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Changes in potentials due to changes in the point spectrum: Anharmonic oscillators with exact solutions

P. B. Abraham
Naval Underwater Systems Center, New London Laboratory, New London, Connecticut 06320

H. E. Moses
University of Lowell, Center for Atmospheric Research, College of Pure and Applied Science, Lowell, Massachusetts 01854

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Assume a solved quantum-mechanical problem for the one-dimensional Schrödinger equation, which has a discrete spectrum. An algorithm is presented to calculate exactly the change in the original potential and eigenfunctions brought about by arbitrary changes in the positions of the original eigenvalues and/or the normalizations of the corresponding eigenfunctions. As a first example, we consider the modification of the harmonic oscillator and thereby obtain potentials for anharmonic oscillators with exact eigenvalues and eigenfunctions. Next, we introduce potentials in the one-dimensional box with rigid walls which alter the usual spectrum in a predetermined way. We also sketch the process of obtaining a change in the Coulomb potential which deletes the lowest eigenvalue for the zero-angular-momentum equation.

I. INTRODUCTION

It is well known that the number of one-dimensional Schrödinger equations having exact point eigenvalues is quite small. Indeed, if no continuous spectrum is present, the only three examples with infinite discrete spectra usually discussed in the literature are the particle in a box, the harmonic oscillator, and the symmetric Pöschl-Teller potential.[1] (Other potentials are also discussed in Ref. 1.)

The intent of the present work is to enlarge this number through the systematic use of the Gelfand-Levitan equation.[2-4] This approach allows us to generate exactly solvable potentials from the potentials mentioned above by adding or subtracting a finite number of eigenvalues and/or by changing the normalizations of a finite number of eigenfunctions. The Gelfand-Levitan equation which appears here makes use of comparison potentials and comparison measures. These concepts have been discussed in full generality by Moses.[4] However, for the purposes of the present paper, we shall give an independent derivation of the algorithm.

After presenting the algorithm in Sec. II, we illustrate the method in subsequent sections. In Sec. III, we exhibit a potential whose spectrum coincides with that of the harmonic oscillator except that the lowest eigenvalue has been removed. We thus have obtained an anharmonic oscillator with known eigenvalues and exact corresponding eigenfunctions, both in closed form.

As a further illustration, we present in Sec. IV the modified potential for a particle in a box, when again the lowest eigenvalue has been omitted. The same procedure is then applied in Sec. V to get the potential for the Coulomb problem in the zero-angular-momentum state.

From these examples it is clear how to generate other potentials with prescribed spectra. To the best of our knowledge, this class of potentials represents the first novel, nontrivial addition to the list of potentials which support known spectra with an infinite number of point eigenvalues. In the concluding Sec. VI, we discuss the results obtained and indicate what generalizations are possible. In the Appendix the algorithm is derived and a proof of the completeness relation for the new eigenfunctions is provided.

II. THE ALGORITHM

Let us consider a one-dimensional Hamiltonian H_0,

$$H_0 = -\frac{d^2}{dx^2} + V_0(x), \quad -\infty \leq x \leq \infty, \tag{1}$$

with a discrete and (generally) a continuous spectrum. Let the eigenfunctions corresponding to the discrete spectrum be denoted by $\Psi_n(x)$. These eigenfunctions satisfy the equation

$$H_0\Psi_n = E_n\Psi_n, \tag{2}$$

where the E_n's are the point eigenvalues and the Ψ_n's have the normalizations C_n,

$$\int_{-\infty}^{\infty} \Psi_n^2(x)\,dx = C_n. \tag{3}$$

In addition, there may be a continuous spectrum, with eigenvalues E and corresponding eigenfunctions $\Psi(x|E, \alpha)$, where α denotes a degeneracy variable (e.g., for the direction of momentum).

We shall require the eigenfunctions to satisfy the completeness relation:

$$\sum_n \frac{\Psi_n(x)\Psi_n(x')}{C_n} + \sum_{\alpha,\alpha'} \int \Psi(x|E,\alpha)\Psi^*(x'|E,\alpha')W(E|\alpha,\alpha')dE = \delta(x-x'). \quad (4)$$

In Eqs. (3) and (4) we have assumed $\Psi_n(x)$ to be real. In Eq. (4) $W(E|\alpha,\alpha')$ is a positive weighting function. For further details concerning this function see Kay and Moses,[3] and Moses.[4]

