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Quadratic forms and solutions of the Schrödinger equation

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Abstract. The spectral theory for the Schrödinger equation on the half-line is treated through an analysis of the asymptotics of quadratic forms in a pair of solutions. Solutions of the second- and third-order differential equations for these forms are derived. In the case of the second-order DE (Milne's equation), it is shown that a single solution leads to the determination of the singular spectrum; this generalizes previous results which applied only to isolated points of the discrete spectrum. For the absolutely continuous spectrum, it is shown that a single solution allows one not only to locate the spectrum, but also to determine the spectral density function explicitly.

1. Introduction

The time-independent Schrödinger equation at energy λ, for a quantum mechanical particle moving in a potential $V(x)$ is given, in suitable units, by

$$-\frac{\mathrm{d}^2 f(x,\lambda)}{\mathrm{d}x^2} + V(x)f(x,\lambda) = \lambda f(x,\lambda).$$

This equation is fundamental to quantum mechanics in one dimension, and with appropriate modification of the potential also applies to three-dimensional problems with spherical symmetry. From the solution of the equation one can deduce, in principle, the energy levels of the Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

the location and nature of continuous spectrum, scattering amplitudes and cross-sections, and so on.

This paper is concerned with the spectral analysis of the Schrödinger Hamiltonian H, and in particular with the connection between spectral analysis and asymptotics of solutions $f(x,\lambda)$ of the time-independent Schrödinger equation at spectral parameter λ. We have three principal aims in mind.

Our first aim is to show how recent developments in spectral analysis imply that it is the square of the wavefunction $f^2(x,\lambda)$, and the integral of the square of the wavefunction, rather than the wavefunction itself, which plays the key role in spectral analysis. This is already well known in the case of the discrete spectrum. An eigenvalue of the Hamiltonian can occur only at an energy λ at which the solution $f(x,\lambda)$ is square integrable (and satisfies some boundary conditions which may be imposed). However, it is possible to go further and show how a complete spectral analysis, including both continuous and singular spectrum, is a consequence of the asymptotics of the squares of the solutions $f^2(x,\lambda)$ and their integrals.

In view of the fundamental role of f^2 rather than f, our second aim is to derive a third-order equation satisfied by quadratic forms of the solutions, and to explore the algebraic structure of both this and related equations satisfied by the squared wavefunction. In the simplest case of zero potential, with $\lambda = k^2 > 0$, a straightforward argument will lead to this third-order equation. A linear homogeneous DE in this case satisfied by the squares of all solutions of the Schrödinger equation must have as solutions $\cos^2 kx$, $\sin^2 kx$ and $\sin kx \cos kx$, and hence by linearity a basis for the solution set will be 1, $\cos 2kx$, $\sin 2kx$. The third-order DE with this solution set is

$$\frac{\mathrm{d}^3 Y(x,\lambda)}{\mathrm{d}x^3} + 4\lambda \frac{\mathrm{d}Y(x,\lambda)}{\mathrm{d}x} = 0.$$

For extension to general potentials $V(x)$ see [1]; the equation can be obtained either from the Schrödinger equation, by substitution for f^2, or as a consequence of Milne's nonlinear DE (see section 3). Our own derivation is new, and brings out more clearly the algebraic structure of this and related equations (including Milne's equation) which follow as a consequence.

Finally we show how the asymptotics of solutions of the third-order DE for f^2 and Milne's equation may be used to derive not only the location of the singular and continuous spectrum, but also an explicit formula for the spectral density function itself. We believe that these results, which generalize previous arguments in the physics literature, are not only useful in themselves, but point the way to possible future developments in spectral theory.

2. Analysis of singular and continuous spectra

We assume the Schrödinger equation in the form

$$\frac{-\mathrm{d}^2 f(x,\lambda)}{\mathrm{d}x^2} + V(x) f(x,\lambda) = \lambda f(x,\lambda)$$

on the interval $0 \leqslant x < \infty$, where both λ and the potential function $V(x)$ are assumed real. To simplify matters, we assume that V is integrable over any finite interval $0 \leqslant x \leqslant N$, though most of the theory can be extended to a wider class of potentials or to Hamiltonians defined on either finite intervals or in the whole real line $\mathbb{R}$.

It is convenient to define two solutions $u(x,\lambda)$, $v(x,\lambda)$ of (1), subject respectively to the initial conditions

$$u = 1 \qquad \frac{\mathrm{d}u}{\mathrm{d}x} = 0 \qquad \text{at} \quad x = 0$$

and

$$v = 0 \qquad \frac{\mathrm{d}v}{\mathrm{d}x} = 1 \qquad \text{at} \quad x = 0\,.$$

The Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

is a differential operator acting in the Hilbert space $L^2(0,\infty)$, subject to a boundary condition at $x = 0$, which we take to be $f(0) = 0$. In most cases of relevance to physics, we are in the so-called limit-point case (see [2], for example) for which no boundary condition at infinity is required; this will be so, for example, if V is bounded at infinity, but also under much more general conditions.

A given value of λ will be an eigenvalue of H provided $\int_0^\infty v^2(x,\lambda)\,\mathrm{d}x < \infty$; $v(x,\lambda)$ will then be the corresponding eigenfunction. Eigenvalues λ are said to belong to the discrete spectrum of H. For definitions of other types of spectrum, for example singular and absolutely continuous spectrum, see [3, 4].

The Hamiltonian H is unitarily equivalent to the multiplication operator $\phi \to \lambda\phi$ on a Hilbert space $L^2(\mathbb{R};\mu)$ where μ is the spectral measure and the norm is given by $\|\phi\|^2 = \int_0^\infty \phi^2(\lambda)\,\mathrm{d}\mu$. The various types of measure then correspond to a decomposition of the spectral measure $\mu = \mu_s + \mu_{ac}$ into its singular and absolutely continuous components.

