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Solution of $\partial_t\phi = [\partial^2_\Omega - V(\Omega)]\phi$ in an arbitrary interval by the method of primitive propagators

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Abstract. A method of solving the initial value problem $\partial_t\phi = [\partial^2_\Omega - V(\Omega)]\phi$ in an arbitrary interval is presented, given auxiliary boundary conditions which induce a unique solution. Although the Green propagator for the problem may be impossible to find directly, progress is made by finding the propagator for the same evolution equation in a different interval and with simpler boundary conditions. This primitive propagator propagates the Green propagator for the actual problem forward from its initial value. The initial value is chosen outside the interval so as to satisfy the actual boundary conditions. Examples are presented.

1. The equations and their solution

We consider the evolution equation

$$\frac{\partial\phi}{\partial\tau} = \left(\frac{\partial^2}{\partial\Omega^2} - V(\Omega)\right)\phi(\Omega, \tau) \tag{1}$$

with the 'potential' $V(\Omega)$ given by

$$V(\Omega) = \frac{1}{\rho}\frac{d^2\rho}{d\Omega^2} \tag{2}$$

and $\rho(\Omega)$ real. Our aim is to solve (1) as an initial value problem in the interval [0, 1], with homogeneous boundary conditions at either end of the interval:

$$\frac{\partial}{\partial\Omega}\rho^{-1}\phi(\Omega, \tau) = 0 \qquad \forall\tau > 0 \text{ at } \Omega = 0, 1. \tag{3}$$

Generalisation to any other finite interval is achieved by rescaling and translating. On substituting for $V(\Omega)$ in (1) from (2), we have

$$\rho\frac{\partial\phi}{\partial\tau} = \frac{\partial}{\partial\Omega}\left(\rho\frac{\partial\phi}{\partial\Omega} - \phi\frac{d\rho}{d\Omega}\right) \tag{4}$$

$$= \frac{\partial}{\partial\Omega}\rho^2\frac{\partial}{\partial\Omega}(\rho^{-1}\phi) \tag{5}$$

so that, provided $\rho(\Omega)$ is sufficiently regular at $\Omega = 0, 1$, boundary conditions (3) imply the integral conservation condition

$$\frac{d}{d\tau}\int_0^1 d\Omega\, \rho(\Omega)\phi(\Omega, \tau) = 0. \tag{6}$$

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The initial value problem is tackled by constructing the Green propagator $G(\Omega, \bar{\Omega}; \tau)$, which solves the same problem with initial value

$$G(\Omega, \bar{\Omega}; 0) = \delta(\Omega - \bar{\Omega}) \qquad \Omega, \bar{\Omega} \in [0, 1]. \tag{7}$$

The solution of (1) is then given by

$$\phi(\Omega, \tau) = \int_0^1 \mathrm{d}\bar{\Omega}\, G(\Omega, \bar{\Omega}; \tau)\phi(\bar{\Omega}, 0). \tag{8}$$

The crucial step is to continue the propagator $G(\Omega, \bar{\Omega}; \tau)$ beyond the interval [0, 1] in Ω space. (The dummy variable $\bar{\Omega}$ is always taken within this interval, from (8).) The initial value $G(\Omega, \bar{\Omega}; 0)$, which is of delta function form within the interval, is chosen outside it so as to satisfy boundary conditions (3).

The first stage is to construct the primitive propagator $G_{\mathrm{p}}(\Omega, \bar{\Omega}; \tau)$, which has initial value $\delta(\Omega - \bar{\Omega})$ everywhere, not merely in [0, 1]. We assume that $V(\Omega)$ is sufficiently regular for the eigenfunctions Π_j of $[-\mathrm{d}^2/\mathrm{d}\Omega^2 + V(\Omega)]$ to be orthonormal and complete in $(-\infty, \infty)$:

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\Omega^2} + V(\Omega)\right)\Pi_j(\Omega) = \lambda_j \Pi_j(\Omega) \tag{9}$$

$$\int_{-\infty}^{\infty} \mathrm{d}\Omega\, \Pi_j^*(\Omega)\Pi_k(\Omega) = \delta_{jk}. \tag{10}$$

The primitive propagator is constructed from the eigenfunctions as

$$G_{\mathrm{p}}(\Omega, \bar{\Omega}; \tau) = \sum_j \Pi_j(\Omega)\Pi_j^*(\bar{\Omega}) \exp(-\lambda_j \tau). \tag{11}$$

