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FAST TRACK COMMUNICATION

On a class of integral equations having application in quantum dynamics

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Abstract
A class of Fredholm integral equations of the second kind is studied, with kernel separable outside the basic interval (a, b). Using theorems of matrix algebra, the solution for x outside (a, b) is found in terms of the Fredholm determinants in a simple and compact form. As a particular case, the quantum propagator for one-dimensional problems is obtained.

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The use of integral equations is ubiquitous in physics [1]. Fixing non-local properties of the unknown functions, they allow the study of a large variety of phenomena. In most possible cases an integral equation reduces to a differential equation with a boundary problem; therefore, boundary conditions are automatically taken into account. In particular, the Fredholm integral equation of the second kind

$$\psi(x) + \lambda \int_a^b \mathrm{d}\xi\, K(x, \xi)\psi(\xi) = \phi(x) \tag{1}$$

is often encountered, and in many problems the solution is required when x lies outside the basic interval (a, b). This is the typical case of scattering, when the details of the wavefunction inside the potential are not needed, but we are mainly interested in the behaviour at large distances. In general, the properties of the kernel K inside (a, b) are different from the outside ones; in particular, outside, it is separable (unfortunately, only in the one-dimensional case, see, e.g., [2]).

We will show that, if the kernel K is separable outside (a, b) (but not inside), it is possible to obtain this solution in a simple form by finding formally ψ inside (a, b) and introducing it into equation (1). Obviously, if K is everywhere separable, this equation is of the Pincherle–Goursat type and the solution is well known [3].

By discretizing in the basic interval (a, b) [3], equation (1) takes the form (being understood that $N \to \infty$)

$$\psi_j + \lambda \sum_{i=1}^{N} K_{ji} \psi_i \, \mathrm{d}x = \phi_j \tag{2}$$

where $\psi_i = \psi(x_i), \phi_i = \phi(x_i), K_{ji} = K(x_j, x_i), \mathrm{d}x = (b - a)/N$. Therefore, the solution is, for $x \in (a, b)$,

$$\vec{\psi} = \mathbf{A}^{-1} \vec{\phi} \tag{3}$$

with $\vec{\psi}$ and $\vec{\phi}$ being two column vectors with components ψ_i, ϕ_i, and

$$\mathbf{A}_{ij} = \delta_{ij} + K_{ij} \, \mathrm{d}\lambda, \qquad \mathrm{d}\lambda = \lambda \, \mathrm{d}x. \tag{4}$$

When the kernel K is separable outside (a, b), namely

$$K(x, \xi) = H(x) F(\xi), \qquad x \notin (a, b), \tag{5}$$

equation (1) reads

$$\psi(x) + H(x) \sum_{i=1}^{N} F_i \psi_i \, \mathrm{d}\lambda = \phi(x), \tag{6}$$

and, by introducing the column vector $\vec{v}$ with components $F_i \mathrm{d}\lambda$,

$$\psi(x) = \phi(x) - H(x)(\vec{v}^T \cdot \vec{\psi}) = \phi(x) - H(x)(\vec{v}^T \mathbf{A}^{-1} \vec{\phi}) \tag{7}$$

where T denoting transpose vector or matrix. It is easy to recognize that the quantity $\vec{v}^T \mathbf{A}^{-1} \vec{\phi}$ can be written in the form

$$\vec{v}^T \mathbf{A}^{-1} \vec{\phi} = \mathrm{Tr}(\mathbf{A}^{-1} \mathbf{V}) \tag{8}$$

where $\mathbf{V}$ is given by

$$\mathbf{V} = \vec{\phi} \vec{v}^T = \begin{pmatrix} \mathrm{d}\lambda \phi_1 F_1 & \mathrm{d}\lambda \phi_1 F_2 & \dots & \mathrm{d}\lambda \phi_1 F_N \\ \mathrm{d}\lambda \phi_2 F_1 & \mathrm{d}\lambda \phi_2 F_2 & \dots & \mathrm{d}\lambda \phi_2 F_N \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{d}\lambda \phi_N F_1 & \mathrm{d}\lambda \phi_N F_2 & \dots & \mathrm{d}\lambda \phi_N F_N \end{pmatrix}, \tag{9}$$

and we are led to

$$\begin{aligned} &\psi(x) = \phi(x)[1 - g(x)\mathrm{Tr}(\mathbf{A}^{-1}\mathbf{V})] = \phi(x)[1 - \mathrm{Tr}(\mathbf{A}^{-1}\mathbf{W})], \\ &g(x) = \frac{H(x)}{\phi(x)}, \qquad \mathbf{W} = g(x)\mathbf{V}. \end{aligned} \tag{10}$$