Recent work in spectral theory has recently identified criteria for points λ to belong to the singular or absolutely continuous spectrum, based in each case on estimates of integrals of the squares of solutions of (1); it is these results, in part due to the present authors, which motivate the work presented in this paper. The main results can be summarized under two headings, results based on the idea of subordinacy, and results based on the so-called condition (A).

(i) Subordinacy (see [5, 6])

A (non-trivial) solution $f(x,\lambda)$ of (1) is said to be *subordinate* if

$$\lim_{N\to\infty} \int_0^N f^2(x,\lambda)\,\mathrm{d}x \Bigg/ \int_0^N g^2(x,\lambda)\,\mathrm{d}x = 0$$

for any solution $g(x,\lambda)$ of (1) which is not a constant multiple of $f(x,\lambda)$.

It may be shown that the singular part μ_s of the spectral measure is concentrated on those points λ at which the solution $v(x,\lambda)$ is subordinate. Certainly, any eigenvalue is a point of subordinacy, but there may be other points λ of the singular spectrum for which $v(x,\lambda)$ is subordinate but not square integrable. (The solution $v(x,\lambda)$ in such cases is often described as a semi-bound state).

The points λ at which *no* solution $f(x,\lambda)$ is subordinate belong to the absolutely continuous spectrum of H.

(ii) Condition (A) (see [7, 8])

This condition is analogous to that of subordinacy, but relates to complex valued solutions $f(x,\lambda)$ of (1).

A solution $f(x,\lambda)$ of (1) is said to satisfy condition (A) if

$$\lim_{N\to\infty} \int_0^N f^2(x,\lambda)\,\mathrm{d}x \Big/ \int_0^N |f^2(x,\lambda)| dx = 0. \tag{1}$$

The points λ at which condition (A) is satisfied, for some (complex valued) solution of (1), may be shown [8] to belong to the absolutely continous spectrum of H. At points of the absolutely continuous spectrum, the Radon–Nikodym derivative $\mathrm{d}\mu/\mathrm{d}\lambda$ defines an absolutely continous measure, with density $p(\lambda)$; thus one has $\mathrm{d}\mu/\mathrm{d}\lambda = p(\lambda)$ in that case, where the density function p characterizes the energy distribution of continuum states such as scattering states. If the solution $f(x,\lambda)$ satisfying condition (A) is 'normalized' so that $f(0,\lambda) = 1$, we can define a coefficient $M(\lambda)$ by the equation

$$f(x,\lambda) = u(x,\lambda) + M(\lambda)v(x,\lambda) \tag{2}$$

where u and v are the two solutions defined earlier. The coefficient $M(\lambda)$, closely related to the Weyl–Titchmarsh m-coefficient (see [2]) leads to a direct determination of the spectral density function $p(\lambda)$, through the formula

$$\frac{\mathrm{d}\mu}{\mathrm{d}\lambda} = \frac{1}{\pi}\,\mathrm{Im}\,M(\lambda) \tag{3}$$

These two approaches, through subordinacy and condition (A), show that spectral analysis may be closely linked to a study of the behaviour of the square of solutions f of the Schrödinger equation, and together suggest that the differential equations satisfied by these squared solutions, or more generally by quadratic forms in the solutions u, v, may have an important role. For example, $|f(x,\lambda)|^2$ in the integrand of the denominator of condition (A) may be expressed, through (2), as such a quadratic form.

In section 3 we shall consider these differential equations and their solutions. In section 4 we shall show how the asymptotics of quadratic forms govern the location of singular spectrum, and in section 5 we shall apply condition (A) and (3) in order to relate the asymptotics of quadratic forms to the spectral density of absolutely continuous spectrum, in a specially simple case. For some recent applications of subordinacy see, for example, [9–11].

3. A Schrödinger equation for the squared wavefunction

Given the solutions $u(x,\lambda)$, $v(x,\lambda)$ of (1) which we defined in section 2, we derive the third-order DE having as solutions all quadratic forms in u and v. The solution set of this DE is spanned by the functions u^2, uv and v^2, and hence contains any squared solution $(au+bv)^2$ of the original Schrödinger equation. Since any two linearly independent solutions of (1) could be used instead of u, v, we prefer to start from a basis independent characterization of the third-order DE. This can be done as follows.

Consider the third-order DE satisfied by the product

$$f_1(x,\lambda) f_2(x,\lambda)$$

of any pair of solutions f_1, f_2 of (1). We also consider the product

$$\frac{\mathrm{d}f_1}{\mathrm{d}x}\frac{\mathrm{d}f_2}{\mathrm{d}x}$$

of the derivatives. The following lemma described the resulting system of coupled DEs.

Lemma 1. Let $f_1(x,\lambda)$, $f_2(x,\lambda)$ be any two solutions of (1) ($f_1 = f_2$ is allowed), and define functions $Y(x,\lambda)$, $Z(x,\lambda)$ by

$$Y(x,\lambda) = f_1(x,\lambda) f_2(x,\lambda) \qquad Z(x,\lambda) = \frac{\mathrm{d}f_1(x,\lambda)}{\mathrm{d}x}\frac{\mathrm{d}f_2(x,\lambda)}{\mathrm{d}x}.$$

Then Y, Z satisfy the coupled differential equations

$$\left.\begin{aligned} &\frac{\mathrm{d}^2Y(x,\lambda)}{\mathrm{d}x^2} - 2(V(x)-\lambda)Y(x,\lambda) = 2Z(x,\lambda) \\ &\frac{\mathrm{d}Z(x,\lambda)}{\mathrm{d}x} = (V(x)-\lambda)\frac{\mathrm{d}Y(x,\lambda)}{\mathrm{d}x} \end{aligned}\right\}. \tag{4}$$

Moreover, Y satisfies the third-order DE

$$\frac{\mathrm{d}^3Y(x,\lambda)}{\mathrm{d}x^3} + 4(\lambda - V(x))\frac{\mathrm{d}Y(x,\lambda)}{\mathrm{d}x} - 2\frac{\mathrm{d}V(x)}{\mathrm{d}x}Y(x,\lambda) = 0 \tag{5}$$

which is also satisfied by all linear combinations of $u^2(x,\lambda)$, $u(x,\lambda)v(x,\lambda)$ and $v^2(x,\lambda)$.

