Time dependent Schrödinger Equation (TDSE)

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$$i\hbar \frac{\partial}{\partial t}|\phi(t)\rangle = \mathcal{H}|\phi(t)\rangle$$

where $|\phi\rangle$ represents the state of the system described by the hamiltonian $\mathcal{H}$.

This has the formal solution $|\phi(m\tau)\rangle = e^{-im\tau\mathcal{H}}|\phi(t=0)\rangle$ where $m = 0, 1, 2, \dots$ is the number of timesteps τ.

- For a charged particle in a static magnetic field

$$\mathcal{H} = \frac{1}{2m^*}(\underline{p} - e\underline{A})^2 + V$$

where m^* is the effective mass of the particle with charge e and:

$\underline{p} = -i\hbar\nabla$ is the momentum operator

V and $\underline{A}$ are the scalar and vector potentials which encapsulate the effect of the electromagnetic field, via

$$\underline{B} = \nabla \times \underline{A} \quad , \quad \underline{E} = -\nabla V - \frac{\partial \underline{A}}{\partial t}$$

2-D ➡ given $\underline{A} = [A_x(x,y), 0, 0]$

we have that $A_x(x,y) = -\int_0^y B(x,y)\,dy$

☆ We will, however, set $\underline{A} = 0$ in our simplified derivation of the method!

Fixing the unit of length by the wavelength λ and energy in units of $E = \frac{\hbar^2 k^2}{2m^*}$ $(k = 2\pi/\lambda)$ and time in units of $\hbar/E$. These dimensionless variables simplify the hamiltonian to:

$$\mathcal{H} = -\frac{1}{4\pi^2}\left[\left(\frac{\partial}{\partial x} - iA_x(x,y)\right)^2 + \frac{\partial^2}{\partial y^2}\right] + V(x,y)$$

So far this is the same as in [Raedt & Michielsen '94] but now we will continue by simplifying a lot!

1. Set $\underline{B} = 0$!
2. Discretize the operator ∇^2 to 2^{nd} order on the grid, instead of 4^{th} order!
3. Use 2^{nd} order in time, instead of 4^{th} order!
4. Start developing the method in 1-D.

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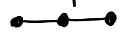
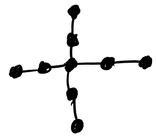
$$\nabla^2 u_\ell = \frac{1}{\Delta^2}\left(u_{\ell+1} + u_{\ell-1} - 2u_\ell\right) + \mathcal{O}(\Delta^2)$$

template 

(instead of 2-D 4th order stencil )

Now: $\mathcal{H} = -\frac{1}{4\pi^2}\frac{\partial^2}{\partial x^2} + V(x)$

$$\mathcal{H}\phi_\ell(t) = \frac{1}{4\pi^2\Delta^2}\Big\{-\phi_{\ell+1}(t) - \phi_{\ell-1}(t) + (2 + 4\pi^2\Delta^2 V_\ell)\,\phi_\ell(t)\Big\}$$

(compare this to equation 1.9 from the paper)

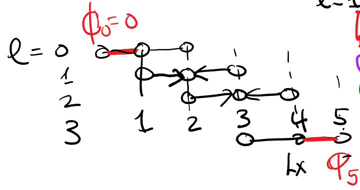
$$|\Phi(t)\rangle = \sum_{\ell=1}^{L_x} \Phi_\ell(t)\,\underbrace{c_\ell^+}_{\text{creation operator at grid point } \ell}|0\rangle$$

state vector

It is far easier to express the formal solution using the creation, c_ℓ^+, and annihilation, c_ℓ, operators:

$$|\Phi(m\tau)\rangle = e^{-im\tau H}|\Phi(t=0)\rangle \quad \text{where}$$

$$H = -\frac{1}{4\pi^2\Delta^2}\sum_{\ell=1}^{L_x-1}\left(c_\ell^+ c_{\ell+1} + c_{\ell+1}^+ c_\ell\right) + \frac{1}{4\pi^2\Delta^2}\sum_{\ell=1}^{L_x}(2 + 4\pi^2\Delta^2 V_\ell)$$



$c_1^+c_0$ | $c_1^+c_2$ | $\ell = 1$
$c_2^+c_1$ | $c_2^+c_3$ | $\ell = 2$
$c_3^+c_2$ | $c_3^+c_4$ | $\ell = 3$
$c_4^+c_3$ | $c_4^+c_5$

$\Big\}\ L_x = 4$

★ Note that the fact that the red contributions are missing is an implicit application of the free boundary cond. $\Phi_0 = \Phi_5 = 0$!

