Physics 242
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Final Report

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1 Symmetries, conservation laws, degeneracies

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

Consider the symmetry operator, $\mathscr{L}$, which either translates or rotates. This symmetry operator can be written as

$$\mathscr{L} = 1 - \frac{i\epsilon}{\hbar}G$$

where G is the Hermitian generator of $\mathscr{L}$. If a Hamiltonian is invariant with respect to the symmetry operator, we will have

$$\mathscr{L}H\mathscr{L}^{\dagger} = H$$

which leads us to the equation

$$\left(1 - \frac{i\epsilon}{\hbar}G\right) H \left(1 - \frac{i\epsilon}{\hbar}G\right) = H$$

or

$$H + \frac{i\epsilon}{\hbar}[G, H] + ... = H$$

and so we conclude that $[G, H] = 0$. Since we know the Heisenberg equations of motion to be

$$\frac{dA}{dt} = \frac{1}{i\hbar}[A, H]$$

then we conclude that

$$\frac{dG}{dt} = 0.$$

Therefore the associated generator G is conserved.

2 Spatial inversion, parity

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

We use the explicit form of spherical harmonics

$$Y_l^m = (-1)^m \sqrt{\frac{(2l+!)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta)e^{im\phi}$$

We also have the definition

$$Y_l^{-m}(\theta,\phi) = (-1)^m[Y_l^m(\theta,\phi)]^*$$

and

$$P_l^m(\cos\theta) = \frac{(-1)^{m+1}}{2^l l!}\frac{(l+|m|)!}{(l-|m|)!}\sin^{-|m|}\theta\left(\frac{d}{d(\cos\theta)}\right)^{l-|m|}\sin^{2l}\theta$$

applying the following transformations,

$$\begin{aligned}
&r \to r \\
&\theta \to \pi - \theta \quad (\cos\theta \to -\cos\theta) \\
&\phi \to \phi + \pi \quad (e^{im\phi} \to (-1)^m e^{im\phi})
\end{aligned}$$

Notice that we'll get a $(-1)^{l-m}$ which comes from the derivative with respect to $\cos\theta$ from the $P_l^m(\cos\theta)$ factor. Therefore,

$$Y_l^m \to (-1)^l Y_l^m$$

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

One selection rule that arise is the Laporte's selection rule. This arose from the analysis of the structure of the spectrum of iron where there are two kinds of terms named, "primed" and "unprimed". The transitions are always from primed to unprimed terms or vice versa. This is also later observed for the atomic spectra of other elements. After quantum mechanics is developed, it is found to be a consequence of the parity operator.

3 Lattice translations, time reversal

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

We start with the fact that the Hamiltonian isn't invariant under a translation $\tau(l)$ but is is invariant when the arbitrary variable l coincides with the lattice spacing a.

$$\tau^\dagger(a)V(x)\tau(a) = V(x+a) = V(a)$$

since we defined our potential to be periodic $V(x \pm a) = V(x)$ and where we have the properties of our translation operator to be

$$\tau^\dagger(l)x\tau(l) = x + l, \quad \tau(l)|x'\rangle = |x + l\rangle.$$

Since the kinetic energy term of a Hamiltonian is invariant under translations, the Hamiltonian satisfies

$$\tau^\dagger(a)H\tau(a) = H$$

Since $\tau(a)$ is unitary, we find that it commutates with the Hamiltonian

$$[H, \tau(a)] = 0$$

The generator of the lattice translations is the crystal momentum k so following our method in our week 1 learning task can use the Heisenberg equations of motion

$$\frac{dk}{dt} = \frac{1}{i\hbar}[k, H],$$

and we similarly conclude that

$$\frac{dk}{dt} = 0.$$

Thus, the crystal momentum is conserved.

3.b 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.

One such example is entropy, as we define entropy to increase as time progresses into the future and in general the macroscopic universe isn't symmetric with respect to time.
Another such example are charged particles exposed to an external magnetic field. The Hamiltonian of these particles would have terms that contain factors such as the spin $\vec{S}$, magnetic field $\vec{B}$, and linear momentum of the particles $\vec{p}$ which are odd under time reversal which then lead for the time symmetry of the motion of the particles to be broken.

4 Perturbation theory (non-degenerate)

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

Degeneracy happens when more than one eigenstate share the same energy. Therefore, in non-degenerate perturbation theory, there are no eigenstates sharing the same energy. Every eigenstate correspond to a unique eigenenergy. We are then allowed to focus on the small corrections of the perturber on the eigenenergies and eigenstates with respect to the powers of λ, which is defined as a continuous real parameter.

