \tilde{f}^2(k)}{2k} \tag{5.12}$$

we see that separable potentials are invertible.

We consider two examples:  $f(x) = \delta(x)$  and  $f(x) = e^{-|x|}$ . In the case of the delta potential we have as our starting point the well known one-dimensional Coulomb-like energy trajectory  $F(v) = -v^2/4$ . Hence  $u(r) = (2r)^{-1}$  and (5.9) becomes

$$\frac{1}{2r} = \int \frac{\tilde{f}^2(k)}{k^2 + r^2} dk. \tag{5.13}$$

We can immediately invert this transform using the potential-transform pair [20]

$$\{\phi(k), u(r)\} = \{k^{-1}, r^{-1}\}$$

to find  $\tilde{f}(k) = 1/\sqrt{2\pi}$ . That is to say,  $f(x) = \delta(x)$  and  $\langle x|V|x' \rangle = -v\delta(x)\delta(x')$ .

Similarly, in the exponential case  $f(x) = e^{-|x|}$  a straightforward solution to the ‘forward’ problem (5.9) yields  $\tilde{f}(k) = \sqrt{2/\pi}(1+k^2)^{-1}$  and

$$u(r) = \frac{2+r}{2r(1+r)^2} = \int \frac{\tilde{f}^2(k)}{k^2 + r^2} dk. \tag{5.14}$$

Again, if in addition to the potential-transform pair mentioned above we also use the pairs

$$\{k(1+k^2)^{-1}, 2k(1+k^2)^{-2}\} \leftrightarrow \{(1+r)^{-1}, (1+r)^{-2}\} \tag{5.15}$$

provided by Widder [20] and the linearity of the transform, we find from (5.14) that  $\tilde{f}(k) = (1+k^2)^{-1}$ ; hence the potential shape  $f(x) = e^{-|x|}$  is recovered.

It is reasonable to expect that this analysis could be extended to potentials in the form of sums of products such as  $\langle x|V|x' \rangle = v \sum_{i=1}^n f_i(x)f_i(x')$ , and even further to  $L^2$  kernels. This might be an interesting area to explore. However, the class of potentials reached in this way does not include the ‘usual’ multiplicative potentials of quantum mechanics with operator kernels in the general form (5.1).

## 6. Uniqueness

We now turn to the question of uniqueness. If we consider, for example, the potential-trajectory pair  $\{x^2, v^{1/2}\}$  generated in the forward direction by the harmonic oscillator, the question arises as to whether the inverse  $v^{1/2} \rightarrow x^2$  is the only possibility (up to shifts). In the case of a fixed coupling it is known [21] that there is a large class of non-symmetric potentials, each element of which generates a Schrödinger spectrum identical to that of the harmonic oscillator: a nice discussion of this may be found in the book by de Lange and Raab [22, ch 3]. In view of such interesting possibilities, uniqueness would at first sight seem to be an unlikely prospect. However, under the assumptions of symmetry and monotonicity, the harmonic oscillator is the unique potential with trajectory  $v^{1/2}$ , and similarly we have uniqueness for the sech-squared potential. More generally, we are able to prove the following theorem.

*Theorem 6.1.*

- (i)  $f$  is symmetric;
- (ii)  $f(x) \geq f(0)$ ;
- (iii)  $f$  is non-decreasing on  $[0, \infty)$ ;

$\Rightarrow$  the potential shape  $f$  corresponding to the trajectory  $F$  is unique.

Our proof of this theorem leans heavily on the monotonicity of the potential. We shall first establish some preliminary results. By theorem 2.1  $F(v)/v$  has the limit  $f(0)$  as  $v \uparrow \infty$ . This limit is approached monotonically, since by (4.4) we have

$$\frac{d}{dv} \left( \frac{F(v)}{v} \right) = \frac{vF'(v) - F(v)}{v^2} = -\frac{s}{v^2} < 0. \quad (6.1)$$

By (4.1) and (4.2) we know that

$$\frac{F(v)}{v} \geq F'(v) = (\psi, f\psi) \geq f(0) \quad (6.2)$$

and also that  $F'(v)$  decreases monotonically to  $f(0)$  because  $F''(v) < 0$ . Thus, for each  $v > 0$  there exists a number  $a(v) > 0$  such that  $f(a) = F'(v)$  and  $f(a) > F'(u)$ ,  $\forall u > v$ . For symmetric semi-monotone potentials it is known that the ground-state probability becomes monotonically more concentrated in an interval about  $x = 0$  as  $v \rightarrow \infty$ . In fact if we define  $q(v)$  to be the probability in the interval  $[-a, a]$ , that is to say

$$q(v) = \int_{-a}^a \psi^2(x, v) dx \quad (6.3)$$

then for each  $a$  such that  $f(a) > f(0)$  and for all  $v$  sufficiently large we have proved [1] the *concentration lemma*:

$$q(v) = \int_{-a}^a \psi^2(x, v) dx \geq \frac{f(a) - F'(v)}{f(a) - f(0)} \rightarrow 1 \quad v \rightarrow \infty. \quad (6.4)$$

If the potential has a constant 'patch'  $f(x) = f(0)|x| < b$  at the centre, then in the limit of large  $v$  the probability is concentrated to this interval, *not* to a point. This particular effect is discussed in detail in [1]. We are now ready for the following proof.