Each term in the first sum involves an interaction between a pair of lattice sites $(\ell, \ell+1)$.

The aim now is to express the solution as a product of 2×2 matrix operation acting on pairs of lattice sites. Each 2×2 matrix op can be computed analytically. We do this calculation now.

Recall $e^y = 1 + y + \frac{y^2}{2!} + \frac{y^3}{3!} + \frac{y^4}{4!} + \frac{y^5}{5!}$

$y = ix$, then

$$e^{ix} = 1 + ix - \frac{x^2}{2} - i\frac{x^3}{3!} + \frac{x^4}{4!} + i\frac{x^5}{5!} - \cdots$$

$$= \left(1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} + \cdots\right)$$

$$+ i\left(x - \frac{x^3}{3!} + \frac{x^5}{5!} - \frac{x^7}{7!}\right)$$

$$= \cos x + i \sin x$$

Now to calculate the exponentials of the fermi operators c_ℓ, c_ℓ^+:

$$|\phi\rangle = \sum_\ell \phi_\ell c_\ell^+ |0\rangle \qquad \{c_\ell^+, c_\ell^+\}=0 \quad \{c_\ell, c_\ell\}=0$$
$$\{c_\ell^+, c_{\ell'}\} = \delta_{\ell\ell'}$$

$$e^{-i\tau(\alpha c_\ell^+ c_{\ell+1} + \alpha^* c_{\ell+1}^+ c_\ell)}|\phi\rangle$$

$$= |\phi\rangle - i\tau(\alpha c_\ell^+ c_{\ell+1} + \alpha^* c_{\ell+1}^+ c_\ell)|\phi\rangle + \dots$$

Let $x = -\tau(\alpha c_\ell^+ c_{\ell+1} + \alpha^* c_{\ell+1}^+ c_\ell)$

$$x|\phi\rangle = -\tau \sum_n \phi_n \alpha c_\ell^+ \underbrace{c_{\ell+1} c_n^+}_{=\delta_{\ell+1\,n} - c_n^+ c_{\ell+1}}|0\rangle - \tau\sum_n \phi_n \alpha^* c_{\ell+1}^+ \underbrace{c_\ell c_n^+}_{=\delta_{\ell n} - c_n^+ c_\ell}|0\rangle$$

Trick to move c_ℓ so it acts on $|0\rangle$:

$c|0\rangle = 0$! $c|0\rangle = 0$!

$$x|\phi\rangle = -\tau\alpha\phi_{\ell+1} c_\ell^+|0\rangle - \tau\alpha^*\phi_\ell c_{\ell+1}^+|0\rangle$$

$$x^2|\phi\rangle = x(x|\phi\rangle) = +\tau^2\alpha^2 c_\ell^+ c_{\ell+1}\phi_{\ell+1}c_\ell^+|0\rangle + \tau^2|\alpha|^2 c_\ell^+ c_{\ell+1}\phi_\ell c_{\ell+1}^+|0\rangle$$
$$+ \tau^2|\alpha|^2 c_{\ell+1}^+ c_\ell \phi_{\ell+1} c_\ell^+|0\rangle + \tau^2\alpha^{*2} c_{\ell+1}^+ c_\ell \phi_\ell c_{\ell+1}^+|0\rangle$$

$$= \tau^2\alpha^2 c_\ell^+\phi_{\ell+1}(\delta_{\ell\,\ell+1} - c_\ell^+ c_{\ell+1})|0\rangle$$
$$+ \tau^2|\alpha|^2 c_\ell^+\phi_\ell(\boxed{\delta_{\ell+1\,\ell+1}} - c_{\ell+1}^+c_{\ell+1})|0\rangle$$
$$+ \tau^2|\alpha|^2 c_{\ell+1}^+\phi_{\ell+1}(\boxed{\delta_{\ell\ell}} - c_\ell^+ c_\ell)|0\rangle$$
$$+ \tau^2\alpha^{*2}c_{\ell+1}^+\phi_\ell(\delta_{\ell\,\ell+1} - c_{\ell+1}^+ c_\ell)|0\rangle$$

