Advanced Quantum Mechanics: Quick Guide

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Abstract

This is a quick guide – a summary – of the Advanced Quantum Mechanics course at the University of Manchester, taught by S.Grigorenko between Sept '08 and Dec '08. These summary notes are based upon his lecture notes. A copy of my full lecture notes, on this topic, may be found at www.jpoffline.com.

Keywords:

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Contents

I. BASIC FORMALISM

The approaches we have considered are:

- In **Copenhagen** formalism the objects we work with are the **wavefunctions** $\psi(x)$, in **coordinate-space**. The **Schrodinger equation** is $i\hbar\dot{\psi} = \hat{\mathcal{H}}\psi$. This approach is good for one-body problems, but pretty much fails when including constraints, and for many-body problems.

- **Dirac** formalism has the objects being **abstract vectors** $|\psi\rangle$ in **Hilbert space**. This approach is good for many-body problems; but fails upon inclusion of constraints.

- The **path integral** approach is good when working with **fields**, but is mathematically vulnerable.

It should be noted that all formalisms are essentially the same, but use different tools to get a result.

The **Schrodinger picture** of quantum mechanics has the states of a system evolving, with operators having no explicit time dependance.

The **Heisenberg picture** has operators evolving, and states staying constant; with the equation of motion

$$\frac{d}{dt}\hat{Q}_{\mathcal{H}}(t) = \frac{\partial \hat{Q}}{\partial t} - \frac{i}{\hbar}\left[\hat{Q}, \hat{\mathcal{H}}\right].$$

II. FORMALISM OF VECTOR SPACES

In the **coordinate basis** $|x\rangle$, we expand a wavefunction in **ket-space**,

$$|\psi\rangle = \sum_x \psi_x |\psi\rangle,$$

where we make the identification

$$\psi_x = \langle x|\psi\rangle = \psi(x).$$

Similarly, we expand in **bra-space**,

$$\langle\psi| = \sum_x \psi_x^* \langle x|.$$

The coordinate basis is **orthonormal**,

$$\langle x|x'\rangle = \delta_{xx'}.$$

By forming the scalar product of two states, we see that

$$\begin{aligned}\langle\chi|\psi\rangle &= \sum_{x,x'} \chi^*_{x'}\langle x'|x\rangle\psi_x \\ &= \sum_x \chi^*_x \psi_x \\ &= \int dx\, \chi^*(x)\psi(x).\end{aligned}$$

The **completeness of the basis** is the statement that

$$\sum_x |x\rangle\langle x| = 1.$$

If instead of using the coordinate basis, we use the **orthonormal** $|n\rangle$-basis, then everything still holds:

$$|\psi\rangle = \sum_n a_n|n\rangle \quad \Rightarrow \quad a_n = \langle n|\psi\rangle \quad \Rightarrow \quad \sum_n |n\rangle\langle n| = 1.$$

Operators are linear, $|\chi\rangle = \hat{Q}|\psi\rangle$. An operator can be expressed in a basis by inserting the unity operator,

$$\begin{aligned}\hat{Q} &= 1.\hat{Q}.1 \\ &= \sum_{m,n} |m\rangle\langle m|\hat{Q}|n\rangle\langle n| \\ &= \sum_{m,n} Q_{mn}|m\rangle\langle n|.\end{aligned}$$

We have arrived at the **matrix representation** of the operator

$$Q_{mn} = \langle m|\hat{Q}|n\rangle.$$

In a different basis, the matrix representation is

$$\begin{aligned}Q_{\tilde{m}\tilde{n}} &= \langle\tilde{m}|\hat{Q}|\tilde{n}\rangle \\ &= \sum_{m,n} \langle\tilde{m}|m\rangle\langle m|\hat{Q}|n\rangle\langle n|\tilde{n}\rangle \\ &= \sum_{m,n} Q_{mn}\langle\tilde{m}|m\rangle\langle n|\tilde{n}\rangle,\end{aligned}$$

which bears resemblance to tensor transformations.

