Deriving a Solution to the Linear Schrödinger Equation and Discussion on Soliton Solutions to the Nonlinear Schrödinger Equation

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Outline

1. Linear Schrödinger Equation
   - History
   - Hydrogen Atom Solution
     - Strauss Solution
     - Griffiths Solution
2. Non-Linear Schrödinger Equation + Soliton Solutions
   - Physical Interest
   - Mathematical Interest

Linear Schrödinger Equation

W.A. Strauss, "Partial Differential Equations" [6]

$$-ih\frac{\partial}{\partial t}u = \frac{h^2}{2m}\Delta u + \frac{e^2}{r}u$$

David J. Griffiths, "Introduction to Quantum Mechanics" [3]

$$i\hbar\frac{\partial}{\partial t}\Psi = -\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi$$

Note: $u = \Psi$, $V = \frac{e^2}{r}$ and $h = \hbar$. (In physics, the bar through the h denotes division by 2π, to differentiate it from Planck's constant.)

Linear Schrödinger Equation

- Louie deBroglie suggested that small particles could be thought of as guided by 'matter waves', but did not develop mathematical formalism for the idea - hence "Schrödinger Equation", rather than "De Broglie Equation".
- Probability of finding a particle between points a and b at a specified time t.

$$\int_a^b |\Psi(x,t)|^2 dx$$

- Defined energy states

$$\hat{H}\psi = E\psi$$

Linear Schrödinger Equation

The Hydrogen Atom

$$iu_t = -\frac{1}{2}\Delta u - \frac{1}{r}u$$

Boundary Condition:

$$\iiint |u(\vec{x}, t)|^2 \, d\vec{x} < \infty$$

Linear Schrödinger Equation: Hydrogen Atom

Let's suppose a solution exists such that

$$u(t, \vec{x}) = T(t)v(\vec{x}).$$

Then

$$\begin{aligned} \frac{\partial}{\partial t} u &= T'(t)v(\vec{x}) + T(t)\frac{\partial}{\partial t} v(\vec{x}) \\ &= T'(t)v(\vec{x}) \end{aligned}$$

and

$$\begin{aligned} \Delta u(\vec{x}, t) &= \Delta(v(\vec{x})T(t)) \\ &= \Delta v(\vec{x})T(t) \end{aligned}$$

Linear Schrödinger Equation: Hydrogen Atom

Substituting:

$$iT'(t)v(\vec{x}) = -\frac{1}{2}\Delta v(\vec{x})T(t) - \frac{1}{r}v(\vec{x})T(t)$$

Divide by $\frac{1}{2}T(t)v(\vec{x}) = \frac{1}{2}u(\vec{x}, t)$:

$$2i\frac{T'}{T} = \frac{-\Delta v - \frac{2}{r}v}{v} = \lambda$$

Linear Schrödinger Equation: Hydrogen Atom

$$2i\frac{T'}{T} = \lambda \Leftrightarrow T' = \frac{-i}{2}\lambda T$$

Linear Schrödinger Equation: Time Component

$$T(t) = e^{-i\lambda t/2}$$

Linear Schrödinger Equation: Hydrogen Atom

$$\frac{-\Delta v - \frac{2}{r}v}{v} = \lambda \Leftrightarrow -\Delta v - \frac{2}{r}v = \lambda v$$

Find *A* Solution

- Impose radial symmetry, $v(\vec{x}) = R(r)$
- Use spherical Laplacian in 3D:

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin(\theta)}\frac{\partial}{\partial \theta} + \frac{1}{r^2}\sin^2(\theta)\frac{\partial^2}{\partial \phi^2}$$

