Problem 1: 1.

Galerkin method:

We want $f(x)$, $x \in [0,1]$ from:

$$\frac{d^2 f(x)}{dx^2} = x+1,$$

with b.c.: $f(0) = f(1) = 0$.

Basis functions: $\varphi_i(x) = x(1-x)^i$ satisfy boundary conditions.

Use $N=2$ and scalar product:
number of basis functions

$$(g,h) = \int_0^1 dx\, g(x)h(x).$$

inspection methods
$\downarrow$
weighted residuals

Galerkin (weak form) | collocation (strong)

$f(x) = \sum_{j=1}^{2} w_j \cdot x_j(x)$

$= w_1 \cdot x_1(x) + w_2\, x_2(x) =$

$= w_1\, x(1-x) + w_2\, x(1-x)^2.$

$L[f] = g \Rightarrow$

$\Rightarrow L\left[\sum_{j=1}^{2} w_j\, x_j(x)\right] = g \Rightarrow$

$\Rightarrow \sum_{j=1}^{2} w_j \underbrace{\left(x_k, L[x_j]\right)}_{r_{kj}} = \underbrace{(x_k, g)}_{g_k} \Rightarrow \boxed{\vec{w} = r^{-1}\, \vec{g}}$

passage in lecture notes...

$\vec{g} = \begin{pmatrix} (x_1, g) \\ (x_2, g) \end{pmatrix} = \begin{pmatrix} \frac{1}{4} \\ \frac{7}{60} \end{pmatrix}$

$(x_1, g) = \int_0^1 \underbrace{x(1-x)}_{x_1}\underbrace{(1+x)}_{g}\, dx =$

$= \int_0^1 x\, dx - \int_0^1 x^3\, dx =$

$= \left(\frac{x^2}{2}\right)\Big|_0^1 - \left(\frac{x^4}{4}\right)\Big|_0^1 = \frac{1}{2} - \frac{1}{4} = \boxed{\frac{1}{4}}$

$(x_2, g) = \int_0^1 x(1-x)^2(1+x)\, dx =$

$= \int_0^1 (x + x^2)(x^2 - 2x + 1)\, dx =$

$= \int_0^1 x^3 - 2x^2 + x + x^4 - 2x^3 + x^2\, dx = \boxed{\frac{7}{60}}$

Analytic:

$\frac{df}{dx} = \frac{x^2}{2} + x + C_1$

$f(x) = \frac{x^3}{6} + \frac{x^2}{2} + C_1 x + C_2.$

$f(0) = C_2 = 0$

$f(1) = \frac{1}{6} + \frac{1}{2} + C_1 = 0$

$\Rightarrow C_1 = -\frac{2}{3}.$

$r_{kj} = (x_k, L[x_j]).$

$r_{11} = (x_1, L[x_1]).$

$L[x_1] = \frac{d^2}{dx^2}\left(x(1-x)\right) = -2$

$L[x_2] = \frac{d^2}{dx^2}\left(x(1-x)^2\right) = 6x - 4.$

$r_{11} = (x_1, L[x_1]) = -2 \int_0^1 x(1-x)\, dx = \boxed{-\frac{1}{3}}$

$r_{12} = (x_1, L[x_2]) = \int_0^1 x(1-x)(6x-4)\, dx = \boxed{-\frac{1}{6}}$

$r_{21} = (x_2, L[x_1]) = -2 \int_0^1 x(1-x)^2\, dx = \boxed{-\frac{1}{6}}$

$r_{22} = (x_2, L[x_2]) = \int_0^1 x(1-x)^2(6x-4)\, dx = \boxed{-\frac{2}{15}}$

these are all simple polynomial integrals, to save time I used Mathematica.