Proof. Using

$$\frac{\mathrm{d}^2 f_1}{\mathrm{d}x^2} = (V-\lambda)f_1 \qquad \text{and} \qquad \frac{\mathrm{d}^2 f_2}{\mathrm{d}x^2} = (V-\lambda)f_2$$

we have

$$\frac{\mathrm{d}^2Y}{\mathrm{d}x^2} = f_1\frac{\mathrm{d}^2 f_2}{\mathrm{d}x^2} + f_2\frac{\mathrm{d}^2 f_1}{\mathrm{d}x^2} + 2\frac{\mathrm{d}f_1}{\mathrm{d}x}\frac{\mathrm{d}f_2}{\mathrm{d}x}$$

$$= f_1(V-\lambda)f_2 + f_2(V-\lambda)f_1 + 2\frac{\mathrm{d}f_1}{\mathrm{d}x^2}\frac{\mathrm{d}f_2}{\mathrm{d}x} = 2(V-\lambda)Y + 2Z$$

which is the first of the two equations in (4).

We also have

$$\frac{\mathrm{d}Z}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\mathrm{d}f_1}{\mathrm{d}x}\frac{\mathrm{d}f_2}{\mathrm{d}x}\right) = \frac{\mathrm{d}f_1}{\mathrm{d}x}\frac{\mathrm{d}^2 f_2}{\mathrm{d}x^2} + \frac{\mathrm{d}f_2}{\mathrm{d}x}\frac{\mathrm{d}^2 f_1}{\mathrm{d}x^2}$$

$$= \frac{\mathrm{d}f_1}{\mathrm{d}x}(V-\lambda)f_2 + \frac{\mathrm{d}f_2}{\mathrm{d}x}(V-\lambda)f_1 = (V-\lambda)\frac{\mathrm{d}}{\mathrm{d}x}(f_1f_2) = (V-\lambda)\frac{\mathrm{d}Y}{\mathrm{d}x}$$

which is the second equation in (4). These two coupled equations are of some interest in themselves. Here we use them to derive a third-order DE for Y. For another proof of (5), see [1].

To obtain equation (5), we must eliminate Z from from equations (4). This can be done by differentiating the first equation and substituting from the second for $\mathrm{d}Z/\mathrm{d}x$, giving

$$\frac{\mathrm{d}^3Y}{\mathrm{d}x^3} - 2\frac{\mathrm{d}}{\mathrm{d}x}((V-\lambda)Y) - 2(V-\lambda)\frac{\mathrm{d}Y}{\mathrm{d}x} = 0 \tag{6}$$

which reduces to equation (5) on simplification. □

Since u, v are solutions of (1), it follows that the products u^2, uv, v^2 satisfy (5). Hence $au^2+buv+cv^2$ satisfies this equation for any real numbers a, b, c. It follows from general uniqueness theorems for linear DEs that this is in fact the general solution. The general solution for Y, Z of the coupled equation is

$$Y = au^2 + buv + cv^2 \qquad Z = a\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)^2 + b\left(\frac{\mathrm{d}u}{\mathrm{d}x}\right)\left(\frac{\mathrm{d}v}{\mathrm{d}x}\right) + c\left(\frac{\mathrm{d}v}{\mathrm{d}x}\right)^2.$$

Strictly, equation (6) is to be preferred to (5), which implies differentiability of the potential, though this is not an important restriction in practice.

Although we can express the general solution of (5) in terms of solutions u, v of the Schrödinger equation, it is more in keeping with the theory presented here to solve equation (5) directly, and to express the solution in terms of quadratic forms directly without having to introduce the solutions u, v of the Schrödinger equation explicitly. That this can be done is a consequence of the fact that (6) is in anti-self-adjoint form; that is, the corresponding adjoint equation is the same as the original DE, apart from an overall change of sign. It follows that any solution of (5) may be used as an integrating factor, converting the third-order DE into a one parameter family of second-order equations.

To verify this, first of all note the identities

$$2Y\frac{\mathrm{d}^3Y}{\mathrm{d}x^3} = \frac{\mathrm{d}}{\mathrm{d}x}\left\{2Y\frac{\mathrm{d}^2Y}{\mathrm{d}x^2} - \left(\frac{\mathrm{d}Y}{\mathrm{d}x}\right)^2\right\}$$

$$Y\left\{\frac{\mathrm{d}}{\mathrm{d}x}((V-\lambda)Y) + (V-\lambda)\frac{\mathrm{d}Y}{\mathrm{d}x}\right\} = \frac{\mathrm{d}}{\mathrm{d}x}\left\{(V-\lambda)Y^2\right\}.$$

Multiplying equation (6) through by $2Y$, we then have

$$\frac{\mathrm{d}}{\mathrm{d}x}\left\{2Y\frac{\mathrm{d}^2Y}{\mathrm{d}x^2} - \left(\frac{\mathrm{d}Y}{\mathrm{d}x}\right)^2 - 4(V-\lambda)Y^2\right\} = 0$$

from which it follows that

$$2Y(x,\lambda)\frac{\mathrm{d}^2}{\mathrm{d}x^2}Y(x,\lambda)-\left(\frac{\mathrm{d}Y(x,\lambda)}{\mathrm{d}x}\right)^2-4(V(x)-\lambda)(Y(x,\lambda))^2=\beta \tag{7}$$

where β is a constant.

