Wave Equations with the Exponential of a Quadratic as a Solution

Stephen Brooks

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1 Motivation

Numerical simulations are typically done with points (macroparticles or grid meshes), or infinite plane waves (Fourier space) as a basis. However, for some applications involving wave equations, something in between is needed, which is infinite in neither frequency space nor real space. This motivates the use of wavelets or wavepackets. In this note, a simple wavepacket that can be displaced in both frequency and position space (while being localised in both) is described. By letting the parameters of the wavepacket vary in time, it is already an exact solution of many non-interacting wave equations.

2 Wavepackets in Wave Equations

In one dimension (x), consider functions of the form e^{ax^2+bx+c}, where a, b, c may be complex. Typically $\mathrm{Re}\, a \geq 0$ so the function does not tend to infinity. The centre of the wavepacket is at $x = -\mathrm{Re}\, b/(2\mathrm{Re}\, a)$. The spatial frequency $k = (2\mathrm{Im}\, a)x + \mathrm{Im}\, b$, where a can be chosen to be real if no chirp is required. The overall constant multiplier of e^c may be used for normalisation purposes.

If the parameters vary as a function of time, functions of the following form are obtained:

$$f(x,t) = e^{a(t)x^2+b(t)x+c(t)}.$$

Using prime for ∂_x and dot for ∂_t, derivatives of f have a fairly simple form:

$$\begin{aligned} \dot{f} &= (\dot{a}x^2 + \dot{b}x + \dot{c})f \\ f' &= (2ax+b)f \\ f'' &= (2a + (2ax+b)^2)f = (4a^2x^2 + 4abx + (2a+b^2))f. \end{aligned}$$

Consider differential equations of the general form below, which is first-order in time:

$$\dot{f} = Af'' + (B_1x + B_0)f' + (C_2x^2 + C_1x + C_0)f.$$

Substituting the above expressions for the derivatives and dividing throughout by f gives:

$$\dot{a}x^2 + \dot{b}x + \dot{c} = A(4a^2x^2 + 4abx + (2a+b^2)) + (B_1x + B_0)(2ax+b) + C_2x^2 + C_1x + C_0,$$

which must be true for all x, so coefficients of powers of x may be equated to give

$$\begin{aligned}\dot{a} &= 4Aa^2 + 2B_1 a + C_2 \\ \dot{b} &= 4Aab + B_1 b + 2B_0 a + C_1 \\ \dot{c} &= A(2a + b^2) + B_0 b + C_0.\end{aligned}$$

The equations above determine the time evolution of the parameters a, b, c for $f(x,t)$ to be a solution of the differential equation; they are mildly nonlinear but are easily integrated numerically on a computer. Simulating the evolution of three numbers takes much less computational effort than a whole mesh of numbers, so if the state is well approximated by the sum of a few wavepackets (the original equation was linear in f), then this is a good basis to use.

The above derivation also explains why certain length polynomials (such as $B_1 x + B_0$) were allowed as coefficients in the differential equation: if the highest order term of the derivative of f in question is below x^2, additional factors of x are allowed. The zero-order derivative allows a quadratic function to be multiplied by f, such as a quadratic potential used in quantum theory.

2.1 Example: Time-Dependent Schrödinger Equation in 1D

The wavefunction $\psi(x,t)$ of a single, non-relativistic quantum (scalar) particle in 1D satisfies the equation below:

$$i\hbar\dot{\psi} = \left(\frac{-\hbar^2}{2m}\partial_x^2 + V(x,t)\right)\psi,$$

which can be rearranged into the form

$$\dot{\psi} = \frac{i\hbar}{2m}\psi'' + \frac{-i}{\hbar}V\psi.$$

This is an example of the general form in the previous section if

$$A = \frac{i\hbar}{2m}, \qquad B_1 = B_0 = 0, \qquad C_2 x^2 + C_1 x + C_0 = \frac{-i}{\hbar}V.$$

Note that this is only an exact solution for potentials V that are quadratic in x. Behaviour in other potentials could be approximated by using small wavepackets and approximating V by its local second-order Taylor series. However, time-varying potentials are allowed, since having the C_n vary with time does not invalidate the derivation of $\dot{a}, \dot{b}, \dot{c}$.

