Time Independent Perturbation

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1 What: What are we doing

We are calculating the eigenvalues for non-analytic potentials, or more accurately for potentials that have a small deviation that makes them no longer analytic.

We are using time independent non degenerative perturbation theory

2 Why: Why are we doing it

This is a solver that provides an alternative to the direct eigensolver that we see in the 1D eigensolver. This calculates for a single (non degenerate) state the eigenvectors using a perturbative approach. This allows us to see the beam profile in a single slice of our laser

3 How: How are we designing this?

We begin by enumerating the perturbative approach beginning from the Schödinger equation

$$\hat{\mathbf{H}} |\psi_n\rangle = E_n |\psi_n\rangle \tag{1}$$

Where our full Hamiltonian is equal to some (usually analytic) $\hat{\mathbf{H}}_\mathbf{o}$, plus an additional perturbative Hamiltonian, $\hat{\mathbf{H}}'$. Our analytic Hamiltonian obeys the following, which will establish our notation

$$\hat{\mathbf{H}} = \hat{\mathbf{H}}_\mathbf{o} + \hat{\mathbf{H}}' \tag{2}$$

$$\hat{\mathbf{H}}_\mathbf{o} |\psi_n^{(0)}\rangle = E_n^{(0)} |\psi_n^{(0)}\rangle \tag{3}$$

Because the eigenvalues of our hamiltonian form a complete basis set, we can write the eigenvectors of our full hamiltonian as a linear combination of them

$$|\psi_n\rangle = \sum_k c_{kn} |\psi_n^{(0)}\rangle \tag{4}$$

plugging this into our equation gives

$$(\hat{\mathbf{H_o}} + \hat{\mathbf{H}'}) \sum_k c_{kn} \left|\psi_k^{(0)}\right\rangle = E_n \sum_k c_{kn} \left|\psi_k^{(0)}\right\rangle \tag{5}$$

$$\sum_k c_{kn} (E_k^{(0)} + \hat{\mathbf{H}'}) \left|\psi_k^{(0)}\right\rangle = E_n \sum_k c_{kn} \left|\psi_k^{(0)}\right\rangle \tag{6}$$

$$\sum_k c_{kn} \hat{\mathbf{H}'} \left|\psi_k^{(0)}\right\rangle = \sum_k (E_n - E_n^{(0)}) c_{kn} \left|\psi_k^{(0)}\right\rangle \tag{7}$$

now, since we have an operator and our ultimate goal is to calculate it's matrix elements, we take the inner product of both sides with a bra vector, another eigenvector of our analytic hamiltonian. The index is arbitrary in the same sense that n is arbitrary, and simply refers to two different energy levels, and so 2 different indices in our matrix

$$\sum_k c_{kn} \left\langle\psi_m^{(0)}\right| \hat{\mathbf{H}'} \left|\psi_k^{(0)}\right\rangle = \sum_k c_{kn} \left\langle\psi_m^{(0)}\right| (E_n - E_n^{(0)}) \left|\psi_k^{(0)}\right\rangle \tag{8}$$

$$\sum_k c_{kn} \left\langle\psi_m^{(0)}\right| \hat{\mathbf{H}'} \left|\psi_k^{(0)}\right\rangle = \sum_k c_{kn} (E_n - E_k^{(0)}) \delta_{mk} \tag{9}$$

$$\sum_k c_{kn} \left\langle\psi_m^{(0)}\right| \hat{\mathbf{H}'} \left|\psi_k^{(0)}\right\rangle = c_{mn} (E_n - E_m^{(0)}) \tag{10}$$

Here we begin to apply some useful approximations. We assume that both c_{kn} and E_n can be written as an infinite series of contributions, each decreasing in size. In order to represent the magnitude of the 'smallness' in a clear way, we introduce λ in order to keep track of the order of 'smallness.' Powers of λ indicate the orders of smallness, however λ is unitary the true size is indicated by the superscript. We assume any arbitrary variable ξ obeys

$$\xi^{(0)} > \xi^{(1)} > \xi^{(2)} > \dots$$

as well as

$$\xi^{(n)} \eta^{(m)} \sim \xi^{(n+m)} \tag{11}$$

and again with $\lambda = 1$ we write

$$c_k n = c_{kn}^{(0)} + \lambda c_{kn}^{(1)} + \lambda^2 c_{kn}^{(2)} + \lambda^3 c_{kn}^{(3)} + \dots \tag{12}$$

$$= \delta_{kn} + \lambda c_{kn}^{(1)} + \lambda^2 c_{kn}^{(2)} + \lambda^3 c_{kn}^{(3)} + \dots \tag{13}$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \lambda^3 E_n^{(3)} + \dots \tag{14}$$

