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Final Report

Week 1: Symmetries, conservation laws, degeneracies

- **Show that if a Hamiltonian is invariant with respect to a symmetry operator, then the associated generator is a constant of the motion (is conserved).**

If H is invariant with respect to a symmetry operator U, then $[H, U] = 0$ or $H = U^\dagger H U$. This implies $U^\dagger U = 1$, or that U is unitary. We can then expand the unitary operator U using the same arguments in showing the generator of an operator:

$$U = 1 - \frac{i\epsilon}{\hbar} G + \mathcal{O}(\epsilon^2) \tag{1}$$

Then, since U is unitary, G is left unchanged by the conjugation, implying G is a Hermitian operator. Then, expanding the invariance statement earlier made,

$$\begin{aligned} \left(1 + \frac{i\epsilon}{\hbar} G + \mathcal{O}(\epsilon^2)\right) H \left(1 - \frac{i\epsilon}{\hbar} G + \mathcal{O}(\epsilon^2)\right) &= H \\ \epsilon^0 : \qquad H &= H \\ \epsilon^1 : \qquad \frac{i}{\hbar} GH \frac{-i}{\hbar} G &= H \end{aligned} \tag{2}$$

so that $[G, H] = 0$. Then, we can use Heisenberg's equation of motion for G since it's a Hermitian observable:

$$\frac{dG}{dt} = \frac{1}{i\hbar}[G, H] = 0 \tag{3}$$

implying G as a constant of motion. (cf. Noether's theorem)

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Week 2: Spatial inversion, parity

- **Give the relationship between the parity of the angular momentum eigenfunctions (spherical harmonics) and the quantum number ℓ.**

Given π as the parity operator, we know that the eigenvalue equation for the spherical harmonics eigenfunctions are

$$\pi \left| n\ell m \right\rangle = (-1)^\ell \left| n\ell m \right\rangle, \tag{4}$$

thus the eigenvalues of π are $(-1)^\ell$.

- **Provide physical situations in which matrix elements between parity eigenstates vanish and lead to convenient selection rules.**

  Laporte's rule: radiative transitions take place between states of opposite parity as a consequence of multipole expansion formalism. First shown by Wigner to be a consequence of the parity-selection rule.

  Nondegenerate energy eigenstates cannot possess a permanent electric dipole moment, if their Hamiltonian is invariant under parity. A direct contradiction is the Stark effect, which is degenerate.

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Week 3: Lattice translations, time reversal

- **Show that a discrete lattice translational invariance leads to conserved crystal momentum.**

  Since discrete lattice translational invariance is observed, Bloch's theorem applies. From Bloch's theorem, $\psi_k(x) = e^{ikx}u(x)$ where $u(x)$ is also periodic (or lattice translational invariant). Then, for one k, several E_k may show up (cf. band structures), which leads to Bragg's law, where we have the same k value (crystal momentum) modulo a reciprocal lattice vector g, but translated energies (and therefore translation in the lattice).

- **Provide some examples of physical systems with broken time reversal symmetry. It would be instructive if you describe how the symmetry is broken when the arrow of time is reversed in some of these examples.**

  1. Introducing an external magnetic field: breaks the symmetry by introducing the extra kinetic energy term from the magnetic vector potential (which does not commute with the time reversal operator).
  2. Existence of a nonzero electric dipole moment in the nucleus. Gives a Hamiltonian term proportional to $\mathbf{S}$ which is odd under time reversal.

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Week 4: Perturbation theory (non-degenerate)

- **What conditions need to be satisfied for non-degenerate perturbation theory to be applicable to a given Hamiltonian?**

  Perturbation can be characterized by some parameter $\lambda << 1$ for which we can write the Hamiltonian as a sum of the unperturbed part (assumed to be time-independent) having known eigenvalues and eigenstates, and the small perturbation term: $H = H_0 + \lambda H'$. We also make sure that the unperturbed part satisfies an eigenvalue problem that contains eigenstates with no degenerate eigenvalues. We can then apply non-degenerate perturbation theory.

