How to obtain the gradients

Note Title 4/1/2009

In your fitting routine, you are trying to minimize the mean square deviation between data, $\{d_i\}$, and theory, $\{t_i\}$, i.e.

$$\min_{E_J, E_L, E_C} f(E_J, E_C, E_L) = \frac{1}{N}\sum_{i=1}^{N}(d_i - t_i)^2.$$

Minimization may be quicker if there is an efficient way to provide the partial derivatives

$$\partial f/\partial E_J, \quad \partial f/\partial E_C, \quad \text{and} \quad \partial f/\partial E_L.$$

We have

$$\frac{\partial f}{\partial E_*} = \frac{2}{N}\sum_{i=1}^{N}(d_i - t_i)\cdot\frac{\partial t_i}{\partial E_*}$$

Each theory value t_i is obtained as an eigenvalue of our CPBL Schrödinger eq. for some specific flux,

$$(*) \qquad H|\psi\rangle = E|\psi\rangle \qquad \text{and} \qquad t_i = E.$$

Note: This is the case where you fit the levels themselves. There will be small modifications for the case where you fit to the energy differences $E_j - E_0$. Try whether you can figure this out based on the case I am treating here.

The Hamiltonian H, its eigenvalue E and the eigenstate $|\psi\rangle$ all depend on E_L, E_J, and E_C. Let us consider the partial derivative of $(*)$:

$$\frac{\partial}{\partial E_*}\left[H|\psi\rangle\right] = \frac{\partial}{\partial E_*}\left[E|\psi\rangle\right]$$

$$\Leftrightarrow \quad \frac{\partial H}{\partial E_*}|\psi\rangle + H\frac{\partial}{\partial E_*}|\psi\rangle = \frac{\partial E}{\partial E_*}|\psi\rangle + E\frac{\partial}{\partial E_*}|\psi\rangle$$

Now let us multiply the whole equation with the bra $\langle\psi|$ from the left:

$$\Rightarrow \quad \langle\psi|\frac{\partial H}{\partial E_*}|\psi\rangle + \langle\psi|H\frac{\partial}{\partial E_*}|\psi\rangle = \langle\psi|\frac{\partial E}{\partial E_*}|\psi\rangle + \langle\psi|E\frac{\partial}{\partial E_*}|\psi\rangle$$

$$\Rightarrow \quad \langle\psi|\frac{\partial H}{\partial E_*}|\psi\rangle + E\langle\psi|\frac{\partial}{\partial E_*}|\psi\rangle = \frac{\partial E}{\partial E_*} + E\langle\psi|\frac{\partial}{\partial E_*}|\psi\rangle$$

$$\Rightarrow \quad \boxed{\frac{\partial E}{\partial E_*} = \langle\psi|\frac{\partial H}{\partial E_*}|\psi\rangle}$$

This is what you need to provide the partial derivatives!

Note:

- Here, $|\psi\rangle$ is the eigenstate that you already calculated when diagonalizing the CPBL Hamiltonian.
- The partial derivatives are simple matrix elements of $\partial H/\partial E_*$ with respect to $|\psi\rangle$.
- You will have to generate the matrices $\partial H/\partial E_*$. For example:

$$H = -4E_C\frac{d^2}{d\varphi^2} - E_J\cos\left(\varphi + \frac{2\pi\phi}{\phi_0}\right) + \frac{E_L}{2}\varphi^2$$

$$\Rightarrow \frac{\partial H}{\partial E_J} = -\cos\left(\varphi + \frac{2\pi\phi}{\phi_0}\right)$$

For the numerics, you will proceed to rewrite this in your harmonic oscillator basis!