KEY CONCEPTS AND EQUATIONS

What is this ?

This document highlights some key concepts and equations from each week. In addition it gives pointers to specific sections of the recommended books for further reading. With the help of the notes you take in class and the recommended reading, you should be able to explain the meaning of each concept listed here, know the meaning of every symbol in the equations, including the relevant units and dimensions.

1 Week 1 : Blackbody radiation and the origins of quantum theory

Reading : Krane Section 3.3. Brandsden-Joachain Section 1.1.

Key concepts and Equations

- What is a Black body ? A black body is an ideal object that absorbs all the radiation incident on it at any temperature, any wavelength, any angle of incidence. It does not transmit or reflect any of the incident radiation.
- A black body also emits the maximum amount of radiant energy for a given temperature.
- The spectral emittance $R(\lambda, T)$ is the power radiated per unit area of emitting surface, per unit small wavelength range around wavelength λ. Thus $R(\lambda, T)d\lambda$ is the power radiated per unit area of emitter in the wavelength range λ to $\lambda + d\lambda$.
- Planck's formula for the spectral emittance of a black body. Also called Planck spectral distribution formula or Planck distribution formula.

$$R(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} \frac{1}{(\exp(\frac{hc}{\lambda kT}) - 1)}$$

where

$\lambda \rightarrow$ wavelength

$T \rightarrow$ temperature

$c \rightarrow$ speed of light

$k \rightarrow$ Boltzmann's constant

$h \rightarrow$ Planck's constant

Quiz : What are the dimensions and SI units of $R(\lambda, T)$?

- Stefan-Boltzmann Law

$$P = \sigma T^4$$

  Derivation from Planck Distribution by integrating over wavelengths.
  $\sigma = 5.67 \times 10^{-8} W m^{-2} K^{-4}$.

- Wien's displacement Law.

$$\lambda_{max} T = b$$

  where the constant $b = 2.898 \times 10^{-3}\ m\ K$.

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$$c = f\lambda$$

- The high frequency (small wavelength) limit (Wien's approximation)

$$R(\lambda, T) = \frac{2\pi hc^2}{\lambda^5} e^{\frac{-hc}{\lambda kT}}$$

- The low frequency (long wavelength) limit - Rayleigh-Jeans formula.

$$R(\lambda, T) = \frac{2\pi ckT}{\lambda^4}$$

- Spectral distribution in frequency space :

$$\tilde{R}(f, T) df = R(\lambda, T) d\lambda$$

  Hence, using $f\lambda = c$ calculate $\tilde{R}(f, T)$.

- **Further Reading related to this week's material**
  Radiation Heat transfer (Siegel and Howell)
  Wikipedia : Kirchhoff's Law of thermal radiation

2 Week 2 : Blackbody radiation and the origins of quantum theory

Reading Krane Section 3.1,3.2 ; Bransden-Joachain Section 1.2

- Relation between spectral emittance and energy density :

$$R(\lambda, T) = \frac{c}{4} u(\lambda, T)$$

- For a laser beam,

$$\text{Power per unit area} = uc$$

- The above two equations are closely related. The 1/4 is a geometrical factor which requires some care.

- Translating between books : $R(\lambda, T)$ in Bransden-Joachain is $I(\lambda)$ in Krane. $\rho(\lambda, T)$ in Bransden-Joachain is $u(\lambda)$ in Krane.

- The Rayleigh-Jeans derivation :

  (A) Modes for waves in a box of size L, with conducting walls. E is zero at the boundaries.

  $$E = \sin(\frac{n_x \pi x}{L}) \sin(\frac{n_y \pi y}{L}) \sin(\frac{n_z \pi z}{L})$$

  where n_x, n_y, n_z are natural numbers, i.e belong to the set $\{0, 1, 2, 3, \cdots\}$.

  (B) Number of modes in wavelength range $(\lambda, \lambda + d\lambda)$, including factor of 2 for polarization

  $$\frac{8\pi L^3 d\lambda}{\lambda^4}$$

  Average energy per mode $k_B T$.