$$\tag{15}$$

And substituting into Eq.10

$$\sum_k (c_{kn}^{(0)} + \lambda c_{kn}^{(1)} + \lambda^2 c_{kn}^{(2)} + \lambda^3 c_{kn}^{(3)} + \dots) \left\langle\psi_m^{(0)}\right| \hat{\mathbf{H}'} \left|\psi_k^{(0)}\right\rangle \tag{16}$$

$$= (c_{mn}^{(0)} + \lambda c_{mn}^{(1)} + \lambda^2 c_{mn}^{(2)} + \dots)(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots - E_m^{(0)}) \tag{17}$$

grouping into powers of λ is ~~a pain in the ass~~ left as an exercise to the reader

$$\hat{\mathbf{H}'}_{kn} = \langle \psi_k^{(0)} | \, \hat{\mathbf{H}'} \, | \psi_n^{(0)} \rangle \tag{18}$$

$$\langle \psi_k | \hat{\mathbf{H}'} | \psi_n \rangle \neq \langle \psi_k^{(0)} | \, \hat{\mathbf{H}'} \, | \psi_n^{(0)} \rangle \tag{19}$$

$$\tag{20}$$

When solving for the cases $k = n$ and $k \neq n$, the following results are obtained, that

$$c_{mk}^{(1)} = \frac{\hat{\mathbf{H}'}_{mk}}{E_n^{(0)} - E_m^{(0)}} \tag{21}$$

$$E_k^{(1)} = \hat{\mathbf{H}'}_{kk} \tag{22}$$

This allows for us to finally calculate the first degree solutions, that

$$c_{kn} = c_{kn}^{(0)} + \frac{\hat{\mathbf{H}'}_{mk}}{E_n^{(0)} - E_m^{(0)}} \tag{23}$$

$$E_n = E_n^{(0)} + \hat{\mathbf{H}'}_{kk} \tag{24}$$

$$\tag{25}$$

we now have our eigenvalues for our full Hamiltonian, as well as a way to construct our eigenstates. With einstein notation (summing over repeated indices)

$$|\psi_n\rangle = c_{kn} \, |\psi_k\rangle \tag{26}$$

in einstein notation this has the form of a matrix-vector multiplication. In numpy (as returned from eigh), our eigenstate set is in a matrix whose column vectors are (in order) our eigenstates.

This allows us to write out our set of true eigenstates as a matrix multiplication from our unperturbed eigenstates

$$\big[\psi\big] = \big[\psi_o\big] \, \big[\mathbf{c}\big] \tag{27}$$

The order of multiplication comes from our intended result, and since we don't treat our c_{mn} coefficients as an operator, this is ok

to actually calculate c_{mn} we preform the following matrix operations, mized in with a bit of numpy's element-wise vector operations

we preform a normal change of basis operator going from our perturbed to unperturbed basis

$$\big[\hat{\mathbf{H}'}\big]_o = \big[\boldsymbol{\psi}\big]^T \, \big[\hat{\mathbf{H}'}\big] \, \big[\boldsymbol{\psi}\big] \tag{28}$$

next (using $\cdot$ to indicate an element wise operation) we produce

$$E_n, E_m = \text{Meshgrid}(\mathbf{E}, \mathbf{E}) \tag{29}$$

$$\implies \big[\hat{\mathbf{H}'}\big]_o \cdot \frac{1}{(E_n - E_m + \hat{\mathbf{1}})} \cdot \hat{\boldsymbol{\Upsilon}} \tag{30}$$

$$\tag{31}$$

where Υ is consructed via

$_{mn} = 1 - \delta_m n$

so that by multiplication, it sends the entire diagnoal to zero
the addition of an identity vector removes divide by zeros
finally, we have

$$\left[\mathbf{c_{mn}}\right] = \hat{\mathbf{1}} + \left[\hat{\mathbf{H}'}\right]_o \cdot \frac{1}{(E_n - E_m)} \tag{32}$$

for second order, we have

$$c^{(2)}_{mn} = \frac{1}{E^{(0)}_n - E^{(0)}_m} \left(-\frac{\hat{\mathbf{H}'}_{mn}\hat{\mathbf{H}'}_{nn}}{E^{(0)}_n - E^{(0)}_m} + \sum_{k \neq n} \frac{\hat{\mathbf{H}'}_{mk}\hat{\mathbf{H}'}_{kn}}{E^{(0)}_n - E^{(0)}_k} \right) \tag{33}$$

which we can recognize via index notation can actually be rewritten as

$$c^{(2)}_{mn} = \frac{1}{E^{(0)}_n - E^{(0)}_m} \left(-\left[c^{(1)}_{mn}\right] \cdot \hat{\mathbf{H}'}_{nn} + \left[\hat{\mathbf{H}'}\right]\left[c^{(1)}\right] \right) \tag{34}$$

- The c_{mn} coefficients, at least calculated numerically, do not produced an orthonormal basis
- When using matrix multiplications or element wise applications, it is extremely important to keep track of the row-column meanings of subscripts

4 How: Future steps