A further consequence of the anti-self-adjointness of (6) follows if we take any two solutions $Y_1(x,\lambda)$, $Y_2(x,\lambda)$ and use equation (6) with $Y=Y_1$ and $Y=Y_2$, respectively. Multiply the Y_1 equation by Y_2, the Y_2 equation by Y_1, and add, using the identities

$$Y_2\frac{\mathrm{d}^3Y_1}{\mathrm{d}x^3}+Y_1\frac{\mathrm{d}^3Y_2}{\mathrm{d}x^3}=\frac{\mathrm{d}}{\mathrm{d}x}\left\{Y_2\frac{\mathrm{d}^2Y_1}{\mathrm{d}x^2}-\frac{\mathrm{d}Y_2}{\mathrm{d}x}\frac{\mathrm{d}Y_1}{\mathrm{d}x}+Y_1\frac{\mathrm{d}^2Y_2}{\mathrm{d}x^2}\right\}$$

$$Y_2\frac{\mathrm{d}}{\mathrm{d}x}((V-\lambda)Y_1)+Y_1(V-\lambda)\frac{\mathrm{d}Y_2}{\mathrm{d}x}=\frac{\mathrm{d}}{\mathrm{d}x}\{(V-\lambda)Y_1Y_2\}$$

together with the same identity with Y_1, Y_2 interchanged.

This leads to the result

$$\frac{\mathrm{d}}{\mathrm{d}x}\left\{\left(Y_1\frac{\mathrm{d}^2Y_2}{\mathrm{d}x^2}+Y_2\frac{\mathrm{d}^2Y_1}{\mathrm{d}x^2}\right)-\frac{\mathrm{d}Y_1}{\mathrm{d}x}\frac{\mathrm{d}Y_2}{\mathrm{d}x}-4(V-\lambda)Y_1Y_2\right\}=0$$

from which it follows, for any two solutions, Y_1, Y_2 of (5), that

$$\left(Y_1\frac{\mathrm{d}^2Y_2}{\mathrm{d}x^2}+Y_2\frac{\mathrm{d}^2Y_1}{\mathrm{d}x^2}\right)-\frac{\mathrm{d}Y_1}{\mathrm{d}x}\frac{\mathrm{d}Y_2}{\mathrm{d}x}-4(V-\lambda)Y_1Y_2=\text{constant}. \tag{8}$$

The left-hand side of (8) may be regarded as a kind of second-order Wronskian of a pair of solutions Y_1, Y_2. Equation (7) is the special case $Y_1=Y_2=Y$. (The same strategy, to reduce a *second-order* Sturm–Liouville DE to a one parameter family of first-order equations, will not work since the Wronskian $f_1\mathrm{d}f_2/\mathrm{d}x-f_2\mathrm{d}f_1/\mathrm{d}x$ in that case, being antisymmetric, is zero for $f_1=f_2$).

Equation (7) is a consequence of (5), but also implies (5) on differentiating with respect to x. For $Y(x,\lambda)=f_1(x,\lambda)f_2(x,\lambda)$, the constant β on the right-hand side of (7) is related to the Wronskian $f_1\mathrm{d}f_2/\mathrm{d}x-f_2\mathrm{d}f_1/\mathrm{d}x$. Substituting $Y=f_1f_2$ and using

$$\frac{\mathrm{d}^2f_1}{\mathrm{d}x^2}=(V-\lambda)f_1 \qquad \frac{\mathrm{d}^2f_2}{\mathrm{d}x^2}=(V-\lambda)f_2$$

we find, on simplifying, that

$$\beta=-\left(f_1\frac{\mathrm{d}f_2}{\mathrm{d}x}-f_2\frac{\mathrm{d}f_1}{\mathrm{d}x}\right)^2. \tag{9}$$

If f_1, f_2 are allowed to be complex, then any solution $Y=au^2+buv+cv^2$ of (5) is a product $Y=f_1f_2$, obtained by factorizing into real or complex factors. Carrying out the factorization explicitly, and using the fact that the Wronskian of u with v is 1, equation (9) implies

$$\beta=4ac-b^2. \tag{10}$$

If $\beta=0$, $\pm Y$ is the square of a real linear combination of u and v; in that case we have the following *second-order* DE satisfied by the square of any real solution of the Schrödinger equation:

$$2Y\frac{\mathrm{d}^2Y}{\mathrm{d}x^2}-\left(\frac{\mathrm{d}Y}{\mathrm{d}x}\right)^2-4(V-\lambda)Y^2=0\,. \tag{11}$$

The above results may be used to express the general solution of (5) in terms of just one particular solution of the equation. Let $Y_1(x, \lambda)$ be a particular solution of (5), corresponding to a positive value of the parameter β in (7). Without loss of generality we may suppose that $\beta = 4$; if not take a constant multiple of this solution, for which $\beta = 4$.

(Although we shall not need to consider the explicit expression for Y_1 as a quadratic, we must have, from (10), that

$$Y_1 = au^2 + buv + cv^2 \qquad \text{with } \; b^2 - 4ac = -4.$$

Note that $Y_1(x, \lambda)$ cannot be zero for any x, since $Y_1 = 0$ would imply $u = v = 0$, contradicting the fact that

$$u\frac{\mathrm{d}v}{\mathrm{d}x} - v\frac{\mathrm{d}u}{\mathrm{d}x} = 1.$$

One solution of (5) for which $\beta = 4$ is $Y_1 = u^2 + v^2$).

The following lemma expresses the general solution of (5) in terms of a single solution Y_1.

Lemma 2. Let $Y_1(x, \lambda)$ be any solution of equation (5) such that $\beta = 4$ in (7). Then the general solution of equation (5) is given by

$$Y(x, \lambda) = AY_1(x, \lambda) + BY_1(x, \lambda)\cos\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t + CY_1(x, \lambda)\sin\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t\,. \qquad (12)$$

Proof. If $Y = Y_1 \cos\int_0^x (2/Y_1(t))\,\mathrm{d}t$ then

$$\frac{\mathrm{d}Y}{\mathrm{d}x} = \frac{\mathrm{d}Y_1}{\mathrm{d}x}\cos\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t - 2\sin\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t$$

$$\frac{\mathrm{d}^2Y}{\mathrm{d}x^2} = \frac{\mathrm{d}^2Y_1}{\mathrm{d}x^2}\cos\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t - \frac{2}{Y_1}\frac{\mathrm{d}Y_1}{\mathrm{d}x}\sin\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t - \frac{4}{Y_1}\cos\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t.$$

