1. The matrix method

We want a general method for solving the 1D Schrodinger eqn. (time independent)

$$H \psi_n(x) = E^{(n)} \psi_n(x) \qquad (1.1)$$

where H is the Hamiltonian, and $E^{(n)}$ and $\psi_n(x)$ are the energy eigenvalue and wavefunction of the nth level. We will consider potentials which have discrete spectra. The wavefns are orthonormal,

$$\int_{-\infty}^{\infty} \psi_m^*(x)\, \psi_n(x)\, dx = \delta_{mn} \,. \qquad (1.2)$$

The idea is to expand the wavefn in terms of another orthonormal set of basis functions $\phi_i(x)$. (Later we will choose these to be harmonic oscillator functions, but this isn't relevant yet.) So we have

$$\psi_n(x) = \sum_{i=0}^{\infty} c_i^{(n)} \phi_i(x) \qquad (1.3)$$

$$\int_{-\infty}^{\infty} \phi_j^*(x)\, \phi_i(x)\, dx = \delta_{ij} \qquad (1.4)$$

where c_i is a coefficient. Multiplying (1.3) by $\phi_j^*(x)$ and integrating gives

$$\int_{-\infty}^{\infty} \phi_j^*(x)\, \psi_n(x)\, dx = \sum_{i=0}^{\infty} c_i^{(n)} \delta_{ij} = c_j^{(n)}$$

So the expression for $c_i^{(n)}$ is

$$c_i^{(n)} = \int_{-\infty}^{\infty} \phi_i^* \psi_n \, dx \qquad (1.5)$$

Using (1.3) in (1.1) gives

$$\sum_{i=0}^{\infty} c_i^{(n)} H \phi_i(x) = \cancel{E^{(n)} \psi_n(x)}\; E^{(n)} \psi_n(x) \qquad (1.6)$$

then putting $\phi_j^*(x)$ on the left

$$\sum_{i=0}^{\infty} c_i^{(n)} \phi_j^*(x) H \phi_i(x) = E^{(n)} \cancel{\sum_{i=0}^{\infty}} \phi_j^*(x) \psi_n(x) \qquad (1.7)$$

and integrating,

$$\cancel{\sum_i c_i^{(n)} (H)_{ij}}$$

$$\sum_i c_i^{(n)} \int_{-\infty}^{\infty} \phi_j^*(x) H \phi_i(x)\, dx = E^{(n)} c_j^{(n)} \qquad (1.8)$$

defining

$$H_{ji} = \int_{-\infty}^{\infty} \phi_j^*(x)\, H\, \phi_i(x)\, dx \qquad (1.9)$$

gives

$$\sum_{i=0}^{\infty} c_i^{(n)} H_{ji} = E^{(n)} c_j^{(n)} \qquad (1.10)$$

This is a set of equations for each j, ie

$$c_1^{(n)} H_{11} + c_2^{(n)} H_{12} + \dots = E^{(n)} c_1^{(n)}$$

$$c_1^{(n)} H_{21} + c_2^{(n)} H_{22} + \dots = E^{(n)} c_2^{(n)}$$

$$\vdots \qquad\qquad\qquad \vdots$$

which is a matrix equation,

$$\begin{pmatrix} H_{11} & H_{12} & \cdots \\ H_{21} & H_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} c_1^{(n)} \\ c_2^{(n)} \\ \vdots \end{pmatrix} = E^{(n)} \begin{pmatrix} c_1^{(n)} \\ c_2^{(n)} \\ \vdots \end{pmatrix} \qquad (1.11)$$

Eqn. (1.10) is exact but for the matrix eqn (1.11) we need matrices of finite size, which is the same as truncating the sum in (1.10); thus is no longer exact. Eqn (1.11) can be written

$$\underline{\underline{H}}\, \underline{x}^{(n)} = E^{(n)} \underline{x}^{(n)} \qquad (1.12)$$

So for a given problem we construct the matrix $\underline{\underline{H}}$ by filling out its entries using (1.9). We would then use a software package to find the eigenvalues $E^{(n)}$ and eigenvectors $\underline{x}^{(n)}$ of $\underline{\underline{H}}$. If we choose $\underline{\underline{H}}$ to be an $N \times N$ matrix, then we will have N eigenvalues and N eigenvectors, namely

n will run from 1 to N. We are most interested in the eigenvalues, but also the eigenvectors are interesting, because these are column vectors of coefficients

$$\underline{x}^{(n)} = \begin{pmatrix} c_1^{(n)} \\ c_2^{(n)} \\ \vdots \\ \vdots \end{pmatrix} \qquad (1.13)$$

and so are equivalent to the wavefunctions, due to (1.3).

Note that if we increase the size of the matrix (N) we will get more accurate results.