Linear Schrödinger Equation: Hydrogen Atom

The Hydrogen Atom: Spacial Component

$$-R_{rr} - \frac{2}{r}R_r - \frac{2}{r}R = \lambda R$$

Boundary Condition:

$$\int_0^\infty |R(r)|^2 r^2 dr < \infty$$

Linear Schrödinger Equation: Hydrogen Atom

Note:

$$\lim_{r\to\infty}(-R_{rr} - \frac{2}{r}R_r - \frac{2}{r}R) \approx -R_{rr},$$

Then, as $r \to \infty$,

$$-R_{rr} = \lambda R$$

$$\Rightarrow R = e^{-\beta r}$$

Where $-\beta = -\sqrt{-\lambda}$; sign satisfies boundary conditions.
Idea: Define a new function, $w(r) = e^{\beta r}R(r)$

Linear Schrödinger Equation: Hydrogen Atom

$$
\begin{aligned}
w(r) = e^{\beta r}R(r) \Rightarrow R = we^{-\beta r},& \\
R_r = (w_r - \beta w)e^{-\beta r},& \\
R_{rr} = (w_{rr} - 2\beta w_r + \beta^2 w)e^{-\beta r}&
\end{aligned}
$$

Substitute into Hydrogen equation:

$$
\begin{aligned}
&- R_{rr} - \frac{2}{r}R_r - \frac{2}{r}R = \lambda R \\
\rightarrow &- w_{rr} + 2(\beta - \frac{1}{r})w_r + (2(\beta - 1)\frac{1}{r})w = 0
\end{aligned}
$$

Linear Schrödinger Equation: Hydrogen Atom

Theorem [6]

$$a(t)u'' + b(t)u' + c(t)u = 0$$

$\beta = \lim_{t\to 0} t\frac{b(t)}{a(t)}$, $\gamma = \lim_{t\to 0} t^2\frac{c(t)}{a(t)}$
r, s solutions to the equation $x(x-1) + \beta x + \gamma = 0$.
If $r - s \notin \mathbb{Z}$, all solutions are of the form

$$Ct^r \sum_{n=0}^{\infty} p_n t^n + Dt^s \sum_{n=0}^{\infty} q_n t^n$$

$$-w_{rr} + 2(\beta - \frac{1}{r})w_r + (2(\beta - 1)\frac{1}{r})w = 0$$

At $r = 0$, $\frac{2(\beta - \frac{1}{r})}{(-1)}$ "behaves no worse than $[r]^{-1}\ldots$" and $\frac{2(\beta-1)\frac{1}{r}}{(-1)}$ "behaves no worse than $[r]^{-2}$ near $t = 0$" [6], so $r = 0$ is a *regular singular point.*
$\Rightarrow$ Use power series!

$$w(r) = \sum_{k=0}^{\infty} a_k r^k$$

$$\frac{1}{2}\sum_{k=0}^{\infty} k(k-1)a_k r^{k-1} - \beta \sum_{k=0}^{\infty} k a_k r^k + \sum_{k=0}^{\infty} k a_k r^{k-1} + (1-\beta)\sum_{k=0}^{\infty} a_k r^k = 0$$

Shift $k \to k-1$ in second and third sums:

$$\sum_{k=0}^{\infty}\left[\frac{1}{2}k(k-1)+k\right] a_k r^{k-1} + \sum_{k=1}^{\infty}\left[-\beta(k-1)+(1-\beta)\right] a_{k-1} r^{k-1} = 0$$

In order for this to be true for all r, need coefficients to be zero

Linear Schrödinger Equation: Hydrogen Atom

$$\frac{k(k+1)}{2} a_k = (\beta_k - 1) a_{k-1}$$

$R(r) = w(r)e^{-\beta r}$,

$$a_1 = (\beta - 1)a_0 \qquad 3a_2 = (2\beta - 1)a_1$$
$$6a_3 = (3\beta - 1)a_2 \qquad 10a_4 = (4\beta - 1)a_3$$
$$15a_5 = (5\beta - 1)a_4 \qquad 21a_6 = (6\beta - 1)a_5$$

n	β	λ	$w(r)$	$v(x)$
1	1	-1	1	e^{-r}
2	$\frac{1}{2}$	$-\frac{1}{4}$	$1 - \frac{1}{2}r$	$e^{-r/2}(1 - \frac{1}{2}r)$
3	$\frac{1}{3}$	$-\frac{1}{9}$	$1 - \frac{2}{3}r + \frac{2}{27}r^2$	$e^{-r/3}[1 - \frac{2}{3}r + \frac{2}{27}r^2]$
4	$\frac{1}{4}$	$-\frac{1}{16}$		