  C) Hence energy per unit volume per unit wavelength range ;

  $$u(\lambda, T) = \frac{8\pi L^3}{\lambda^4} \times k_B T$$

  (D) Then use $R = \frac{uc}{4}$ and simplify to get $R(\lambda, T) = \frac{2\pi c k_B T}{\lambda^4}$.

- Classical formula for average energy

$$< E >= \frac{\int_0^\infty E e^{\frac{-E}{kT}} dE}{\int_0^\infty e^{\frac{-E}{kT}} dE}$$

- Useful rewriting. With $\beta = \frac{1}{kT}$

$$< E >= \frac{\int_0^\infty E e^{-\beta E}}{\int_0^\infty e^{-\beta E} dE} = -\frac{d}{d\beta} Log \left(\int_0^\infty e^{-\beta E} dE \right)$$

- Planck's modification : Energy discretized.$E = n\epsilon_0$.

$$< E >= \frac{\sum_{n=0}^\infty n\epsilon_0 e^{-n\beta\epsilon_0}}{\sum_{n=0}^\infty e^{-n\beta\epsilon_0}} = -\frac{d}{d\beta} Log \left(\sum_{n=0}^\infty e^{-\beta n \epsilon_0} \right)$$

- For **further reading** on derivation of the mode counting formula see, for example, Chapter 9 of the book by Reif "Fundamentals of statistical and thermal physics"

3 Week 3 : Review of electromagnetic waves, including Poynting vector + Photo-electric effect

Reading
Krane Section 3.1 : Light as waves - Review of Electromagnetic waves.
Krane Section 3.2 : Light as photons - Photo-electric effect.
Bransden-Joachain Section 1.2 :

Equations describing the $\vec{E}, \vec{B}$ fields for a plane wave, Poynting vector, Intensity from Poynting vector (including time-averaging), Plane wave-fronts.

Photo-electric effect. work function. Stopping potential. The equations

$$\begin{aligned} & hf - \phi = K_{\max} \\ & K_{\max} = eV_s \\ & \phi = hf_c \end{aligned}$$

Cutoff frequency (threshold frequency) in photo-electric effect - explained by quantum physics but not classical physics.

4 Week 4 : More on particle-like properties of light - Compton scattering ; Interference; Wave-particle duality

Reading : Krane Section 3.4-3.6 and 3.1 ; Feynman Lectures Volume 3 - Chapter 1,2.
Compton scattering : Photon (e.g. X-ray) scatters off a loosely bound electron.
Expectation from wave picture of light : Intensity in direction of incoming wave decreases, frequency unchanged.
Photon picture leads to an increase in wavelength of outgoing photon, due to energy conservation
Energy and momentum conservation equations

Derivation of

$$\lambda' - \lambda = \frac{h}{m_e c}(1 - \cos\theta)$$

Bremsstrahlung. Electrons accelerated through a positive potential difference ΔV. Then deceleration through interaction with matter. Energy delivered to photons. Minimum wavelength :

$$\frac{hc}{\lambda_{min}} = e\Delta V$$

Maxwell's equations and EM waves. The equations relating frequency and wave-vector for a wave propagating in general direction. Wave-vector $\vec{k} = (k_x, k_y, k_z)$.

$$\begin{aligned}\omega^2 &= c^2(k_x^2 + k_y^2 + k_z^2) \\ \lambda &= \frac{2\pi}{k} = \frac{2\pi}{\sqrt{k_x^2 + k_y^2 + k_z^2}}\end{aligned}$$

Photon energy, momentum

$$\begin{aligned}E &= \hbar\omega = hf \\ \vec{p} &= \hbar\vec{k}\end{aligned}$$

for photons where $\hbar = \frac{h}{2\pi}$.
Superposition property of the solutions to Maxwell's equations.
Revisiting interference : Young's double slit experiment. Bright fringes at :

$$y_n = \frac{n\lambda D}{d}$$

5 Week 5 : Wave nature of matter and diffraction

Reading : Krane Chapter 4 on wave nature of matter + Krane Section 3.1 (X-ray diffraction and Bragg's Law) +. Bransden and Joachain Section 1.6
De Broglie's formula.

$$\lambda = \frac{h}{p}$$

The formulae from relativity

$$\begin{aligned}&p = \gamma m v \\ &E = \gamma m c^2 \\ &K = E - mc^2 = (\gamma - 1)mc^2\end{aligned}$$

The non-relativistic limit : $v/c << 1$.
Equivalently $K << mc^2$.
The ultra-relativistic limit : v close to c ; $\gamma >> 1$ or $K >> mc^2$.