Now we show that it is possible to add a potential $V'(x)$ to H_0, so that the new Hamiltonian H,

$$H = H_0 + V' \quad (5)$$

has the same continuous spectrum as H_0, and its discrete spectrum coincides with that of H_0, except for a finite number of eigenvalues and/or a finite number of normalizations. Explicitly, let $\chi_n(x)$ be the eigenfunctions for the point eigenvalues of H, now denoted by $\hat{E}_n$, and having normalizations $\hat{C}_n$. The continuous spectrum eigenfunctions of H will be denoted by $\chi(x|E,\alpha)$ which, by the assumption that the continuous spectra of H and H_0 coincide, have associated with them the same continuous measure function $W(E|\alpha,\alpha')$. Thus, for the Hamiltonian H, the completeness relation is

$$\sum_n \frac{\chi_n(x)\chi_n(x')}{\hat{C}_n} + \times \sum_{\alpha,\alpha'} \int \chi(x|E,\alpha)\chi^*(x'|E,\alpha')W(E|\alpha,\alpha')dE = \delta(x-x'). \quad (6)$$

By our assumption, all but a finite number of $\hat{E}_n$'s, and similarly the number of $\hat{C}_n$'s not identical to the C_n's is finite. In particular, there may be no continuous spectrum at all, as in the case of the three potentials mentioned in the Introduction.

To exhibit the algorithm, we start by introducing the formal eigenfunction $\hat{\Psi}_n$ of H_0, which corresponds to the eigenvalue $\hat{E}_n$,

$$H_0\hat{\Psi}_n = \hat{E}_n\hat{\Psi}_n. \quad (7)$$

It should be noted that those $\hat{E}_n$'s which do *not* coincide with any of the E_n's, may be completely arbitrary real numbers. Therefore Eq. (7) is an ordinary differential equation with two linearly independent solutions. We select that solution of Eq. (7) which satisfies the boundary condition

$$\lim_{x\to-\infty} \hat{\Psi}_n(x) = 0. \quad (8)$$

We remark that $\hat{\Psi}_n(x)$ will coincide with $\Psi_n(x)$ if $\hat{E}_n$ is equal to E_n, and Ψ_n is constrained to satisfy the same boundary conditions as Ψ_n.

Now let us construct the function

$$\Omega(x,y) = \sum_n \frac{\hat{\Psi}_n(x)\hat{\Psi}_n(y)}{\hat{C}_n} - \sum_n \frac{\Psi_n(x)\Psi_n(y)}{C_n}. \quad (9)$$

Our previous assumptions imply that $\Omega(x,y)$ contains only a finite number of terms.

The Gelfand-Levitan kernel $K(x,y)$ is defined as the (unique) solution of the integral equation

$$K(x,y) = -\Omega(x,y) - \int_{-\infty}^{x} K(x,z)\Omega(z,y)dz. \quad (10)$$

Note that, for fixed x, $K(x,y)$ is the solution of a Fredholm integral equation. In terms of $\hat{\Psi}_n$, Ψ, Ω, and K, the algorithm for the determination of V', χ_n, and χ is

$$V'(x) = 2\frac{d}{dx}K(x,x), \quad (11)$$

$$\chi_n(x) = \hat{\Psi}_n(x) + \int_{-\infty}^{x} K(x,y)\hat{\Psi}_n(y)dy, \quad (12)$$

$$\chi(x|E,\alpha) = \Psi(x|E,\alpha) + \int_{-\infty}^{x} K(x,y)\Psi(y|E,\alpha)dy. \quad (13)$$

The Gelfand-Levitan equation is easily solved for K because the kernel $K(x,y)$ is separable, as seen from its definition in Eq. (9). The derivation of this algorithm is presented in the Appendix, where a proof of the completeness relation satisfied by the χ_n's is also given.

Having found K, it is useful to introduce the operator U acting on functions belonging to the Hilbert space $L_2(-\infty,\infty)$, and defined as

$$Uf(x) = f(x) + \int_{-\infty}^{x} K(x,y)f(y)dy. \quad (14)$$

Then Eqs. (12) and (13) can be written as

$$\chi_n(x) = U\hat{\Psi}_n(x), \quad \chi(x|E,\alpha) = U\Psi(x|E,\alpha). \quad (15)$$

It is clear that the roles of H and H_0 can be interchanged. When this is done, a new Gelfand-Levitan kernel $\hat{K}(x,y)$ is obtained and corresponding to it an operator $\hat{U}$. It is not difficult to show that

$$\hat{U}U = I, \quad (16)$$

where I is the identity operator. Equation (16) makes it evident that the interchange of H and H_0 allows us to obtain U^{-1}, the inverse of U.

III. EXACT ANHARMONIC OSCILLATORS

We shall now give examples of anharmonic oscillators with exact eigenvalues and eigenfunctions. To the best of our knowledge these are the first examples of such oscillators, with infinite discrete spectra.