$r = \begin{pmatrix} -\frac{1}{3} & -\frac{1}{6} \\ -\frac{1}{6} & -\frac{2}{15} \end{pmatrix} \Rightarrow r^{-1} = \frac{1}{ad - bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix} = \begin{pmatrix} -8 & 10 \\ 10 & -20 \end{pmatrix}$

o Finally:

$$\vec{B} = K^{-1}\cdot\vec{F} = \begin{pmatrix} -8 & 10 \\ 10 & -20 \end{pmatrix}\begin{pmatrix} \frac{1}{4} \\ \frac{7}{60} \end{pmatrix} = \begin{pmatrix} -\frac{5}{6} \\ \frac{1}{6} \end{pmatrix} \Rightarrow$$

$$\Rightarrow p(x) = -\frac{5}{6}x(1-x) + \frac{1}{6}x(1-x)^2.$$

. Analytical solution is: $\boxed{u(x) = \frac{x^3}{6} + \frac{x^2}{2} - \frac{2}{3}x}$.

. Galerkin:

$$p(x) = -\frac{5}{6}x(1-x) + \frac{1}{6}x(1-x)^2 =$$

Simplification...

$$= \boxed{\frac{x^3}{6} + \frac{x^2}{2} - \frac{2}{3}x} \rightarrow$$ Same as the exact analytical solution

Problem 2:

$$i\frac{\partial \Psi}{\partial t} + \nabla^2 \Psi - (V_1 + V_2)\Psi = 0.$$

(a) Using the standard solver, we would have $A = i(V_1+V_2)$. The condition that $e^{tA} \approx 1$ (required to have the operator close to commute: $e^{tA}e^{tB} = e^{tB}e^{tA}$) implies that:

$$tA << 1 \Rightarrow t\,|i(V_1+V_2)| << 1 \Rightarrow$$

$$\Rightarrow t\,|V_1+V_2| << 1 \Rightarrow \text{stronger restriction.}$$

$$\Rightarrow t(|V_1|+|V_2|) << 1 \Rightarrow$$

$$\Rightarrow t << \frac{1}{|V_1|+|V_2|} \Rightarrow t << \frac{1}{\frac{1}{a\sqrt{x^2+y^2+z^2+w^2}} + |\alpha(t)x|}.$$

Idea: Consider operator $e^{i\alpha(t)\cdot x}$ rather restrictive condition...

$\Psi(\vec r,t) \to e^{i\alpha(t)\cdot x}\,\varphi(\vec r,t)$.

The TDSE becomes:

$$i\frac{\partial}{\partial t}\left(e^{i\alpha(t)\cdot x}\varphi\right) + \nabla^2\left(e^{i\alpha(t)\cdot x}\varphi\right) - \left(V_1(\vec r) + V_2(\vec r,t)\right)\left(e^{i\alpha(t)\cdot x}\varphi\right) = 0 \Rightarrow$$

$$\Rightarrow i\Big(i x \underbrace{\cancel{\dot\alpha(t)}}_{=-a(t)} e^{i\alpha(t)x}\varphi + e^{i\alpha(t)x}\dot\varphi\Big) + e^{i\alpha(t)x}\nabla^2\varphi + \varphi\nabla^2\left(e^{i\alpha(t)x}\right) + 2\partial_x\left(e^{i\alpha(t)x}\right)\nabla\varphi - V_1 e^{i\alpha(t)x}\varphi - \cancel{V_2 e^{i\alpha(t)x}\varphi} = 0 \Rightarrow$$

$$\Rightarrow i\cancel{e^{i\alpha(t)x}}\dot\varphi + \cancel{e^{i\alpha(t)x}}\nabla^2\varphi - \alpha^2(t)\cancel{e^{i\alpha(t)x}}\varphi + 2i\alpha(t)\cancel{e^{i\alpha(t)x}}\frac{\partial\varphi}{\partial x} - V_1\cancel{e^{i\alpha(t)x}}\varphi = 0 \Rightarrow$$

$$\Rightarrow i\frac{\partial\varphi}{\partial t} = \underbrace{-\nabla^2\varphi - 2i\alpha(t)\frac{\partial\varphi}{\partial x} + \alpha^2(t)\varphi}_{B} + \underbrace{V_1\varphi}_{A}$$

· **For B:** $i\frac{\partial \psi}{\partial t} = -\nabla^2\psi - 2i\alpha(t)\frac{\partial \psi}{\partial x} + \alpha^2(t)\psi \Rightarrow$ 3.