Principle of superposition and Linearity of equations :
If $\vec{E}^{(1)}$ and $\vec{E}^{(2)}$ are two solutions of

$$\nabla^2 \vec{E} = \frac{1}{c^2}\frac{\partial^2 \vec{E}}{\partial t^2}$$

then the $\vec{E}^{(1)} + \vec{E}^{(2)}$ is also a solution.

Young's double slit interference pattern as an application of superposition principle. Derivation of

$$y_n = \frac{n\lambda D}{d}$$

Single slit diffraction pattern : Minima at

$$a \sin\theta = n\lambda$$

This shows that a has to be comparable to λ for observable diffraction
Multi-slit diffraction pattern. The n'th order maximum as

$$d \sin\theta = n\lambda$$

The Davisson-Germer experiment : electron diffraction
Futher Reading : Bragg's Law - X-ray diffraction.

One photon double-slit interference experiment.

6 Week 6 : Wavepackets and Heisenberg Uncertainty

Reading : Chapter 4 of Krane. Chapter 2 (and Appendix) of Bransden and Joachain.

- Electron 2-slit experiment and interference. Photon interfence : superpose $E^{(1)}, E^{(2)}$ solutions to linear Maxwell's equations and $I \propto E^2$. Electron interfence : Superpose $\Psi^{1)}(x,t), \Psi^{(2)}(x,t)$ - solutions to linear equations of QM (mention Schrodinger to be studied later).

- $\Psi(\vec{x},t)$ is complex, and $\Psi^*\Psi$ is a probability density. In one dimensional case $\Psi(x,t)$. If a particle is described by wavefunction $\Psi(x,t)$, then the probability of finding the particle in the region between x and $x+dx$ is $\Psi^*(x,t)\Psi(x,t)dx$.

- In two slit experiment, we add the wavefunctions due to the two slits

  $$\begin{aligned} \Psi &= (\Psi_1 + \Psi_2) \\ \Psi^*\Psi &= \Psi_1^*\Psi_1 + \Psi_2^*\Psi_2 + \Psi_1^*\Psi_2 + \Psi_2^*\Psi_1 \end{aligned}$$

  The probability density is NOT the sum of the probability densitites due to the two slits. Hence the maxima and minima of the interference pattern.

- The wavefunction for a free particle of definite wavenumber.

  $$\Psi_{free}(x,t) = Ae^{i(kx-\omega t)}$$

  for some constant A, and $p = \hbar k = \frac{h}{\lambda}$ (de Broglie) with $E = hf = \hbar\omega$. Motivated by de Broglie equation and Planck/Einstein equations. Later we will see that it solves the Schrodinger equation for free particle.

- Observe $\Psi^*\Psi = A^*A$ Uses $e^{i\theta}(e^{i\theta})^* = e^{i\theta}e^{-i\theta} = 1$ for any real θ. Probability density independent of position - equallly likely to be anywhere. First sign of Heisenberg Uncertainty, which *implies* that, for a wavefunction where momentum is completely certain, the position is completely uncertain.

- Definition of a normalized wavefunction.

- Observe, using formula for $\Psi_{free}(x,t)$, that

$$-i\hbar\frac{\partial}{\partial x}\Psi_{free}(x,t) = \hbar k\Psi_{free}(x,t) = p\Psi_{free}(x,t)$$

  This is an example of a general correspondence in Quantum Mechanics :

$$p \leftrightarrow -i\hbar\frac{\partial}{\partial x}$$

- Start studying Gaussian wave-packets to describe localised objects. Sketch the probability density as a function of x. Then Calculate $< x >, < x^2 >, \Delta x$.