The equation for the evolution of a is

$$\dot{a} = \frac{2i\hbar}{m}a^2 + \frac{-i}{\hbar}V_2,$$

where V_2 is the coefficient of x^2 in the potential.

2.2 Higher-order Generalisation

The wavepacket definition may be extended so that the exponent is a polynomial of order N, in which case the method for calculating the time derivatives of the coefficients is analogous. The expression for $f^{(n)}$ contains an nth order polynomial, so its coefficient in the differential equation can be an $(N-n)$th order polynomial.

2.3 Generalisation to Multiple Dimensions

In multiple dimensions, where $\mathbf{x}$ is a vector, wavepackets can be defined in the following way:

$$\exp\left(\sum_{i,j} a_{ij}x_i x_j + \sum_i b_i x_i + c\right) = e^{\mathbf{x}^T A\mathbf{x}+\mathbf{b}\cdot\mathbf{x}+c}.$$

Here $A = (a_{ij})$ is a matrix, which can be chosen to be symmetric, while $\mathbf{b} = (b_i)$ is a vector. Defining

$$f(\mathbf{x}, t) = e^{\mathbf{x}^T A(t)\mathbf{x}+\mathbf{b}(t)\cdot\mathbf{x}+c(t)}$$

gives analogous expressions for the partial derivatives of f:

$$\begin{aligned}
\dot{f} &= (\mathbf{x}^T\dot{A}\mathbf{x} + \dot{\mathbf{b}}\cdot\mathbf{x} + \dot{c})f \\
\partial_i f &= \left(2\sum_j a_{ij}x_j + b_i\right) f = (2\mathbf{a}_i\cdot\mathbf{x} + b_i)f \\
\partial_i\partial_j f &= \partial_i((2\mathbf{a}_j\cdot\mathbf{x} + b_j)f) \\
&= (2a_{ij} + (2\mathbf{a}_i\cdot\mathbf{x} + b_i)(2\mathbf{a}_j\cdot\mathbf{x} + b_j))f \\
&= (\mathbf{x}^T(4\mathbf{a}_i\mathbf{a}_j^T)\mathbf{x} + (2b_i\mathbf{a}_j + 2b_j\mathbf{a}_i)\cdot\mathbf{x} + (2a_{ij} + b_ib_j))f.
\end{aligned}$$

The general differential equation in 3D to the same order as the one used in 1D is:

$$\begin{aligned}
\dot{f} &= \sum_{i,j} p_{0,ij}\partial_i\partial_j f + \sum_i\left(\sum_j q_{1j,i}x_j + q_{0,i}\right)\partial_i f + \left(\sum_{i,j} r_{2ij}x_ix_j + \sum_i r_{1i}x_i + r_0\right) f \\
&= \nabla^T P_0\nabla f + \mathbf{x}^T Q_1\nabla f + \mathbf{q}_0\cdot\nabla f + \left(\mathbf{x}^T R_2\mathbf{x} + \mathbf{r}_1\cdot\mathbf{x} + r_0\right) f.
\end{aligned}$$

Equating terms of the same order in $\mathbf{x}$ (after dividing by f) gives:

$$\begin{aligned}
\dot{A} &= 4AP_0A + 2\,\mathrm{sym}(Q_1A) + R_2 \\
\dot{\mathbf{b}} &= 4AP_0\mathbf{b} + Q_1\mathbf{b} + 2A\mathbf{q}_0 + \mathbf{r}_1 \\
\dot{c} &= 2\,\mathrm{tr}(AP_0) + \mathbf{b}^TP_0\mathbf{b} + \mathbf{q}_0\cdot\mathbf{b} + r_0,
\end{aligned}$$

where $\mathrm{tr}(A) = \sum_i a_{ii}$ and $\mathrm{sym}(A) = \frac{1}{2}(A + A^T)$. The symmetrisation is used to keep the derivative of A symmetrical even though Q_1 may not be.

