Green Solver FD

$$\begin{array}{cccc} & i-1 & i & i+1 \\ \phi(x_i) & \cdot & \cdot & \cdot \end{array}$$

$$\begin{array}{ccccc} & i-\tfrac{3}{2} & i-\tfrac{1}{2} & i+\tfrac{1}{2} & i+\tfrac{3}{2} \\ \phi'(x_i) & \cdot & \cdot & \cdot & \cdot \end{array}$$

① $(\phi_{i+1} - \phi_i) - \phi'_{i+\frac{1}{2}}\, dx = 0$

② $(\phi'_{i+\frac{1}{2}} - \phi'_{i-\frac{1}{2}}) + 2(E - V_i)\phi_i\, dx = 0$

solution vector ↳ $X = \begin{bmatrix} \phi_i \\ \phi'_i \end{bmatrix} \begin{array}{l} \} \text{ Nelem} \\ \} \text{ Nelem+1} \end{array}$

Nelem is # of grid points in our mesh.

Eq. 1 represents Nelem -1 linear equations and are represented ~~[illegible]~~ as a matrix:

$$\text{Nelem}-1 \left\{ \left[ \underbrace{D1}_{\text{Nelem}} \,,\, \underbrace{-MID}_{\text{Nelem+1}} \right] \right. \left[ x \right] = 0$$

Eq 2 represents Nelem linear equations:

$$\text{Nelem} \left\{ \left[ \underbrace{2 \cdot [E - V_i]}_{\text{Nelem}} \,,\, \underbrace{D1}_{\text{Nelem+1}} \right] \right. \cdot \left[ x \right] = 0$$

↳ diagonal matrix w/ $2 \cdot (E - V_i)\, dx$ along the diagonal

Additionally 2 boundary conditions are required which adds 2 more equations. Thus we end up w/ 2*Nelem+1 Eqs. + 2*Nelem+1 variables greensolvefd combines these equations into a single matrix with the structure:

$$A(E) = \begin{bmatrix} [\ bc\phi\ ,\ bc\phi'\ ] & \\ DI & -MID \\ 2*[E-V_i] & DI \end{bmatrix} * X = 0$$

This would be a linear eigenvalue problem in E except that the boundary conditions are nonlinear. To zeroeth order (in dx) they depend on $K = \sqrt{-2E}$. $\rightarrow E = \frac{k^2}{2}$

The initial greensolvefd solution is to convert to a quadratic eigenvalue problem in K:

$$\left[ \underbrace{K^2}_{=2\cdot E} \underbrace{\begin{bmatrix} 0 & 0 \\ \underset{\text{identity}}{I} & 0 \end{bmatrix}}_{A_2} + k \cdot \underbrace{\overset{\text{k dependent BC}}{\begin{bmatrix} [\ bc\ \ 0\ ] \\ 0 \end{bmatrix}}}_{A_1} + \underbrace{\overset{\text{k independent BC}}{\begin{bmatrix} [\ 0\ ] & [\ BC\ ] \\ DI & -MID \\ -2*V_i & DI \end{bmatrix}}}_{A_0} \right] X = 0$$

This quadratic eig problem is converted to generalized linear eig problem. (of 2* dimension)

$$\begin{pmatrix} A_0 & O \\ O & I \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = k \begin{pmatrix} -A_1 & -A_2 \\ I & O \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

this is setup so that $y = kx$

$$\phi \qquad \overset{i-1}{\bullet} \quad \overset{i}{\bullet} \quad \overset{i+1}{\bullet} \quad \overset{i+2}{\bullet}$$

$$\phi' \qquad \underset{i-\frac{3}{2}}{\bullet} \quad \underset{i-\frac{1}{2}}{\bullet} \quad \underset{i+\frac{1}{2}}{\bullet} \quad \underset{i+\frac{3}{2}}{\bullet} \quad \underset{i+\frac{5}{2}}{\bullet}$$

Equations:

① $(\phi_{i+1} - \phi_i) - \phi'_{i+\frac{1}{2}} dx = 0$

② $-\frac{1}{2}(\phi'_{i+\frac{1}{2}} - \phi'_{i-\frac{1}{2}}) + (v_i - E)\phi_i dx = 0$

Asymptotic Behavior: $v_i = \text{const}$

ansatz: $\phi_{i+1} = e^{ikdx}\phi_i \rightarrow \phi_i = e^{-ikdx}\phi_{i+1}$

plug ansatz into ①:

③ $$(e^{ikdx} - 1)\phi_i - \phi'_{i+\frac{1}{2}} dx = 0$$

and:

④ $$(1 - e^{-ikdx})\phi_i - \phi'_{i-\frac{1}{2}} = 0$$

③ - ④:

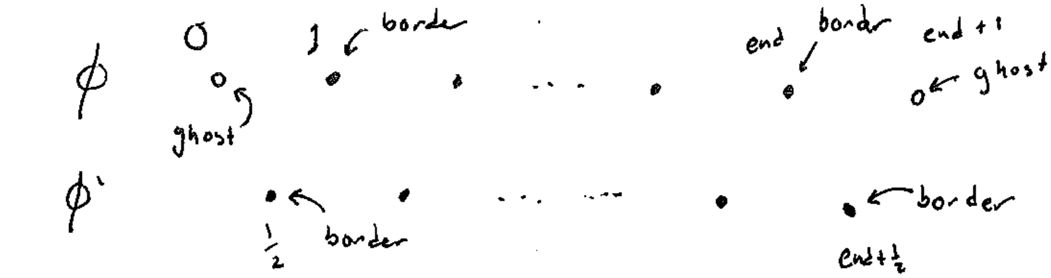
$$(e^{ikdx} + e^{-ikdx} - 2)\phi_i - (\phi'_{i+\frac{1}{2}} - \phi'_{i-\frac{1}{2}})dx = 0$$

$$\frac{1}{dx}(\cos kdx - 1)\phi_i - \frac{1}{2}(\phi'_{i+\frac{1}{2}} - \phi'_{i-\frac{1}{2}}) = 0$$

compare to ②:

$$E - v = \frac{1}{dx^2}(1 - \cos kdx) \approx \frac{k^2}{2}$$

Corrected boundary conditions:




from ansatz:

$$\phi_0 = e^{-ik_L dx}\phi_1 \quad \text{and} \quad \phi_{end+1} = e^{ik_R dx}\phi_{end}$$

+ eq (1):

$$\left(1 - e^{-ik_L dx}\right)\phi_1 - \phi'_{\frac{1}{2}}dx = 0 \qquad \left(e^{ik_R dx} - 1\right)\phi_{end} - \phi'_{end+\frac{1}{2}}dx = 0$$

so:

$$\phi'_{\frac{1}{2}} = \frac{1}{dx}\left(1 - e^{-ik_L dx}\right)\phi_1 \simeq +ik_L\phi_1$$

$$\phi'_{end+\frac{1}{2}} = \frac{1}{dx}\left(e^{ik_R dx} - 1\right)\phi_{end} \simeq ik_R\phi_{end}$$