We begin by choosing for the unperturbed system the usual harmonic oscillator whose Hamiltonian H_0 is taken to be

$$H_0 = \frac{1}{2}\left(-\frac{d^2}{dx^2}+x^2\right). \tag{17}$$

The well-known eigenfunctions $\Psi_n(x)$ and eigenvalues E_n are

$$\Psi_n(x) = \frac{1}{(\sqrt{\pi}\,2^n n!)^{1/2}}\, e^{x^2/2} H_n(x), \tag{18}$$

$$E_n = n+\tfrac{1}{2}, \quad C_n = 1. \tag{19}$$

We have followed Messiah[5] in our choice of units and definition of the Hermite polynomials $H_n(x)$.

To obtain an exact perturbed system, we change a finite number of the eigenvalues and/or the normalizations of the eigenfunctions. The simplest cases occur when we delete or add one eigenvalue, or alternatively, the spectrum is left unchanged but the normalization of a single eigenfunction is altered.

In detail, let us consider the dynamical system obtained when the spectrum of the perturbed system is identical with that of the harmonic oscillator, except for the absence of the lowest eigenvalue $E_0 = \frac{1}{2}$. The eigenfunctions of the perturbed system are assumed to have the same normalizations as the Ψ_n's in Eq. (18).

According to our assumptions, we have in the present case

$$\hat{\Psi}_n(x) \equiv \Psi_n(x), \quad n = 1, 2, 3, \ldots . \tag{20}$$

Moreover, it is clear from Eq. (9) that

$$\Omega(x,y) = -\Psi_0(x)\Psi_0(y). \tag{21}$$

The Gelfand-Levitan kernel is readily shown to be

$$K(x,y) = \frac{2}{\sqrt{\pi}}\,\frac{e^{-(x^2+y^2)/2}}{\operatorname{erfc}(x)}, \tag{22}$$

where $\operatorname{erfc}(x)$ is defined by[6]

$$\operatorname{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}dt. \tag{23}$$

The potential $V'(x)$ that is to be added to $V_0 = \frac{1}{2}x^2$ is, by virtue of Eqs. (11) and (22),

$$V'(x) = -2\,\frac{d^2}{dx^2}\ln[\operatorname{erfc}(x)]$$

$$= \frac{4}{\sqrt{\pi}}\,\frac{e^{-x^2}}{\operatorname{erfc}(x)}\left(\frac{e^{-x^2}}{\sqrt{\pi}\operatorname{erfc}(x)} - x\right). \tag{24}$$

The eigenfunctions of $H = H_0 + V'$, are

$$\chi_n(x) = \Psi_n(x) - \left(\frac{2}{n\pi}\right)^{1/2}\frac{e^{-x^2}}{\operatorname{erfc}(x)}\Psi_{n-1}(x), \quad n = 1, 2, 3, \ldots . \tag{25}$$

This set of eigenfunctions is complete and $\hat{C}_n = 1$ for $n = 1, 2, 3, \ldots$. Therefore the χ_n's satisfy the relation

$$\sum_{n=1}^{\infty}\chi_n(x)\chi_n(y) = \delta(x-y). \tag{26}$$

In deriving our results we have made use of Eq. (20).

The addition of $V'(x)$ to H_0 means that H is the Hamiltonian of an anharmonic oscillator, whose spectrum is the discrete set ($E_n = n+\frac{1}{2}$; $n = 1, 2, 3, \ldots$) with corresponding eigenfunctions given explicitly by Eq. (25).

The foregoing has treated the case of deletion of one eigenvalue. An example of the addition of one eigenvalue is provided by the interchange of H and H_0. In this case, the algorithm demands that we solve the ordinary differential equation

$$H\hat{\chi}_0 = \hat{\epsilon}_0\hat{\chi}_0, \tag{27}$$

where $\hat{\epsilon}_0 = E_0 = \frac{1}{2}$ and $(\hat{\chi}, \hat{\epsilon})$ are the counterparts of $(\hat{\Psi}, \hat{E})$ in the original formulation.

It turns our that a $\hat{\chi}_0$ satisfying Eq. (27) and the boundary condition of Eq. (18) can be found and is given by

$$\hat{\chi}_0 = U\hat{\Psi}_0. \tag{28}$$

The apparent contradiction that $\hat{\chi}_0$ is an eigenfunction of H and yet does not appear in the completeness relation of Eq. (26), is resolved simply by noting that $\hat{\chi}_0$ is only a formal eigenfunction, since it is not quadratically integrable [and thus it is outside the space $L_2(-\infty, \infty)$].