If the eigenvalue spectrum includes a continuum, this must be included in (11). The eigenvalues λ_j are real and, moreover, non-negative; for on multiplying (9) by $\Pi_j(\Omega)$ and integrating by parts, we have

$$\int_{-\infty}^{\infty} \mathrm{d}\Omega \left| \rho \frac{\mathrm{d}}{\mathrm{d}\Omega}(\rho^{-1}\Pi_j) \right|^2 = \lambda_j \int_{-\infty}^{\infty} \mathrm{d}\Omega |\Pi_j(\Omega)|^2. \tag{12}$$

It has been assumed that $\rho(\Omega)$ is sufficiently regular for the integrated term to vanish. Finally, we know by inspection of (3) and (5) that the zeroth eigenfunction is

$$\Pi_0(\Omega) \propto \rho(\Omega) \tag{13}$$

with eigenvalue zero.

The primitive propagator is used to propagate the initial value of the true propagator forwards in time:

$$G(\Omega, \bar{\Omega}; \tau) = \int_{-\infty}^{\infty} \mathrm{d}y\, G_{\mathrm{p}}(\Omega, y; \tau)G(y, \bar{\Omega}; 0). \tag{14}$$

This superposition satisfies the evolution equation and the initial condition (7). $G(y, \bar{\Omega}; 0)$ is now chosen outside [0, 1] to make it satisfy the boundary conditions (3):

$$\frac{\partial}{\partial\Omega} \rho^{-1} G(\Omega, \bar{\Omega}; \tau) = 0 \qquad \forall \tau > 0 \text{ at } \Omega = 0, 1. \tag{15}$$

Define the quantities

$$K_{0,1}(y, \tau) = \frac{\partial}{\partial\Omega} \rho(\Omega)^{-1} G_{\mathrm{p}}(\Omega, y; \tau) \qquad \text{at } \Omega = 0, 1 \tag{16}$$

respectively, and

$$g(y,\bar\Omega) = G(y,\bar\Omega;0) - \delta(y-\bar\Omega). \tag{17}$$

It follows from (14)-(17) that

$$\int_{-\infty}^{\infty} \mathrm{d}y\, K_{0,1}(y,\tau) g(y,\bar\Omega) = -K_{0,1}(\bar\Omega,\tau). \tag{18}$$

From (7), $g(y,\bar\Omega)$ is zero in $0<y<1$, ruling out the naive solution $g(y,\bar\Omega) = -\delta(y-\bar\Omega)$. The integral transforms are to be solved for $g(y,\bar\Omega)$ at all values of y. Although there are two transforms (one for K_0, one for K_1), the problem is not automatically overdetermined; in fact we shall prove uniqueness of any solution found.

The solution of (9) for $G(y,\bar\Omega;0)$ is then substituted into (14) and the quadrature performed to give the propagator.

2. Symmetry and uniqueness

Let us take the Laplace transform with respect to time of the evolution equation, and define

$$\overset{+}{G}(\Omega,\bar\Omega;s) = \int_0^{\infty} \mathrm{d}\tau \exp(-s\tau) G(\Omega,\bar\Omega;\tau). \tag{19}$$

Then

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}\Omega^2} + V(\Omega) + s\right)\overset{+}{G}(\Omega,\bar\Omega;s) = \delta(\Omega-\bar\Omega) \qquad \Omega,\bar\Omega \in [0,1]. \tag{20}$$

On integrating the identity

$$\begin{aligned}\overset{+}{G}(y,\bar\Omega;s)&\left(-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + V(y) + s\right)\overset{+}{G}(y,\Omega;s) - \overset{+}{G}(y,\Omega;s)\left(-\frac{\mathrm{d}^2}{\mathrm{d}y^2} + V(y) + s\right)\overset{+}{G}(y,\bar\Omega;s)\\ &\equiv -\frac{\mathrm{d}}{\mathrm{d}y}\left(\rho(y)\overset{+}{G}(y,\bar\Omega;s)\frac{\mathrm{d}}{\mathrm{d}y}[\rho(y)^{-1}\overset{+}{G}(y,\Omega;s)]\right.\\ &\qquad \left.-\rho(y)\overset{+}{G}(y,\Omega;s)\frac{\mathrm{d}}{\mathrm{d}y}[\rho(y)^{-1}\overset{+}{G}(y,\bar\Omega;s)]\right)\end{aligned} \tag{21}$$

over y from 0 to 1, the LHS simplifies using (20) to

$$\overset{+}{G}(\Omega,\bar\Omega;s) - \overset{+}{G}(\bar\Omega,\Omega;s) \tag{22}$$

while the RHS vanishes as a consequence of boundary conditions (15). This confirms the symmetry of $\overset{+}{G}$ and hence of G in Ω and $\bar\Omega$. A similar argument applied to two proposed distinct solutions $\overset{+}{G}_1(y,\bar\Omega;s)$ and $\overset{+}{G}_2(y,\bar\Omega;s)$ causes their difference to vanish, confirming uniqueness.