- **Identify the quantities needed to calculate first- and second-order energy corrections.**

  To find the first-order energy correction, we need an eigenfunction $|E_0'\rangle$ corresponding to an eigenvalue other than E_0. Then,

$$E_1 = \langle\psi_0|H'|\psi_0\rangle \tag{5}$$

  and for the second-order energy correction,

$$E_2 = \sum_{E_0' \neq E_0} \frac{|\langle\psi_0|H'|E_0'\rangle|^2}{E_0 - E_0'} \tag{6}$$

- **Identify the quantities needed to calculate first-order eigenfunction corrections.**

  The first-order correction $|\psi_1\rangle$ coming from the perturbative expansion $|\psi(\lambda)\rangle = |\psi_0\rangle + \lambda\,|\psi_1\rangle$ will be

$$|\psi_1\rangle = \sum_{E_0' \neq E_0} |E_0'\rangle \frac{\langle E_0'|H'|\psi_0\rangle}{E_0 - E_0'} \tag{7}$$

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Week 6: Perturbation theory (degenerate)

- **What conditions need to be satisfied for degenerate perturbation theory apply to a given energy level?**

  From the three previous bullets, we now take E_n to be g-fold degenerate so that we denote its corresponding state by $|E_{n,a}\rangle$ for another quantum number $a \in [1, g]$. We also need to have a perturbing potential V that must completely lift this degeneracy once it is turned on.

- **Outline the calculation of the first-order energy corrections due to a perturbation that splits a degenerate energy level.**

  Suppose we take a from the previous bullet as doubly degenerate, taking on two values (say, 1 and 2). Then as we did to arrive at the necessary quantities from non-degenerate perturbation theory (PT), we first expand $E(\lambda)$ from $H(\lambda)\,|\psi(\lambda)\rangle = E(\lambda)\,|\psi(\lambda)\rangle$ as $E(\lambda) = E_0 + \lambda E_1 + \ldots$ so that to first order in λ,

$$H_0\,|\psi_1\rangle + H'\,|\psi_0\rangle = E_0\,|\psi_1\rangle + E_1\,|\psi_0\rangle \tag{8}$$

  Projecting this equation onto $\langle E_{n,a}|$, we then arrive at two equations, one for each a:

$$\langle E_{0,a}|H'|\psi_0\rangle = E_1 \langle E_{0,a}|\psi_0\rangle \tag{9}$$

But then $\psi_0 = \alpha_1 |E_{0,1}\rangle + \alpha_2 |E_{0,2}\rangle$ for some complex α_i so that we obtain a matrix equation

$$H' \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = E_1 \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} \tag{10}$$

from which we can derive a characteristic equation $|H' - E_1 \mathbb{I}| = 0$ that allows us to solve for the two unknown eigenvalues and eigenstates. In this case, we take H' to be the V in the previous bullet.

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Week 7: Perturbation theory (examples)

- **Work on applications of perturbation theory given in Problem Set 2.**

  PS2 #1 is a problem on degenerate perturbation theory for a particle confined to a ring, and was solved in the passed problem set, following the prescriptions of the bullets in the previous week (diagonalization, solving for eigenvectors).

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Week 8: Perturbation theory (time-dependent)

- **Distinguish the interaction picture from the Schrodinger and Heisenberg pictures of quantum dynamics.**

  While the Schrodinger picture lets the state kets evolve in time using the solution to the time-dependent Schrodinger equation, and the Heisenberg picture lets the operators to evolve in time instead, the interaction (or Dirac) picture separates the Hamiltonian into a time-independent (and exactly solvable) term as well as a "perturbative" term which carries all the time dependence. In this picture, both the state kets and operators evolve in time.

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Week 9: Variational methods

- **Outline the technique of obtaining a variational estimate for the ground state energy of a given Hamiltonian.**

  Suppose the Hamiltonian $H = \dfrac{p^2}{2m} + V(\mathbf{r})$ has a set of eigenstates that are unknown to us, i.e. it satisfies $H|n\rangle = E_n |n\rangle$ for unknown E_n and $|n\rangle$. To use the variational method for estimating the ground state energy, we introduce a trial wavefunction $|\psi, \alpha\rangle$ having a trial parameter α which we could vary in order to get an estimate for E_0. This is done by expanding $|\psi, \alpha\rangle$ in the state space of $|n\rangle$:

$$|\psi, \alpha\rangle = \sum_n a_n(\alpha) |n\rangle \tag{11}$$

Letting $\langle\psi, \alpha| H$ act on both sides (and normalizing) gives us

$$\begin{aligned} \langle\psi, \alpha|H|\psi, \alpha\rangle &= \sum_n a_n(\alpha) \langle\psi, \alpha|H|n\rangle = \sum_n a_n(\alpha) E_n \langle\psi, \alpha|n\rangle \\ \frac{\langle\psi, \alpha|H|\psi, \alpha\rangle}{\langle\psi, \alpha|\psi, \alpha\rangle} &= \sum_n |a_n|^2(\alpha) E_n \geqslant E_0 \end{aligned} \tag{12}$$

which gives us a lower bound for the ground state energy E_0 (see Figure 1).