3 Operations on Wavepackets

3.1 Pointwise Operations

3.1.1 Addition

The sum of two wavepackets is in general not another wavepacket (with some exceptions below), so more complex functions must be represented by a sum

$$f(x) = \sum_n e^{a_nx^2+b_nx+c_n}.$$

A constant k can be represented as $e^{\ln k}$ where $\ln k$ is a suitable version of the complex natural logarithm, so setting $a = b = 0$, $c = \ln k$ gives a wavepacket that can be added to the sum.

3.1.2 Simplification of Sums

If two wavepackets have equal a and b, then they can be combined:

$$e^{ax^2+bx+c_1} + e^{ax^2+bx+c_2} = e^{ax^2+bx}\left(e^{c_1} + e^{c_2}\right) = e^{ax^2+bx+\ln(e^{c_1}+e^{c_2})}.$$

If $e^{c_1} + e^{c_2} = 0$ then the two wavepackets cancel.

3.1.3 Scalar Multiplication

$$ke^{ax^2+bx+c} = e^{ax^2+bx+(c+\ln k)}$$
$$-e^{ax^2+bx+c} = e^{ax^2+bx+(c+\pi i)}$$

3.1.4 Multiplication of Two Wavepackets

$$e^{a_1x^2+b_1x+c_1}e^{a_2x^2+b_2x+c_2} = e^{(a_1+a_2)x^2+(b_1+b_2)x+(c_1+c_2)}$$

3.1.5 Powers

For real integer k,

$$\left(e^{ax^2+bx+c}\right)^k = e^{kax^2+kbx+kc}.$$

3.1.6 Modulus and Phase

For real x,

$$\left|e^{ax^2+bx+c}\right| = e^{(\operatorname{Re} a)x^2+(\operatorname{Re} b)x+\operatorname{Re} c};$$
$$\arg e^{ax^2+bx+c} = (\operatorname{Im} a)x^2 + (\operatorname{Im} b)x + \operatorname{Im} c.$$

3.1.7 Complex Conjugate

For real x,

$$\overline{e^{ax^2+bx+c}} = e^{\bar{a}x^2+\bar{b}x+\bar{c}}.$$

3.1.8 Real and Imaginary Parts

For real x,

$$\operatorname{Re} e^{ax^2+bx+c} = e^{ax^2+bx+(c-\ln 2)} + e^{\bar{a}x^2+\bar{b}x+(\bar{c}-\ln 2)};$$
$$\operatorname{Im} e^{ax^2+bx+c} = e^{ax^2+bx+(c-\ln 2-\frac{\pi}{2}i)} + e^{\bar{a}x^2+\bar{b}x+(\bar{c}-\ln 2+\frac{\pi}{2}i)}.$$

3.2 Geometrical Operations

3.2.1 Centre

Every wavepacket with a finite integral has a single point where its modulus is a maximum. This is

$$\arg\max\left|e^{ax^2+bx+c}\right| = \arg\max e^{(\operatorname{Re} a)x^2+(\operatorname{Re} b)x+\operatorname{Re} c} = \arg\max((\operatorname{Re} a)x^2 + (\operatorname{Re} b)x + \operatorname{Re} c).$$

At the maximum, the derivative $2(\operatorname{Re} a)x + \operatorname{Re} b$ will be equal to zero, thus $x = \frac{-\operatorname{Re} b}{2\operatorname{Re} a}$.