3. Generalisations

The method of solution set out above remains useful when the evolution equation is supplemented by different constraints from the boundary conditions (15). The primitive propagator is again used to propagate the initial value of the desired propagator forward in time. The initial value $G(y,\bar\Omega;0)$ is chosen by substituting (14) into the new constraints. Existence and uniqness should be investigated first in such cases.

4. Examples

To illustrate this procedure we consider first the simplest possible case: $\rho(\Omega)=1$, $V(\Omega)=0$, so that

$$\frac{\partial G}{\partial \tau}=\frac{\partial^2 G}{\partial \Omega^2}(\Omega, \bar{\Omega}; \tau) \tag{23}$$

with boundary conditions

$$\frac{\partial G}{\partial \Omega}(\Omega, \bar{\Omega}; \tau)=0 \qquad \forall \tau>0 \text{ at } \Omega=0, 1. \tag{24}$$

The sum over all modes giving the primitive propagator in this case is continuous and can be integrated explicitly:

$$G_{\mathrm{p}}(\Omega, \bar{\Omega}; \tau)=\frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k \exp(\mathrm{i}k\Omega)\exp(-\mathrm{i}k\bar{\Omega})\exp(-k^2\tau) \tag{25}$$

$$=(4\pi\tau)^{-1/2}\exp[-(\Omega-\bar{\Omega})^2/4\tau]. \tag{26}$$

The integral transforms (18) simplify to

$$\int_{-\infty}^{\infty} \mathrm{d}y\, y \exp[-y^2/4\tau] g(y, \bar{\Omega})=-\bar{\Omega}\exp[-\bar{\Omega}^2/4\tau] \tag{27}$$

$$\int_{-\infty}^{\infty} \mathrm{d}y(y-1)\exp[-(y-1)^2/4\tau] g(y, \bar{\Omega})=(1-\bar{\Omega})\exp[-(1-\bar{\Omega})^2/4\tau]. \tag{28}$$

In the first of these, define a new dummy variable of integration z by $y=-\sqrt{2z}$ in $y<0$ and $y=\sqrt{2z}$ in $y>0$, to give

$$\int_0^{\infty} \mathrm{d}z \exp(-z/2\tau)[-g(-\sqrt{2z}, \bar{\Omega})+g(\sqrt{2z}, \bar{\Omega})]=-\bar{\Omega}\exp[-\bar{\Omega}^2/4\tau]. \tag{29}$$

This is a Laplace transform with conjugate variables z and $(2\tau)^{-1}$. It is trivially inverted to give

$$-g(-\sqrt{2z}, \bar{\Omega})+g(\sqrt{2z}, \bar{\Omega})=-\bar{\Omega}\delta(z-\tfrac{1}{2}\bar{\Omega}^2) \qquad z\geqslant 0 \tag{30}$$

or, putting $z=\frac{1}{2}y^2$,

$$-g(-y, \bar{\Omega})+g(y, \bar{\Omega})=-\bar{\Omega}\delta(\tfrac{1}{2}y^2-\tfrac{1}{2}\bar{\Omega}^2) \qquad y\geqslant 0. \tag{31}$$

Similarly, by putting $(y-1)=-\sqrt{2z}$ in $y<1$ and $(y-1)=\sqrt{2z}$ in $y>1$, we find from (28) that

$$-g(1-y, \bar{\Omega})+g(1+y, \bar{\Omega})=(1-\bar{\Omega})\delta[\tfrac{1}{2}y^2-\tfrac{1}{2}(1-\bar{\Omega})^2] \qquad y\geqslant 0. \tag{32}$$

These two equations, taken with the condition that $g(y, \bar{\Omega})=0$ for $y\in[0, 1]$, are to be solved for g. Leaving aside the delta functions on the RHS, they state that $g(y, \bar{\Omega})$ is even about $y=0$ and $y=1$.

