Physics 242: Final Report

Janna May Z. Angeles
2015-09948

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).

A symmetry operator $\mathscr{S}$ can be written as

$$\mathscr{S} = 1 - \frac{i\varepsilon}{\hbar} G \tag{1}$$

where G is the associated Hermitian generator of this operator. If we suppose that H is invariant under $\mathscr{S}$, then we have

$$\mathscr{S}^\dagger H \mathscr{S} = H. \tag{2}$$

From this, we can infer that

$$[\mathscr{S}, H] = 0 \tag{3}$$

by multiplying both sides of Eq. (2) with $\mathscr{S}$. Equivalently, due to the relation of $\mathscr{S}$ and G, we can say that,

$$[G, H] = 0 \tag{4}$$

Now, using the Heisenberg equation of motion, we get

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{1}{i\hbar} \cancelto{0}{[G, H]} = 0 \tag{5}$$

which means that G is unchanging with respect to time. Thus, G is a constant of the motion.

2 Spatial inversion, parity

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

Generally, the parity of the spherical harmonics Y_ℓ^m is $(-1)^\ell$ which can be obtained by applying parity transformation to the spherical angles:

$$(\theta, \phi) \to (\pi - \theta, \phi + \pi) \tag{6}$$

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

An example would be the change in the dipole moment of centrosymmetric molecules after the absorption of a photon excites an electron in said molecules from one energy state to another. Laporte's rule, a selection rule that arises from this situation and serves as guideline on whether the given transition is allowed or not, states that transitions between states of the same parity are forbidden.

Another example is rotational transitions in diatomics that can be described by rigid motors. Symmetries from the rotational wave functions of the rigid motor gives rise to the selection rule $\delta J = \pm 1$.

3 Lattice translations, time reversal

(a) **Show that a discrete lattice translational invariance leads to conserved crystal momentum (Bloch wavevector).**

Consider a periodic wavefunction $V(x \pm a) = V(x)$. Also, recall the translation operator and how it acts on a state ket

$$\tau^{\dagger}(l) x \tau(l) = x + l, \quad \tau(l) \left|x'\right\rangle = \left|x' + l\right\rangle . \tag{7}$$

Let this displacement l be a to reflect the structure of the crystal. Since the potential is periodic, we know that

$$\tau^{\dagger}(a) V(x) \tau(a) = V(x + a) = V(x) \tag{8}$$

which represents a discrete lattice translational invariance. Let $|\theta\rangle$ be defined as

$$|\theta\rangle \equiv \sum_{n=-\infty}^{\infty} e^{in\theta} |n\rangle \tag{9}$$

where θ is a real parameter with $-\pi \leq \theta \leq \pi$. Note that applying $\tau(a)$ to the state $|n\rangle$ results to

$$\tau(a)|n\rangle = |n+1\rangle \tag{10}$$

Then, applying the translation operator to $|\theta\rangle$ leads to

$$\tau(a)|\theta\rangle = \sum_{n=-\infty}^{\infty} e^{in\theta}|n+1\rangle = \sum_{n=-\infty}^{\infty} e^{i(n-1)\theta}|n\rangle = e^{-i\theta}|\theta\rangle \tag{11}$$

Note that we can apply the translation operator to $\langle x'|$ so

$$\langle x'|\tau(a)|\theta\rangle = \langle x' - a \mid \theta\rangle \tag{12}$$

On the other hand, we can also apply translation operator to $|\theta\rangle$ using the earlier relation:

$$\langle x'|\tau(a)|\theta\rangle = e^{-i\theta} \langle x' \mid \theta\rangle \tag{13}$$

We can then infer that

$$\langle x' - a \mid \theta\rangle = \langle x' \mid \theta\rangle e^{-\imath\theta} \tag{14}$$

This equation can be solved by setting

$$\langle x' \mid \theta\rangle = e^{ikx'} u_k\left(x'\right) \tag{15}$$

with $\theta = ka$ and $u_k\left(x'\right)$ being a periodic function with period a. This is the Bloch wavevector.