In multiple dimensions we need to find $\arg\max(\mathbf{x}^T(\operatorname{Re} A)\mathbf{x}+(\operatorname{Re}\mathbf{b})\cdot\mathbf{x}+\operatorname{Re} c)$. Assuming that $A = A^T$, the vector gradient of this is $2(\operatorname{Re} A)\mathbf{x}+\operatorname{Re}\mathbf{b}$. This is zero when $\mathbf{x} = -\frac{1}{2}(\operatorname{Re} A)^{-1}\operatorname{Re}\mathbf{b}$.

3.2.2 Translation

3.2.3 Rotation

3.3 Integral Operations

3.3.1 Integral Over All Space

This can be computed by using the identity $\int_{-\infty}^{\infty} e^{-\pi x^2}\,\mathrm{d}x = 1$.

$$\begin{aligned}
\int_{-\infty}^{\infty} e^{ax^2+bx+c}\,\mathrm{d}x &= \int_{-\infty}^{\infty} e^{a\left(x^2+\frac{b}{a}x+\frac{c}{a}\right)}\,\mathrm{d}x \\
&= \int_{-\infty}^{\infty} e^{a\left(\left(x+\frac{b}{2a}\right)^2-\frac{b^2}{4a^2}+\frac{c}{a}\right)}\,\mathrm{d}x \\
&= e^{c-\frac{b^2}{4a}}\int_{-\infty}^{\infty} e^{a\left(x+\frac{b}{2a}\right)^2}\,\mathrm{d}x \\
&= e^{c-\frac{b^2}{4a}}\int_{-\infty}^{\infty} e^{ax^2}\,\mathrm{d}x \\
&= e^{c-\frac{b^2}{4a}}\sqrt{\frac{-\pi}{a}}\int_{-\infty}^{\infty} e^{-\pi x^2}\,\mathrm{d}x \\
&= e^{c-\frac{b^2}{4a}}\sqrt{\frac{-\pi}{a}}.
\end{aligned}$$

In the case of complex coefficients, the identity $\int_{-\infty}^{\infty} e^{ax^2}\,\mathrm{d}x = \sqrt{\frac{-\pi}{a}}$ holds as long as $\operatorname{Re} a < 0$. The shift of origin $\int_{-\infty}^{\infty} e^{a\left(x+\frac{b}{2a}\right)^2}\,\mathrm{d}x = \int_{-\infty}^{\infty} e^{ax^2}\,\mathrm{d}x$ is not intuitively true if b/a is not real. However, a contour integration argument shows the infinite line of integration can also be moved in the imaginary direction without affecting the integral so long as it does not cross a pole (there are no poles in $e^{Q(x)}$) and the integral remains convergent.

The case for multiple dimensions is analogous but slightly more complicated; three dimensions will be used here as an example. The basic identity works in multiple dimensions:

$$\int_{-\infty}^{\infty} e^{-\pi x^2}\,\mathrm{d}x = \int_{-\infty}^{\infty} e^{-\pi y^2}\,\mathrm{d}y = \int_{-\infty}^{\infty} e^{-\pi z^2}\,\mathrm{d}z = 1$$

$$\Rightarrow \quad \int_{-\infty}^{\infty} e^{-\pi x^2}\,\mathrm{d}x \int_{-\infty}^{\infty} e^{-\pi y^2}\,\mathrm{d}y \int_{-\infty}^{\infty} e^{-\pi z^2}\,\mathrm{d}z = 1$$

$$\Rightarrow \quad \int_{\mathbb{R}^3} e^{-\pi x^2} e^{-\pi y^2} e^{-\pi z^2}\,\mathrm{d}V = \int_{\mathbb{R}^3} e^{-\pi \mathbf{x}\cdot\mathbf{x}}\,\mathrm{d}V = 1.$$

$$\Rightarrow \quad \int_{\mathbb{R}^3} e^{-\mathbf{x}\cdot\mathbf{x}}\,\mathrm{d}V = \pi^{3/2},$$

where the final step is done by a scaling of $\sqrt{\pi}$ in each axis.