The explicit form of $\hat{\chi}_0(x)$ is

$$\hat{\chi}_0(x) = \frac{2e^{-1/2x^2}}{\pi^{1/4}\operatorname{erfc}(x)}. \tag{29}$$

The Gelfand-Levitan kernel for this case is

$$\hat{K}(x,y) = -\frac{2}{\sqrt{\pi}}\,\frac{e^{-1/2(x^2+y^2)}}{\operatorname{erfc}(y)}. \tag{30}$$

Explicit computation then shows that

$$\hat{U}U = U\hat{U} = I, \tag{31}$$

where I is the identity operator.

A second example which is also easily treated is the case where the normalization of one eigenfunction is modified while the spectra of H_0 and H are assumed identical. The unperturbed system is the harmonic oscillator as before, and we take

$$\hat{C}_n = C_n = 1, \quad n = 1, 2, 3, \ldots . \tag{32}$$

For brevity we write

$$\hat{C}_0 = C . \tag{33}$$

Our formalism then yields for this case

$$\Omega(x, y) = -D\Psi_0(x)\Psi_0(y), \tag{34}$$

where

$$D = 1 - 1/C . \tag{35}$$

The kernel $K(x, y)$ is easily seen to be

$$K(x, y) = \frac{2}{\sqrt{\pi}} \frac{e^{-1/2(x^2+y^2)}}{\lambda + \operatorname{erfc}(x)} \tag{36}$$

with λ defined by

$$\lambda = \frac{2(1-D)}{D} = \frac{2}{C-1} . \tag{37}$$

It is of interest to note that in the limit $\lambda \to 0$ (i.e., $C \to \infty$), we recover from Eq. (36) the kernel in Eq. (22). This is as expected, since $C \to \infty$ implies that the lowest eigenvalue does not belong to the spectrum of the new Hamiltonian H. For $\lambda \neq 0$, Eq. (36) yields in the usual way explicit expressions for both $V'(x)$ and $\chi_n(x)$. This example shows that it is possible for two Hamiltonians to have identical spectra, and yet the two may not be unitarily equivalent. This is an analog of a well-known result in inverse scattering theory.[7]

Another class of potentials which support the same spectrum as that of the harmonic oscillator is obtained by deleting the lowest m eigenvalues to obtain in the manner described above a Hamiltonian $H^{(m)}$ with eigenfunctions $\chi_n(x)$ $(n = m, m+1, \ldots)$. Let us define a new Hamiltonian

$$\hat{H}^{(m)} = H^{(m)} - m$$

and eigenfunctions $\gamma_n(x) = \chi_{m+n}(x)$. Then $\hat{H}^{(m)}$ has the same spectrum as the harmonic oscillator H_0. Its eigenfunctions $\gamma_n(x)$ with $n = 0, 1, 2, \ldots$ are associated with the eigenvalues $E_n = n + \frac{1}{2}$. In the present case $\hat{H}^{(m)}$ *is* unitarily equivalent to the harmonic-oscillator Hamiltonian H_0. The unitary operator giving the transformation can be constructed from the kernel $K(x, y)$. We refrain from details. In the present case the ambiguity of the potential differs from that discussed above.

Another question of interest which we may deal with in later papers is the effect of scaling the potential $V'(x)$, i.e., replacing $V'(x)$ by $\epsilon V'(x)$. It appears that the spectrum of $H_0 + \epsilon V'(x)$ is a discontinuous function of ϵ. Close analogs to this problem are discussed in Ref. 8.

IV. PARTICLE IN A BOX

In this section we apply our method to the Hamiltonian H_0 associated with a particle in a box. The limits $-\infty$ and $+\infty$ of the previous example are replaced by $-(\pi/2)$ and $+(\pi/2)$, respectively. Thus, following Messiah,[5] we have

$$H_0 = -\frac{d^2}{dx^2}, \quad -\tfrac{1}{2}\pi \leq x \leq \tfrac{1}{2}\pi . \tag{38}$$

The eigenfunctions $\Psi_n(x)$ are given by

$$\Psi_n(x) = \begin{cases} \sqrt{2/\pi}\sin(nx), & n \text{ even} \\ \sqrt{2/\pi}\cos(nx), & n \text{ odd} . \end{cases} \tag{39}$$