Substituting Y, $\mathrm{d}Y/\mathrm{d}x$ and $\mathrm{d}^2Y/\mathrm{d}x^2$ into the left-hand side of (7) leads, on simplification, to

$$\left(2Y_1\frac{\mathrm{d}^2Y_1}{\mathrm{d}x^2} - \left(\frac{\mathrm{d}Y_1}{\mathrm{d}x}\right)^2 - 4(V-\lambda)Y_1^2 - 8\right)\cos^2\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t - 4\sin^2\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t\,.$$

Since, by hypothesis,

$$2Y_1\frac{\mathrm{d}^2Y_1}{\mathrm{d}x^2} - \left(\frac{\mathrm{d}Y_1}{\mathrm{d}x}\right)^2 - 4(V-\lambda)Y_1^2 = 4$$

the left-hand side of (7), with

$$Y = Y_1\cos\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t$$

is just

$$-4\left(\cos^2\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t + \sin^2\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t\right) = -4\,.$$

Hence

$$Y = Y_1\cos\int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t$$

satisfies (7), with a β constant equal to -4, and similarly $Y_1\sin\int_0^x (2/Y_1(t))\,\mathrm{d}t$ satisfies the same equation, again with $\beta = -4$. Since equation (7) implies (5) on differentiation, it follows that these two functions are both solutions of the third-order DE. We therefore have three solutions of this DE, which may be verified to be linearly independent. Hence the result of the lemma. □

Starting from a particular solution Y_1 of (5), the two other linearly independent solutions exhibited on the right-hand side of (12) may be identified, as quadratic forms in u and v, through their initial values, at $x = 0$, of Y, $\mathrm{d}Y/\mathrm{d}x$ and $\mathrm{d}^2Y/\mathrm{d}x^2$, using standard uniqueness theorems applied to third-order linear equations.

For example, with $Y_1 = u^2 + v^2$, in this way we find

$$\left.\begin{aligned} Y_1 \cos \int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t &= u^2 - v^2 \\ Y_1 \sin \int_0^x \frac{2}{Y_1(t)}\,\mathrm{d}t &= 2uv \end{aligned}\right\} .$$

4. Milne's equation and the singular spectrum

The nonlinear differential equation known as Milne's equation is usually derived from the polar decomposition of the pair of solutions u, v of the Schrödinger equation.

That is, we define functions $R(x, \lambda),\ \theta(x, \lambda)$ by

$$\left.\begin{aligned} u &= R\cos\theta \\ v &= R\sin\theta \end{aligned}\right\} \tag{13}$$

so that $R = \sqrt{u^2 + v^2}$ and $\tan\theta = v/u$.

The constancy of the Wronskian $u\mathrm{d}v/\mathrm{d}x - v\mathrm{d}u/\mathrm{d}x = 1$ then implies $R^2\mathrm{d}\theta/\mathrm{d}x = 1$.

Differentiating either of equations (13) and substituting into the Schrödinger equation, we arrive at Milne's equation for the function R, namely

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}R(x,\lambda) + (V(x) - \lambda)R(x,\lambda) + \frac{1}{R^3(x,\lambda)} = 0. \tag{14}$$

Equation (14) is closely related to the solution of the Schrödinger equation, in that a single solution R of Milne's equation will lead to the general solution of Schrödinger's equation, thus

$$f(x,\lambda) = cR(x,\lambda)\sin\left(\int_0^x \frac{1}{R^2(t,\lambda)}\,\mathrm{d}t - b\right)$$

where b and c are constants.

For this and related results see the review article [12].

Of course, $R = \sqrt{u^2 + v^2}$ is not the only solution of Milne's equation. For the general solution in terms of square roots of quadratic forms see Eliezer and Gray [13]. We can derive Milne's equation from the second-order DE for $Y(x, \lambda)$ in (7), with the parameter β taken to have the value $\beta = 4$. With $\beta > 0$, we cannot have $Y = 0$, so we assume $Y > 0$. (Otherwise replace Y with $-Y$). Dividing equation (7) by $4Y^{3/2}$ we have

$$-\frac{1}{2}Y^{-1/2}\frac{\mathrm{d}^2Y}{\mathrm{d}x^2} + \frac{1}{4}Y^{-3/2}\left(\frac{\mathrm{d}Y}{\mathrm{d}x}\right)^2 + (V - \lambda)Y^{1/2} + \frac{\beta}{4}Y^{-3/2} = 0$$

where the first two terms on the left-hand side may be written

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left\{\frac{1}{2}Y^{-1/2}\frac{\mathrm{d}Y}{\mathrm{d}x}\right\} \qquad \text{or} \qquad -\frac{\mathrm{d}^2}{\mathrm{d}x^2}Y^{1/2}.$$

Hence $R = Y^{1/2}$ satisfies

$$-\frac{\mathrm{d}^2 R}{\mathrm{d}x^2} + (V - \lambda)R + \frac{\beta}{4R^3} = 0$$

which becomes Milne's equation in the case $\beta = 4$.

It follows from (10) that if $Y = au^2 + buv + cv^2$ is a quadratic form for which $a > 0$ and $4ac - b^2 = 4$, then $R = \sqrt{Y}$ satisfies Milne's equation. We may use this result to write down the solution of Milne's equation subject to the initial conditions

$$R = A(>0) \qquad \frac{\mathrm{d}R}{\mathrm{d}x} = B \qquad \text{at} \quad x = 0$$

namely

$$R(x, \lambda) = \sqrt{(Au(x, \lambda) + Bv(x, \lambda))^2 + A^{-2}v^2(x, \lambda)}\,. \tag{15}$$

The original solution $R = \sqrt{u^2 + v^2}$ corresponds to the special case $A = 1,\ B = 0$; solutions for which $R < 0$ initially are given by the negative of the right-hand side of (15), now with $A < 0$. Through these two families of solutions, respectively with $R > 0,\ R < 0$, we have the general solution of Milne's equation.