$$x^2|\phi\rangle = \tau^2|\alpha|^2(\phi_\ell c_\ell^+ + \phi_{\ell+1}c_{\ell+1}^+)|0\rangle$$

$$x^3|\phi\rangle = x(x^2|\phi\rangle)$$
$$= -\tau^3\alpha|\alpha|^2(c_\ell^+c_{\ell+1}\phi_\ell c_\ell^+ + c_\ell^+ c_{\ell+1}\phi_{\ell+1}c_{\ell+1}^+)|0\rangle$$
$$-\tau^3\alpha^*|\alpha|^2(c_{\ell+1}^+c_\ell\phi_\ell c_\ell^+ + c_{\ell+1}^+c_\ell\phi_{\ell+1}c_{\ell+1}^+)|0\rangle$$
$$= -\tau^3\alpha|\alpha|^2(\phi_\ell c_\ell^+(\delta_{\ell+1\,\ell} - c_\ell^+ c_{\ell+1})|0\rangle +$$
$$\phi_{\ell+1}c_\ell^+(\boxed{\delta_{\ell+1\,\ell+1}} - c_{\ell+1}^+c_{\ell+1})|0\rangle)$$
$$-\tau^3\alpha^*|\alpha|^2(\phi_\ell c_{\ell+1}^+(\boxed{\delta_{\ell\ell}} - c_\ell^+ c_\ell)|0\rangle +$$
$$\phi_{\ell+1}c_{\ell+1}^+(\delta_{\ell\,\ell+1} - c_{\ell+1}^+ c_\ell)|0\rangle)$$

$$x^3|\phi\rangle = -\tau^3\alpha|\alpha|^2\phi_{\ell+1}c_\ell^+|0\rangle - \tau^3\alpha^*|\alpha|^2\phi_\ell c_{\ell+1}^+|0\rangle$$
$$= \tau^2|\alpha|^2(x|\phi\rangle) \;!$$

$$x^4|\phi\rangle = x(x^3|\phi\rangle) = \tau^2|\alpha|^2 x(x|\phi\rangle) = \tau^2|\alpha|^2 x^2|\phi\rangle$$
$$= \tau^4|\alpha|^4(\phi_\ell c_\ell^+ + \phi_{\ell+1}c_{\ell+1}^+)|0\rangle$$

$$\cos x|\phi\rangle = \left(1 - \frac{x^2}{2} + \frac{x^4}{4!} - \frac{x^6}{6!} + \dots\right)|\phi\rangle$$

For: $|\phi\rangle = (\phi_\ell c_\ell^+ + \phi_{\ell+1}c_{\ell+1}^+)|0\rangle \longleftarrow$ state of the pair of lattice sites.

$$\cos x|\phi\rangle = \left(1 - \tfrac12\tau^2|\alpha|^2 + \tfrac{1}{4!}\tau^4|\alpha|^4 - \dots\right) = \cos(\tau|\alpha|)|\phi\rangle$$

$$\sin x|\phi\rangle = \left(1 - \frac{\tau^2|\alpha|^2}{3!} + \frac{\tau^4|\alpha|^4}{5!} - \dots\right)x|\phi\rangle$$
$$= \left(\tau|\alpha| - \frac{\tau^3|\alpha|^3}{3!} + \frac{\tau^5|\alpha|^5}{5!} - \dots\right)\frac{1}{\tau|\alpha|}x|\phi\rangle$$

$$\sin x|\Phi\rangle = \left(1 - \frac{\tau^2|\alpha|^2}{3!} + \frac{\tau^4|\alpha|^4}{5!} - \dots\right) x|\Phi\rangle$$

$$= \left(\tau|\alpha| - \frac{\tau^3|\alpha|^3}{3!} + \frac{\tau^5|\alpha|^5}{5!} - \dots\right)\frac{1}{\tau|\alpha|}\, x|\Phi\rangle$$

$$= \sin(\tau|\alpha|)\frac{1}{\tau|\alpha|}\, x|\Phi\rangle$$

$$= \sin(\tau|\alpha|)\left(-\frac{\alpha}{|\alpha|}\Phi_{\ell+1}c_\ell^{+}|0\rangle - \frac{\alpha^*}{|\alpha|}\Phi_\ell c_{\ell+1}^{+}|0\rangle\right)$$