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

For the first- and second- order correction to the energy, we need the form of the perturbation, V, and calculate its taylor series expansion until the highest significant order. We are then therefore required to evaluate for the expectation value of V with respect to the unperturbed ket. The first-order energy correction is the found by evaluating

$$\Delta_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$$

where $|n^{(0)}\rangle$ is our energy eigenket. The second-order expansion needs to calculate for the 1st order eignenket given by

$$|n^{(1)}\rangle = \frac{\phi_n}{E_n^{(0)} - H_0}|n^{(0)}\rangle$$

where ϕ_n is the complementary projection operator given by

$$\phi_n = 1 - |n^{(0)}\rangle\langle n^{(0)}| = |k^{(0)}\rangle\langle k^{(0)}|$$

We can then compute for the second-order energy corrections given by

$$\Delta_n^{(2)} = \langle n^{(0)}|V\frac{\phi_n}{E_n^{(0)} - H_0}V|n^{(0)}\rangle$$

4.c Identify the quantities needed to calculate first-order eigenfunction corrections?

The first order correction to the wave function is given by

$$\psi_n^{(1)} = \sum_{n\neq k}\frac{V_{kn}}{E_n^{(0)} - E_k^{(0)}}\psi_k^{(0)}$$

where $V_{nk} = \langle n^{(0)}|V|k^{(0)}\rangle$. Therefore we need to evaluate first the matrix elements of V_{nk} with respect to the unperturbed kets. Additionally, we need the ground state energy, $E_n^{(0)}$, and the energy $E_k^{(0)}$.

5 Problem Set 1

6 Perturbation theory (degenerate)

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

The non-degenerate case of perturbation theory assumes that there is a unique energy that corresponds to every eigenket. When the factor λ approaches zero, the perturbed ket would simplify into a well-defined unperturbed ket. In the degenerate case, any linear combination of the unperturbed kets result to the same energy. When a perturbing potential is applied that destroys the symmetry that permits the degeneracy, the energy levels splits into different distinct energy levels. We apply the degenerate perturbation theory to help evaluate the different energy levels.

6.b Outline the calculations of the first-order energy corrections due to a perturbation that splits a degenerate energy level?

We first start by defining $|l\rangle$ as the set of g perturbed eigenstates of unique energies. As the $\lambda \to 0$, this set approaches $|l^{(0)}\rangle$. We write this as

$$|l^{(0)}\rangle = \sum_{m \in D} \langle m^{(0)}|l^{(0)}\rangle |m^{(0)}\rangle$$

where the sum is over the degenerate subspace, D. We define the projection operator P_0 and P_1 to define the projection onto the space defined by $|m^{(0)}\rangle$ and the projection to the remaining states, respectively. We can rewrite the Schrodinger equation for the states $|l\rangle$ as

$$\begin{aligned} 0 &= (E - H_0 - \lambda|V\rangle \\ 0 &= (E - E_D^{(0)} - V)P_0|l\rangle + (E - H_0 - \lambda V)P_1|l\rangle \end{aligned}$$

We can then write

$$P_1|l\rangle = P_1 \frac{\lambda}{E - H0 - \lambda P_1 V P_1} P_1 V P_0 |l\rangle$$

or

$$P_1|l^{(l)}\rangle = \sum_{k \in D} \frac{|k^{(0)}\rangle V_{kl}}{E_D^{(0)} - E_k^{(0)}}$$

We then solve for $P_0|l\rangle$ by substituting $P_1|l\rangle$ into $(E - E_D^{(0)} - \lambda P_0 V)P_0|l\rangle - \lambda P_0 V P_1|l\rangle = 0$ which we can derive from the equations above. We then obtain

$$(E - E_D^{(0)} - \lambda P_0 V P_0 - \lambda^2 P_0 V P_1 \frac{1}{E - H_0 - \lambda V} P_1 V P_0) P_0 |l\rangle = 0$$

We then focus our attention to the first few terms of the above equation

$$(E - E_D^{(0)} - \lambda P_0 V P_0) P_0 |l\rangle = 0$$

This is an equation in the g dimensional degenerate subspace. This means that the eigenvectors of this equation are the eigenvectors of the $g \times g$ matrix $P_0 V P_0$ and the eigenvalues $E^{(1)}$ are the roots of the equation

$$det[V - (E - E_D^{(0)})] = 0, \quad V = \text{matrix of } P_0 V P_0$$

The roots determine the eigenvalues $\Delta_l^{(1)}$ which are the first-order energy shifts given by

$$\Delta_l^{(1)} = \langle l^{(0)}|V|l^{(0)}\rangle$$

7 Perturbation theory (examples)

7.a Work on applications of perturbation theory given in Problem Set 2.

