

Linear and Nonlinear Schrödinger Equations

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The Schrödinger equation for a point particle in a quartic potential and a non-linear Schrödinger equation are solved by the decomposition method yielding convergent series for the solutions which converge quite rapidly in physical problems involving bounded inputs and analytic functions. Several examples are given to demonstrate use of the method.

The Schrödinger equation

$$(-\hbar^2/2m) d^2\psi/dx^2 + (1/2) ax^4\psi = E_i\psi$$

describes a point particle in a quartic potential $V(x) = (1/2) ax^4$. If we let $\alpha = -ma/\hbar^2$ and $\beta = 2mE_i/\hbar^2$, the equation becomes

$$d^2\psi/dx^2 + \alpha x^4\psi + \beta\psi = 0$$

Assume the energy of each eigenstate has been determined as discussed in Ref. 1. Now, if $L = d^2/dx^2$, we can write

$$L\psi + \alpha x^4\psi + \beta\psi = 0$$

or

$$L\psi = -(\alpha x^4 + \beta)\psi$$

Denoting by Φ the solution of $L\psi = 0$, we have

$$\psi = \Phi - L^{-1}(\alpha x^4 + \beta)\psi$$

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so that, using the decomposition method⁽²⁾

$$\begin{aligned} \psi_0 &= \Phi \\ \psi_{n+1} &= -L^{-1}(\alpha x^4 + \beta) \psi_n \end{aligned}$$

for $n \geq 0$. Then $\psi = \sum_{n=0}^{\infty} \psi_n$ is the solution.

In three dimensions with $V(\bar{x}) = (1/2)\alpha |\bar{x}|^4 \psi$, writing $L_x = \partial^2/\partial x^2$, $L_y = \partial^2/\partial y^2$, $L_z = \partial^2/\partial z^2$, letting Φ_x , Φ_y , Φ_z denote the solutions of $L_x\psi = 0$, $L_y\psi = 0$, $L_z\psi = 0$, respectively, the decomposition procedure yields

$$[L_x + L_y + L_z]\psi + \alpha x^4\psi + \beta\psi = 0$$

Solving for the linear operator terms, we obtain

$$\begin{aligned} L_x\psi &= -L_y\psi - L_z\psi - \alpha x^4\psi - \beta\psi \\ L_y\psi &= -L_x\psi - L_z\psi - \alpha x^4\psi - \beta\psi \\ L_z\psi &= -L_x\psi - L_y\psi - \alpha x^4\psi - \beta\psi \end{aligned}$$

With the inversions, we have

$$\begin{aligned} L_x^{-1}L_x\psi &= -(L_x^{-1}L_y + L_x^{-1}L_z)\psi - L_x^{-1}\alpha x^4\psi - L_x^{-1}\beta\psi \\ L_y^{-1}L_y\psi &= -(L_y^{-1}L_x + L_y^{-1}L_z)\psi - L_y^{-1}\alpha x^4\psi - L_y^{-1}\beta\psi \\ L_z^{-1}L_z\psi &= -(L_z^{-1}L_x + L_z^{-1}L_y)\psi - L_z^{-1}\alpha x^4\psi - L_z^{-1}\beta\psi \end{aligned}$$

and so

$$\begin{aligned} \psi &= \Phi_x - (L_x^{-1}L_y + L_x^{-1}L_z)\psi - L_x^{-1}\alpha x^4\psi - L_x^{-1}\beta\psi \\ \psi &= \Phi_y - (L_y^{-1}L_x + L_y^{-1}L_z)\psi - L_y^{-1}\alpha x^4\psi - L_y^{-1}\beta\psi \\ \psi &= \Phi_z - (L_z^{-1}L_x + L_z^{-1}L_y)\psi - L_z^{-1}\alpha x^4\psi - L_z^{-1}\beta\psi \end{aligned}$$

