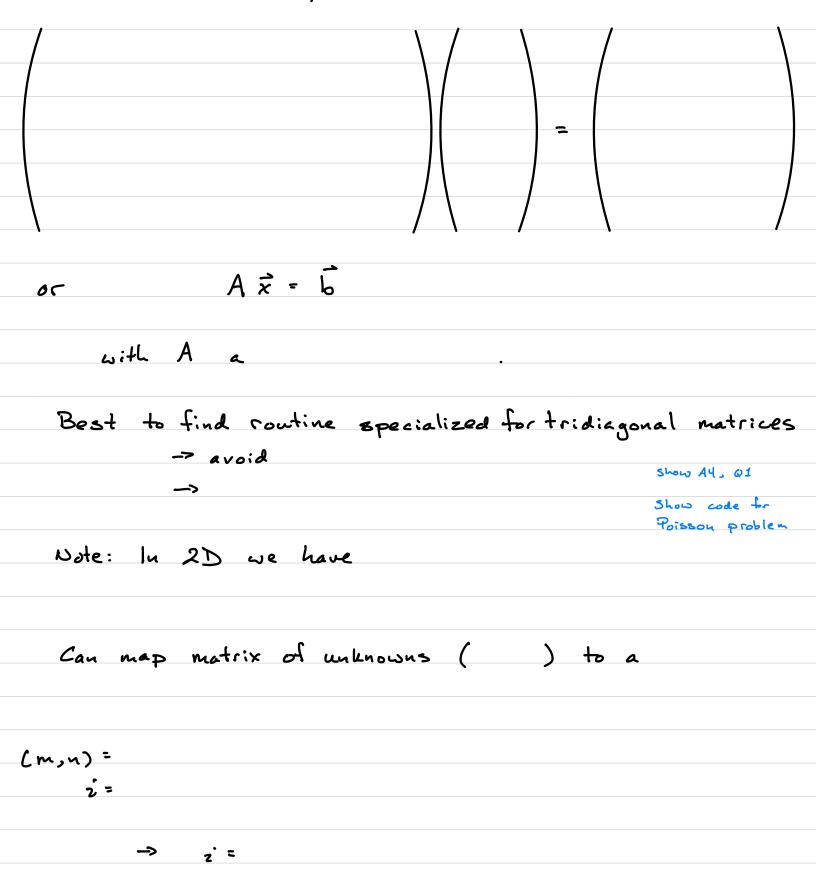
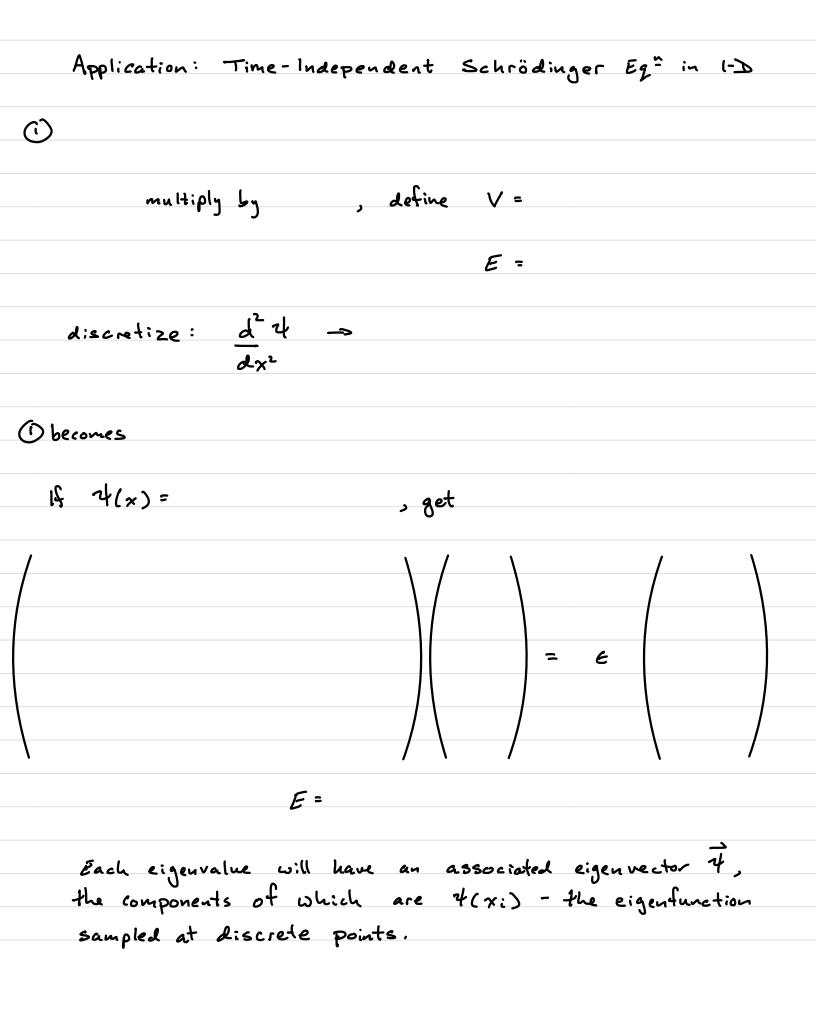
Application of solving a linear system: 1-D Poisson Equation V is electrostatic potential associated with or gravitational potential with Discretize second derivative and get ______ fu = h = , n= X0 < and we assume that we know V0 = VN+1 = We get NSI n=2 **Ν·3** : n=N