- The Gaussian wavepacket

$$\psi_{k_0,d}(x) = \frac{1}{\pi^{1/4}\sqrt{d}}\ \ e^{ik_0x-\frac{x^2}{2d^2}}$$

  Expectation values

$$\begin{aligned}
< x > &= \int_{-\infty}^{\infty} \psi^*_{k_0,d}(x)\ x\ \psi_{k_0,d}(x) \\
< x^2 > &= \int_{-\infty}^{\infty} \psi^*_{k_0,d}(x)\ x^2\ \psi_{k_0,d}(x) \\
< p > &= -i\hbar\int_{-\infty}^{\infty} \psi^*_{k_0,d}(x)\ \frac{\partial}{\partial x}\ \psi_{k_0,d}(x) \\
< p^2 > &= -\hbar^2\int_{-\infty}^{\infty} \psi^*_{k_0,d}(x)\ \left(\frac{\partial}{\partial x}\right)^2\ \psi_{k_0,d}(x)
\end{aligned}$$

- Hence $\Delta x\Delta p = \frac{\hbar}{2}$ for Gaussian wave-packets. And $\Delta x\Delta p \geq \frac{\hbar}{2}$ for general wave-packets. Hesienberg-Uncertainty principle - A fundamental limitation on accuracy of simultaneous measurements of x, p. Some examples with macroscopic and microscopic objects.

7 Week 8 : Heisenberg Uncertainty Principle and Applications; Complementarity

Reading : Chapter 4 of Krane. Chapter 2 (and Appendix) of Bransden and Joachain.

- Heisenberg Uncertainty Principle (HUP) continued.

$$\begin{aligned}
\Delta p_x \Delta x &\geq \frac{\hbar}{2} \\
\Delta p_y \Delta y &\geq \frac{\hbar}{2} \\
\Delta p_z \Delta z &\geq \frac{\hbar}{2} \\
\Delta E \Delta t &\geq \frac{\hbar}{2}
\end{aligned}$$

- HUP in terms of wavelengths :

$$\Delta x \Delta \lambda \geq \frac{1}{4\pi} \lambda^2$$

- Application of HUP to single slit experiment. Heisenberg uncertainty explains the spread in directions of outgoing particles from the slit.

- Application of HUP to double slit experiment. Measurement of position of particle as it is going through the slits - if it has enough precision to distinguish which slit particle goes through, then it produces an uncertainty in momentum large enough to destroy the interference pattern. This is complementarity : cannot simultaneously observe the wave property of interference and the trajectory of the particle.

- In Quantum mechanics, we have particles, but not particle trajectories. This is related to the quantum mechanical wave-behaviour of particles. In classical mechanics, the state at a given time is described by $(x(t), p(t))$ equivalently by $(x(t), \dot{x}(t))$. In quantum mechanics, the state is described by a wave function $\Psi(x, t)$. The properties of waves imply the Heisenberg uncertainty principle : positions and momenta cannot be determined with certainty at a given time.

- Energy-time uncertainty relation : Relating lifetimes and widths of particles.

- Diffraction limit of microscopes. Heisenberg's thought experiment - The Heisenberg microscope. (see Bransden-Joachain page 70).

- Group Velocity of de Broglie Waves

  $$v_g = \frac{d\omega}{dk}$$

  Using the equations

  $$\begin{aligned}
  E &= \hbar\omega = \gamma m c^2 \\
  p &= \hbar k = \gamma m v
  \end{aligned}$$

  we can show that $v_g = v$: group velocity is equal to particle velocity.

Some further reading : Experimental verification of Heisenberg uncertainty relation for hot Fullerene molecules by Nairz, Arndt, Zeilinger - available online (Google it).

8 Week 9: Quantum Postulates and Schrodinger's Equation

Reading : Chapter 5 of Krane + Parts of Chapter 3 and 5 of Bransden and Joachain.

- Postulates of quantum physics (Reading - Bransden and Joachain - Chapter 5).

