

Physics 310 Cheat Sheet

The Schrödinger equation,

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

relates a particle's (possibly complex-valued) wave function, Ψ to its potential energy.

$$H\psi(x) = E\psi(x) \quad \text{for } H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2}.$$

Probability Density Function (PDF): $\rho(x, t)$.

The statistical interpretation: $\rho(x, t) = |\Psi(x, t)|^2$.

$$\int_a^b |\Psi(x, t)|^2 dx = \text{Prob. of finding the particle between } a \text{ and } b, \text{ at time } t.$$

In QM, measurement and physical system are separated. Measuring collapses the particle's wave function to a spike because the act of measuring changes the amount of energy in the system.

Standard deviation (measures spread of PDF):

$$\sigma_j = \sqrt{\langle j^2 \rangle - \langle j \rangle^2}.$$

Einstein's idea for photon energy:

$$E = h \frac{c}{\lambda} = hf = \hbar 2\pi f = \hbar \omega.$$

de Broglie's idea of the matter wave:

$$p = \frac{h}{\lambda} = \frac{2\pi\hbar}{\lambda} = \hbar k \quad \left(k \equiv \frac{2\pi}{\lambda}, \text{ wave number} \right).$$

In QM, 'matter wave' \rightarrow 'wave-function'.
Schrödinger's idea of the momentum operator:

$$\underbrace{\frac{\hbar}{i} \frac{d}{dx}}_{\text{operator}} \underbrace{e^{i\frac{p}{\hbar}x}}_{\text{operand}} = \underbrace{p}_{\text{value}} \underbrace{e^{i\frac{p}{\hbar}x}}_{\text{operand}}.$$

In general,

$$\langle Q(x, p) \rangle = \int_{-\infty}^{\infty} \Psi^* Q \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \Psi dx.$$

Ehrenfest's Theorem: $\frac{d}{dt} \langle p \rangle = - \left\langle \frac{dV}{dx} \right\rangle$.

Uncertainty principle: $\sigma_x \sigma_p \geq \frac{\hbar}{2}$

Through separation, we find the solution to be

$$\Psi(x, t) = \sum_{\text{all } n} c_n e^{-iE_n t/\hbar} \psi_n(x)$$

Normalization condition (time independent)

$$1 = \int_{-\infty}^{\infty} |\Psi(x, 0)|^2 dx \implies 1 = \sum_n |c_n|^2.$$

Kronecker delta and the orthonormality of the Energy eigenfunction:

$$\int_{-\infty}^{\infty} \psi_n(x)^* \psi_m(x) dx = \delta_{mn} = \begin{cases} 1 & m = n \\ 0 & m \neq n \end{cases}$$

Physical interpretation of c_n : $\langle E \rangle = \langle H \rangle = \sum_n |c_n|^2 E_n$, so $|c_n|^2$ is the probability of observing E_n .

$$c_n = \int_{-\infty}^{\infty} \psi_n^*(x) \Psi(x, 0) dx$$

The relation $P_n = |c_n|^2$ is time independent: $\Psi(x, t)$ will change over time by $e^{-iE_n t/\hbar}$. c_n is dependent of t and x so

$$\frac{dc_n}{dt} = 0 \implies \frac{d\langle E \rangle}{dt} = 0 \leftarrow \text{Conservation of Energy}$$

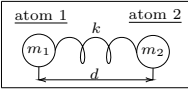
Conservation of Probability

$$\frac{d}{dt} \int_{-\infty}^{\infty} |\Psi(x, t)|^2 dx = 0.$$

For the continuity equation $\frac{\partial |\Psi|^2}{\partial t} + \frac{\partial J}{\partial x} = 0$,

$$J = \frac{-\hbar}{2mi} \left(\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right)$$

is the probability current.