$$\left(-\frac{\alpha}{|\alpha|}c_\ell^+c_{\ell+1} - \frac{\alpha^*}{|\alpha|}c_{\ell+1}^+c_\ell\right)|\Phi\rangle = -\frac{\alpha}{|\alpha|}c_\ell^+c_{\ell+1}\Phi_\ell c_\ell^+|0\rangle$$

$$-\frac{\alpha}{|\alpha|}c_\ell^+c_{\ell+1}\Phi_{\ell+1}c_{\ell+1}^+|0\rangle$$

$$-\frac{\alpha^*}{|\alpha|}c_{\ell+1}^+c_\ell\Phi_\ell c_\ell^+|0\rangle$$

$$-\frac{\alpha^*}{|\alpha|}c_{\ell+1}^+c_\ell\Phi_{\ell+1}c_{\ell+1}^+|0\rangle$$

$$= \underbrace{-\frac{\alpha}{|\alpha|}\Phi_{\ell+1}c_\ell^+|0\rangle - \frac{\alpha^*}{|\alpha|}\Phi_\ell c_{\ell+1}^+|0\rangle}_{=}$$

So $$\sin x|\Phi\rangle = \left(-\frac{\alpha}{|\alpha|}c_\ell^+c_{\ell+1} - \frac{\alpha^*}{|\alpha|}c_{\ell+1}^+c_\ell\right)\sin(\tau|\alpha|)|\Phi\rangle$$

For $|\Phi\rangle = \Phi_\ell c_\ell^+|0\rangle + \Phi_{\ell+1}c_{\ell+1}^+|0\rangle$ we have that:

$$e^{-i\tau(\alpha c_\ell^+c_{\ell+1} + \alpha^* c_{\ell+1}^+c_\ell)}|\Phi\rangle =$$

$$\left[\cos(\tau|\alpha|) - i\left(\frac{\alpha}{|\alpha|}c_\ell^+c_{\ell+1} + \frac{\alpha^*}{|\alpha|}c_{\ell+1}^+c_\ell\right)\sin(\tau|\alpha|)\right]|\Phi\rangle$$

$$c_\ell^+c_{\ell+1}(c_{\ell+1}^+|0\rangle) = c_\ell^+|0\rangle \Rightarrow \Phi_{\ell+1} \rightarrow \Phi_\ell'$$

$$c_\ell^+c_{\ell+1}(c_\ell^+|0\rangle) = 0$$

new states

$$c_{\ell+1}^+c_\ell(c_{\ell+1}^+|0\rangle) = 0$$

$$c_{\ell+1}^+c_\ell(c_\ell^+|0\rangle) = c_{\ell+1}^+|0\rangle \Rightarrow \Phi_\ell \rightarrow \Phi_{\ell+1}'$$

Using matrix notation $|\Phi\rangle = \begin{pmatrix}\Phi_\ell \\ \Phi_{\ell+1}\end{pmatrix}$

this operation results in the following:

$$\begin{pmatrix} \cos(\tau|\alpha|) & -i\frac{\alpha}{|\alpha|}\sin(\tau|\alpha|) \\ -i\frac{\alpha^*}{|\alpha|}\sin(\tau|\alpha|) & \cos(\tau|\alpha|)\end{pmatrix}\begin{pmatrix}\Phi_\ell \\ \Phi_{\ell+1}\end{pmatrix} = \begin{pmatrix}\Phi_\ell' \\ \Phi_{\ell+1}'\end{pmatrix}$$

Note: $$\frac{\alpha}{|\alpha|} = \frac{\alpha|\alpha|}{|\alpha|^2} = \frac{\alpha|\alpha|}{\alpha\,\alpha^*} = \alpha^{*-1}|\alpha|\,, \quad \frac{\alpha^*}{|\alpha|} = \alpha^{-1}|\alpha|$$

$$
M = \begin{pmatrix} \cos(\tau|\alpha|) & -i\,\alpha^{*-1}|\alpha|\sin(\tau|\alpha|) \\ -i\,\alpha^{-1}|\alpha|\sin(\tau|\alpha|) & \cos(\tau|\alpha|) \end{pmatrix}
$$

$$
\begin{pmatrix} \phi_\ell' \\ \phi_{\ell+1}' \end{pmatrix} = M \begin{pmatrix} \phi_\ell \\ \phi_{\ell+1} \end{pmatrix}
$$