(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 example is by applying a uniform magnetic field on a moving electron (in the absence of an external electric field). Also, we can infer that the initial velocity of the electron is reversed ($\mathbf{v} \to -\mathbf{v}$) when we run this experiment backwards in time as velocity is proportional to the momentum which is odd under time reversal. On the other hand, the magnetic field remains unchanged. This results to the Lorentz force felt by the electron, given by

$$\mathbf{F} = q\mathbf{v} \times \mathbf{B} \tag{16}$$

for this case, to be negative compared to the original picture. As the the time-reversed picture is not equal to the original picture, such systems break time symmetry.

Another interesting system that breaks time symmetry is a discrete time crystal. These are created when a driving force is applied periodically to a quantum many-body system. This can lead to the system's period of oscillations being longer than that of the driving force. The period of the force should be followed by the Schrödinger equation's stationary solutions. With the system exhibiting stationary motion with a different period, time symmetry is broken. In an experimental setting, an example of this is a constantly rotating ring of charged ions in an otherwise lowest-energy state.

4 Perturbation theory (non-degenerate)

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

The conditions are:

1. The perturbation V must be Hermitian and be sufficiently small/ weak compared to the entire energy scale.
2. Each energy eigenstate should correspond to a unique energy eigenvalues.

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

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

It would be better to perform these objectives simultaneously. For calculating the first-order correction to the energy eigenvalue, we need the perturbation itself and the unperturbed wave functions as this correction is just the expectation value of the perturbation in the uncorrected state:

$$E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle \tag{17}$$

On the other hand, second-order energy correction is given by

$$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle \tag{18}$$

We see here that we need the first-order correction to the wavefunction which is given by

$$|n^{(1)}\rangle = -\sum_{k\neq n} \frac{V_{kn}}{E_k^{(0)} - E_n^{(0)}} |k^{(0)}\rangle \tag{19}$$

In calculating for $|n^{(1)}\rangle$, we required the unperturbed energies in addition to the the perturbation and the unperturbed wave functions. From Eq. (19), we obtain for the second-order energy correction:

$$E_n^{(2)} = -\sum_{k\neq n} \frac{\langle n^{(0)}|V|k^{(0)}\rangle\, V_{kn}}{E_k^{(0)} - E_n^{(0)}} = -\sum_{k\neq n} \frac{|V_{kn}|^2}{E_k^{(0)} - E_n^{(0)}} \tag{20}$$

since $\langle n^{(0)}|V|k^{(0)}\rangle = V_{nk} = V_{kn}^*$.

5 Perturbation theory (degenerate)

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

The conditions are:

1. The perturbation V must be Hermitian and be sufficiently small/ weak compared to the entire energy scale.
2. The spectrum of the unperturbed Hamiltonian $H^{(0)}$ has energy eigenstates with the same energy (degenerate states).

(b) **Outline the calculation of the first-order energy corrections due to a perturbation that splits a degenerate energy level?**

1. Identify the degenerate unperturbed energy eigenstates $|n^0\rangle$ and normalize them with the use of the normalization condition.
2. Construct the perturbation matrix $\mathbf{V}$, a $g \times g$ matrix if the degeneracy is g -fold, with its elements given by:

$$\mathbf{V}_{nk} = \langle n^{(0)}|V|k^{(0)}\rangle \tag{21}$$

3. Diagonalize the perturbation matrix by taking the eigenvalue problem

$$\mathbf{V} |v\rangle = E_n^{(1)} |v\rangle \tag{22}$$

where $|v\rangle = \alpha |n^0\rangle + \beta |k^0\rangle + \ldots$ which has g terms. The eigenvector $|v\rangle$ is a general linear combination of the degenerate states. We then evaluate the determinant

$$|\mathbf{V} - E_n^{(1)} \mathbf{I}| = 0 \tag{23}$$

where $\mathbf{I}$ is the $g \times g$ identity matrix.

4. Solve for the energy eigenvalues $E_n^{(1)}$ from the expression resulting from the previous step

6 Perturbation theory (examples)

Work on applications of perturbation theory given in Problem Set 2

This is given in the solution of PS2.