$\mathcal{F}$:

$\Rightarrow i\frac{\partial \psi_k}{\partial t} = k^2\psi_k + 2k_x\alpha(t)\psi_k + \alpha^2(t)\psi_k \Rightarrow$

$\Rightarrow \frac{\partial \psi_k}{\partial t} = -i\left(k^2 + 2k_x\alpha(t) + \alpha^2(t)\right)\psi_k \Rightarrow$

$\Rightarrow \psi_k(t) = e^{-i\int_0^t k^2 + 2k_x\alpha(\tau) + \alpha^2(\tau)\,d\tau} \approx$

$= e^{-i\left(k^2 + 2k_x\alpha(t) + \alpha^2(t)\right)t}$

· For sufficiently small t. (Assumption).

· **For A:** $i\frac{\partial \psi}{\partial t} = V_i\psi \Rightarrow$

$\Rightarrow \partial_t\psi = -iV_i\psi \Rightarrow \psi(t) = e^{-iV_it}\psi(0).$

Final solution (propagator):

$P_{AB}(t,0) = e^{-iV_i\frac{t}{2}}\mathcal{F}^{-1}\left[e^{-i\left(k^2+2k_x\alpha(t)+\alpha^2(t)\right)t}\mathcal{F}\left[e^{-iV_i\frac{t}{2}}\cancel{\psi(0)}\right]\right].$

· Same that:

$\psi(t) = e^{-iV_i\frac{t}{2}}\mathcal{F}^{-1}\left[e^{-i\left(k^2+2k_x\alpha(t)+\alpha^2(t)\right)t}\mathcal{F}\left[e^{-iV_i\frac{t}{2}}\psi(0)\right]\right] + O(t^3).$

· Now, the time step:

$|V_it| \ll 1 \Rightarrow t \ll \frac{1}{\frac{1}{\sqrt{x^2+y^2+z^2+\varepsilon^2}}} = \sqrt{x^2+y^2+z^2+\varepsilon^2}$

· Not as strong of a restriction as before!

Also, before we had

$t \ll \frac{1}{\frac{1}{\sqrt{x^2+y^2+z^2+\varepsilon^2}} + |\alpha(t)\cdot x|}$

At worst:

$t \ll \frac{1}{\frac{1}{\sqrt{x^2+y^2+z^2+\varepsilon^2}} + E_{max}\cdot\omega}$

· Before:

· Since $E_{max}\cdot\omega$ is big,

· the time step had to be small.

·· Now: it can be bigger.

·· good! (Advantage)

Q1. Now, we have a different problem: the wavefunction will spread long distances due to the "prominent" displacement of the electric field. We can alter our wavefunction in a way such that we don't need as big of a simulation box. This will be done by the application of the translation operator $e^{\alpha(t)\partial_x}$.

(equivalent to changing the reference frame...)

$$e^{\alpha(t)\partial_x} = \sum_{n=0}^{+\infty} \frac{(\alpha(t)\frac{\partial}{\partial x})^n}{n!} = \underbrace{\hat{I}}_{\text{identity}} + \underbrace{i\alpha(t)\frac{\partial}{\partial x} + \frac{\alpha^2(t)}{2}\frac{\partial^2}{\partial x^2} + \dots}_{\text{Taylor Series}}$$

To verify that this corresponds to a translation, we can do:

$$\psi(\vec r, t) = \int d\vec k \, e^{-i\vec k\cdot\vec r}\, \psi_k(\vec k, t)$$

