Time-Independent Perturbation Theory

Qualitative Aspects

As you know, the most important application of time-independent perturbation theory is the calculation of the fine and hyperfine structure of atoms and molecules.

- (a) Hydrogen Fine Structure. Explain the physical origins of the fine structure of hydrogen. Explain how TIPT is used to calculate the fine-structure energy corrections.
- (b) Hydrogen Hyperfine Structure. Explain the physical origins of the hyperfine structure of hydrogen. Explain how TIPT is used to calculate the hyperfine-structure energy corrections.
- (c) Applied Magnetic Fields. Explain the application of TIPT to the Zeeman effect in hydrogen.
- (d) Applied Electric Fields. Explain the application of TIPT to the Stark effect in hydrogen.

As you know, time-independent perturbation theory gives us a wonderful, systematic method to calculate the changes in the eigenenergies and the eigenkets when a perturbation Hamiltonian H_1 is applied to a known Hamiltonian H_0 .

- (e) Write down the time-independent perturbation theory equation that describes the perturbed energy as a series of corrections to the unperturbed energy.
- (f) Write down the time-independent perturbation theory equation that describes the perturbed wavefunction as a series of corrections to the unperturbed wavefunction.

Write both of these equations down to as high an order as you remember, or to as high an order as you have in your notes, or

- (g) Explain in detail what these equations mean, and how we use them to solve interesting problems.
- (h) Explain degenerate-state time-independent perturbation theory: How does it work? Why do we need it? What is the most interesting problem that you've solved (or seen solved) using it? What equations do you know that apply to it, and how do they work?

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Quantitative Aspects 1

Consider the perturbation caused by putting a "quantum mechanical potential brick" with potential V into the center of an infinite square well. Let your well extend from -a to +a, so the unperturbed wavefunctions are given by

$$\psi_n(x) = \sqrt{\frac{1}{a}} \cos\left(\frac{n\pi x}{2a}\right)$$
 for n odd
 $\psi_n(x) = \sqrt{\frac{1}{a}} \sin\left(\frac{n\pi x}{2a}\right)$ for n even

and let the perturbation extend from -b to +b, so the perturbation is given by

$$V_0(x) = 0 \quad \text{for } -\mathbf{a} \le \mathbf{x} < -\mathbf{b}$$
$$V_0(x) = V \quad \text{for } -\mathbf{b} \le \mathbf{x} \le +\mathbf{b}$$
$$V_0(x) = 0 \quad \text{for } +\mathbf{b} < \mathbf{x} \le +\mathbf{a}.$$

- (a) Calculate the first-order TIPT correction to the ground state energy.
- (b) Calculate the first-order TIPT correction to the ground state wavefunction.
- (c) Calculate the second-order TIPT correction to the ground state energy.
- (d) Calculate the second-order TIPT correction to the ground state wavefunction.
- (e) Sketch and explain the shape of the perturbed ground state wavefunction compared to the unperturbed ground state wavefunction. Treat both cases, namely V > 0 and V < 0.

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Quantitative Aspects 2

Consider a two-level system described by the unperturbed Hamiltonian H_0

$$H_0 = \begin{pmatrix} 3000 & 0\\ 0 & 1000 \end{pmatrix}$$

that is perturbed by a time-independent H_1

$$H_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

- (a) Calculate the first-order TIPT corrections to the ground state energy.
- (b) Calculate the first-order TIPT corrections to the ground state eigenvector.
- (c) Calculate the second-order TIPT corrections to the ground state energy.
- (d) Calculate the second-order TIPT corrections to the ground state eigenvector.
- (e) Find the exact eigenvalues and eigenvectors of H_0 .
- (f) Find the exact eigenvalues and eigenvectors of $H = H_0 + H_1$.
- (g) Compare your TIPT ground state energy and eigenvector with the exact ground state energy and eigenvector.