	$V(x)$	Energy and Eigenfunction	Application
Infinite Square Well	$\begin{cases} 0 & (0, a); \\ \infty & \text{o/w.} \end{cases}$	$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) & (0, a); \\ 0 & \text{o/w.} \end{cases}$ $E_n = \frac{\pi^2 \hbar^2}{2ma^2} n^2 \quad \Delta E = E_1(2n+1)$ $n \in \mathbb{N}$	<u>Molecular Energy Absorption</u> : N free electrons ($N/2$ double bonds), l = bond length, n is the number corresponding to the Highest Occupied Molecular Orbit (HOMO). $a = (N-1)l$. $E_1(2n+1) = \Delta E = \frac{\hbar c}{\lambda} \implies \lambda = \frac{8cm(N-1)^2 l^2}{(2n+1)\hbar}$ <small>photon</small> <i>Pauli exclusion principle</i> : only two electrons can occupy the same energy level.
Simple Harmonic Oscillator	$\frac{m\omega^2 x^2}{2}$	$\psi_n(x) = C_n H_n(\xi) e^{-\xi^2/2}$ $\xi = \sqrt{\frac{m\omega}{\hbar}} x$ $H_0(\xi) = 1, H_1(\xi) = 2\xi$ $H_{n+1}(\xi) = 2\xi H_n(\xi) - 2n H_{n-1}(\xi)$ $n \in \mathbb{N}_0$ $E_n = \hbar\omega \left(n + \frac{1}{2} \right)$ $\Delta E = \hbar\omega$ $\bar{E} = \frac{\sum_n P_n E_n}{\sum_n P_n}$	<u>Molecular Vibration</u> : Diatomic Molecule's potential energy (nuclear interaction) can be modeled with a parabola $V(x)$. $E_n = \frac{\hbar c}{\lambda_n}$ for $n \in \mathbb{N}_0 \implies \Delta E = \hbar c \left(\frac{1}{\lambda_{n+1}} - \frac{1}{\lambda_n} \right)$.  $\omega = \sqrt{\frac{k}{m}}, m = \frac{m_1 m_2}{m_1 + m_2}$ the 'reduced mass' $\hbar\omega = \Delta E = \hbar c \left(\frac{1}{\lambda_{n+1}} - \frac{1}{\lambda_n} \right)_{\text{avg}} \implies \omega = 2\pi c \left(\frac{1}{\lambda_{n+1}} - \frac{1}{\lambda_n} \right)_{\text{avg}}$ <u>Ensemble of SHO's</u> : Will reach thermal equilibrium, $P_n \propto e^{E_n/k_B T}$. Write $\beta = \frac{1}{k_B T}$, $Z \equiv \sum_n P_n = \sum_{n=0}^{\infty} e^{-\hbar\omega(n+\frac{1}{2})\beta} \therefore \frac{1}{2 \sinh\left(\frac{\beta\hbar\omega}{2}\right)}$ $\bar{E} = \frac{-1}{Z} \frac{\partial Z}{\partial \beta} \doteq \frac{\hbar\omega}{2} + \frac{\hbar\omega}{e^{\hbar\omega/k_B T} - 1}$ <u>Black Body Radiation</u> : Radiation from a cavity with wall temperature T and volume $V = L^3$. Vacuum is filled with SHO's. Dispersion relation of EM wave: $\omega = c \vec{k} \doteq \frac{c\pi r}{L}$ with $k_u = \frac{2\pi}{\lambda_u}$, (where $\lambda_u = \frac{2L}{n_u}$), \vec{k} is the propagation vector, and $r = \sqrt{n_x^2 + n_y^2 + n_z^2}$. Twice the number of modes (n_x, n_y, n_z) in between r and $r + \Delta r$ is the number of EM wave modes in between ω and $\omega + \Delta\omega$, $n(\omega)\Delta\omega \doteq \frac{L^3}{c^3 \pi^2} \omega^2 \Delta\omega$. The total mean energy in the cavity is $E = \int_0^{\infty} \rho(\omega) d\omega = \int_0^{\infty} \bar{E}(\omega, T) n(\omega) d\omega.$
Free Particle	0	Plane wave solution: $\Psi(x, t) = e^{-iEt/\hbar} \left(\underbrace{A e^{ikx}}_{x \text{ drctn.}} + \underbrace{B e^{-ikx}}_{-x \text{ drctn.}} \right)$ $E = \frac{(\hbar k)^2}{2m}$	$\frac{\partial \rho}{\partial t} = 0 \implies \frac{dJ}{dx} = 0$ by the continuity equation. This means that $J(b, t) = J(a, t)$, 'conservation of J '. We can find $J = \frac{-\hbar}{2mi} \left(\frac{\partial \Psi^*}{\partial x} \Psi - \Psi^* \frac{\partial \Psi}{\partial x} \right) = \frac{\hbar}{mk} (A ^2 - B ^2).$ Wave packet solution: $\Psi(x, t) = \int_0^{\infty} c(E) e^{-iEt/\hbar} \psi(E, x) dE$.
Step Potential	$\begin{cases} 0 & x < 0 \\ V_0 & \text{o/w} \end{cases}$	$\Psi(x, t) = e^{-iEt/\hbar} \left\{ \begin{aligned} & A e^{ikx} + B e^{-ikx} \\ & F e^{i\ell x} \end{aligned} \right.$ $\frac{(\hbar k)^2}{2m} = E_1 = E_{II} = \frac{(\hbar \ell)^2}{2m} + V_0$	$J_I = J_{II} \implies \underbrace{\frac{\hbar k}{m} A ^2}_{J_{\text{inc}}} - \underbrace{\frac{\hbar k}{m} B ^2}_{J_{\text{ref}}} = \underbrace{\frac{\hbar \ell}{m} F ^2}_{J_{\text{trans}}} \implies J_{\text{inc}} - J_{\text{ref}} = J_{\text{trans}} \implies 1 - \underbrace{\frac{J_{\text{ref}}}{J_{\text{inc}}}}_R = \underbrace{\frac{J_{\text{trans}}}{J_{\text{inc}}}}_T \implies R + T = 1$ R is the reflection coefficient and T is the transmission coefficient, which give the probability of reflection and transmission, probability. The boundary conditions, $\psi_I(0) = \psi_{II}(0)$ and $\psi'_I(0) = \psi'_{II}(0)$ yield $A + B = F$ and $ik(A - B) = i\ell F$.