You should repeat all of this in Dirac notation, and make sure you understand that. I suggest you use round brackets for the wavefns you are trying to find, and angled brackets for the (harmonic oscillator) basis functions, ie

$$\langle x | n) = \psi_n(x) \qquad (1.14)$$

$$\langle n | i \rangle = \phi_i(x)$$

In Dirac notation the previous steps are

$$H | n) = E^{(n)} | n) \qquad (1.1^*)$$

$$(m | n) = \delta_{mn} \qquad (1.2^*)$$

$$| n) = \sum_{i=0}^{\infty} | i \rangle \langle i | n) \qquad (1.3^*)$$

$$\langle j | i \rangle = \delta_{ij} \qquad (1.4^*)$$

$$\langle i | n) = \int_{-\infty}^{\infty} \langle i | x \rangle \langle x | n) \qquad (1.5^*)$$

$$\sum_i H | i \rangle \langle i | n) = \sum_i E^{(n)} | n) \qquad (1.6^*)$$

$$\sum_i \langle j | H | i \rangle \langle i | n) = \sum_i E^{(n)} \langle j | n) \qquad (1.8^*)$$

$$\langle j | H | i \rangle = \int_{-\infty}^{\infty} \langle j | x \rangle H \langle x | i \rangle \, dx \qquad (1.9^*)$$

$$\sum_i \langle j | H | i \rangle \langle i | n) = E^{(n)} \langle j | n) \qquad (1.10^*)$$

$$\begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle & \cdots \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \langle 1|n\rangle \\ \langle 2|n\rangle \\ \vdots \end{pmatrix} = E^{(n)} \begin{pmatrix} \langle 1|n\rangle \\ \langle 2|n\rangle \\ \vdots \end{pmatrix} \quad (1.11^*)$$

$$x^{(n)} = \begin{pmatrix} \langle 1|n\rangle \\ \langle 2|n\rangle \\ \vdots \end{pmatrix} \quad (1.13^*)$$

2. Harmonic oscillators

We will use HOs for the basis functions, so you should review and understand the treatment of HOs particularly in terms of ladder operators. As described in several textbooks (eg Griffiths) it is convenient to make everything dimensionless. Then the Hamiltonian is

$$H = \frac{1}{2}\left(-\frac{d^2}{dx^2} + x^2\right) \qquad (2.1)$$

and the Schrodinger eqn

$$H \phi_i(x) = E_i \phi_i(x) \qquad (2.2)$$

has solns with energies

$$E_i = i + 1/2 \qquad (2.3)$$

Better to write it in terms of Dirac notation,

$$H|i\rangle = E_i |i\rangle \qquad (2.4)$$

In terms of operators

$$H = a^+ a + \frac{1}{2} \qquad (2.5)$$

with

$$\left.\begin{aligned} a &= \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right) \\ a^+ &= \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right) \end{aligned}\right\} \qquad (2.6)$$

Later you will definitely need

$$\left.\begin{aligned} a\,|i\rangle &= \sqrt{i}\,|i-1\rangle \\ a^{+}\,|i\rangle &= \sqrt{i+1}\,|i+1\rangle \end{aligned}\right\} \quad (2.7)$$

3. Power series potential

Consider a Hamiltonian where everything is dimensionless, so

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + V(x) , \tag{3.1}$$

where $V(x)$ is some power series

$$V(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + \ldots \tag{3.2}$$
$$= \sum_k^{k_{max}} a_k x^k$$

We want a general method for ~~finding~~ solving the Schrodinger eqn for such a potential. Why is this interesting?

(i) Some potentials which explicitly have this form are interesting in their own right. Eg the "double-well" potential can be written

$$V(x) = \alpha x^2 + \beta x^4 \tag{3.3}$$

with $\alpha < 0$ and $\beta > 0$. It would be nice to have a general method for solving such potentials.

(ii) More importantly, we can take any potential and do a Taylor Series expansion

$$V(x) = V(x_0) + (x - x_0) V'(x_0) + \frac{(x-x_0)^2}{2} V''(x_0) + \frac{(x-x_0)^3}{6} V'''(x_0) + \ldots \qquad (3.4)$$

and so re-cast it in the form (3.2). So in principle we can then use the technique to solve for any potential, provided it is well represented by a Taylor series.

Often we expand about the minimum, so $V'(x_0)=0$, and can choose the minimum to be at $x_0 = 0$, so that

$$V(x) = V(x_0) + \frac{V''(0)}{2} x^2 + \frac{V'''(0)}{6} x^3 + \ldots \qquad (3.5)$$

So. We want to solve

$$H = -\frac{1}{2}\frac{d^2}{dx^2} + \sum_{k=0}^{k_{max}} a_k x^k \qquad (3.6)$$

How to proceed?

The only thing you need to solve your problem is to construct the matrix $\underline{\underline{H}}$. In other words, you need to find a general expression for the matrix elements

$$\langle j | H | i \rangle .$$

These matrix elements are actually integrals — see eqn (1.9*) — but there is a clever way of avoiding the integrals all together.

Start by inverting eqns (2.6), so that you have an expression for x and $\frac{d}{dx}$ in terms of operators a and a^+. Then you can re-write Hamiltonian (3.6) in terms of a and a^+.

[redacted]

Then you can evaluate $\langle j | H | i \rangle$ using relations (2.7) and orthogonality (1.4*).

So, I suggest [redacted] you derive a general expression for $\langle j | H | i \rangle$ with $k_{max} = 4$, say. Good luck!