which is a matrix equation



Eigenvalue Problems especially from QM, can be Many physics problems, expressed as \bigcirc $a_{11} \times_1 + a_{12} \times_2 + \ldots + a_{1N} \times_N = \lambda \times_1$ like system of linear eq=s, except and solutions exist only for - Solutions are () can be rewritten as For non-trivial solution (), this implies , for which an NXN matrix leads to an which has N solutions for), i.e., Finding all roots for an N-Legree polynomial

Rather than solving the difficult polynomial problem, e.g. see Jacobi method for symmetric matrices (which employs "Givens rotations") or a general method based on QR decomposition. Let A_o = A k = Q -R-upper triangular set Ak+1 = Ak converges to an - eigenvalues of an upper triangular matrix are LAPACK : Different routines for different types of matrices.



Shows code for AU Q2 Notes on A4 Q2 For harmonic potential i) V(x) = 1 m w² x², energy eigenvalues are 2) $E_n = t_{12} (n - \frac{1}{2}), n = 1, 2, ...$ Here h= , m= 30 V(x)= En= Now V(x) = ω: : تك

For 3D problems, having
$$N^3$$
 gridpoints makes
the problem difficult.
Alternative: write wavefunctions as a linear
combination of
 $\psi(\vec{r}) =$
The $\psi_{\mathcal{B}}(\vec{r})$'s are known functions that solve part of
the problem. E.g.
Goal is to find coefficients that solve the S.G.
 $-\nabla^2 t + V(\vec{r})t = E t$
multiply by $\psi_{\mathcal{A}}^*$ and integrate
 $\sum_{\mathcal{A}} \int d^{2\vec{r}} \psi_{\mathcal{A}}^*(\vec{r}) (-\nabla^2 + V(\vec{r})) \psi_{\mathcal{B}}(\vec{r}) \alpha_{\mathcal{B}}$
 $= E \sum_{\mathcal{A}} \int d^{2\vec{r}} \psi_{\mathcal{A}}^*(\vec{r}) \psi_{\mathcal{B}}(\vec{r}) \alpha_{\mathcal{B}}$
Define elements of two matrices
 $H_{\mathcal{A}\mathcal{B}} = \int d^{3\vec{r}}$ (overlap matrix)

Schrödinger Equation becomes $\sum_{\beta} = E \sum_{\beta}$ or A - generalized eigenvalue problem -If q's are orthonormal, then and we get If not, need to transform #, as through a Cholesky factorization, an LU decomposition of a positive-definite Hermitian matrix S: S = L L (Lij = Lji) lower triangular * becomes HIA = ELLTA $H(L^{\dagger})^{-1}L^{\dagger}a^{\dagger} = EL(L^{\dagger}a)$ $L'H(L^{\dagger})'(L^{\dagger}\bar{a}) = E(L^{\dagger}\bar{a})$