One of the main applications of Milne's equation in the literature (see [12], for example) has been to the eigenvalue problem for the Schrödinger operator on the real line. Here the solution $R = \sqrt{u^2 + v^2}$ of Milne's equation has been used to determine the ground state and excited energy levels through the solution $\lambda = \lambda_n$ of the equation

$$\int_{-\infty}^{\infty} \frac{1}{R^2(t, \lambda)}\, \mathrm{d}t = (n+1)\pi \qquad (n = 0, 1, 2, \ldots). \tag{16}$$

The corresponding equation for λ_n if the Schrödinger operator is defined on the half-line becomes

$$\int_{0}^{\infty} \frac{1}{R^2(t, \lambda)}\, \mathrm{d}t = (n+1)\pi \qquad (n = 0, 1, 2, \ldots) \tag{17}$$

where we have again assumed the boundary condition $f(0) = 0$. Equations (16) and (17) are not, strictly, equations for eigenvalues at all, but may be regarded as sufficient (but not necessary) conditions for a point λ to belong to the singular spectrum. For example, equation (16) holds with $n = 0$ at zero energy if we take $V(x) = 0$; however $\lambda = 0$ is not an eigenvalue but the energy of a semi-bound state. Similarly equation (17) for the differential operator on the half-line, shows that the solution $v(x, \lambda)$, given by

$$v(x, \lambda) = R(x, \lambda) \sin\left(\int_0^x \frac{1}{R^2(t, \lambda)}\, \mathrm{d}t\right)$$

is subordinate at $\lambda = \lambda_n$. According to the discussion of section 2, such points λ_n will belong to the support of the singular measure μ_{s}, though they will only be eigenvalues if v is square integrable.

Neither equation (16) nor equation (17) holds in the case of potentials $V(x)$ for which the Schrödinger equation is oscillatory. This is because, for example in (17), the convergence of the integral implies that the solutions u and v have only a finite number of zeros, in which case the DE is said to be non-oscillatory. The integral in (17) will certainly diverge whenever there is an absolutely continous spectrum. However, any potential for which the Hamiltonian has singular spectrum not consisting of isolated eigenvalues will also lead to the divergence of the integral. Such potentials are of considerable current interest in spectral theory; see [14], for example, where it is shown that the potential $V(x) = \cos\sqrt{x}$ has singular spectrum which is dense in the interval $-1 \leqslant \lambda \leqslant 1$, a situation which may be likened to that of an operator for which every rational number in this finite interval is an eigenvalue.

To deal with examples such as these, it is necessary to find an equation which generalizes (17) and which may be used to characterize the singular spectrum of the Hamiltonian, even if the integral on the left-hand side of (17) diverges.

This can be done as follows. Suppose for simplicity that there is an interval $\lambda_1 \leqslant \lambda \leqslant \lambda_2$ on which the Hamiltonian has no absolutely continuous spectrum. In that case, on $[\lambda_1, \lambda_2]$ the spectrum must be purely singular, consisting either of eigenvalues, or of a singular continuous spectrum, or of some mixture of these two. Define, for $N > 0$ and $\lambda_1 \leqslant \lambda \leqslant \lambda_2$, the function $\theta(N, \lambda)$ by

$$\theta(N, \lambda) = \int_0^N \frac{1}{R^2(t, \lambda)}\, \mathrm{d}t \tag{18}$$

and let $\theta_\pi(N, \lambda) = \theta(N, \lambda)|_{\mathrm{mod}\,\pi}$; the right-hand side of of this equation means subtracting from $\theta(N, \lambda)$ for a given N and λ, an integral multiple of π, to arrive at a number in the interval $-\pi/2 < \theta_\pi(N, \lambda) \leqslant \pi/2$. Now define a function $\theta_\pi(\lambda)$, for (Lebesgue) almost all $\lambda \in [\lambda_1, \lambda_2]$, by

$$\theta_\pi(\lambda) = \operatorname*{lim\text{-}meas}_{N\to\infty} \theta_\pi(N, \lambda). \tag{19}$$

The limit on the right-hand side of (19) may be shown to exist for almost all $\lambda \in [\lambda_1, \lambda_2]$, using arguments based on value distribution; see [15, 16] for a discussion of value distribution applied to the spectral theory of Herglotz functions and of differential operators—the complete proof of (19) and further consequences of this result will be published elsewhere.

The limit on the right-hand side is a limit in measure. We say that $\theta_\pi(N, \lambda)$ converges in measure to $\theta_\pi(\lambda)$ if, for every $\epsilon > 0$, the Lebesgue measure of the set of points λ at which $|\theta_\pi(N, \lambda) - \theta_\pi(\lambda)| > \epsilon$ converges to zero in the limit as $N \to \infty$; roughly this means that, for large N, $\theta_\pi(N, \lambda)$ will be close to $\theta_\pi(\lambda)$ except at a set of λ having small Lebesgue measure. Note that if the Schrödinger equation is oscillatory then $\theta_\pi(N, \lambda)$ will not converge to $\theta_\pi(\lambda)$ in the ordinary sense, since $\theta_\pi(N, \lambda)$ will then assume every value in the interval $[-\pi/2, \ \pi/2]$ infinitely often, for large N.

Equation (19) defines the function $\theta_\pi(\lambda)$ almost everywhere on the interval $[\lambda_1, \lambda_2]$. (As a technical point on which we shall not dwell here, for any point λ at which $\theta_\pi(\lambda)$ has an approximate limit, we can identify the value of $\theta_\pi(\lambda)$ with that approximate limit—this makes $\theta_\pi(\lambda)$ approximately continuous at all such points λ. For definitions of the notions of approximate limit and approximate continuity, see [17], for example).

The following theorem now provides a characterization of the singular spectrum which holds for oscillatory as well as non-oscillatory DEs.