  P1. An ensemble of systems is described by a wavefunction. For a particle in one dimension, the wavefunction is a function of x, t, written as $\Psi(x,t)$. Discussion :

  - Indeterminacy and ensembles - recall single slit or double slit experiment.
  - normalization
  - $c\Psi$ describes same physics as Ψ for any complex number c.

  Contrast with classical mechanics where classical state is described by $(x(t), \cdot x(t))$. Newton's equations allow us to calculate the future positions and velocities, given the initial positions and velocities. Schrodinger equation allows us to calculate the evolution in time of the wavefunction.

  P2. Principle of superposition. If Ψ_1 and Ψ_2 are wavefunctions for a system, then $c_1\Psi_1 + c_2\Psi_2$ is another wavefunction.

  P3. Observables A correspond to operators $\hat{A}$.

$$\begin{aligned}
&x\text{-momentum}, p_x \rightarrow \hat{p}_x : \psi(x,t) \rightarrow \frac{-i\hbar\partial\psi(x,t)}{\partial x} \\
&\text{position}, x \rightarrow \hat{x} : \psi(x,t) \rightarrow x\psi(x,t) \\
&\text{Energy}, E \rightarrow \hat{E} : \psi(x,t) \rightarrow i\hbar\frac{\partial\psi(x,t)}{\partial t}
\end{aligned}$$

  These equations - applied to $e^{i(kx-\omega t)}$ describing a wave propagating in the x-direction - allow us to recover de Broglie's equations :

$$\begin{aligned}
E &= \hbar\omega \\
p &= \hbar k
\end{aligned}$$

  now as applications of the general framework of quantum mechanics.

  The operators corresponding to observables correspond to *lnear hermitian* operators. Linear means that :

$$\hat{A}(c_1\Psi_1 + c_2\Psi_2) = c_1(\hat{A}\Psi_1) + c_2(\hat{A}\Psi_2)$$

  for aribtrary constants c_1, c_2. You will see mathematical definition of *hermitian* in QMB and MT3.

P4. Operators, expectation values, eigenvalues.

Expectation value of observable A

$$< A >= \frac{\int \Psi^* \hat{A} \Psi}{\int \Psi^* \Psi}$$

Eigenvalue equation for operator $\hat{A}$

$$\hat{A}\Psi_a = a\Psi_a$$

Ψ_a is an eigenfunction or eigenstate. a is an eigenvalue. In the state ψ_a the measured value of the observable A.

Linear hermitian operators have real eigenvalues.

Born Rule If we have $\Psi = c_1\Psi_{a_1} + c_2\Psi_{a_2}$ where

$$\begin{aligned} \hat{A}\Psi_{a_1} &= a_1\Psi_{a_1} \\ \hat{A}\Psi_{a_2} &= a_2\Psi_{a_2} \end{aligned}$$

i.e Ψ_{a_1}, Ψ_{a_2} are eigenfunctions of an operator $\hat{A}$ with distinct eigenvalues a_1, a_2 (i.e $a_1 \neq a_2$), then a measurement of A can give either a_1 or a_2. The respective probabilities P_1, P_2 are :

$$\begin{aligned} P_1 &= \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} \\ P_2 &= \frac{|c_1|^2}{|c_1|^2 + |c_2|^2} \end{aligned}$$

P5. The collapse of the wavefunction. If $\Psi = c_1\Psi_{a_1} + c_2\Psi_{a_2}$ as above (in P4) is the quantum state of a system, then two possible values for measurement of A are a_1, a_2. IF at time t_0, the measured value if a_1, then the wavefunction immediately after measurement is Ψ_{a_1}. If the measured value at time t_0 is a_2, then the wavefunction immediately after is Ψ_{a_2}.

- The time-dependent Schrodinger's equation for a non-relativistic particle in presence of potential energy function $V(x)$:

$$\frac{-\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$

- The time-independent Schrodinger equation

$$\frac{-\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x)$$

This is used to calculate the possible energy levels of a system.

- Free Particle in an infinite potential well. Derivation of energy level formula

$$E_n = \frac{n^2h^2}{8mL^2}$$

(See Krane section 5.4).