The Φ_x , Φ_y , Φ_z are completely specified by initial/boundary conditions. Assuming these are all nonzero, any one of those equations can be used for obtaining the solution.⁽³⁾ Or, we can add the three equations and divide by three to get a single equation where $\psi_0 = (1/3)(\Phi_x + \Phi_y + \Phi_z)$:

$$\begin{aligned} \psi &= \psi_0 - (1/3)[L_x^{-1}L_y + L_x^{-1}L_z + L_y^{-1}L_x + L_y^{-1}L_z + L_z^{-1}L_x + L_z^{-1}L_y]\psi \\ &\quad - (1/3)[L_x^{-1} + L_y^{-1} + L_z^{-1}]\alpha x^4\psi - (1/3)[L_x^{-1} + L_y^{-1} + L_z^{-1}]\beta\psi \end{aligned}$$

If, for convenience in writing, we let

$$K = -(1/3)[L_x^{-1}L_y + L_x^{-1}L_z + L_y^{-1}L_x + L_y^{-1}L_z + L_z^{-1}L_x + L_z^{-1}L_y]$$

$$G = -(1/3)[L_x^{-1} + L_y^{-1} + L_z^{-1}]$$

we have

$$\psi = \psi_0 + K\psi + G\alpha x^4\psi + G\beta\psi$$

Letting $\psi = \sum_{n=0}^{\infty} \psi_n$, we have ψ_0 given and

$$\psi_{n+1} = K\psi_n + G(\alpha x^4 + \beta)\psi_n$$

for $n \geq 0$, yielding the components of ψ . The n -term expression $\varphi_n = \sum_{i=0}^{n-1} \psi_i$ forms a convergent expression for ψ which becomes $\psi = \sum_{n=0}^{\infty} \psi_n$ as $n \rightarrow \infty$.

It is generally much easier to consider the individual equations for ψ rather than their sum since if the boundary conditions fixing Φ_x , Φ_y , and Φ_z are general, i.e., when conditions for one independent variable depend on the other variables, the solutions for each equation are identical.⁽³⁾ We also note that if an initial term (Φ_x , Φ_y , or Φ_z) is zero, that particular equation cannot be used (and the sum of the equations also cannot be used).

Supposing, for example, we use the equation for which Φ_x can be determined from known conditions; then

$$\psi = \Phi_x - (L_x^{-1}L_y + L_x^{-1}L_z) \sum \psi_n - L_x^{-1}\alpha x^4 \sum \psi_n - L_x^{-1}\beta\psi$$

Then

$$\psi_0 = \Phi_x$$

$$\psi_{n+1} = -(L_x^{-1}L_y + L_x^{-1}L_z) \psi_n - L_x^{-1}\alpha x^4 \psi_n - L_x^{-1}\beta\psi_n$$

for $n \geq 0$ and $\varphi_n = \sum_{i=0}^{n-1} \psi_i$ is an n -term approximation converging to $\psi = \sum_{n=0}^{\infty} \psi_n$.

Consider the nonlinear Schrödinger equation

$$iu_t + 2u|u|^2 + u_{xx} = 0$$

which we write

$$iL_t u + Nu + L_x u = 0$$

where $L_t = \partial/\partial t$ and $L_x = \partial^2/\partial x^2$, $Nu = 2u|u|^2$. We can solve for either linear operator. Thus

$$L_t u = iNu + iL_x u \quad (1)$$

$$L_x u = -iL_t u - Nu \quad (2)$$

To solve these equations, we apply L_t^{-1} to (1) and L_x^{-1} to (2). Equation (1) becomes

$$u = u(x, 0) + iL_t^{-1}Nu + iL_t^{-1}L_x u \quad (3)$$

and (2) becomes

$$u = \alpha(t) + x\beta(t) - iL_x^{-1}L_t u - L_x^{-1}Nu \quad (4)$$

Solving (3) by decomposition, we obtain

$$u = u_0 + iL_t^{-1} \sum_{n=0}^{\infty} A_n - iL_t^{-1}L_x \sum_{n=0}^{\infty} u_n$$

where $u_0 = u(x, 0)$ and the A_n are the polynomials defined by Adomian.^(2,4) Now

$$\begin{aligned} u_1 &= iL_t^{-1}A_0 + iL_t^{-1}L_x u_0 \\ u_2 &= iL_t^{-1}A_1 + iL_t^{-1}L_x u_1 \\ &\vdots \\ u_{n+1} &= iL_t^{-1}A_n + iL_t^{-1}L_x u_n \end{aligned}$$

Then the solution is $u = \sum_{n=0}^{\infty} u_n$, and $\varphi_n = \sum_{i=0}^{n-1} u_i$ is an n -term approximation converging to u .