The matrix A in the exponent $\mathbf{x}^T A\mathbf{x}$ can be symmetric without loss of generality, thus $-A$ is also symmetric. Symmetric matrices always factorise as $-A = B^T B$. This means that

$$\int_{\mathbb{R}^3} e^{\mathbf{x}^T A\mathbf{x}}\,\mathrm{d}V = \int_{\mathbb{R}^3} e^{-\mathbf{x}^T B^T B\mathbf{x}}\,\mathrm{d}V = \int_{\mathbb{R}^3} e^{-(B\mathbf{x})^T B\mathbf{x}}\,\mathrm{d}V.$$

If A was real, then B is real and this is equal to

$$\frac{1}{\det B}\int_{\mathbb{R}^3} e^{-\mathbf{x}^T\mathbf{x}}\,\mathrm{d}V = \frac{\pi^{3/2}}{\sqrt{\det(-A)}} = \sqrt{\frac{\pi^3}{\det(-A)}} = \sqrt{\frac{(-\pi)^3}{\det A}},$$

where we have used $\det(-A) = \det B^T \det B = (\det B)^2$ and the fact that $\det(-A) = (-1)^3 \det A$ where 3 is the number of dimensions of space. The general version of this result incorporates the value $\sqrt{\frac{-\pi}{a}}$ for one dimension. Subtle point: both B and $-B$ work in the factorisation of $-A$, so we choose the one with positive determinant that will not invert the sign of the volume element and also ensures $\det B$ is the positive root $\sqrt{\det(-A)}$.

If A has complex entries, similar matrix factorisations are possible but it is not intuitively clear that arguments about scaling the volume element with the determinant work. However, it is probably correct to rely on the analytic continuation of the real result into the complex plane.

The final step to integrating the full exponent $\mathbf{x}^T A\mathbf{x} + \mathbf{b}\cdot\mathbf{x} + c$ is 'completing the square' in multiple dimensions. Assuming $A = A^T$, consider a displacement $\mathbf{d}$ to the quadratic term:

$$(\mathbf{x}+\mathbf{d})^T A(\mathbf{x}+\mathbf{d}) = \mathbf{x}^T A\mathbf{x} + 2\mathbf{d}^T A\mathbf{x} + \mathbf{d}^T A\mathbf{d}$$

and note that the linear term is reconstructed if $2\mathbf{d}^T A\mathbf{x} = \mathbf{b}^T\mathbf{x}$, which is true if $\mathbf{d} = \frac{1}{2}A^{-1}\mathbf{b}$. Now we have

$$\mathbf{x}^T A\mathbf{x} + \mathbf{b}\cdot\mathbf{x} + c = (\mathbf{x}+\mathbf{d})^T A(\mathbf{x}+\mathbf{d}) - \mathbf{d}^T A\mathbf{d} + c$$

and

$$\begin{aligned}
\int_{\mathbb{R}^3} e^{\mathbf{x}^T A\mathbf{x}+\mathbf{b}\cdot\mathbf{x}+c}\,\mathrm{d}V &= \int_{\mathbb{R}^3} e^{(\mathbf{x}+\mathbf{d})^T A(\mathbf{x}+\mathbf{d})-\mathbf{d}^T A\mathbf{d}+c}\,\mathrm{d}V \\
&= e^{c-\mathbf{d}^T A\mathbf{d}}\int_{\mathbb{R}^3} e^{(\mathbf{x}+\mathbf{d})^T A(\mathbf{x}+\mathbf{d})}\,\mathrm{d}V \\
&= e^{c-\frac{1}{4}\mathbf{b}^T A^{-1}\mathbf{b}}\int_{\mathbb{R}^3} e^{\mathbf{x}^T A\mathbf{x}}\,\mathrm{d}V \\
&= e^{c-\frac{1}{4}\mathbf{b}^T A^{-1}\mathbf{b}}\sqrt{\frac{(-\pi)^3}{\det A}}.
\end{aligned}$$

The complex shifts of the range of integration are allowed as before and note that this formula incorporates the one-dimensional result (if 3 is replaced by 1).

