An Inversion Inequality for Potentials in Quantum Mechanics

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Abstract

We suppose: (1) that the ground-state eigenvalue $E = F(v)$ of the Schrödinger Hamiltonian $H = -\Delta + vf(x)$ in one dimension is known for all values of the coupling $v > 0$; and (2) that the potential shape can be expressed in the form $f(x) = g(x^2)$, where g is monotone increasing and convex. The inversion inequality $f(x) \leq \bar{f}(\frac{1}{4x^2})$ is established, in which the 'kinetic potential' $\bar{f}(s)$ is related to the energy function $F(v)$ by the transformation: $\{\bar{f}(s) = F'(v), \quad s = F(v) - vF'(v)\}$. As an example f is approximately reconstructed from the energy function F for the potential $f(x) = ax^2 + b/(c + x^2)$.

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1. Introduction

We suppose that a discrete eigenvalue $E = F(v)$ of the Schrödinger Hamiltonian

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

is known for all sufficiently large values of the coupling parameter $v > v_c$ and we try to use this data to reconstruct the potential shape f. Here v_c is the critical value of the coupling parameter for the eigenvalue considered. For the present discussion we shall assume that the potential shape $f(x)$ is non-constant, symmetric, and monotone increasing for $x > 0$. The usual 'forward' problem would be: given the potential (shape) f, find the energy trajectory F; 'geometric spectral inversion' is the inverse of this, that is to say $F \to f$.

This problem should be distinguished from the 'inverse problem in the coupling constant' discussed, for example, by Chadan and Sabatier [1]. In this latter problem, the discrete part of the 'input data' is a set $\{v_n\}$ of values of the coupling constant that all yield the identical energy eigenvalue E. The index n might typically represent the number of nodes in the corresponding eigenfunction. In contrast, for the problem discussed in the present paper, n is kept fixed and the input data is the graph $(F_n(v), v)$, where the coupling parameter has any value $v > v_c(n)$, and $v_c(n)$ is the critical value of v for the support of a discrete eigenvalue with n nodes; for the ground state in one dimension we have in general $v_c(0) = 0$. For the excited states, the critical coupling depends on the potential shape; for example, in the case of the square well, $v_c(n) = (n\pi/2)^2$; for the sech-squared potential with shape $f(x) = -\text{sech}^2(x)$, we have [2] $v_c(n) = n(n+1)$. There are strong indications on the basis of studies involving the inversion of the WKB approximation [3] that inversion from a single fixed energy trajectory F_n becomes more efficient as n increases (and the problem becomes more classical). However, the present paper will be concerned only with inversion from the ground-state energy function $F_0(v) = F(v)$ for the problem in one spatial dimension.

By making suitable assumptions concerning the class of potential shapes, theoretical progress has already been made with this inversion problem [4-7]. In Ref. [5]

a 'concentration lemma' is proved. If we suppose that $H\psi = E\psi$ and $||\psi|| = 1$, this lemma quantifies the monotone increase in concentration towards $x = 0$ of the probability density $\psi^2(x, v)$ with increasing v. In Ref. [6] this lemma is used to establish the uniqueness of the potential shape f corresponding to a given energy function F. The class of potentials for which this uniqueness proof applies are those non-constant potential shapes f which are symmetric, continuous at $x = 0$, piecewise analytic [8], and monotone increasing for $x > 0$. The 'envelope inversion' discussed in Ref. [6] involved a class of potentials that could be expressed as a smooth monotone transformation $f(x) = g(h(x))$ of a soluble potential $h(x)$. The approximation obtained was *ad hoc* in the sense that nothing was known *a priori* concerning the relationship between the approximation and the (unknown) exact potential corresponding to the given energy function $F(v)$. In the present paper we establish an inversion *inequality* for a special case of envelope inversion, namely the case in which the 'envelope basis' is the harmonic-oscillator shape $h(x) = x^2$. Thus we assume that the potential shape $f(x)$ has the representation

$$f(x) = g(x^2), \tag{1.2}$$

where g is monotone increasing and convex ($g'' > 0$). This is a strong assumption but, as we prove in Section (2), it yields a corresponding strong result, that is to say:

$$f(x) \leq \bar{f}\left(\frac{1}{4x^2}\right), \tag{1.3}$$

where $\bar{f}(s)$ is the 'kinetic potential' corresponding to the potential $f(x)$. The parameter s is equal to the mean kinetic energy $< -\Delta >$ and, in terms of s, the eigenvalue $F(v)$ may be represented [9] *exactly* by the semi-classical expression:

$$E = F(v) = \min_{s>0} \left\{ s + v\bar{f}(s) \right\}. \tag{1.4}$$

The transformations $F \leftrightarrow \bar{f}$ are essentially Legendre transformations [10]. This is so because we know [5] that F and $\bar{f}$ have definite and opposite convexity; more particularly, we know

$$\bar{f}''(s)F''(v) = -\frac{1}{v^3} < 0. \tag{1.5}$$

The transformation in the direction needed here $F \to \bar{f}$ will be given explicitly in Section (2) below where we also prove the inequality (1.3), the main result of this paper. In Section (3) we discuss an example for which we compare the upper approximation given by (1.3) with the corresponding exact result.

2. Proof of the inversion inequality

We suppose that the exact normalized wave function corresponding to the potential $vf(x)$ is given by $\psi(x, v)$, where the coupling parameter $v > 0$. Thus $(\psi, H\psi) = F(v)$. We know how this total expectation value is divided between kinetic and potential energies for, in more detail, we have

$$< -\Delta> = (\psi, -\Delta\psi) = F(v) - vF'(v) = s,$$

$$<f> = (\psi, f\psi) = F'(v) = \bar{f}(s). \tag{2.1}$$

These equations also define the kinetic potential $\bar{f}(s)$ parametrically in terms of the parameter $v > 0$. We first use Heisenberg's uncertainty inequality which gives us

$$< -\Delta><x^2> = s<x^2> \ \geq \ \frac{1}{4}. \tag{2.2}$$

We now consider

$$\bar{f}(s) = <f(x)> = <g(x^2)> \ \geq \ g(<x^2>). \tag{2.3}$$

This inequality follows from Jensen's inequality [11] and the fact that g is convex. By applying (2.2) in (2.3) we find

$$\bar{f}(s) \ \geq g\left(\frac{1}{4s}\right) = f\left(\frac{1}{2\sqrt{s}}\right). \tag{2.4}$$

Finally by letting $x = \frac{1}{2\sqrt{s}}$ we establish the inversion inequality

$$f(x) \ \leq \ \bar{f}\left(\frac{1}{4x^2}\right). \tag{2.5}$$

$\square$

Since the transformation in the direction $F \to \bar{f}$ is already expressed by (2.1), the upper approximation provided by the inversion inequality is now completely determined.

3. An example

We consider the potential shape given by

$$f(x) = ax^2 + b/(c + x^2), \quad a, b, c > 0. \tag{3.1}$$

The case $a = b = c = 1$ is illustrated in Fig.(1) which shows the potential shape $f(x)$, in the inset graph, and also the ground-state energy function $F(v)$ generated from it. In Fig.(2) the upper approximation A obtained by the inversion inequality is shown along with the exact potential shape f itself. The set of corresponding 'exact' wave functions $\psi(x, v)$ are also shown for $3 \times 10^{-4} \le v \le 10$. The wave-function normalization is arbitrarily taken here to be $\psi(0, v) = 20$, so that the graphs fit on the same figure as the potentials. As the coupling v increases, the wave functions become monotonically more concentrated near zero, in agreement with the 'concentration lemma' mentioned in Section (1).

3. Conclusion

Although the assumption behind the inversion inequality is strong, the fact that such an inequality exists may be important, especially if it can eventually be generalized. The expression of this result in terms of kinetic potentials could be avoided in principle. However, the representation of the energy functions $F(v)$ in terms of $\bar{f}(s)$ has already yielded some very effective bounds in the forward direction and it is natural to explore this same apparatus for the more difficult inversion problem. For example, in the forward direction the envelope method [9] may be expressed

succinctly as

$$f(x) = g(h(x)) \quad \Rightarrow \quad \bar{f}(s) \approx g(\bar{h}(s)), \tag{3.1}$$

where $\approx=\geq$ if g is convex and $\approx=\leq$ if g is concave. Once one has such an approximation for $\bar{f}(s)$, it can immediately be inserted in the expression (1.4) to yield an approximation for the corresponding eigenvalue $E = F(v)$. In the present paper we have found one case $h(x) = x^2$ for which an inequality is retained for the inverse problem. In Ref. [6] we also explored the idea of inverting the Rayleigh-Ritz variational method and we obtained an inversion approximation with respect to a chosen family of 'trial' functions. However, unlike the situation in the forward direction, the inversion approximation obtained was again *not* an inequality. Our experience with this problem so far suggests that it is difficult to generate potential inequalities for geometric spectral inversion.