Operators in **their basis** are simple,

$$\hat{x}|x\rangle = x|x\rangle, \quad \hat{p}|p\rangle = p|p\rangle.$$

To get an eigenstate in a different basis, one projects onto the basis required. For example, the momentum eigenstate, in coordinate representation:

$$\begin{aligned}
\hat{p}|p\rangle &= p|p\rangle \\
\Rightarrow \langle x|\hat{p}|p\rangle &= p\langle x|p\rangle \\
\Rightarrow \sum_{x'} \langle x|\hat{p}|x'\rangle\langle x'|p\rangle &= p\langle x|p\rangle \\
\Rightarrow \sum_{x'} \langle x|\hat{p}|x'\rangle P(x') &= pP(x) \\
\Rightarrow -i\hbar\frac{d}{dx}P(x) &= pP(x) \\
\Rightarrow P(x) &= \frac{1}{(\sqrt{2\pi\hbar})^n}e^{\frac{ipx}{\hbar}}
\end{aligned}$$

The **properties of operators** are

- **Hermitian**: $\hat{Q}^\dagger = \hat{Q}$. Such operators have real eigenvalues.
- **Anti-Hermitian**: $\hat{Q}^\dagger = -\hat{Q}$. One can make an anti-Hermitian operator Hermitian, by multiplying by i.
- **Unitary**: $\hat{U}^\dagger\hat{U} = 1$.
- The **eigenvalue equation** is such that $\hat{Q}|\psi\rangle = \lambda|\psi\rangle$, whereby states are normalised $\langle\psi|\psi\rangle = 1$.

Raising and lowering operators for the Harmonic oscillator have the following relations:

$$\begin{aligned}
\left[\hat{a}, \hat{a}^\dagger\right] &= 1 \\
\hat{\mathcal{H}} &= \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right) \\
\hat{a}|n\rangle &= \sqrt{n}|n-1\rangle \\
\hat{a}^\dagger|n\rangle &= \sqrt{n+1}|n+1\rangle
\end{aligned}$$

The **vacuum state** is such that $\hat{a}|0\rangle = 0$. In **coordinate representation**, one has

$$\sum_{x'} \langle x|\hat{a}|x'\rangle\langle x'|0\rangle = 0 \quad \Rightarrow \quad \sum_{x'} a_{xx'}\psi_0(x') = 0.$$

Furthermore, as $\hat{a} = \alpha\hat{p} + \beta\hat{x}$, then

$$a_{xx'} = \alpha\left(-i\hbar\frac{d}{dx}\right)\delta_{xx'} + \beta x\delta_{xx'},$$

which fairly easily allows one to find that the vacuum state, in coordinate representation, is

$$\psi_0(x) = C.e^{-\frac{m\omega x^2}{2\hbar}}.$$

In **momentum representation**, one has

$$\sum_{p'}\langle p|\hat{a}|p'\rangle\langle p'|0\rangle = 0 \quad\Rightarrow\quad \sum_{p'} a_{pp'}\psi_0(p') = 0.$$

To find $\psi_0(p)$, we must compute $x_{pp'}$, as

$$a_{pp'} = p\delta_{pp'} - im\omega x_{pp'}.$$

So, the position operator, in momentum representation:

$$\begin{aligned}
x_{pp'} &= \langle p|\hat{x}|p'\rangle \\
&= \sum_{x,x'}\langle p|x\rangle\langle x|\hat{x}|x'\rangle\langle x'|p'\rangle \\
&= \sum_{x} x\langle p|x\rangle\langle x|p'\rangle \\
&= \int dx\, xP^*(x)P'(x) \\
&= C\int dx\, x\, e^{\frac{ix}{\hbar}(p'-p)} \\
&= D\frac{d}{dp'}\int dx\, e^{\frac{ix}{\hbar}(p'-p)} \\
&= i\hbar\delta_{pp'}\frac{d}{dp'}.
\end{aligned}$$