The normalizations C_n are

$$C_n = 1, \quad \text{all } n, \tag{40}$$

and the $\Psi_n(x)$ have been chosen to satisfy the boundary conditions

$$\Psi_n(\pm\tfrac{1}{2}\pi) = 0 . \tag{41}$$

Finally, the eigenvalues of H_0 are

$$E_n = n^2, \quad n = 1, 2, 3, \ldots . \tag{42}$$

The simplest way of obtaining a new dynamical system is to delete the lowest eigenvalue $E_1 = 1$ and require $\hat{C}_n = 1$ for $n > 1$. In this case

$$\Omega(x, y) = -(2/\pi)\cos x \cos y . \tag{43}$$

The kernel obtained from Eqs. (10) and (43) is

$$K(x, y) = -4\cos x \cos y/(2x - \pi - \sin 2x) \tag{44}$$

and the resulting $V'(x)$ is

$$V'(x) = 8(2x - \pi)/(2x - \pi - \sin 2x)^2 . \tag{45}$$

The new eigenfunctions have the form

$$\chi_n(x) = \Psi_n(x) + (-1)^n \frac{2\cos x}{2x - \pi - \sin 2x} \times \left(\frac{\Psi_{n+1}(x)}{n+1} + \frac{\Psi_{n-1}(x)}{n-1} \right), \quad n = 2, 3, \ldots . \tag{46}$$

Equation (46) shows immediately that $\chi_n(x)$ satisfies the boundary conditions (41). Furthermore, the algorithm implies that these $\chi_n(x)$'s satisfy the completeness relation. Again, other generalizations are possible for the present case as well, but we refrain from pursuing this here.

V. MODIFICATION OF THE COULOMB POTENTIAL

The algorithm for one-dimensional problems developed above, holds also for the radial equation corresponding to an arbitrary angular momentum.

We can therefore introduce a new Hamiltonian for each angular momentum.

In particular, let us consider the zero-angular-momentum case and take the H_0 to correspond to the Coulomb potential with $Z=1$ and a_0 (the Bohr radius) = 1.

If we delete the ground state of the hydrogen atom, we obtain the potential

$$V'(r)=16r(r+1)/(2r^2+2r+1)^2. \tag{47}$$

We note that as $r\to\infty$, $V'(r)\sim 4/r^2$. Thus $V'(r)$ represents a screening potential such that the spectrum of the zero-angular-momentum equation coincides with that of the unperturbed hydrogen atom, except for the ground state. For higher angular momenta, the spectra of the new Hamiltonian may not correspond to the original hydrogen spectrum.

VI. GENERALIZATIONS

It is of interest to write down the solutions of the Gelfand-Levitan equation for the two cases of deletion and addition of a single, arbitrary point eigenvalue, with all normalizations taken equal to one.

In case we delete the eigenvalue E_d, we obtain

$$\Omega_d(x,y)=-\Psi_d(x)\Psi_d(y), \tag{48}$$

$$K_d(x,y)=\Psi_d(x)\Psi_d(y)\Big/\left(1-\int_{-\infty}^{x}\Psi_d^2(z)dz\right), \tag{49}$$

$$V_d'=-2\frac{d^2}{dx^2}\ln\left(1-\int_{-\infty}^{x}\Psi_d(z)dz\right). \tag{50}$$

If the point eigenvalue $\hat{E}_a$ is added to the spectrum, the results are

$$\Omega_a(x,y)=\hat{\Psi}_a(x)\hat{\Psi}_a(y), \tag{51}$$

$$K_a(x,y)=-\hat{\Psi}_a(x)\hat{\Psi}_a(y)\Big/\left(1+\int_{-\infty}^{x}\hat{\Psi}_a^2(z)dz\right), \tag{52}$$

$$V_a'(x)=-2\frac{d^2}{dx^2}\ln\left(1+\int_{-\infty}^{x}\hat{\Psi}_a^2(z)dz\right). \tag{53}$$

As a consequence of the above equations, it is possible to exhibit, without further quadrature, the forms of $\chi_d(x)$ and $\chi_a(x)$.

Use of Eqs. (42), (49), and (52) yields

$$\chi_d(x)=\Psi_d(x)\Big/\left(1-\int_{-\infty}^{x}\Psi_d^2(z)dz\right). \tag{54}$$

As mentioned previously, $\chi_d(x)$ is only a formal eigenfunction of H, since it is not quadratically integrable (the denominator vanishes when $x\to+\infty$).

On the other hand, note that

$$\chi_a(x)=\hat{\Psi}_a(x)\Big/\left(1+\int_{-\infty}^{x}\hat{\Psi}_a^2(z)dz\right) \tag{55}$$

is an actual eigenfunction.