The solution to (4) is carried out the same way:

$$\begin{aligned} u_0 &= \alpha + \beta x \\ u_{n+1} &= -iL_x^{-1}L_t u_n - L_x^{-1}A_n \end{aligned}$$

for $n \geq 0$. The quantities α , β are fixed by the boundary conditions on x .

For example, α is fixed by a given condition at $x=0$. If a second condition was $u \rightarrow 0$ as $x \rightarrow \infty$, then $\beta=0$. Or, we could have conditions on u given at $x=0$ and $x=1$. The solution to either equation (called a partial solution) is the same and represents the solution of the original differential equation so long as $u(x, 0) = \gamma(x) \neq 0$ and $\alpha = \alpha(t)$, $\beta = \beta(t)$.^(3,4) Thus we can solve either to get the solution. Which we choose depends on the best

known conditions or which offers the least effort. In this case L_t^{-1} is a single integration while L_x^{-1} is a two-fold integration, so (3) is simpler.

Some specific examples with known solutions may serve to further demonstrate use of the decomposition method.

(1) $d^2u/dx^2 - kx^p u = g$ with $u(1) = u(-1) = 0$. Using the decomposition method, write $L = d^2/dx^2$ and $Lu = g + kx^p u$. Operating with L^{-1} , we have $L^{-1}Lu = L^{-1}g + L^{-1}kx^p u$. Then if, for convenience, we take g as a constant,

$$u = c_1 + c_2 x + gx^2/2 + L^{-1}kx^p u$$

Let $u = \sum_{n=0}^{\infty} u_n$ with $u_0 = c_1 + c_2 x + gx^2/2$. Then $u_{m+1} = L^{-1}kx^p u_m$ with $m \geq 0$. Thus $u = \sum_{m=0}^{\infty} (L^{-1}kx^p)^m u_0$ or $u = \sum_{m=0}^{\infty} (L^{-1}kx^p)^m c_1 + \sum_{m=0}^{\infty} (L^{-1}kx^p)^m c_2 x + \sum_{m=0}^{\infty} (L^{-1}kx^p)^m gx^2/2$, and finally $u = c_1 \xi(x) + c_2 \eta(x) + \zeta(x)$, where

$$\xi(x) = \sum_{m=0}^{\infty} k^m x^{mp+2m} / (mp+2m-1)(mp+2m)$$

$$\eta(x) = \sum_{m=0}^{\infty} k^m x^{mp+2m+1} / (mp+2m)(mp+2m+1)$$

$$\zeta(x) = \sum_{m=0}^{\infty} (1/2) g k^m x^{mp+2m+2} / (mp+2m+1)(mp+2m+2)$$

Since $u(1) = u(-1) = 0$, we have $c_1 \xi(1) + c_2 \eta(1) + \zeta(1) = 0$ and $c_1 \xi(-1) + c_2 \eta(-1) + \zeta(-1) = 0$ or

$$\begin{vmatrix} \xi(1) & \eta(1) \\ \xi(-1) & \eta(-1) \end{vmatrix} \cdot \begin{vmatrix} c_1 \\ c_2 \end{vmatrix} = \begin{vmatrix} -\zeta(1) \\ -\zeta(-1) \end{vmatrix}$$

Thus

$$c_1 = [\eta(1) \zeta(-1) - \eta(-1) \zeta(1)] / [\xi(1) \eta(-1) - \eta(1) \xi(-1)]$$

$$c_2 = [\xi(-1) \zeta(1) - \eta(1) \zeta(-1)] / [\xi(1) \eta(-1) - \eta(1) \xi(-1)]$$

and the complete solution has been determined. Numerical computation for the case $g = 2, k = 40, p = 1$ verified accuracy to seven digits. In numerical computation, we see results stabilizing quickly to the required accuracy. For analytical results, the solution can be verified by substitution. The given examples here are linear; in nonlinear cases, the A_n polynomials used to represent nonlinearities⁽²⁾ by writing $f(u) = \sum_{n=0}^{\infty} A_n$ for an analytic function $f(u)$ have been shown in Ref. 5 to form a generalized Taylor series about the function u_0 and are convergent, of course.