Theorem 1. Suppose the spectrum is purely singular on some interval $[\lambda_1, \lambda_2]$, and define $\theta_\pi(\lambda)$ for almost all λ in this interval by equations (18) and (19) (with $\theta_\pi(\lambda)$ approximately continous where the approximate limit exists). Then the singular measure μ_{s} is supported on the set of all $\lambda \in [\lambda_1, \lambda_2]$ for which $\theta_\pi(\lambda) = 0$.

Although we shall not provide the proof of this result here, it may be helpful in understanding the implications of the theorem to give a more intuitive interpretation. A point λ_0 will belong to the singular spectrum provided that, for large N, the integral $\int_0^N \left(1/R^2(t, \lambda)\right)\, \mathrm{d}t$ is to be found very close to an integer multiple of π, for 'most' λ near to $\lambda = \lambda_0$. For example, if λ_0 is any eigenvalue of H, we can expect in the oscillatory case, as N goes to infinity, that, except for shorter and shorter intervals of N values, the integral will be close to some multiple of π. On these short intervals in N, which will be centred on the values of N for which $u(N, \lambda_0) = 0$, the integral will be very rapidly varying as a function of N, and will approximate to a step function having jump π. Except on these short intervals of rapid increase, the integral will be relatively slowly varying. Only in this way can a continuous, increasing function of N, which diverges in the limit $N \to \infty$, nevertheless be found predominantly close to a multiple (but not a *fixed* multiple!) of π.

The function $\theta_\pi(\lambda)$ defined by (16) can also be used to characterize the singular spectrum for the operator $-\mathrm{d}^2/\mathrm{d}x^2 + V(x)$ subject to a general boundary condition at $x = 0$. If, for example, we define the Hamiltonian $H_\alpha = -\mathrm{d}^2/\mathrm{d}x^2 + V(x)$ subject to the boundary condition $(\cos\alpha) f + (\sin\alpha) f' = 0$ at $x = 0$, then the singular measure of H_α will be concentrated on the set of all λ at which $\theta_\pi = \alpha$.

We claim that an analysis of the solutions of the Schrödinger equation through a study of quadratic forms, integrals involving quadratic forms, and the differential equations which govern them, provides an important tool in spectral theory, which will have many theoretical and computational implications. To provide further justification, we apply these methods in the following section to the absolutely continuous part of the spectrum.

5. Quadratic forms and the absolutely continuous spectrum

If, as we have maintained in this paper, the third-order differential equation (5) in section 3, satisfied by all quadratic forms $Y(x, \lambda)$ in the basic solutions $u(x, \lambda)$, $v(x, \lambda)$ is fundamental to spectral theory for the Schrödinger equation, it should be possible to derive spectral properties from a knowledge of the asymptotics of solutions $Y(x, \lambda)$ in the limit as $x \to \infty$. Here we shall provide just one example of this kind of result, based on the hypothesis that there is a solution $Y(x, \lambda)$ of (5) which approaches a non-zero value in the limit $x \to \infty$, for some value of λ. Note first of all the following result, where again we distinguish between the oscillatory and non-oscillatory case.

Lemma 3. Suppose the Schrödinger equation is oscillatory, for some value of λ. Then, for this value of λ, there can be at most one linearly independent solution $Y(x, \lambda)$ of (5), having the property that $\lim_{x\to\infty} Y(x, \lambda)$ exists and is non-zero.

Proof. Suppose there are two such linearly independent solutions, Y_1 and Y_2. Then a suitable linear combination Y_0 of Y_1 and Y_2, not identically zero, has the property $Y_0(x, \lambda) \to 0$ as $x \to \infty$.

Let us write $Y_0 = a_0 u^2 + b_0 uv + c_0 v^2$.

Now $R = \sqrt{u^2 + v^2}$ is non-zero for $x > 0$. Nor can R become arbitrarily small, for large values of x, since this would imply u, v arbitrarily small, and so contradict the hypothesis that the quadratic form Y_1 have a non-zero limit as $x \to \infty$. Hence, say for $x \geqslant 1$, we have $R(x, \lambda) \geqslant$ constant > 0, for fixed λ, implying that $1/R^2$ is bounded on $x \geqslant 1$. Multiplying the quadratic form Y_0 by $1/R^2$ and substituting $u = R\cos\theta$, $v = R\sin\theta$, it follows that

$$\lim_{x\to\infty} a_0 \cos^2\theta + b_0 \cos\theta \sin\theta + c_0 \sin^2\theta = 0.$$

However, this can only hold for θ monotonic increasing and differentiable ($\mathrm{d}\theta/\mathrm{d}x = 1/R^2 > 0$), if $\theta(x, \lambda)$ approaches a limit as $x \to \infty$. But this would imply that both $u(x, \lambda)$ and $v(x, \lambda)$ have a finite number of zeros, whereas by hypothesis the DE is oscillatory.

Hence there can be at most one solution $Y(x, \lambda)$ having a non-zero limit as $x \to \infty$, and the lemma is proved. □

(Note the assumption that the equation is oscillatory cannot be dropped. For example, with $V(x)$ identically zero and $\lambda = -1$, there are two solutions $u = \cosh x$, $v = \sinh x$, such that, in the limit $x \to \infty$, we have both $u^2 - v^2 \to 1$ and $u^2 - v^2 + C(u - v)^2 \to 1$, for any constant C.)

Consider, then, a solution $Y(x, \lambda)$ of (5), such that $Y(x, \lambda)$ approaches a non-zero limit as $x \to \infty$. We suppose that the DE is oscillatory for this value of λ. We may also assume that Y approaches a *positive* limit, since if not we could consider $-Y$ rather than Y.

The value of β in (7) will also be positive, since with $\beta \leqslant 0$ in (10) the quadratic form defining Y factorizes into a product of real solutions of the Schrödinger equation. For Y to have a non-zero limit, these factors would then be non-vanishing for sufficiently large x, contradicting the assumption that the DE is oscillatory. By taking a constant multiple of Y if necessary, we may therefore assume without loss of generality that $\beta = 4$.

The following theorem describes the spectral properties of the Hamiltonian in terms of the behaviour of $Y(x, \lambda)$ at $x = 0$ and $x = \infty$.