Therefore, the vacuum state, in momentum representation:

$$p\psi_0(p) = -\hbar m\omega\frac{d}{dp}\psi_0(p) \quad\Rightarrow\quad \psi_0(p) = e^{-\frac{p^2}{2m\omega\hbar}}.$$

The **evolution operator** is

$$\hat{U}(t) = \sum_{n} e^{-\frac{iE_n t}{\hbar}}|n\rangle\langle n|$$

III. MANY BODY PROBLEMS

Bosons are **symmetric** under exchange of two particles,

$$\psi(x_1, x_2, \ldots) = \psi(x_2, x_1, \ldots).$$

Fermions are **anti-symmetric** under the exchange

$$\psi(x_1, x_2, \ldots) = -\psi(x_2, x_1, \ldots).$$

The state $|n_0, n_1, n_2 \ldots\rangle$ tells us about the number of particles in a particular state, whereby n_k is the **occupancy number** of state k. The total number of particles in a system is then just

$$N = \sum_{i=0}^{\infty} n_i.$$

The different states with different N produce the **Fock space**.

The action of the **creation and annihilation** operators on **Bosons** are such that

$$\begin{aligned} \hat{a}_i^+ |n_0, \ldots, n_i, \ldots\rangle &= \sqrt{n_i + 1} |n_0, \ldots, n_i + 1, \ldots\rangle, \\ \hat{a}_i |n_0, \ldots, n_i, \ldots\rangle &= \sqrt{n_i} |n_0, \ldots, n_i - 1, \ldots\rangle. \end{aligned}$$

Fermions are the same, but have a transposition sign-factor outfront.

Commutators for **Bosons** are such that the **only non-zero** commutator is

$$\left[\hat{a}_i^+, \hat{a}_j\right] = \delta_{ij}.$$

Fermions have **anti-commutators**, whereby the **only non-zero** anti-commutator is

$$\left\{\hat{a}_i^+, \hat{a}_j\right\} = \delta_{ij}.$$

States may be generated from the vacuum, by applying the creation operator many times;

$$|n_0, n_1, \ldots\rangle = \prod_j \frac{\left(\hat{a}_j^+\right)^{n_j}}{\sqrt{n_j!}} |0\rangle.$$

The Hamiltonian, under **secondary quantisation** is

$$\hat{\mathcal{H}} = \sum_n \varepsilon_n \hat{a}_n^+ \hat{a}_n + \frac{1}{2} \sum_{i,j,n,m} V_{ij,nm} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_n \hat{a}_m,$$

where the **number of states** operator

$$\hat{n}_i = \hat{a}_i^+ \hat{a}_i,$$

and returns the number of particles in state i. This secondary quantisation is good for many-body problems.

IV. SYMMETRY IN QUANTUM MECHANICS

The symmetry operator commutes with the Hamiltonian,

$$\left[\hat{\mathcal{H}}, \hat{O}\right] = 0.$$

As they commute, the symmetry operator and Hamiltonian share a basis in which they are diagonal. Hence,

$$\frac{d}{dt}\langle\hat{O}\rangle = 0,$$

which means that $\langle\hat{O}\rangle$ is **conserved** and quantum numbers associated with $\hat{O}$ are **good quantum numbers**. If the symmetry operator is Hermitian, then there is a conserved measurable quantity.

The **translation operator** has a few representations,

$$\hat{T}_a = \sum_x |x\rangle\langle x+a|, \quad \left(\hat{T}_a\right)_{xx'} = e^{a\frac{d}{dx}}\delta_{xx'}, \quad \left(\hat{T}_a\right)_{xx'} = \delta(x+a-x).$$

The translation operator is unitary,

$$\hat{T}_a^\dagger \hat{T}_a = 1.$$

Expanding the translation operator, for small a,

$$\hat{T}_{\delta a} = 1 + \hat{U}\delta a, \quad \hat{U} = \left.\frac{\partial \hat{T}_{\delta a}}{\partial a}\right|_{a=0}.$$

Directly following from the unitarity of $\hat{T}_a$, one can show that

$$\hat{U}^\dagger = -\hat{U},$$

so that $\hat{R} = -i\hbar\hat{U}$ is unitary and Hermitian. Hence,

$$\hat{R} = -i\hbar\left.\frac{\partial \hat{T}}{\partial a}\right|_{a=0}.$$

$\hat{R}$ is an operator that describes a conserved symmetry quantity, and will provide good quantum numbers.