Figure: Selected Coefficients + Solutions [6]

Linear Schrödinger Equation: Hydrogen Atom

$$\frac{-\Delta v - \frac{2}{r} v}{v} = \lambda \Leftrightarrow -\Delta v - \frac{2}{r} v = \lambda v$$

If I was a physicist...

- Assume Separation of Variables Again! $v(\vec{x}) = R(r) Y(\theta, \phi)$
- Use spherical Laplacian in 3D:

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2 \sin(\theta)}\frac{\partial}{\partial \theta} + \frac{1}{r^2}\sin^2(\theta)\frac{\partial^2}{\partial \phi^2}$$

Linear Schrödinger Equation: Hydrogen Atom

$$-\frac{1}{2}\left[\frac{Y}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{R}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{R}{r^2\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]-\frac{1}{r}RY = \lambda RY$$

Divide by RY, multiply by $2r^2$:

$$\left\{\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)-2r^2[\frac{1}{r}-\lambda]\right\} + \frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = 0$$

Linear Schrödinger Equation: Hydrogen Atom

Again, only works if we have

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - 2r^2[\frac{1}{r} - \lambda] = l(l+1)$$

and

$$\frac{1}{Y}\left\{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right) + \frac{1}{sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right\} = -l(l+1)$$

Linear Schrödinger Equation: Hydrogen Atom

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - 2r^2[\frac{1}{r} - \lambda]R = l(l+1)R$$

Define $u(r) = rR(r)$

$$\Rightarrow R = u/r,$$
$$\frac{dR}{dr} = [r\frac{du}{dr} - u]\frac{1}{r^2},$$
$$\frac{d}{dr}\left[r^2\frac{dR}{dr}\right] = \frac{rd^2u}{dr^2}$$

$$-\frac{1}{2}\frac{d^2u}{dr^2} + \left[\frac{1}{r} + \frac{1}{2}\frac{l(l+1)}{r^2}\right]u = \lambda u$$

Linear Schrödinger Equation: Hydrogen Atom

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r}$$

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + \left[-\frac{e}{4\pi\epsilon_0}\frac{1}{r} + \frac{\hbar^2}{2m}\frac{l(l+1)}{r^2}\right]u = Eu$$

Define $\kappa = \frac{\sqrt{-2mE}}{\hbar}$, $\rho = \kappa r$, and $\rho_0 = \frac{me^2}{2\pi\epsilon_0\hbar^2\kappa}$

$$\frac{d^2u}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2}\right]u$$

Linear Schrödinger Equation: Hydrogen Atom

Examine behavior as $\rho \to \infty$,

$$\frac{d^2 u}{d\rho^2} = u$$

So $u(\rho) \sim Ae^{-\rho}$ as ρ goes to infinity. Introduce $\nu(\rho)$

$$u(\rho) = \rho^{l+1} e^{-\rho} \nu(\rho)$$

Oh look! It's what Strauss did. (Good)

Linear Schrödinger Equation: Hydrogen Atom

$$\sin\theta \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial Y}{\partial\theta}\right) + \frac{\partial^2 Y}{\partial\phi^2} = l(l+1)\sin^2\theta\, Y$$

Separation of Variables Again! $Y(\theta, \phi) = \Theta(\theta)\Phi(\phi)$

$$\left\{\frac{1}{\Theta}\left[\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right)\right] + l(l+1)\sin^2\theta\right\} = m^2$$