The results above can be extended to any number of additions or deletions of point eigenvalues. Since $\Omega(x,y)$ is taken from the outset to be separable, $K(x,y)$ will also be separable. Aside from the quadratures involved, the only difficulty in this approach is algebraic, since we have to solve a system of linear equations. This approach is close to that for obtaining the reflectionless potentials of Ref. 9. An alternative approach is to proceed one step at a time and then the difficulty is in performing appropriate quadratures which may become progressively more complicated.

The exact anharmonic oscillator, found in Sec. III, can lend itself easily to a perturbation analysis. This follows from a comparison of $V'(x)$ of Eq. (24) with x^2. A modest numerical effort showed that $V'(x)$ represents a very slight perturbation to x^2. Since we know the exact eigenvalues and eigenfunctions of the perturbed problem, we can check the effectiveness of various perturbation theories on using this anharmonic-oscillator model.

In conclusion, we feel that the ability to generate novel, exactly solvable models with the aid of the present algorithm, is quite significant and has many possible ramifications. Some of these will be explored in future work.

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APPENDIX: DERIVATION OF THE FUNDAMENTAL ALGORITHM

For the sake of simplicity, let us assume in what follows that H_0 (and hence H) has a purely discrete spectrum. The generalization to the case of a spectrum possessing also a continuous part is immediate.

For reasons that will become apparent in the sequel, we define

$$H_0^u=-\frac{d^2}{du^2}+V_0(u). \tag{A1}$$

To derive the algorithm, we want to show that the function $(H_0^x-\hat{E}_n)\chi_n(x)$ is equal to a function of x multiplying $\chi_n(x)$ itself. This so far unknown function will then be equal to $-V'(x)$, and thus will lead to the new Hamiltonian H we wish to determine. Applying the operator $H_0^x-\hat{E}_n$ on $\chi_n(x)$, where the latter is as defined in Eq. (12), we ob-

tain

$$(H_0^x - \hat{E}_n)\chi_n(x) = (H_0^x - \hat{E}_n)\hat{\Psi}_n(x) + (H_0^x - \hat{E}_n)\int_{-\infty}^{x} K(x,y)\hat{\Psi}_n(y)dy . \tag{A2}$$

The first term on the right-hand side (rhs) of Eq. (A2) is zero by Eq. (7). Also,

$$\frac{d^2}{dx^2}\int_{-\infty}^{x} K(x,y)\hat{\Psi}_n(y)dy = \left(\frac{d}{dx}K(x,x)\right)\hat{\Psi}_n(x) + K(x,x)\frac{d\hat{\Psi}_n}{dx} + \frac{\partial}{\partial x}K(x,y)\Big|_{y=x}\hat{\Psi}_n(x) + \int_{-\infty}^{x}\frac{\partial^2 K(x,y)}{\partial x^2}\hat{\Psi}_n(y)dy . \tag{A3}$$

Now we make use of the identity

$$\frac{dK(x,x)}{dx} = \frac{\partial K(x,y)}{\partial x}\Big|_{y=x} + \frac{\partial K(x,y)}{\partial y}\Big|_{y=x} \tag{A4}$$

and of Eq. (A3) to write

$$H_0^x\int_{-\infty}^{x} K(x,y)\hat{\Psi}_n(y)dy = -2\left(\frac{d}{dx}K(x,x)\right)\hat{\Psi}_n(x) - K(x,x)\frac{d\hat{\Psi}_n}{dx} + \frac{\partial K(x,y)}{\partial y}\Big|_{y=x}\hat{\Psi}_n(x) - \int_{-\infty}^{x}[H_0^x K(x,y)]\hat{\Psi}_n(y)dy . \tag{A5}$$

In addition, we use Eq. (7) once more to obtain

$$\hat{E}_n\int_{-\infty}^{x} K(x,y)\hat{\Psi}_n(y)dy = \int_{-\infty}^{x} K(x,y)H_0\hat{\Psi}_n(y)dy . \tag{A6}$$

The form of the term on the rhs of Eq. (A6) can be changed if we use the definition of H_0^y and integrate repeatedly by parts. Thus,

$$\int_{-\infty}^{x} K(x,y)\frac{d^2\hat{\Psi}_n}{dy^2}dy = K(x,x)\frac{d\hat{\Psi}_n}{dx} - \frac{\partial K(x,y)}{\partial y}\Big|_{y=x}\hat{\Psi}_n(x) + \int_{-\infty}^{x}\frac{\partial^2 K(x,y)}{\partial y^2}\hat{\Psi}_n(y)dy . \tag{A7}$$

In Eq. (A7) the effect of the lower limit in the integrated terms has been eliminated with the aid of the boundary condition (8) and of

$$\lim_{y\to\infty} K(x,y) = 0 , \tag{A8}$$

which follows easily from the same property of $\Omega(x,y)$.