From Homework # 1

Problem 1.3: $\rho(x) = Ae^{-\lambda|x-a|}$

A = sqrt(lambda/pi) (x) = a (x^2) = 1/2lambda + a^2 sigma = 1/sqrt(2lambda)

Problem 1.5: Psi(x,t) = Ae^{-lambda|x|}e^{-iwt}

A = sqrt(lambda) (x) = 0 (x^2) = 1/2lambda^2 sigma = 1/sqrt(2lambda)

P(x) = [-1/sqrt(2lambda), 1/sqrt(2lambda)] = e^{-sqrt(2)}

Problem 1.9: psi(x,t) = Ae^{-a[(mx^2)/h + it]}

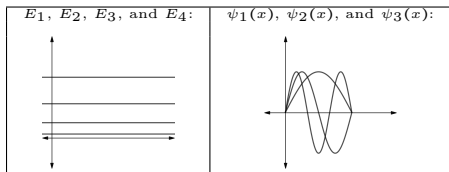
A = sqrt(2am/h*pi) (x) = 0 (x^2) = h/4am (p) = 0 (p^2) = ham sigma_x = sqrt(h/4am) sigma_p = sqrt(ham) sigma_x sigma_p = h/2

From Exercise #1 (Infinite Square Well)

0 <= x <= a and 0 <= E

n > 0, since if n = 0, the wave function would be 0 everywhere, so the particle would not be found anywhere.