To find g, let y vary first between 0 and 1 in (31). There can be no contribution from the $g(y, \bar{\Omega})$ term on the LHS, so the delta function must arise from the $g(-y, \bar{\Omega})$ term. Thus, sending $y\to -y$,

$$g(y, \bar{\Omega})=\delta(y+\bar{\Omega}) \qquad -1<y<0. \tag{33}$$

Now vary y between 0 and 1 in (32). This gives, similarly,

$$g(y, \bar{\Omega}) = \delta(y - (2 - \bar{\Omega})) \qquad 1 < y < 2. \tag{34}$$

Next we vary y within $[1, 2]$ in (31) and (32). The information this yields, together with (33) and (34), allows us to find $g(y, \bar{\Omega})$ in $-2 < y < -1$ and $2 < y < 3$. The process is repeated to build up g outwards to $y = \pm\infty$. The result is

$$G(y, \bar{\Omega}; 0) = g(y, \bar{\Omega}) + \delta(y - \bar{\Omega}) = \sum_{n=-\infty}^{\infty} [\delta(y + 2n - \bar{\Omega}) + \delta(y + 2n + \bar{\Omega})]. \tag{35}$$

This is depicted in figure 1. On substitution into (14), the propagator emerges as

$$G(\Omega, \bar{\Omega}; \tau) = (4\pi\tau)^{-1/2} \sum_{n=-\infty}^{\infty} \{\exp[-(\Omega - \bar{\Omega} + 2n)^2/4\tau] + \exp[-(\Omega + \bar{\Omega} + 2n)^2/4\tau]\}. \tag{36}$$

The series is clearly convergent. Its terms satisfy the boundary conditions in pairs.

Our solution for $G(y, \bar{\Omega}; 0)$ might conceivably have been found by using the 'method of images' between two parallel mirrors (for a related example of its use in the diffusion equation, see [1]). This is inconceivable in more difficult problems; the next most easy model problem is for $\rho(\Omega) = a + b\Omega$, for which $V(\Omega)$ is still zero and the primitive propagator still (26). The equations which generalise (31) and (32) are

$$a\frac{\mathrm{d}}{\mathrm{d}y}[g(y, \bar{\Omega}) - g(-y, \bar{\Omega})] - b[g(y, \bar{\Omega}) + g(-y, \bar{\Omega})] = -a\bar{\Omega}\frac{\mathrm{d}}{\mathrm{d}y}\delta(\tfrac{1}{2}y^2 - \tfrac{1}{2}\bar{\Omega}^2) + b\bar{\Omega}\delta(\tfrac{1}{2}y^2 - \tfrac{1}{2}\bar{\Omega}^2) \qquad y > 0 \tag{37}$$

and

$$(a+b)\frac{\mathrm{d}}{\mathrm{d}y}[g(1+y, \bar{\Omega}) - g(1-y, \bar{\Omega})] - b[g(1+y, \bar{\Omega}) + g(1-y, \bar{\Omega})] = (a+b)(1-\bar{\Omega})\frac{\mathrm{d}}{\mathrm{d}y}\delta(\tfrac{1}{2}y^2 - \tfrac{1}{2}(1-\bar{\Omega})^2) + b(1-\bar{\Omega})\delta(\tfrac{1}{2}y^2 - \tfrac{1}{2}(1-\bar{\Omega})^2) \qquad y > 0. \tag{38}$$

Constants of integration are chosen by demanding the solution reduce, as $b \to 0$, to that of (31) and (32). We do not examine this problem further, since it is a limiting case of the next.

The propagator has also been found for constant potential, trivially scaled to $V(\Omega) = 1$. From (2), $\rho(\Omega)$ is a linear combination of $\exp(\pm\Omega)$. Although the primitive propagator is only $\exp(-\tau)$ times its value in the problem above (expression (26)), and the integral transforms are again Laplace's, the ρ-dependent boundary conditions

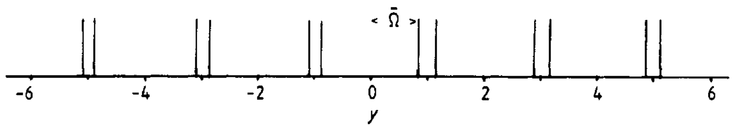

Figure 1. $G(y, \bar{\Omega}; 0)$.

render the problem extremely complicated. The initial value $G(y, \bar{\Omega}; 0)$ is a mixture of delta functions, step functions, polynomials and exponentials and even to quote the propagator $G(\Omega, \bar{\Omega}; \tau)$ (let alone the working) takes several pages. The analysis is given in [2, 3], and the result summarised in [3], equations (145)-(151). Simplification of this takes place when $\rho(\Omega) = \exp(\Omega)$ or $\exp(-\Omega)$, rather than a general linear combination. For $\exp(-\Omega)$, the result is [2, 3]