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Week 11: Identical particles

- **Outline the distinguishing characteristics between bosons and fermions.**

  (a) Spins: bosons have integer spin, while fermions have half-integer spin
  (b) Wave functions: those whose wavefunctions are symmetric after acting the exchange operator E_{12} are bosons, while those whose wavefunctions are antisymmetric after acting are fermions
  (c) Pauli's exclusion principle (restriction on number of particles occupying the same quantum state): fermions are affected by this principle while bosons are not
  (d) purpose: bosons hold matter together, while fermions make up the matter.

- **Describe the symmetry/antisymmetry of many-particle bosonic/fermionic wavefunctions under particle interchange. How are these features captured by commutation/anti-commutation relations?**

  For many-particle wavefunctions, we use second quantization (which is a prerequisite to proving Dirac's spin-statistics theorem). The symmetry and antisymmetry of a wavefunction of many particles can then be captured by using creation/annihilation operators $a_i^\dagger$ and a_i which follow

$$a_i |k_j\rangle = \delta_{ij} |\mathbf{0}\rangle \tag{13}$$

  For $|\mathbf{0}\rangle = |0, 0, \ldots\rangle$ being the vacuum state. For a two-particle state, we see that

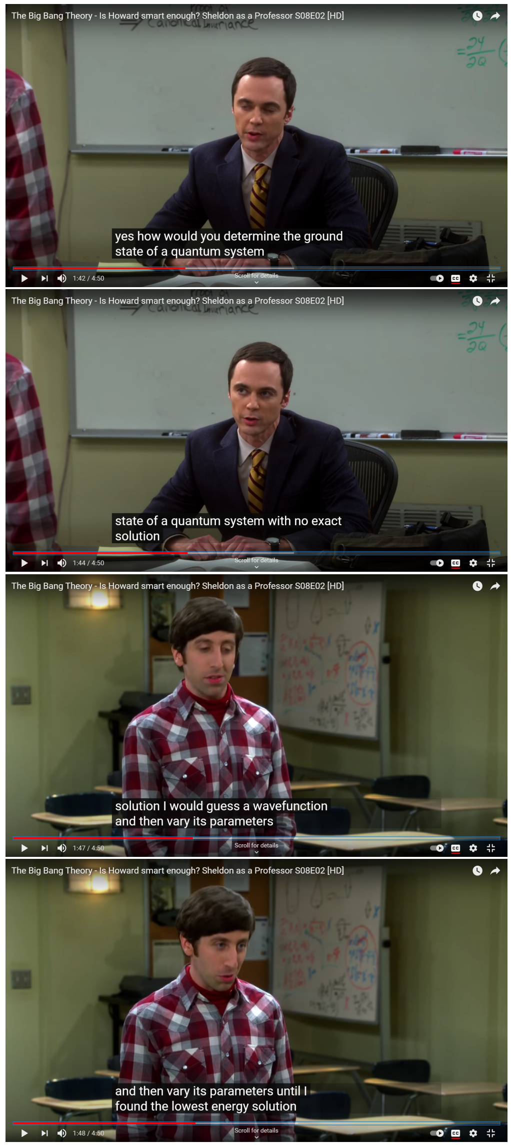

Figure 1: TBBT being accurate in its graduate-level physics sources. From https://www.youtube.com/watch?v=61FasQ6KQCI

$$a_i^\dagger a_j^\dagger |\mathbf{0}\rangle = \pm a_j^\dagger a_i^\dagger |\mathbf{0}\rangle \tag{14}$$

where $+$ is for bosons and $-$ is for fermions. Then, extending this to many particles and getting their respective adjoints,

$$[a_i^\dagger, a_j^\dagger] = 0 \qquad \text{for bosons,} \tag{15}$$
$$\{a_i^\dagger, a_j^\dagger\} = 0 \qquad \text{for fermions.} \tag{16}$$

where $\{\}$ is the anticommutator, $\{A, B\} = AB + BA$.

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Week 12: Scattering

- **Briefly discuss the significance of the cross-section in scattering experiments.**

  The (differential) cross-section $d\sigma$ relates the scattering amplitude to the (differential) flux, given by

$$\frac{d\sigma}{d\Omega} = |f(\mathbf{k}', \mathbf{k})|^2 \tag{17}$$

  It serves as a measure of strength of the interaction between the scattered particle/s and the scattering center. It is the effective area for collision.

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