Since for $f(u) = u$, the $\sum_{n=0}^{\infty} A_n$ becomes $\sum_{n=0}^{\infty} u_n$ or u , the series obtained are convergent.

(2) The special case of Airy's equation $y'' - ty = 0$, $y(0) = 1$, $y'(0) = 1$ can be simply written in the form $Ly - Ry = 0$ with $L = d^2/dt^2$, $R = t$. Then operating with L^{-1} , a twofold integration from 0 to t , we obtain $y(t) = y(0) + ty'(0) + L^{-1}Ry$. The solution is $y = \sum_{n=0}^{\infty} y_n$, where the y_n are defined by

$$\begin{aligned}
 y_0 &= 1 + t \\
 y_1 &= L^{-1}Ry_0 = L^{-1}t(1 + t) = \frac{t^3}{2 \cdot 3} + \frac{t^4}{3 \cdot 4} = \frac{1 \cdot t^3}{3!} + \frac{2 \cdot t^4}{4!} \\
 y_2 &= L^{-1}Ry_1 = \frac{t^6}{2 \cdot 3 \cdot 5 \cdot 6} + \frac{t^7}{3 \cdot 4 \cdot 6 \cdot 7} = \frac{1 \cdot 4 \cdot 6 \cdot t^6}{6!} + \frac{2 \cdot 5 \cdot t^7}{7!} \\
 &\vdots \\
 y_n &= \frac{1 \cdot 4 \cdot 7 \cdots (3n - 2) t^{3n}}{(3n)!} + \frac{2 \cdot 5 \cdot 8 \cdots (3n - 1) t^{3n+1}}{(3n + 1)!}
 \end{aligned}$$

(3) $u_{xx} - u_{yy} = 0$ on $0 \leq x \leq \pi/2$, $0 \leq y \leq \pi/2$ given the conditions

$$\begin{aligned}
 u(0, y) &= 0, & u(\pi/2, y) &= \sin y \\
 u(x, 0) &= 0, & u(x, \pi/2) &= \sin x
 \end{aligned}$$

Let $L_x = \partial^2/\partial x^2$ and $L_y = \partial^2/\partial y^2$ and write the above equations as $L_x u = L_y u$.

As usual in the decomposition method,⁽¹⁾ we solve for each linear operator term, $L_x u$ and $L_y u$, in turn and then apply the appropriate inverse to each:

$$\begin{aligned}
 L_x^{-1}L_x u &= u - c_1 k_1(y) - c_2 k_2(y)x = L_x^{-1}L_y u \\
 L_y^{-1}L_y u &= u - c_3 k_3(x) - c_4 k_4(x)y = L_y^{-1}L_x u
 \end{aligned}$$

or

$$u = c_1 k_1(y) + c_2 k_2(y)x + L_x^{-1}L_y u \tag{5}$$

$$u = c_3 k_3(x) + c_4 k_4(x)y + L_y^{-1}L_x u \tag{6}$$

Define $\Phi_x = c_1 k_1(y) + c_2 k_2(y)x$ and $\Phi_y = c_3 k_3(x) + c_4 k_4(x)y$ to rewrite (1) and (2) as

$$u = \Phi_x + L_x^{-1}L_y u \tag{7}$$

$$u = \Phi_y + L_y^{-1}L_x u \tag{8}$$

One-term approximants to the solution u are $u_0 = \Phi_x$ in (3) and $u_0 = \Phi_y$ in (4). Two-term approximants are $u_0 + u_1$, where $u_1 = L_x^{-1}L_y u_0$ in (3) and $L_y^{-1}L_x u_0$ in (4), etc. Thus $u_{n+1} = L_x^{-1}L_y u_n$ in (3) and $L_y^{-1}L_x u_n$ in (4) for $n \geq 0$.