(x)_n = a/2 (x^2)_n = a^2/3 - a^2/(2(pi*n)^2)



From Exercise #2 (General solution and Infinite square well)

2. (a) Pn = |cn|^2 = |int from -inf to inf psi* Psi(x,0) dx|^2 = 480/(pi^6 * n^6) ((-1)^(n+1) + 1)

(b-c) Since cn does not depend on t, P1 approx 0.998555, P2 = 0, P3 approx 0.001369759, P4 = 0.

From Homework #2 (Infinite square well)

Vitamin A1: We assume a bond length of l = 0.1 nm and since Vitamin A1 has 5 double bonds in a chain, there are N = 10 free electrons. Because of the Pauli exclusion principle, HOMO is E5 so n = 5 (LUMO is E6). The (absorption) wavelength needed to excite an electron from E5 to E6 is lambda approx 243 nm.

Problem 2.4 (x)_n = a/2 (x^2)_n = a^2/3 - a^2/(2(pi*n)^2 (p)_n = d(x)/dt = 0 (p^2)_n = h^2 * (pi/n)^2 sigma_x,n = a * sqrt(1/12 - 1/(2pi*n)^2) sigma_p,n = h*pi/n/a (sigma_x sigma_p)_n approx h/2

Table with 7 columns: n, 1, 2, 3, 4, 5, 6 and 7 rows: sigma_x sigma_p/h, 0.57, 1.67, 2.63, 3.56, 4.48, 5.40

Clearly, (sigma_x sigma_p)_n comes closest to h/2 at n = 1.

Problem 2.5. Psi(x,0) = A[psi1(x) + psi2(x)]

(a) 1 = sum from n of |cn|^2 = |c1|^2 + |c2|^2 = A^2 + A^2 = 2A^2 => A = 1/sqrt(2)

(b) Psi(x,t) = 1/sqrt(a) * (e^{-iwt} sin(pi/a * x) + e^{-i4wt} sin(2pi/a * x))

|Psi(x,t)|^2 = 1/a * (sin^2(pi/a * x) + sin^2(2pi/a * x) + 2 sin(pi/a * x) sin(2pi/a * x) cos(3wt))

(c) (x) = int from -inf to inf x |Psi(x,t)|^2 dx = a/2 * (1 - 32/(9pi^2) cos(3wt))

Angular frequency is 3w = 3 * pi * 2h/2m * a^2. Amplitude is a/2 * 32/(9pi^2)

(d) (p) = m * d(x)/dt = m * a/2 * 32/(9pi^2) sin(3wt) * (3w) = 16amw/3pi^2 sin(3wt)

Exercise #3 (S.H.O.)

(1) H2(x) = 4x^2 - 2, H3(x) = 8x^3 - 12x, H4(x) = 16x^4 - 48x^2 + 8

(2.c) psi0(x) = C0 e^{-x^2/2}, psi1(x) = C1 2xi e^{-xi^2/2}, psi2(x) = C2 (4xi^2 - 2) e^{-xi^2/2}

(d) We will show that H*psi_n - En*psi_n = 0 for n = 0 and n = 1:

H*psi_n - En*psi_n = Cn * h^2/2m * d^2/dx^2 [Hn(xi) * e^{-xi^2/2}] + cn * Hn(xi) * e^{-xi^2/2} - En * Cn * e^{-xi^2/2} = 0

e. C0 = sqrt(h*pi/mw), C1 = 1/sqrt(2) * sqrt(h*pi/mw)

Homework # 3 (S.H.O.)

Problem 1. Psi(x,0) = c0 psi0(x) + c1 psi1(x)

(a) Defining xi = sqrt(mw/h) * x and Cn = (mw/h)^{1/4} * 1/sqrt(2^n * n!),

Psi = c0 e^{-itw/2} * (mw/h)^{1/4} * e^{-xi^2/2} + c1 e^{-i3tw/2} * (mw/h)^{1/4} * 2xi e^{-xi^2/2}

(b) (x) = sqrt(h/2mw) * (c0* c1 e^{-iwt} + c0* c1* e^{iwt})

Problem 2

(a) When c0 = 0 and c1 = 1, (x) = 0, so the particle is not vibrating.