9 Week 10 :Particle in a box - illustrating the principles of Quantum Physics.

Reading : Krane Chapter 5, Parts of Chapter 3 and 5 of Bransden and Joachain.

- Recall that $\psi_n(x)$ are eigenfunctions of the Hamiltonian operator (which is the energy operator expressed in terms of position and momentum operators).

  $$\hat{H}\psi_n = E_n\psi_n$$
  $$\hat{H} = \frac{-\hbar^2}{2m}\frac{\partial^2\psi_n}{\partial x^2}$$

  Equivalently

  $$\frac{-\hbar^2}{2m}\frac{\partial^2\psi_n(x)}{\partial x^2} = E_n\psi_n(x)$$

  where

  $$E_n = \frac{n^2h^2}{8mL^2}$$

- The normalized energy eigenfunctions :

  $$\psi_n(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi x}{L})$$

- Orthogonality : ψ_n, ψ_m are orthogonal for $n \neq m$, i.e.

  $$\int \psi_n^*\psi_m dx = 0$$

- If we have a superposition of states

  $$\psi(x) = c_m\psi_m + c_n\psi_n$$

  the norm of ψ can be shown to be

  $$\int dx\psi^*(x)\psi(x) = |c_n|^2 + |c_m|^2$$

  To normalize ψ, we define $\hat{\psi}$, related to ψ by an overall constant factor

  $$\hat{\psi}(x) = \frac{1}{\sqrt{|c_n|^2 + |c_m|^2}}\psi$$

  Check that $\hat{\psi}$ is normalized, i.e has unit norm.

- Use the time-dependent Schrodinger equation to calculate the time-dependence of energy eigenstates. Using

  $$\Psi(x, t = 0) = \psi_n(x)$$

  as the "initial condition" we guess that the time dependent wavefunction is

  $$\Psi(x, t) = \psi_n(x) f(t)$$

  Sustitute in the time-dependent Schroedinger equation and use the initial condition to get

  $$\Psi(x, t) = \psi_n(x) e^{\frac{-iE_n t}{\hbar}}$$

- If the initial condition is a superposition of energy eigenstates

  $$\Psi(x, t = 0) = \sum_n c_n \psi_n(x)$$

  then

  $$\Psi(x, t) = \sum_n c_n \psi_n(x) e^{\frac{-iE_n t}{\hbar}}$$

- For superpositions such as $\psi = c_m \psi_m + c_m \psi_n$, we discussed how to calculate the expectation value of the energy

  $$< E >= \frac{|c_m|^2}{|c_n|^2 + |c_m|^2} E_m + \frac{|c_n|^2}{|c_n|^2 + |c_m|^2} E_n$$

- The coefficients of E_m and E_n are the probabilities for finding E_m and E_n when a measurement of energy is made - This is an application of the **Born rule** which gives the probabilities of measurements of different eigenvalues.

- Calculation of uncertainties Δx and Δp in eigenstate $\psi_n(x)$ are developed in exercises/homeworks. These uncertainties are consistent with the Heisenberg uncertainty relation.

10 Week 11 : Simple Harmonic Oscillator

Reading : Krane Sec. 5.5 ; Br and Jo Chapter 4 - see pictures of probability distributions and classical limit ; Dr Russo notes (under the heading "textbooks" in QMPLUS) - see oxygen molecule - for discussion of quantum mechanics of molecule vibrations also see sec 1.3 and 9.4 of Krane.

- Review of the classical mechanics of simple harmonic oscillator. Schrodinger's equation. Energy spectrum. Ground state wavefunction - start with ansatz Be^{-ax^2} and determine a in terms of $k, m, \hbar$ and the ground state energy. Excited states from ladder operator.
- Hamiltonian for oscillations around $x = x_0$ with minumum potential energy U_0. Change of variables and wavefunctions centred on x_0.
- Properties of the energy eigenfunctions under the parity operation P

  $$P\psi(x) = \psi(-x)$$

  Using parity to deduce that $< x >= 0$ for all the energy eigenstates.
- Calculating $\Delta x \Delta p$ for the ground state.
- Time-dependent wavefunctions. Deriving oscillating $< x >$ and $< p >$ in a superposition of energy eigenfunctions.