For the x conditions $u(x, 0) = 0$ and $u(x, \pi/2) = \sin y$ applied to the one-term approximant $u_0 = c_1 k_1(y) + c_2 k_2(y)x$, we have

$$\begin{aligned} c_1 k_1(y) &= 0 \\ c_2 k_2(y) \pi/2 &= \sin y \end{aligned}$$

or $c_2 = 2/\pi$ and $k_2(y) = \sin y$.

For the y conditions $u(x, 0) = 0$ and $u(x, \pi/2) = \sin x$ applied to $u_0 = c_3 k_3(x) + c_4 k_4(x) y$, we get

$$\begin{aligned} c_3 k_3(x) &= 0 \\ c_4 k_4(x) \pi/2 &= \sin x \end{aligned}$$

Thus $c_4 = 2/\pi$ and $k_4(x) = \sin x$.

If a one-term approximant were sufficient, the solution would be²

$$\Phi_1 = (1/2) \{ (2/\pi)x \sin y + (2/\pi)y \sin x \}$$

The next terms for (3) and (4) respectively are

$$\begin{aligned} u_1 &= L_x^{-1}L_y u_0 = L_x^{-1}L_y [c_2 x \sin y] \\ u_1 &= L_y^{-1}L_x u_0 = L_y^{-1}L_x [c_4 y \sin x] \end{aligned}$$

We continue to obtain u_2, u_3, \dots . Clearly, for any n ,

$$\begin{aligned} u_n &= (L_x^{-1}L_y)^n u_0 = c_2 (\sin y) (-1)^n x^{2n+1} / (2n+1)! \\ u_n &= (L_y^{-1}L_x)^n u_0 = c_4 (\sin x) (-1)^n y^{2n+1} / (2n+1)! \end{aligned}$$

Letting φ_m represent the m -term approximant, we have for the two cases:

$$\varphi_m = c_2 \sin y \sum_{n=0}^{m-1} (-1)^n x^{2n+1} / (2n+1)! \tag{9}$$

$$\varphi_m = c_4 \sin x \sum_{n=0}^{m-1} (-1)^n y^{2n+1} / (2n+1)! \tag{10}$$

² An n -term approximant is $\varphi = \sum_{i=0}^{n-1} \psi_i$.

We can now apply the conditions $\varphi_m(\pi/2, y) = \sin y$ for (5); thus

$$c_1 k_1(y) = 0$$

$$c_2 \sin y \sum_{n=0}^{m-1} (\pi/2)^{2n+1}/(2n+1)! = \sin y$$

$$c_2 = \frac{1}{\sum_{n=0}^{m-1} (-1)^n (\pi/2)^{2n+1}/(2n+1)!}$$

As $m \rightarrow \infty$, we get $\sin \pi/2$ so that $c_2 \rightarrow 1$. The sum in (5) approaches $\sin x$ in the limit.

Now applying the conditions $\varphi_m(x, 0) = 0$ and $\varphi_m(x, \pi/2) = \sin x$, we have

$$c_3 k_3(x) = 0$$

$$c_4 \sin x \sum_{n=0}^{m-1} (-1)^n (\pi/2)^{2n+1}/(2n+1)! = \sin x$$

$$c_4 = \frac{1}{\sum_{n=0}^{m-1} (-1)^n (\pi/2)^{2n+1}/(2n+1)!}$$

Again as $m \rightarrow \infty$, $c_4 \rightarrow 1$ and the sum in (6) becomes $\sin y$. We can now write the exact solution

$$u = (1/2)\{\sin y \sin x + \sin x \sin y\}$$

or

$$u = \sin y \sin x$$

since for this case, the series is summed. Thus, we see u is indeed the solution and that the approximation $\varphi_n = \sum_{i=0}^{n-1} u_i$ becomes u in the limit as claimed.

Final Remarks. The principal advantage of the method applied here to Schrödinger's equation is its generality in solving wide classes of problems. The general case in physical systems is nonlinear and stochastic, and the basic method is generalized to solve such cases without linearization, perturbation, closure approximations, and assumptions of special processes not existing in nature, as shown in Refs. 2, 4, and 5. Thus, in a method developed basically for stochastic and nonlinear systems, it is interesting that special cases (linear, deterministic) are handled by the same method. The alternative approach to linear deterministic problems can have computational advantages even when problems are solvable by other methods.

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