Up to this point, it can seem that no good result has been obtained since, as for the solution inside (a, b), the inverse of the matrix $\mathbf{A}$ is needed. A great simplification arises, however, when observing that the matrix $\mathbf{W}$ is of rank 1. This can be seen in the following way: $\mathbf{W}$ is given (see equation (9)) by the product of two $(N \times 1)$ and $(1 \times N)$ matrices, both obviously of rank 1, and therefore their product also has this rank [4]. Now, denoting by $|\mathbf{M}|$ the determinant of the square matrix $\mathbf{M}$, the following theorem holds.

If $\mathbf{A}$ is a non-singular matrix and $\mathbf{W}$ is a matrix of rank 1, then

$$\mathrm{Tr}(\mathbf{A}^{-1}\mathbf{W}) = 1 - \frac{|\mathbf{A} - \mathbf{W}|}{|\mathbf{A}|}. \tag{11}$$

The proof is easy: suffice it to write

$$|\mathbf{A} - \mathbf{W}| = |\mathbf{A}||\mathbf{I} - \mathbf{A}^{-1}\mathbf{W}|, \tag{12}$$

and expanding the last factor by diagonal minors [5], one has

$$|\mathbf{I}-\mathbf{A}^{-1}\mathbf{W}| = 1-\mathrm{Tr}(\mathbf{A}^{-1}\mathbf{W}). \tag{13}$$

Therefore equation (10) takes the simple form

$$\psi(x) = \phi(x)\frac{|\mathbf{A}-\mathbf{W}|}{|\mathbf{A}|}. \tag{14}$$

It is useful to write $\mathbf{W}$ as

$$\mathbf{W} = \alpha(x)\mathbf{U} \tag{15}$$

where $\alpha(x)$ is an adimensional function, in general different from $g(x)$. So,

$$\psi(x) = \phi(x)[1-\alpha(x)\mathrm{Tr}(\mathbf{A}^{-1}\mathbf{U})] = \phi(x)\left[1-\alpha(x)\left(1-\frac{|\mathbf{A}-\mathbf{U}|}{|\mathbf{A}|}\right)\right]. \tag{16}$$

It can be recognized at once that $|\mathbf{A}|$ is the Fredholm determinant $\Delta(\lambda)$ of the integral equation (1). On the other hand, also $\Gamma(\lambda) = |\mathbf{A}-\mathbf{U}|$ is an analogous infinite determinant (be aware that Δ depends only on the kernel, but Γ depends also on the known function ϕ) that can be calculated in a similar way. Infinite determinants of this kind are well known in the literature, and convergent expansions in power series of λ can be obtained [3, 6, 7]. In comparison with the one inside the basic interval, the simplicity of this solution is clearly greater; in order to underline this point, we will explicitly show the formal solution inside the basic interval. Rewriting equation (3), by cofactors $\mathbf{A}^{(ji)}$, as

$$\psi_j = \frac{1}{|\mathbf{A}|}\sum_{i=1}^{N}\mathbf{A}^{(ji)}\phi_i, \tag{17}$$

the limit $N\to\infty$ gives, as shown in [8],

$$\psi(x) = \phi(x) - \frac{1}{\Delta(\lambda)}\int_a^b \mathrm{d}\xi\,\Delta(x,\xi;\lambda)\phi(\xi), \qquad x\in(a,b) \tag{18}$$

where $\Delta(x,\xi;\lambda)$ is a function similar to $\Delta(\lambda)$, although more complicated. The great difference between equation (16) and equation (18) is evident.

This result can be applied to scattering integral equation for a particle with mass m subject to a non-singular potential $V(x)$, different from zero when $x\in(a,b)$. Starting from the Schrödinger equation in integral form and taking as unperturbed Hamiltonian the free one, we are led to the equation for the propagator $G(x,t;\eta)$ [9, 10], where η and x are initial and final positions, respectively; after a Laplace transform, the following equation is obtained (for details, see [11]):

$$\psi(x) + \lambda\int_a^b \mathrm{d}\xi\,\mathrm{e}^{-k|x-\xi|}V(\xi)\psi(\xi) = \phi(x) \tag{19}$$

where $\psi(x)$ is the Laplace transform of the propagator (sometimes called the 'energy propagator' or 'Green function'), and

$$\phi(x) = \frac{c}{2}\frac{\mathrm{e}^{-c|x-\eta|\sqrt{s}}}{\sqrt{s}}, \qquad c=\sqrt{\frac{2m}{\hbar}}, \qquad \lambda = \frac{c}{2\hbar}\frac{1}{\sqrt{s}}, \qquad k = c\sqrt{s}. \tag{20}$$

The kernel outside the main interval has the form

$$K(x,\xi) = \begin{cases}\mathrm{e}^{k(x-\xi)}V(\xi) & \text{for } x<a\\ \mathrm{e}^{-k(x-\xi)}V(\xi) & \text{for } x>b.\end{cases} \tag{21}$$

The quantities s, conjugate to time t by Laplace transform (the energy), and η (the initial position $<a$) play the role of parameters and are omitted in ψ.