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2$$

Linear Schrödinger Equation: Hydrogen Atom

$$\frac{d^2\Phi}{d\phi^2} = -m^2$$

$$\Rightarrow \Phi(\phi) = e^{im\phi}$$

$$\left\{ \frac{1}{\Theta} \left[\sin\theta \frac{d}{d\theta} \left(\sin\theta \frac{d\Theta}{d\theta} \right) \right] + l(l+1)\sin^2\theta \right\} = m^2$$

$$\Rightarrow \Theta(\theta) = AP_l^m(\cos\theta)$$

Linear Schrödinger Equation: Hydrogen Atom

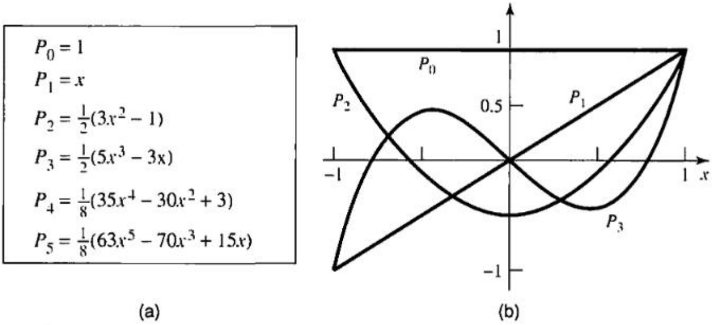
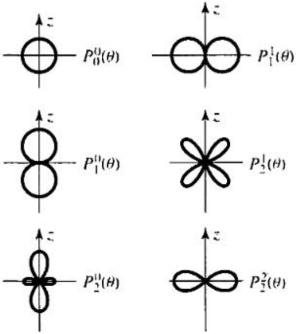


Figure: Legendre Polynomials [3]

Linear Schrödinger Equation: Hydrogen Atom

$P_0^0 = 1$	$P_2^0 = \frac{1}{2}(3\cos^2\theta - 1)$
$P_1^1 = \sin\theta$	$P_3^3 = 15\sin\theta(1 - \cos^2\theta)$
$P_1^0 = \cos\theta$	$P_3^2 = 15\sin^2\theta\,\cos\theta$
$P_2^2 = 3\sin^2\theta$	$P_3^1 = \frac{3}{2}\sin\theta(5\cos^2\theta - 1)$
$P_2^1 = 3\sin\theta\,\cos\theta$	$P_3^0 = \frac{1}{2}(5\cos^3\theta - 3\cos\theta)$

(a)



(b)

Figure: Legendre Functionals $P_l^m(\cos\theta)$ [3]

Linear Schrödinger Equation: Hydrogen Atom

Spherical Harmonics

$$Y_l^m(\theta, \phi) = \epsilon\sqrt{\frac{2l+l}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}e^{im\phi}P_l^m(\cos\theta)$$

l = azimuthal quantum number, m = magnetic quantum number

Non-Linear Schrödinger Equation

General Nonlinear Schrödinger Equation [5]

$$iu_t + p : \nabla\nabla u + f(|u|^2)u = 0$$

$u(x,t)$ is a complex-valued function, p is a dispersion tensor with real-valued elements, $f(s)$ is a differentiable complex-valued functions such that $f(|u|)^2 \,|_{u\to 0} = 0$

Non-Linear Schrödinger Equation

NLS From Laser Propogation [2]

$$2ik_0\psi_z(x, y, z) + \Delta\psi + k_0^2 \frac{4n^2}{n_0} |\psi|^2\psi = 0$$

- The NLS is derived from Maxwell's Equations, classical physics
  - LS can also be derived by Maxwell's Eqs, using parabolic approximation to make a boundary problem

    $$\Delta E(x, y, z) + k_0^2 E = 0 \quad \text{(Helmholtz Eq)}$$

    into an initial value problem
- Describes propogation of linear continuous wave (cw) laser in a homogeneous Kerr medium

Non-Linear Schrödinger Equation

1D Cubical Focusing NLS

$$i\psi_z(z,x) + \psi_{xx} + |\psi|^2\psi = 0$$

Subcritical, allows solitons

- Inverse Scattering Theory developed for KdV applied to 1D Cubical Focusing NLS soliton solutions
- 1D cubic is integrable - 2D is not