- Applying the operator: doing this explicitly

$$e^{\alpha(t)\partial_x}\psi(\vec r,t) = \int d\vec k \, \underline{e^{\alpha(t)\partial_x}}\ \underline{e^{-i\vec k\cdot\vec r}}\ \psi_k(\vec k, t) =$$

$$= \int d\vec k \, \boxed{e^{-i\vec k\cdot\vec r}\cdot e^{-ik_x\alpha(t)}}\ \psi_k(\vec k,t) =$$

$$= \int d\vec k \, e^{-i\vec k\cdot(\vec r+\alpha(t)\hat e_x)}\ \psi_k(\vec k, t) =$$

$$= \psi(\vec r + \alpha(t)\hat e_x, t) = \psi(\vec r + x_0 \hat e_x, t)$$

∴ translation is evident here.

In a classical approximation:

$$\ddot x_0 = -\frac{\partial V}{\partial x} = -\frac{\partial (V_i + V_e)}{\partial x} = -\frac{\partial V_e}{\partial x} = -a(t).$$

we can neglect V_i far away (since the paper assumes: this + external field is stronger than coulombic field)

$$\Rightarrow \boxed{\ddot\alpha(t) = -a(t)}$$ this time.

Finally introducing this in the TDSE:

$$i\frac{\partial}{\partial t}\left(e^{\alpha(t)\partial_x}\psi\right) + \frac{\nabla^2}{2}\left(e^{\alpha(t)\partial_x}\psi\right) - (V_i + V_e)\left(e^{\alpha(t)\partial_x}\psi\right) = 0 \Rightarrow$$

$$\Rightarrow i\dot\alpha\,\partial_x\psi + i\dot\psi + \frac{\nabla^2}{2}\psi - V_i\psi - a(t)\,x\,\psi = 0.$$

(after commuting the translation with $e^{-\alpha(t)\partial_x}$).

$$\Rightarrow i\,\partial_t \psi = -\partial_x^2 \psi - i\dot{\alpha}\,\partial_x \psi + (V_i + V_e)\psi \Rightarrow$$

$$\Rightarrow \partial_t \psi = \underbrace{-i\left(-\partial_x^2 - i\dot{\alpha}\,\partial_x\right)\psi}_{B} \underbrace{- i\left(V_i + V_e\right)\psi}_{A} \quad (4)$$

Part B:

$$\partial_t \psi = -i\left(-\partial_x^2 - i\dot{\alpha}\,\partial_x\right)\psi \overset{F.T.}{\Longrightarrow}$$

$$\Rightarrow \partial_t \psi_k = -i\left(k^2 + k_x \dot{\alpha}\right)\psi_k \Rightarrow$$

$$\Rightarrow \psi_k \propto e^{-i(k^2 + k_x\dot{\alpha})t}$$

Part A:

$$\partial_t \psi = -i\left(V_i + V_e\right)\psi \Rightarrow \psi(t) = e^{-i(V_i+V_e)t}\,\psi(0)$$

$$\Rightarrow \underline{\text{Split}(t=0)}: \; e^{-i(V_i+V_e(t+1))\frac{t}{2}}\, \mathcal{F}^{-1}\!\left[e^{-i(k^2+k_x\dot{\alpha})t}\; \mathcal{F}\!\left[e^{-i(V_i+V_e(0))\frac{t}{2}}\right.\right.$$

(propagator)

Split Step:

$$\psi(t) = e^{-i(V_i+V_e(t))\frac{t}{2}}\, \mathcal{F}^{-1}\!\left[e^{-i(k^2+k_x\dot{\alpha})t}\; \mathcal{F}\!\left[e^{-i(V_i+V_e(0))\frac{t}{2}}\,\psi(0)\right]\right]$$

We have thus solved the problem with this approach. We no longer require an unreasonably large simulation box size.

r: I don't worry much about the time step here, as I reckon that's not the main point of question 6. (that would be 7!).