Use of Eq. (A7) enables us to write

$$\int_{-\infty}^{x} K(x,y)H_0^y\hat{\Psi}(y)dy = -K(x,x)\frac{d\hat{\Psi}_n}{dx} + \frac{\partial K(x,y)}{\partial y}\Big|_{y=x}\hat{\Psi}_n(x) + \int_{-\infty}^{x}[H_0^y K(x,y)]\hat{\Psi}_n(y)dy . \tag{A9}$$

The substitution of all these results in Eq. (A2) yields

$$(H_0^x - \hat{E}_n)\chi_n(x) = -2\frac{dK(x,x)}{dx}\hat{\Psi}_n(x) + \int_{-\infty}^{x}[(H_0^x - H_0^y)K(x,y)]\hat{\Psi}_n(y)dy . \tag{A10}$$

To evaluate the last term on the rhs of Eq. (A10) we use the Gelfand-Levitan Eq. (10). Thus, applying H_0^x and H_0^y on Eq. (1) we obtain

$$H_0^x K(x,y) = -H_0^x\Omega(x,y) + \frac{dK(x,x)}{dx}\Omega(x,y) + K(x,x)\frac{\partial\Omega(x,y)}{\partial x} + \frac{\partial K(x,y)}{\partial y}\Big|_{y=x}\Omega(x,y) - \int_{-\infty}^{x} H_0^x K(x,z)\Omega(z,y)dz , \tag{A11}$$

$$H_0^y K(x,y) = -H_0^x\Omega(x,y) - \int_{-\infty}^{x} K(x,z)H_0^z\Omega(z,y)dz . \tag{A12}$$

In Eq. (A12) we have used in both terms on the rhs, the identity

$$H_0^u\Omega(u,v) = H_0^v\Omega(u,v) , \tag{A13}$$

which follows from the symmetry of Ω, as can be easily verified.

Integration by parts in Eq. (A12) yields

$$H_0^y K(x,y) = -H_0^x\Omega(x,y) + K(x,x)\frac{\partial\Omega(x,y)}{\partial x} - \frac{\partial K(x,y)}{\partial y}\Big|_{y=x}\Omega(x,y) - \int_{-\infty}^{x}[H_0^z K(x,z)]\Omega(z,y)dz . \tag{A14}$$

Equations (A11), (A14), and the identity (A4) yield then

$$(H_0^x - H_0^y)K(x,y) = 2\frac{dK(x,x)}{dx}\Omega(x,y) - \int_{-\infty}^{x}[(H_0^x - H_0^z)K(x,z)]\Omega(z,y)dz . \tag{A15}$$

Let us define now the functions $V'(x)$ and $F(x,y)$:

$$V'(x) = 2\frac{dK(x,x)}{dx}, \tag{A16}$$

$$-V'(x)F(x,y) = (H_0^x - H_0^y)K(x,y) . \tag{A17}$$

Substituting these definitions in Eq. (A15) we obtain

$$F(x,y) = -\Omega(x,y) - \int_{-\infty}^{x} F(x,z)\Omega(z,y)dz . \tag{A18}$$

In deriving Eq. (A18), we have assumed that $V'(x)$ is not identically zero. The truth of this statement follows from the observation that $V'(x) \equiv 0$ would yield a homogeneous integral equation for $(H_0^x - H_0^y)K(x,y)$ in Eq. (A15). But this equation has the same kernel $\Omega(x,y)$ as the inhomogeneous Gelfand-Levitan Eq. (10), which we know to have the unique solution $K(x,y)$. Thus we obtain a contradiction and hence $V'(x)$ cannot be identically zero.

Returning to Eq. (A18) and using again the uniqueness of K as a solution of Eq. (10) [alias Eq. (A18)], we have identically

$$F(x,y) = K(x,y) . \tag{A19}$$

Substitution of this identity in Eq. (A17) yields the equation

$$(H_0^x - H_0^y)K(x,y) = -V'(x)K(x,y) . \tag{A20}$$

We go back now to Eq. (A10), substitute from Eq. (A20), and use Eq. (12) in the resulting expressions. The final result is

$$(H_0^x - \hat{E}_n)\chi_n(x) = -V'(x)\chi_n(x) . \tag{A21}$$

This shows immediately that $\chi_n(x)$ is an eigenfunction of the Hamiltonian

$$H = H_0 + V' . \tag{A22}$$

As promised in the text, the algorithm does indeed yield both the potential $V'(x)$ and the eigenfunctions $\chi_n(x)$.