This was already shown in the first item of Problem Set 2.

8 Perturbation theory (time-dependent)

8.a Distinguish the interaction picture form the Schrodinger and Heisenberg pictures of quantum dynamics.

In the Hamiltonians with time-dependent potentials we have three pictures to consider. First is the interaction picture, which is also called the Dirac picture and the last two are the Heisenberg and Schrodinger picture.
In the Schrodinger picture the operators/observables remain fixed while the state ket/basis are changed with respect to time – or in this case with respect to the Hamiltonian H. In the Heisenberg picture the state ket/basis are kept fixed while the operator/observable are changed in time – more specifically changed with respect to V_1 where V_1 is given by $V_1 = e^{iH_0t/\hbar}V^{-iH_0t/\hbar}$. However, in the Dirac picture, both state kets/basis and operators/observables are evolving in time – to be more specific, with respect to V_1 and H_0, respectively.

9 Variational methods

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

The variational method is an important way to estimate the ground state energy of a trial waveform when we do not know its exact solutions. We start by defining a trial ket, $|\bar{0}\rangle$, that is similar in form to the actual ground-state ket. We then plug this in to

$$\bar{H} = \frac{\langle\bar{0}|H|\bar{0}\rangle}{\langle\bar{0}|\bar{0}\rangle}.$$

and compute for its value. We then solve for the value of the parameter that minimises $\bar{H}$ then plug it back in to our above equation to find the variational estimate for the ground state energy of a given Hamiltonian.

10 Problem Set 2

11 Identical Particles

11.a Outline the distinguishing characteristics between bosons and fermions

We first look at the difference between the connection of spin and to the type of particle. Fermionic particles have half-integer spins while Bosonic particles have integer spins. Another difference between these two kinds of particles lie in its occupied state. It is impossible for 2 fermions to occupy the same states. Meanwhile, for bosons for most of the allowed arrangement, we see that both particles can fill both states.

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

Let's start with a system of two identical particles, one located at x_1 and the other at x_2. The respective wavefunction would then be given by

$$\psi(x_1, x_2) = |x_1, x_2\rangle$$

Let $P_{1,2}$ be the particle interchange operator that changes the particles position with each other. Therefore, we have by intuition

$$P_{1,2}|x_1, x_2\rangle = |x_2, x_1\rangle$$

where we have $P_{1,2}^2 = I$. If we have the Hamiltonian given by

$$H = \frac{1}{2m}(p_1^2 + p_2^2) + V_{pair}(|x_2 - x_1|, t) + V(x_1, t) + V(x_2, t),$$

we will have

$$P_{1,2}HP_{1,2}^{-1} = H \quad \text{or} \quad [P_{1,2}, H] = 0$$

We can then find the simultaneous eigenfunctions of $P_{1,2}$ and H. We let $\psi_\lambda(x_1, x_2)$ be an eigenstate

$$\begin{aligned} P_{1,2}\psi_\lambda(x_1, x_2) &= \lambda\psi_\lambda(x_1, x_2) = \psi_\lambda(x_2, x_1) \\ P_{1,2}^2\psi_\lambda(x_1, x_2) &= \lambda^2\psi_\lambda(x_1, x_2) = \psi_\lambda(x_1, x_2) \end{aligned} \tag{11.b.1}$$

which leads to $\lambda^2 = 1$ or $\lambda = \pm 1$. Therefore we have for $\lambda = 1$ a symmetric state given by $\psi_\lambda(x_1, x_2) = \psi_\lambda(x_2, x_1)$, and an antisymmetric state given by $\psi_\lambda(x_1, x_2) = -\psi_\lambda(x_2, x_1)$. It is found that particles whose wavefunctions are symmetric are under particle interchange have intrinsic spins that are of integer or zero value. Particles that are symmetric under particle interchange are bosons. Meanwhile, it is found that particles that are antisymmetric under particle interchange have half-integer intrinsic spins, and are found to be fermions.

12 Scattering

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

The cross-section acts as the effective area of collision/interaction in scattering experiments. It usually measures the probability that an interaction will take place when when an excitation meets or crosses through a particle or density shift. It can also be thought as the rate per unit area in which interaction occurs in the given set-up.