In the transmission case ($x > b$), one has

$$\phi(x) = \frac{c}{2}\frac{\mathrm{e}^{-c(x-\eta)\sqrt{s}}}{\sqrt{s}}, \qquad \phi_i = \frac{c}{2}\frac{\mathrm{e}^{-c(x_i-\eta)\sqrt{s}}}{\sqrt{s}}, \qquad H(x) = \mathrm{e}^{-kx}, \qquad F_i = \mathrm{e}^{kx_i} V_i \tag{22}$$

so that $\alpha(x) = 1$, and

$$\mathbf{A} = \begin{pmatrix} 1 + \mathrm{d}\lambda_1 & \mathrm{d}\lambda_2\,\mathrm{e}^{-kx_{12}} & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{-kx_{1N}} \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-kx_{12}} & 1 + \mathrm{d}\lambda_2 & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{-kx_{2N}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-kx_{1N}} & d\lambda_2\,\mathrm{e}^{-kx_{2N}} & \dots & 1 + \mathrm{d}\lambda_N \end{pmatrix},$$
$$\mathbf{U}^t = \begin{pmatrix} \mathrm{d}\lambda_1 & \mathrm{d}\lambda_2\,\mathrm{e}^{kx_{12}} & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{kx_{1N}} \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-kx_{12}} & \mathrm{d}\lambda_2 & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{kx_{2N}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-kx_{1N}} & \mathrm{d}\lambda_2\,\mathrm{e}^{-kx_{2N}} & \dots & \mathrm{d}\lambda_N \end{pmatrix}, \tag{23}$$

where $x_{ij} = |x_i - x_j|$, $\mathrm{d}\lambda_i = V_i\,\mathrm{d}\lambda$. Therefore, $|\mathbf{A} - \mathbf{U}^t| = \Gamma^t(\lambda) = 1$ and

$$\psi(x) = \frac{\phi(x)}{\Delta(\lambda)}. \tag{24}$$

The reflection case ($x < a$) is more complicated; now

$$\phi(x) = \frac{c}{2}\frac{\mathrm{e}^{-c|x-\eta|\sqrt{s}}}{\sqrt{s}}, \qquad \phi_i = \frac{c}{2}\frac{\mathrm{e}^{-c(x_i-\eta)\sqrt{s}}}{\sqrt{s}}, \qquad H(x) = \mathrm{e}^{kx}, \qquad F_i = \mathrm{e}^{-kx_i} V_i \tag{25}$$

and it turns out that

$$\alpha(x) = \frac{c}{2}\frac{1}{\phi(x)}\frac{\mathrm{e}^{k(x+\eta)}}{\sqrt{s}}, \qquad \mathbf{U}^r = \begin{pmatrix} \mathrm{d}\lambda_1\,\mathrm{e}^{-2kx_1} & \mathrm{d}\lambda_2\,\mathrm{e}^{-kx_{12}^+} & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{-kx_{1N}^+} \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-kx_{12}^+} & \mathrm{d}\lambda_2\,\mathrm{e}^{-2kx_2} & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{-kx_{2N}^+} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{d}\lambda_1\,\mathrm{e}^{-kx_{1N}^+} & \mathrm{d}\lambda_2\,\mathrm{e}^{-kx_{2N}^+} & \dots & \mathrm{d}\lambda_N\,\mathrm{e}^{-2kx_N} \end{pmatrix}, \tag{26}$$

where $x_{ij}^+ = x_i + x_j$, leading to the result

$$\psi(x) = \phi(x) - \frac{c}{2}\frac{\mathrm{e}^{c(x+\eta)\sqrt{s}}}{\sqrt{s}}\left[1 - \frac{\Gamma^r(\lambda)}{\Delta(\lambda)}\right]. \tag{27}$$