V. ANGULAR MOMENTUM

The **total angular momentum** operator is

$$\hat{\boldsymbol{J}} = \hat{\boldsymbol{L}} + \hat{\boldsymbol{S}}.$$

The **eigenstates** of angular momentum are

$$\hat{J}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle, \quad \hat{J}_z|j,m\rangle = m\hbar|j,m\rangle.$$

Commutators are such that

$$\left[\hat{J}_a, \hat{J}_b\right] = i\hbar\hat{J}_c\,\epsilon_{abc}.$$

Ladder operators are defined such that

$$\hat{J}_\pm = \hat{J}_x + i\hat{J}_y,$$

and that their action on a state is

$$\hat{J}_\pm|j,m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\hbar|j, m\pm 1\rangle.$$

Spin operators are

$$\hat{\boldsymbol{S}} = \frac{\hbar}{2}\hat{\boldsymbol{\sigma}},$$

where the **Pauli-spin matrices** are

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The Pauli matrices can be shown to conform to the commutation and anti-commutation relations:

$$[\hat{\sigma}_a\hat{\sigma}_b] = 2i\sigma_c\,\epsilon_{abc}, \quad \{\hat{\sigma}_a\hat{\sigma}_b\} = 2\delta_{ab}.$$

VI. CHARGED PARTICLES IN EM FIELDS

The **Pauli Hamiltonian** is

$$\hat{\mathcal{H}} = \frac{1}{2m}\left(\hat{\boldsymbol{p}} - \frac{e}{c}\boldsymbol{A}\right)^2 + q\phi - \frac{gq}{2mc}\hat{\boldsymbol{S}} \cdot \boldsymbol{B}.$$

If $\boldsymbol{B}$ is constant, one can extract the **spin equation**,

$$i\hbar|\dot{\eta}\rangle = -\hat{\boldsymbol{\mu}} \cdot \boldsymbol{B}|\eta\rangle, \quad \hat{\boldsymbol{\mu}} = \frac{gq}{2mc}\hat{\boldsymbol{S}}.$$

For electrons,

$$g = 2, \quad \hat{\boldsymbol{\mu}} = \mu_B \hat{\boldsymbol{\sigma}}.$$

The **phase shift**, due to magnetic potential, is

$$\varphi = \frac{q}{\hbar c}\oint_\gamma \boldsymbol{A} \cdot d\boldsymbol{r} = \frac{q\Phi}{\hbar c},$$

where Φ is the magnetic flux through the closed contour γ. This shift of phase, due to non-zero magnetic potential, gives the **Aharonov-Bohm effect**.

Upon quantisation of radiation, one can write the **vector potential operator**:

$$\hat{\boldsymbol{A}} = C\sum_{\boldsymbol{k},\lambda}\left(e^{i\boldsymbol{k}\cdot\boldsymbol{x}}\boldsymbol{\varepsilon}_{\boldsymbol{k},\lambda}\hat{a}_{\boldsymbol{k},\lambda}(t) + e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}\boldsymbol{\varepsilon}^*_{\boldsymbol{k},\lambda}\hat{a}^+_{\boldsymbol{k},\lambda}(t)\right),$$

where the destruction/creation operators conform to the commutation relation

$$\left[\hat{a}_{\boldsymbol{k},\lambda}, \hat{a}^\dagger_{\boldsymbol{k}',\lambda'}\right] = \delta_{\boldsymbol{k},\boldsymbol{k}'}\delta_{\lambda,\lambda'}.$$

This relies upon the **Coulomb gauge** $\nabla \cdot \boldsymbol{A} = 0$. This gives that the EM field is a sum over modes of quantum harmonic oscillators.