*Proof of theorem 6.1.* We suppose that the two potentials  $f(x)$  and  $f(x) + \gamma(x)$  both satisfy the hypotheses of the theorem. Then we have

$$-\psi_{xx}(x, v) + v f(x) \psi(x, v) = F(v) \psi(x, v) \quad v > 0 \tag{6.5}$$

and

$$-\phi_{xx}(x, v) + v(f(x) + \gamma(x))\phi(x, v) = F(v)\phi(x, v) \quad v > 0. \tag{6.6}$$

From (4.5) we have

$$(\psi, f\psi) = \bar{f}(s) = F'(v) = (\phi, (f + \gamma)\phi) \tag{6.7}$$

in which the two wavefunctions are assumed to satisfy  $\|\psi\| = \|\phi\| = 1$ . If we apply each wavefunction as a trial function to 'the other' Hamiltonian, by the min-max definition (4.11) of  $\bar{f}(s)$  we obtain the complementary inequalities

$$(\phi, \gamma\phi) \leq 0 \leq (\psi, \gamma\psi). \tag{6.8}$$

By a sweeping process starting at the origin, we shall show that the inequalities (6.8) force  $\gamma$  to be zero. Theorem 2.1 tells us that  $f(0) = \lim_{v \uparrow \infty} (F(v)/v) = f(0) + \gamma(0)$ . Hence,  $\gamma(0) = 0$ . Since  $\gamma$  is necessarily symmetric, we consider only  $x > 0$ . If  $\gamma(x)$  has only one sign then the complementary inequalities immediately require that  $\gamma = 0$ . Hence, we need only consider the case in which  $\gamma(x)$  changes sign. Let us suppose that the first sign change occurs as  $x$  increases from zero occurs at  $x = a$ . Without loss of generality (because the argument is the same for either case), let us assume that  $\gamma(x)$  is not zero on all of  $[0, a]$  and that  $\gamma(x) \geq 0$  on  $[0, a]$ . We now choose  $v$  so large that  $F'(v) < f(a)$ , which allows us to use the concentration lemma. Whilst keeping  $a$  constant, we increase  $v$  so that  $q$  is sufficiently close to  $q = 1$  for both  $\psi$  and  $\phi$ , so that the signs of both integrals in the complementary inequalities are positive. Since this cannot be if  $\gamma \neq 0$ , we conclude that  $\gamma = 0$ . Therefore, amongst the symmetric non-decreasing potentials, a given energy trajectory  $F$  has the unique inverse  $f$ .  $\square$

The uniqueness problem is related to the notion of a complete set of densities [23–25]. Suppose that for each  $v > 0$ ,  $\rho(x, v)$  is a probability density on  $\mathbb{R}$ , then this set of densities is said to be complete if

$$\int_{-\infty}^{\infty} \rho(x, v) p(x) dx = 0 \quad \forall v > 0 \quad \Rightarrow \quad p = 0 \quad (\text{a.e.}) \tag{6.9}$$

Naturally in quantum mechanics we choose  $\rho(x, v) = |\psi(x, v)|^2$ . It is not difficult to find quantum-mechanical problems with ground-state wavefunctions that generate a complete set of densities in this way. For example, in the case of the harmonic oscillator  $f(x) = x^2$  we have

$$\phi(x) = (v/\pi^2)^{1/8} \exp(-v^{1/2}x^2/2) \tag{6.10}$$

with a corresponding set  $\{\psi^2, v > 0\}$  of densities that may be shown to be complete by the fundamental properties [18] of the Laplace transform: it is sufficient if the Laplace transform

of a function vanishes on any set of points forming an unending arithmetic sequence, to conclude that its pre-image is necessarily zero.

We make the connection with our problem in the following way. We multiply (6.5) by  $\phi$  and (6.6) by  $\psi$ , integrate over  $\mathbb{R}$ , and subtract to obtain

$$(\phi, \gamma\psi) = 0 \quad v > 0. \quad (6.11)$$

Since the two wavefunctions  $\psi$  and  $\phi$  are nodeless ground states, we can construct from them the probability density  $c\psi\phi$ , where  $c$  is a normalization constant. If the set of densities  $\{c\psi\phi, v > 0\}$  is complete, then (6.11) provides another proof of theorem 6.1. Under what circumstances such a set of densities may be shown to be complete is an interesting open question.