11 Week 12 : Quantum Mechanics of atoms and molecules

- Bohr model of the atom

  $$E_n = -\frac{m_e e^4}{8\epsilon_0^2 h^2 n^2}$$

  See Krane section 6.5 for the derivation, as well as the successes and failures of the Bohr model.
- Rotational and Vibrational modes of molecules ; Specific heat capacities. See Krane section 1.3, section 9.4 and 9.5.
- Ehrenfrest theorem (no proof given in this course)- See Bransden and Joachain section 3.4 for the three-dimensional version.

  $$\frac{d < x >}{dt} = \frac{< p >}{m}$$

  can be shown using

  $$\begin{aligned} &< x >= \int \Psi^*(x,t) x \Psi(x,t)\ dx \\ &< p >= -i\hbar \int \Psi^*(x,t) \frac{\partial}{\partial x} \Psi(x,t)\ dx \\ &\left(-\hbar^2 \frac{\partial^2}{\partial x^2} + U(x)\right) \Psi(x,t) = \frac{i\hbar \partial \Psi(x,t)}{\partial t} \end{aligned}$$

The integrals are understood to be from $-\infty$ to ∞. The wavefunctions vanish at infinity, so we can use integration by parts to simplify the answer. Using similar steps, we can show that

$$\frac{d}{dt} < p >= - < \frac{dU}{dx} >$$

The LHS is

$$\begin{aligned}
&\frac{d}{dt} < p >= \frac{d}{dt} \int \Psi^*(x,t) \left(-i\hbar \frac{\partial \Psi(x,t)}{\partial x} \right) \\
&= (-i\hbar) \int \frac{\partial \Psi^*}{\partial t} \frac{\partial \Psi(x,t)}{\partial x} - (i\hbar) \int \Psi^*(x,t) \frac{\partial^2 \Psi(x,t)}{\partial x \partial t} \\
&= \int \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right) \Psi^* \frac{\partial \Psi(x,t)}{\partial x} - \int \Psi^*(x,t) \frac{\partial}{\partial x} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x) \right) \Psi
\end{aligned}$$

The terms involving third derivatives with respect to x cancel after using partial integration twice. We are left with

$$\begin{aligned}
&\frac{d}{dt} < p >= \int \Psi^* U(x) \frac{\partial \Psi}{\partial x} - \Psi^* \frac{\partial}{\partial x} (U\Psi) \\
&= - \int \Psi^* \frac{\partial U}{\partial x} \Psi \\
&= - < \frac{\partial U}{\partial x} >
\end{aligned}$$

This is, at the level of quantum expectation values, the statement that the force is equal to rate of change of momentum.

- A math fact we use in verifying that guesses such as e^{-ax^2} or xe^{-ax^2} solve the SHO schrodinger equation is that if a polynomial function of x vanishes for all x, then all the coefficients vanish. This is intuitively obvious and can be used in this module without proof, but here, just for clarity, we will explain a proof of this math fact. Take for example

  $$\alpha_1 + \alpha_2 x = 0$$

  Assume that α_1, α_2 are independent of x. By setting $x = 0$ we deduce $\alpha_1 = 0$. Taking a derivative with respect to x, and then setting $x = 0$ proves that $\alpha_2 = 0$. Similarly we can show that if this equation

  $$\alpha_1 + \alpha_2 x + \alpha_3 x^2 = 0$$

  holds for all x, then all the x-independent quantities, $\alpha_1, \alpha_2, \alpha_3$ are zero. To prove this : First set $x = 0$ to prove that $\alpha_1 = 0$. Then take one derivative, followed by setting $x = 0$: this shows that $\alpha_2 = 0$. Of we take 2 derivatives before setting $x = 0$, we see that $\alpha_3 = 0$. This clearly generalizes to polynomials of order n where you have $\alpha_1, \cdots, \alpha_n$.