3.3.2 Inner Product

The standard inner product $\langle f, g \rangle$ between complex functions is the integral $\int \bar{f}g$ over the whole space. In one dimension,

$$\begin{aligned}\left\langle e^{a_1x^2+b_1x+c_1}, e^{a_2x^2+b_2x+c_2}\right\rangle &= \int_{-\infty}^{\infty} e^{(\bar{a}_1+a_2)x^2+(\bar{b}_1+b_2)x+(\bar{c}_1+c_2)}\,\mathrm{d}x \\ &= e^{\bar{c}_1+c_2-\frac{(\bar{b}_1+b_2)^2}{4(\bar{a}_1+a_2)}}\sqrt{\frac{-\pi}{\bar{a}_1+a_2}}.\end{aligned}$$

In multiple dimensions, the analogous substitutions are made into the multidimensional integral-over-all-space formula.

3.3.3 L_2 Norm

The 'Euclidean' or L_2 norm is defined via $||f|| = \sqrt{\langle f, f \rangle}$ so that

$$\begin{aligned}||e^{ax^2+bx+c}|| &= \sqrt{\int_{-\infty}^{\infty} e^{(\bar{a}+a)x^2+(\bar{b}+b)x+(\bar{c}+c)}\,\mathrm{d}x} \\ &= \sqrt{e^{2\mathrm{Re}\,c-\frac{(2\mathrm{Re}\,b)^2}{8\mathrm{Re}\,a}}\sqrt{\frac{-\pi}{2\mathrm{Re}\,a}}} \\ &= e^{\mathrm{Re}\,c-\frac{(\mathrm{Re}\,b)^2}{4\mathrm{Re}\,a}}\sqrt[4]{\frac{-\pi}{2\mathrm{Re}\,a}}.\end{aligned}$$

The fact that $\langle f, f \rangle = \int \bar{f}f = \int |f|^2$ means that $||f||^2$ corresponds to the integral of the probability density for quantum wavefunctions.

3.3.4 Fourier Transform

If the Fourier transform is defined by $\tilde{f}(\omega) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} f(x)e^{-i\omega x}\,\mathrm{d}x$, then the transform of a 1D wavepacket, making use of the integral formulae above, is:

$$\begin{aligned}\tilde{f}(\omega) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ax^2+bx+c}e^{-i\omega x}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{ax^2+(b-i\omega)x+c}\,\mathrm{d}x \\ &= \frac{1}{\sqrt{2\pi}}e^{c-\frac{(b-i\omega)^2}{4a}}\sqrt{\frac{-\pi}{a}} \\ &= e^{c-\frac{b^2-2ib\omega-\omega^2}{4a}}\sqrt{\frac{-1}{2a}} \\ &= e^{\frac{\omega^2}{4a}+\frac{ib}{2a}\omega+(c-\frac{b^2}{4a}-\frac{1}{2}\ln(-2a))}.\end{aligned}$$

This has the form of a wavepacket in ω with parameters

$$\tilde{a} = \frac{1}{4a}, \qquad \tilde{b} = \frac{ib}{2a}, \qquad \tilde{c} = c - \frac{b^2}{4a} - \frac{1}{2}\ln(-2a).$$

Applying these formulae twice gives $\tilde{\tilde{a}} = a$, $\tilde{\tilde{b}} = -b$ and $\tilde{\tilde{c}} = c$, consistent with the fact that the transform of the transform is $f(-x)$.

3.4 Splitting/Slicing

3.5 Merging

Although the sum of two (or more) wavepackets is usually not another wavepacket, it may sometimes be desired to merge them if a single wavepacket is a good enough approximation to the sum.