Theorem 2. Suppose that, for all λ in some set $\mathcal{S}$, there exists a solution $Y(x, \lambda)$ of (5) for which $Y(x, \lambda)$ approaches a positive limit as $x \to \infty$ (this limit depending on λ in general); take Y to be 'normalized' so that $\beta = 4$ in (7). Suppose that for $\lambda \in \mathcal{S}$, the DE is oscillatory. Then:
(i) for all $\lambda \in \mathcal{S}$, the spectrum of the differential operator $H = -\mathrm{d}^2/\mathrm{d}x^2 + V(x)$, with boundary condition $f(0) = 0$, is purely absolutely continuous; and
(ii) the spectral density function over this interval is $1/\pi Y(0, \lambda)$.

Proof. Let the quadratic form Y, normalized so that $\beta = 4$, be given by $Y = au^2 + buv + cv^2$.

Here we must have $a > 0$; otherwise there would be a sequence of points $\{x_n\}$ (the zeros of v) for which $x_n \to \infty$ and $Y \leqslant 0$, contradicting the assumption that Y has a positive limit. Since $\beta = 4ac - b^2 = 4$, we also have $c > 0$.

Defining a pair of real numbers A, B, with $A > 0$, by $A^2 = a$, $2AB = b$, $B^2 + 1/A^2 = c$, we can write the solution Y as

$$Y = (Au + Bv)^2 + v^2/A^2 .$$

Equation (15) shows that $R = \sqrt{Y}$ is a solution of Milne's equation, and correspondingly, substituting $R = \sqrt{Y}$ into the general solution of the Schrödinger equation, we can construct two solutions

$$f_1 = \sqrt{Y(x, \lambda)} \cos \int_0^x \frac{1}{Y(t, \lambda)}\, \mathrm{d}t \qquad f_2 = \sqrt{Y(x, \lambda)} \sin \int_0^x \frac{1}{Y(t, \lambda)}\, \mathrm{d}t$$

of (1). From the initial values at $x = 0$, namely $R = A$ and $\mathrm{d}R/\mathrm{d}x = B$, at $x = 0$ we find

$$f_1 = A \quad \frac{\mathrm{d}f_1}{\mathrm{d}x} = B \qquad f_2 = 0 \quad \frac{\mathrm{d}f_2}{\mathrm{d}x} = 1/A .$$

The initial conditions for u and v then imply

$$f_1 = Au + Bv \qquad f_2 = v/A. \tag{20}$$

Let us write $\lim_{x\to\infty} Y(x, \lambda) = 1/q(\lambda)$ $(\lambda \in \mathcal{S})$, for some $q(\lambda) > 0$. From the expressions for f_1 and f_2, using the asymptotic behaviour of Y, as $x \to \infty$ we have

$$f_1 \simeq q^{-1/2} \cos(qx) \qquad f_2 \simeq q^{-1/2} \sin(qx) .$$

These two formulae are to be interpreted to mean, for example, that, as $x \to \infty$,

$$f_1(x, \lambda) = \big(q^{-1/2} + \mathrm{o}(1)\big) \cos\big(qx + \mathrm{o}(x)\big)$$

and it is a straightforward matter to express u, v as linear combinations of f_1, f_2 to determine the asymptotics of these functions too.

One of the solutions of the Schrödinger equation which plays an important role in spectral analysis is the complex linear combination $f = (f_1 + \mathrm{i} f_2)/A$, given here by

$$f(x,\lambda) = A^{-1}\sqrt{Y(x,\lambda)}\exp\left(\mathrm{i}\int_0^x \frac{1}{Y(t,\lambda)}\,\mathrm{d}t\right).$$

From the behaviour of Y for large x, we know that

$$\int_0^N |f(x,\lambda)|^2\,\mathrm{d}x \sim N/A^2q \qquad \text{as} \quad N\to\infty.$$

Since $A^{-2}Y - (Aq)^{-2}Y^{-1} \to 0$ as $x\to\infty$, we also have

$$\left|\int_0^N \left\{\left(A^{-2}Y - (Aq)^{-2}Y^{-1}\right)\exp\left(2\mathrm{i}\int_0^x \frac{1}{Y}\,\mathrm{d}t\right)\right\}\,\mathrm{d}x\right| = \mathrm{o}(N)$$

as $N\to\infty$.

Noting that

$$\int_0^N \left\{Y^{-1}\exp\left(2\mathrm{i}\int_0^x \frac{1}{Y}\,\mathrm{d}t\right)\right\}\,\mathrm{d}x = \frac{1}{2\mathrm{i}}\left\{\exp 2\mathrm{i}\int_0^N \frac{1}{Y}\,\mathrm{d}t - 1\right\}$$

is bounded uniformly in N, it follows that

$$\left|\int_0^N f^2(x,\lambda)\,\mathrm{d}x\right| = \mathrm{o}(N) \qquad \text{as} \quad N\to\infty$$

and hence that

$$\lim_{N\to\infty}\frac{\int_0^N f^2(x,\lambda)\,\mathrm{d}x}{\int_0^N |f(x,\lambda)|^2\,\mathrm{d}x} = 0\,. \tag{21}$$

Equation (21) is just the so-called condition (A) referred to earlier, and the results given in section 2 imply that the points in $\mathcal{S}$ belong to the absolutely continuous spectrum of the Hamiltonian. Using equations (20) to express $f = (f_1 + \mathrm{i} f_2)/A$ as a linear combination of u and v, we can then calculate the $M-$coefficient given by (2), giving $M(\lambda) = B/A + \mathrm{i}/A^2$.

Hence, from (3), the spectral density function for all $\lambda\in\mathcal{S}$ is given by $\mathrm{d}\mu/\mathrm{d}\lambda = 1/\pi A^2$. Since $A^2 = a = Y(0)$, we have finally, $\mathrm{d}\mu/\mathrm{d}\lambda = 1/\pi Y(0,\lambda)$ as stated. □

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