$$\begin{aligned} G(\Omega, \bar{\Omega}; \tau) &= (4\pi\tau)^{-1/2} \exp(-\tau) \sum_{m=-\infty}^{\infty} \exp[-(\Omega+\bar{\Omega}-2m)^2/4\tau] \\ &\quad + (4\pi\tau)^{-1/2} \exp(-\tau) \sum_{m=-\infty}^{\infty} \exp[-(\Omega-\bar{\Omega}-2m)^2/4\tau] \\ &\quad - \sum_{m=1}^{\infty} \exp(2m-\Omega-\bar{\Omega}) \operatorname{erfc}\left(\frac{2m-\Omega-\bar{\Omega}+2\tau}{(4\tau)^{1/2}}\right) \\ &\quad + \sum_{m=1}^{\infty} \exp(-2(m-1)-\Omega-\bar{\Omega}) \operatorname{erfc}\left(\frac{2(m-1)+\Omega+\bar{\Omega}-2\tau}{(4\tau)^{1/2}}\right). \end{aligned} \tag{39}$$

The first two summations correspond to delta functions and the last two to step functions in the initial value $g(\Omega, \bar{\Omega}; 0)$. The problem $V(\Omega) = 0$, $\rho = a + b\Omega$, is retrieved by restoring the constant potential V_0 on dimensional grounds and then shrinking it to zero.

References [2-4] set the problem in the physical context of electron distribution thermalisation by means of contact with a heat bath.

5. Alternative forms of the solution

The boundary conditions (15) ensure self-adjointness of the problem, so that there should exist a complete orthogonal set of eigenfunctions in [0, 1]. Once this eigenproblem is solved, the propagator can be constructed from its solutions in the usual way. The values of the eigenvalue parameter λ are not necessarily equal to the eigenvalues of the primitive problem. The resulting form of the solution is most useful at large times, in contrast with the expression found by the method above.

For the problem $\rho(\Omega) = 1$, normalised eigenfunctions are 1, $\sqrt{2}\cos(n\pi\Omega)$ and the eigenvalue spectrum is discrete. (This is in contrast with the continuum found in $(-\infty, \infty)$ for the primitive problem.) The propagator is therefore

$$G(\Omega, \bar{\Omega}; \tau) = 1 + 2 \sum_{n=1}^{\infty} \cos(n\pi\Omega) \cos(n\pi\bar{\Omega}) \exp(-n^2\pi^2\tau). \tag{40}$$

This series is convergent, reduces to $\delta(\Omega - \bar{\Omega})$ in [0, 1] for $\tau = 0$, and by uniqueness must equal (36), at least within [0, 1]. It is characteristic of a Fourier expansion in an interval of width two, not one; extra eigenvalues are situated midway between those naively expected.

It is easy to confirm that (40) satisfies the requirement

$$G(\Omega, \bar{\Omega}; \infty) = C^{-1}\rho(\Omega)\rho(\bar{\Omega}) \qquad C = \int_0^1 \mathrm{d}\Omega' \rho(\Omega')^2. \tag{41}$$

This breaks down should the eigenproblem be sufficiently irregular. For example, if

$\rho(\Omega)$ has a zero at $\Omega = \omega$, $\omega \in [0, 1]$, (5) implies that the quantities

$$\int_0^\omega d\Omega\, \rho(\Omega)\phi(\Omega, \tau) \qquad \int_\omega^1 d\Omega\, \rho(\Omega)\phi(\Omega, \tau) \tag{42}$$

do not change with time. There is no reason why $\phi(\Omega, 0)$ should be such that they take the value corresponding to $\phi = \rho(\Omega)$. Both the eigenproblem and (41) then fail, although the image method still works.

The two forms (36) and (40) are also related by the following transformation. The Fourier coefficients for expansion of a delta function in an interval of width β all equal β^{-1}. Since the expansion is periodic it must represent a sequence of delta functions, so that

$$\sum_{m=-\infty}^{\infty} \delta(z - m\beta) \equiv \beta^{-1} \sum_{m=-\infty}^{\infty} \exp(2\pi i m z/\beta) \qquad \forall \text{ real } z;\ \beta > 0. \tag{43}$$

On multiplying this by a function $F(z)$ and integrating, the LHS becomes a sum of equally spaced samples of F, and the RHS of $\tilde{F}$, its Fourier transform, with inverse spacing. With appropriate choice of $\tilde{F}$, this transformation (the Poisson summation formula) relates the two forms of the propagator in the present example; in fact it proves them equal everywhere, not just in $[0, 1]$. It also relates the two forms of the propagator for the model problem $V(\Omega) = 1$ [4].

6. Conclusion

The method of solution presented, and its generalisations, significantly widen the classes of linear problems which can be tackled. Although no claim for rigour has been made, any prospective solution can always be tested by direct *a posteriori* substitution into the governing equations.

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