(b) Let c0 = 1/sqrt(2) and c1 = i/sqrt(2), then (x) = sqrt(h/2mw) sin(wt), with A = sqrt(h/2mw) the amplitude of oscillation.

(c) The frequency of molecular vibration of nitrogen (N2) is about 840 GHz. A approx 2.92 * 10^-11 m = 0.292 A.

(d) For carbon monoxide (CO). Then find the amplitude A in units of A for the same state.

f = c * 1/8 * (1/lambda_g - 1/lambda_o) = 790 GHz A approx 3.04 * 10^-11 m.

Exercise # 4 (Black Body)

1. [rho(w)] = [E(w,T)n(w)] = kg * m^2/s

2. u = E/V = 1/V * int from 0 to inf h*w/kBT - 1 * L^3*w^2/(pi^2*c^3) * d*w = h/(pi^2*c^3) * (kBT/h)^4 * int from 0 to inf x^3/(e^x - 1) dx = k^4_B * T^4 * pi^2 / (h^3*c^3*15)

3. The Stefan-Boltzman Constant: sigma = J/T^4 = cu/4T^4 = c*k^4_B * T^4 * pi^2 / (4h^3*c^3*15T^4) = pi^2 * k^4_B / (60 * h^3*c^2) = 5.67 * 10^-8 K^3/s^2

4. [sigma] = [k_B]^4 / [h]^3 [c]^2 = (J/K)^4 / (J^3/s^3 [c]^2) = J^4/K^4 / (J^3/s^3 [c]^2) = Kg m^2/s^2 / (Kg^3 m^2/s^3) = Kg / (Kg^3 m^2/s^3) = Kg / (Kg^3 s^3)

[sigma] = [J]/[T]^4 = (kg/s^3) / (K^4) = Kg / (K^4 s^3)

5. 0 = dp/dw = d/dw [h*w/kBT - 1 * L^3*w^2 / (pi^2*c^3)] = L^3/h * d/dw [w^3 / (e^{h*w/kBT} - 1)] = L^3/h * (3w^2 * e^{h*w/kBT} - w^3 * (h/kBT * e^{h*w/kBT})) / (e^{h*w/kBT} - 1)^2

=> 0 = 3w^2 * e^{h*w/kBT} - 3w^2 - w^3 * (h/kBT) * e^{h*w/kBT}
=> 0 = 3e^{h*w/kBT} - 3 - (h/kBT) * e^{h*w/kBT}
=> 0 = e^{h*w/kBT} * (h/kBT - 3) + 3
using solution x approx 2.824 for 3 + e^x(x-3) = 0,

=> 2.824 = h*w/kBT => w = 2.824 * k_B * T / h

Exercise # 5 (Potential Barriers for hump)

psi(x) = { psi_I(x) = Ae^{ikx} + Be^{-ikx} for x < 0; psi_II(x) = Ce^{ilx} + De^{-ilx} for 0 <= x <= a; psi_III(x) = Fe^{ikx} + Ge^{-ikx} for x > a

1. G is 0 since there is no wave traveling in the -x direction in region III.

2. J_I = J_III => h*k/m * (|A|^2 - |B|^2) = h*k/m * (|F|^2)
=> T = J_trans/J_inc = (h*k/m * |A|^2) / (h*k/m * |F|^2) = |A|^2/|F|^2

3. psi_I(0) = psi_II(0) => A + B = C + D

psi_I'(0) = psi_II'(0) => ikA - ikB = ilC - ilD => k(A - B) = l(C - D)

=> A - B = l/k * (C - D)