Soliton Solutions

- Integrable - " a dynamical system with sufficiently many conserved quantities, or first integrals, such that its behavior has fewer degrees of freedom than the dimensionality of its phase space." [7]
- Completely Integrable: "Existence of a maximal set of conserved quantities." [7]
- Dark Solitons - non-localized solitary wave solutions. Intensity profile exhibit a dip in uniform background [2]
- https://www.youtube.com/watch?v=xPmV2WWwm68

Non-Linear Schrödinger Equation

1D Cubical Schrödinger Eq [5]

$$iu_t + p : \nabla\nabla u + q|u_2|u$$

Where p is the dispersion tensor $p_{ij} = \frac{1}{2}\partial^2\omega/\partial k_i k_j$ and $q = \partial\omega/\partial|u|^2$

- Benjamin-Feir criterion (1967)- instability of Fourier modes creates soliton solutions
- "Breather Solutions" useful in fluid dynamics - see [1]

Soliton Solutions

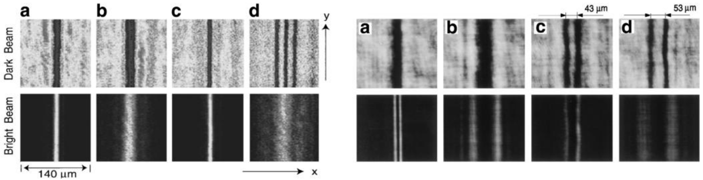


Fig. 1. (Color Online) Formation of DB solitons in photorefractive crystals: the left four panels (adapted from Ref. [27]) showcase the evolution of an initial condition [panel (a)], upon propagation under linear evolution, leading to dispersion [panel (b)], nonlinear evolution of uncoupled components, again leading to breakup/dispersion [panel (d)], and under coupled nonlinear evolution [panel (c)]. A similar case example, but for two bright beams, is shown in the right four panels (adapted from Ref. [28]). The dark (bright) component is shown in the top (bottom) panel.

Figure: From [4]

Soliton Solutions

Recent (2016) Examples [4]

$$i\partial_t\psi = H_0\psi_{\pm1} + \delta[(|\psi_{\pm1}|^2 + |\psi_0|^2 - |\psi_{\mp1}|^2)\psi_{\pm1} + \psi_0^2\psi_{\mp1}^*]$$

$$i\partial_t\psi_0 = H_0\psi_0 + \delta[(|\psi_{-1}|^2 + |\psi_{+1}|^2)\psi_0 + 2\psi_{-1}\psi_0^*\psi_{+1}]$$

$\psi_{0,\pm1}$ are the three vertical spin components, δ is the ratio of strengths of spin-dependent and spin-independent interatomic reactions,

$$H_0 \equiv -(1/2)\partial_x^2 + V(x) + |\psi_{-1}|^2 + |\psi_0|^2 + |\psi_{+1}|^2$$

Not integrable, but reduces to integrable problems when $\delta = 0$ (Manakov), $\delta = 1$ (completely integrable!).

Soliton Solutions

Has two integrals of motion:

- $$N = \int_{-\infty}^{\infty} n_{tot} dx$$

  Where $n_{tot} = n_{-1} + n_0 + n + 1 \equiv |\psi_{-1}|^2 + |\psi_0|^2 + |\psi_{+1}|^2$

- $$E = \int_{-\infty}^{\infty} \epsilon dx$$

  where the density ϵ reads
  $\epsilon = \sum_{j=0,\pm1} (\frac{1}{2}|\partial_x \psi_j|^2 + V(x) n_j + \frac{1}{2} n_j^2) + \sum_{j,k=0,\pm1}^{j \neq k} n_j n_k + \frac{\delta}{2}|f|^2$

Conclusion

- Separation of Variables: Take a PDE and Make it and ODE!
  - Series solutions are your friend, as always
- NLS + KdV are related, have intriguing solutions and applications

Works Cited

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