The effective calculation of the determinants Δ and Γ is, in general, a difficult task. Let us consider the transmission (equation (24)), where only Δ is required; by following, for example, [6], it is easy to show that, for the kernel $K(x,\xi) = \mathrm{e}^{-k|x-\xi|}V(\xi)$, one has

$$\Delta(\lambda) = 1 + \sum_{n=1}^{\infty}\frac{\lambda^n}{n!}D_n, \tag{28}$$

$$D_n = \int_0^a \mathrm{d}x_n \cdots \int_0^a \mathrm{d}x_2 \int_0^a \mathrm{d}x_1 \begin{vmatrix} 1 & \mathrm{e}^{-kx_{12}} & \dots & \mathrm{e}^{-kx_{1n}} \\ \mathrm{e}^{-kx_{12}} & 1 & \dots & \mathrm{e}^{-kx_{2n}} \\ \vdots & \vdots & \ddots & \vdots \\ \mathrm{e}^{-kx_{1n}} & \mathrm{e}^{-kx_{2n}} & \dots & 1 \end{vmatrix} V(x_1)V(x_2)\cdots V(x_n), \tag{29}$$

giving a series expansion that can be useful for approximate calculations. We like to point out another method of calculating Δ; among various interesting analytical properties, it obeys the differential equation [6]

$$\frac{\Delta'(\lambda)}{\Delta(\lambda)} = \sum_{n=0}^{\infty} (-1)^n A_{n+1} \lambda^n \tag{30}$$

where A_n are the so-called traces of iterated kernels:

$$A_n = \int_0^a \mathrm{d}x \int_0^a \mathrm{d}x_{n-1} \cdots \int_0^a \mathrm{d}x_2 \int_0^a \mathrm{d}x_1 K(x, x_{n-1}) K(x_{n-1}, x_{n-2}) \cdots K(x_2, x_1) K(x_1, x). \tag{31}$$

This alternative expression for Δ follows

$$\Delta(\lambda) = \mathrm{e}^{-F(\lambda)}, \qquad F(\lambda) = \sum_{n=1}^{\infty} (-1)^n A_n \frac{\lambda^n}{n}. \tag{32}$$

As a simple example, by considering a delta potential

$$V(x) = V\delta(x - y), \qquad 0 < y < a, \tag{33}$$

$A_n = V^n$ is easily obtained, so that

$$F(\lambda) = \sum_{n=1}^{\infty} (-1)^n V^n \frac{\lambda^n}{n} = -\ln(1 + \lambda V). \tag{34}$$

It follows $\Delta(\lambda) = 1 + \lambda V$, and equation (24) gives the well-known formula for the Laplace transform of the delta potential propagator [12, 13].

These considerations can be extended by observing that a separable kernel has the general form

$$K(x, \xi) = \sum_{l=1}^{M} H^{(l)}(x) F^{(l)}(\xi) \qquad \text{or} \qquad K(x, x_i) = \sum_{l=1}^{M} H^{(l)}(x) F_i^{(l)} \tag{35}$$

and equation (16) becomes, with obvious extension of definitions,

$$\psi(x) = \phi(x) \left[1 - \sum_{l=1}^{M} \alpha_l(x) \left(1 - \frac{|\mathbf{A} - \mathbf{U}^{(l)}|}{|\mathbf{A}|} \right) \right]. \tag{36}$$

The most general kernel behaving as shown in equation (35) outside (a, b), but not inside, seems to be

$$K(x, \xi) = \sum_{l=1}^{M} h^{(l)}(x) f^{(l)}(\xi) \exp(-k_l |x^{\beta_l} - \xi^{\beta_l}|) \tag{37}$$

with $\beta_l > 0 \,\forall\, l, x > 0$, and

$$H^{(l)}(x) = h^{(l)}(x) \exp(\pm k_l x^{\beta_l}), \qquad F^{(l)}(\xi) = f^{(l)}(\xi) \exp(\mp k_l \xi^{\beta_l}), \tag{38}$$

where the upper sign holds when $x < a$ and the lower holds when $x > b$. The case of scattering, given by equation (19), is recovered when $l = 1, h = \text{const}, \beta_l = 1$.

This equation represents a class of kernels that is larger than one could expect. For example, by considering an arbitrary, regular function of $|x - \xi|$: $K = K(|x - \xi|)$, this can be expanded with arbitrary precision in (a, b) through a truncated Fourier series, that is a particular case of equation (37).

To sum up, we have presented a method of obtaining the solution of a class of integral equations, outside the basic interval. The result has a simple form and is expressed by means of the Fredholm determinant Δ and its companion Γ in a direct way, without performing any operation of integration or derivation on them. As an immediate application, the energy propagator for unidimensional problems is found.

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