There is a possible connection, though much less immediate, with the Hohenberg–Kohn theory [26–28] which treats the question of the possible invertibility of the relationship between the potential in a many-body problem and the densities generated by the ground state; this problem has some interesting and complicated aspects [28]. However, in geometric spectral inversion we consider a one-particle problem and we have much more information at our disposal: the ground-state energy trajectory, and a continuous infinity of eigenvalues.

One notable consequence of the inversion theorem is that all the power-law potentials are exactly invertible: once the power-law pre-image is recognized from the correspondence

$$|x|^q = f(x) \quad \leftrightarrow \quad F(v) = F(1)v^{2/(2+q)} \quad (6.12)$$

then uniqueness determines  $f(x)$ . This is true for any potential  $f$  with a trajectory  $F$  that happens to be known. Of course, potential normalization helps with the process of recognition.

## 7. Conclusion

In this paper we have established both abstract and constructive inversion results for symmetric monotonic potentials. For the bounded potentials with area, theorem 3.2 establishes the inequality  $\Lambda(f) = F > F^{\square}$ , where  $F$  is the normalized trajectory for any such potential  $f$  which is not square. We have shown how to normalize a given trajectory so that  $f(0) = -1$ ,  $f(\infty) = 0$ , and so that  $|f(x)|$  has area two. We know [1] that for this class of potentials  $F$  must be monotonically decreasing and concave. In the case of unbounded potentials, it is convenient to normalize a trajectory so that  $f(0) = 0$ ; in this case the trajectory function  $F$  is necessarily monotonically increasing and concave. These results, along with the uniqueness theorem 6.1, are as far as we have been able to go towards a general characterization of  $\Lambda$ . If the constraints of monotonicity and symmetry are relaxed, it may be necessary to consider a generalized (many-valued) inverse  $\Lambda^{-1}$ , but we do not know whether this possibility is ever realized.

We have exact inversion for power laws, square wells and, by uniqueness, for any potential  $f$  with a trajectory  $F$  that is recognized; and also generally for separable potentials. We have also obtained families of approximate reconstruction formulae by Gaussian inversion (4.8) and by envelope inversion (4.17). These inverse approximations lack the ordering that their counterparts in the forward direction have: this most desirable feature awaits further refinements other than theorem 3.1 to the ‘usual’ comparison theorem of quantum mechanics.

Geometric spectral inversion may seem surprising at first sight since knowledge of only the ground state for all values of the coupling  $v$  leads to the potential shape  $f$  from which, in turn, the details of all the states can be found. This result may perhaps appear to be less paradoxical in the light of the following, partly heuristic, remarks. For symmetric potentials, the set of all the (generalized) energy eigenstates corresponding to the set of energies necessary for inversion is a spanning set for the Hilbert (sub) space of symmetric functions. It may be possible to prove, as we have suggested in section 6, that the set of densities  $\{\psi^2, v > 0\}$  derived from all the ground-state wavefunctions is complete: this leads again to such a spanning set for the symmetric part of Hilbert space. An illustration of this completeness idea may be found in the beautiful exposition of the theory of the Laplace transform by Doetsch [18]: the set of nodeless exponential functions

$$\{e^{-r_n|x|}\}_{n=1}^{\infty}$$

spans the symmetric part of the Hilbert space  $L^2(\mathbb{R})$ ; for this spanning purpose any positive unending arithmetic sequence  $\{r_n\}_{n=1}^{\infty}$  will suffice. Much of the current theory [23–25] of complete sets of densities seems to be a generalization, by change of variable, of this fundamental completeness result. It may therefore prove fruitful to explore in detail the connection between the theory of Schrödinger operators and complete sets of densities since the theory of the latter is at present dominated by results obtained for the ‘exponential classes’; however, these densities are much too restrictive for the interesting problems raised by quantum mechanics.

The approximate inversion by potential envelopes is not restricted to the ground-state data. Since the ground-state trajectory alone is already sufficient, the set of all energy trajectories would represent more than enough spectral information for inversion. Indeed, for a single fixed coupling  $v$  (and a symmetric potential) the set of all energy eigenvalues is known [6] to be sufficient for the reconstruction of the potential  $v f(x)$ . If there is only a selection of data available from some of the trajectories, then it is clear in principle that all of these data can be employed to sharpen our picture of the potential shape  $f$ . In the context of an approximation, the consistency question which arises because of overlapping constraints could be used to improve the approximate inversion. If we imagine a diagram with plots of the energy (and resonance) trajectories as functions of coupling  $v$ , then it is natural to ask the general question: how much of this bound-state data is sufficient to reconstruct the potential? More particularly, could one reconstruct the potential knowing only the energy trajectory  $F_n(v)$  for one of the excited states  $n > 0$ , even though such a trajectory might exist only for a sufficiently large coupling  $v$ ? One possible way of exploring this idea approximately is by using the concise envelope inversion (4.17) which is not restricted to the ground state.

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