4. 2A = C + D + l/k * (C - D) => A = C(k+l)/2k + D(k-l)/2k

5. psi_II(a) = psi_III(a) => C + De^{-2ila} = Fe^{i(k-l)a}

psi_II'(a) = psi_III'(a) => C - De^{-2ila} = l/k * Fe^{i(k-l)a}

6. C = (l+k)/2 * e^{i(k-l)a} F and D = (l-k)/2 * e^{i(k+l)a} F

7. T = |F|^2/|A|^2 = [1 + (k^2 - l^2)/(2il) * sin^2(la)]^{-1}

8. E = k^2*h^2/2m = l^2*h^2/2m + V0 => k = sqrt(2mE)/h and l = sqrt(2m(E-V0))/h

9. T = 1 => (k^2 - l^2)/(2k*l) * sin^2(la) = 0 => l = pi*n/a for n in N.

=> En = h^2 * (n*pi/a)^2 / 2m + V0 => E_min = E1 since E > V0

10. R = 1 - T = 1 - [1 + V0^2/(4(E^2 - EV0)) * sin^2(sqrt(2m(E-V0))/h * a)]^{-1}

Homework # 4

Problem 1: The Sun

(a) Using the solution to (5) on Exercise # 4, w = 2.824 * k_B * T / h => T = w * h / (2.824 * k_B) = (2pi * 3.4 * 10^14 Hz) / (1.05457 * 10^-34 Js) = 5778.111 K

(b) Using the Stephan-Boltzman Law (J = sigma T^4), Delta E = P*Delta t = J*A*Delta t = sigma*T^4*4*pi*r_sun^2*Delta t = (5.67 * 10^-8 * K^3/s^2) * (5778K)^4 * 4pi * (7 * 10^8 m)^2 * (86400 s) = 3.362 * 10^31 J

Problem 2: Finding J for Psi(x,t) = e^{-iEt/h} (Ae^{ikx} + Be^{-ikx})

J = -h/(2mi) * (dPsi/dx - Psi* dPsi/dx) = -h/(2mi) * (e^{iEt/h}/h * (A*(-ik)e^{-kx} + B*(ik)e^{ikx})e^{-iEt/h} - e^{-iEt/h}/h * (A*(ik)e^{-kx} + B*(-ik)e^{ikx})e^{-iEt/h}) = -h/(2mi) * ik * (-|A|^2 - A*B*e^{-2ikx} + B*A*e^{2ikx} + |B|^2 - |A|^2) = h/(2mi) * ik * (2|A|^2 - 2|B|^2) = h*k/m * (|A|^2 - |B|^2)

Problem 3: Step Potential

(a) Boundary conditions psi_I(0) = psi_II(0) and psi_I'(0) = psi_II'(0), imply that A + B = F and ik(A - B) = ilF.

F = k/(l) * (A - B) = k/(l) * (A - (F - A)) = k/(l) * (2A - F) => F = k/(l) * (2A) = 2kA/l, and B = 2kA/l - A = (k-l)A/(k+l)

(b) R = J_ref/J_inc = (h*k|B|^2/m) / (h*k|A|^2/m) = |B|^2/|A|^2 = ((k-l)/(k+l))^2 * |A|^2/|A|^2 = ((k-l)/(k+l))^2

T = (h*|F|^2/m) / (h*|A|^2/m) = |F|^2/|A|^2 = (4k^2|A|^2) / (k|A|^2 * (l+k)^2) = 4kk/(k+l)^2

(c) When V0 = 0, E = h^2*k^2/2m = h^2*ell^2/2m + 0 => k^2 = ell^2, and since ell, k > 0, ell = k. So, R = ((k-l)/(k+l))^2 = 0 and T = 1 - R = 1. This means that there is no chance that the particle will be reflected; it will be transmitted.

(d) When E >> V0, h^2*k^2/2m = E approx h^2*ell^2/2m => k^2 approx ell^2 and since ell, k > 0, ell approx k. So, R = ((k-l)/(k+l))^2 approx 0 and T = 1 - R approx 1. This means that the particle will most likely be transmitted, with very little possibility of reflection.

(e) When E = V0, V0 = E = h^2*ell^2/2m + V0 => ell = 0. So, R = ((k-0)/(k+0))^2 = k^2/k^2 = 1 and T = 1 - R = 0. This means that the particle will be reflected, with no possibility of transmission.

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