It remains to show now that the χ_n's are the only eigenfunctions of H. This is equivalent to requiring the χ_n's to satisfy the completeness relation (for the case of a purely discrete spectrum assumed here):

$$\sum_n \frac{\chi_n(x)\chi_n(y)}{\hat{C}_n} = \delta(x-y) . \tag{A23}$$

To derive the completeness relation we substitute for χ_n from Eq. (12) into the sum:

$$\sum_n \frac{\chi_n(x)\chi_n(y)}{\hat{C}_n} = \sum_n \frac{\hat{\Psi}_n(x)\hat{\Psi}_n(y)}{\hat{C}_n} + \int_{-\infty}^{x} dz\, K(x,z)\sum_n \frac{\hat{\Psi}_n(z)\hat{\Psi}_n(y)}{\hat{C}_n} + \int_{-\infty}^{y} d\zeta\, K(y,\zeta)\sum_n \frac{\hat{\Psi}_n(x)\hat{\Psi}_n(\zeta)}{\hat{C}_n} + \int_{-\infty}^{x} dz \int_{-\infty}^{y} d\zeta\, K(x,z)K(y,\zeta)\sum_n \frac{\hat{\Psi}_n(z)\hat{\Psi}_n(\zeta)}{\hat{C}_n} . \tag{A24}$$

We shall now assume that the eigenfunctions $\Psi_k(x)$ of H_0 satisfy the completeness relation

$$\sum_k \frac{\Psi_k(u)\Psi_k(v)}{C_k} = \delta(u-v) . \tag{A25}$$

Then using Eq. (9) defining Ω, and Eq. (A25), we can write

$$\sum_k \frac{\hat{\Psi}_n(u)\hat{\Psi}_n(v)}{\hat{C}_n} = \Omega(u,v) + \delta(u-v) . \tag{A26}$$

In Eq. (A26), the sum on the lhs has an infinite number of terms since it includes also those for which the $\hat{\Psi}_n$'s coincide with the Ψ_n's.

Substitution of Eq. (A26) into Eq. (A24) yields

$$\sum_n \frac{\chi_n(x)\chi_n(y)}{\hat{C}_n} = \delta(x-y) + \Omega(x,y) + \int_{-\infty}^{x} dz\, K(x,z)\Omega(z,y) + \eta(x-y)K(x,y) + \int_{-\infty}^{y} d\zeta\, K(y,\zeta)\Omega(\zeta,x) + \eta(y-x)K(y,x) + \int_{-\infty}^{x} dz \int_{-\infty}^{y} d\zeta\, K(x,z)K(y,\zeta)\Omega(z,\zeta) + \int_{-\infty}^{x} dz \int_{-\infty}^{y} dK(x,z)K(y,\zeta)\delta(z-\zeta) , \tag{A27}$$

where

$$\eta(u) = \begin{cases} 1, & u \geq 0 \\ 0, & u < 0 \end{cases} \tag{A28}$$

is the Heaviside step function. The last integral in Eq. (A27) is easily seen to equal

$$\eta(x-y)\int_{-\infty}^{y} d\xi\, K(x,\xi)K(y,\xi)+\eta(y-x)\int_{-\infty}^{x} dz\, K(x,z)K(y,z). \tag{A29}$$

Now, using the symmetry of Ω, i.e.,

$$\Omega(u,v)=\Omega(v,u)$$

we can write

$$\Omega(u,v)=\eta(u-v)\Omega(u,v)+\eta(v-u)\Omega(v,u). \tag{A30}$$

We substitute Eq. (A30) in Eq. (A27) wherever Ω appears and replace the last integral by its expression in Eq. (A29). In the resulting equation we use the Gelfand-Levitan equation repeatedly to eliminate Ω and obtain without difficulty

$$\begin{aligned}\sum_n \frac{\chi_n(x)\chi_n(y)}{\hat{C}_n} &= \delta(x-y)-\eta(x-y)K(x,y)-\eta(y-x)K(y,x)+\eta(x-y)K(x,y)+\eta(y-x)K(y,x)\\ &\quad -\eta(x-y)\int_{-\infty}^{y} d\xi\, K(y,\xi)K(x,\xi)-\eta(y-x)\int_{-\infty}^{x} dz\, K(x,z)K(y,z)\\ &\quad +\eta(x-y)\int_{-\infty}^{y} d\xi\, K(y,\xi)K(x,\xi)+\eta(y-x)\int_{-\infty}^{x} dz\, K(x,z)K(y,z)\\ &=\delta(x-y).\end{aligned} \tag{A31}$$

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