Acknowledgment

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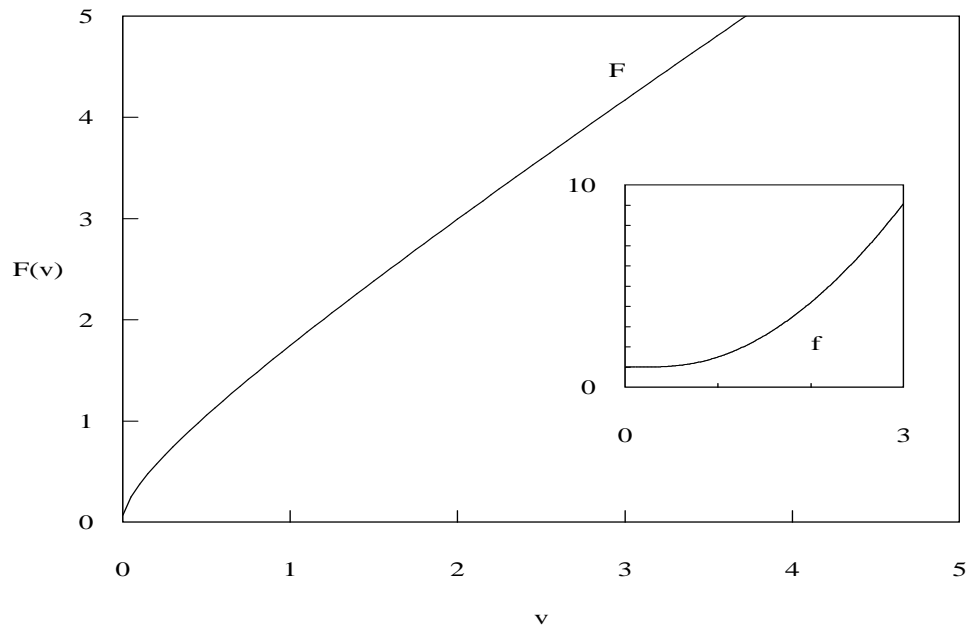
Figure (1) The potential $f(x) = x^2 + 1/(1 + x^2)$ is shown in the inset graph, along with the corresponding ground-state energy function $E = F(v)$. The aim of geometric spectral inversion is to reconstruct f from F.
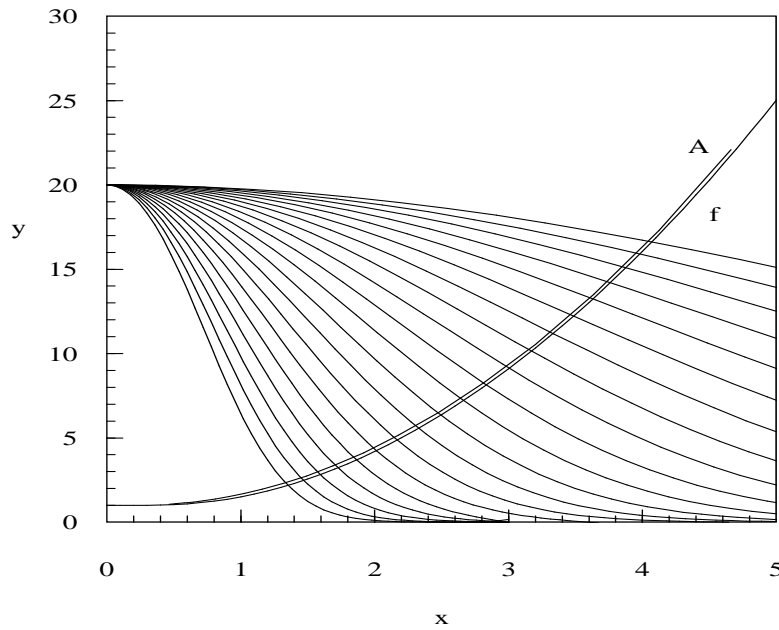
Figure (2) The approximation A obtained from the inversion inequality (2.5) is compared to the exact potential f. The family of corresponding 'exact' wave functions $\psi(x,v)$ satisfying $\psi(0,v) = 20$ is also shown: the wave functions become monotonically concentrated towards zero as v is increased from $v = 3 \times 10^{-4}$ to 10.