7 Perturbation theory (time-dependent)

Distinguish the interaction picture from the Schrödinger and Heisenberg pictures of quantum dynamics.

In the Schrödinger picture, it is the state vectors that exhibit time dependence while it is the operators that carry this dependence for the Heisenberg picture. On the other hand, the interaction picture makes use of elements from both the Schrödinger and Heisenberg pictures. Some Heisenberg operators are constructed, using the known Hamiltonian $H^{(0)}$, which will then be used to write the Schrödinger equation. Also, both state vectors and operators carry time dependence.

8 Variational methods

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

1. Determine the Hamiltonian of the system.

2. Pick a trial wave function and normalize it with the use of the normalization condition.

3. With the relation

$$\langle H \rangle = \langle T \rangle + \langle V \rangle \,, \tag{24}$$

we determine the expectation value of the Hamiltonian by solving for the expectation values of the kinetic and potential energy.

4. Minimize $\langle H \rangle$ since we want to tighten the upper bound on the ground state energy E_{gs} to be as low as possible.

5. Solve the expression arising from the previous step.

6. Substitute the obtained relation back to $\langle H \rangle$ for the variational estimate of E_{gs}.

9 Identical particles

(a) **Outline the distinguishing characteristics between bosons and fermions.**

	Bosons	Fermions
Symmetry	symmetric	antisymmetric
Spin	integer spin	half-integer spin
Statistics	Bose-Einstein (B-E)	Fermi-Dirac (F-D)
Can two identical particles of this kind occupy the same state?	yes	no

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

First, we consider the a two-particle system made up of indistinguishable particles. Let particle 1[2] be at position $\mathbf{r}_{1[2]}$ Then, interchanging the two particles leads to either of the two cases depending on the kind of particles the system has:

$$\text{Symmetric case (bosons):} \qquad \Psi(\mathbf{r}_1, \mathbf{r}_2) = \Psi(\mathbf{r}_2, \mathbf{r}_1) \tag{25}$$

$$\text{Antisymmetric case (fermions):} \qquad \Psi(\mathbf{r}_1, \mathbf{r}_2) = -\Psi(\mathbf{r}_2, \mathbf{r}_1) \tag{26}$$

This can be extended to the many-particle system but we would need to take note of the permutation in which we interchange the particles. Let P be the permutation operator. For fermions, we have

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \sum \text{sign}(P) P\, \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \tag{27}$$

where the summation is a sum over all permutations and $\text{sign}(P) = (\pm 1)^{N_p}$ with N_p $(p = 1, 2, \ldots)$ being the number of successive permutations that P can be decomposed of. The many-particle state $\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N)$ can be in terms of the occupation numbers n_p $(p = 1, 2, \ldots)$ which represents the number of particles in a single-particle state. For bosons, we have

$$\Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \frac{1}{\sqrt{n_1! n_2! \ldots}} \frac{1}{\sqrt{N!}} \sum P\, \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N) \tag{28}$$

There are a lot of derivation involved but, basically, the occupation number operator is related to creation and annihilation operators which must satisfy the commutation relations for bosons:

$$[a_i, a_k] = \left[a_i^\dagger, a_k^\dagger\right] = 0, \quad \left[a_i, a_k^\dagger\right] = \delta_{i,k}, \quad \forall i, k \tag{29}$$

and the anti-commutation relations for fermions

$$[a_i, a_k] + = \left[a_i^\dagger, a_k^\dagger\right] + = 0, \quad \left[a_i, a_k^\dagger\right] + = \delta_{i,k}, \quad \forall i, k. \tag{30}$$

Depending on which of the relations are applicable, they can apply a restriction on the many-particle state. For example, the anti-commutation relations make sure that fermions follow the Pauli's exclusion principle (no two identical fermions can occupy the same state) while the commutation rules for bosons does not lead to such a restriction.

10 Scattering

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

By evaluating for the cross section, we gain a lot of information in scattering experiments like the physical interaction between photons and the physical properties of the scattering center. This variable is relevant in knowing the end state of the incoming particle given a certain trajectory towards the scattering center.