PHYS 121 Quantum Mechanics Equation Sheet

Statistics & Probability
Discrete: $\langle f\rangle = \sum_j f(j)P(j)$, $\sum_j P(j) = 1$.
Continuous: $\langle f(x)\rangle = \int f(x)\rho(x)\mathrm{d}x$, $\int \rho(x)\mathrm{d}x = 1$.
$P(a < x < b) = \int_a^b \rho(x)\mathrm{d}x$.
$\sigma^2 = \langle (x - \langle x\rangle)^2\rangle = \langle x^2\rangle - \langle x\rangle^2$, $\sigma = \sqrt{\sigma^2}$.
$\rho = |\psi|^2$, $\langle A\rangle = \int \psi^* \hat{A}\, \psi\, \mathrm{d}x$.

Operators & Commutators
$\hat{x} = x$, $\hat{p} = -\mathrm{i}\hbar\, \partial_x$, $\hat{H} = \hat{p}^2/2m + V$.
$[A, B] = AB - BA$.
$\sigma_A \sigma_B \geq \frac{1}{2}|\langle [A, B]\rangle|$.
Ehrenfest: $\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{i}}{\hbar}\langle [H, A]\rangle + \langle \partial_t A\rangle$.

Schrödinger Equations
TDSE: $\mathrm{i}\hbar\, \partial_t \psi = \left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi$.
TISE: $\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]\psi = E\psi$.
Stationary: $\psi(\boldsymbol{r}, t) = \psi(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}Et/\hbar}$, $|\psi|^2$ time-independent.

Free Particle & Fourier
$V = 0$: $\psi = (A\mathrm{e}^{\mathrm{i}kx} + B\mathrm{e}^{-\mathrm{i}kx})\mathrm{e}^{-\mathrm{i}\omega t}$, $k = \pm\sqrt{2mE}/\hbar$.
$E = \hbar\omega = \hbar^2 k^2/2m$, $p = \hbar k$.
$\phi(k) = \frac{1}{\sqrt{2\pi}}\int \psi(x, 0)\mathrm{e}^{-\mathrm{i}kx}\mathrm{d}x$.
$\psi(x, t) = \frac{1}{\sqrt{2\pi}}\int \phi(k)\mathrm{e}^{\mathrm{i}(kx-\omega t)}\mathrm{d}k$.
Plancherel: $\int |\psi|^2\mathrm{d}x = \int |\phi|^2\mathrm{d}k$.
Reflection/Transmission: $R = |r|^2$, $T = |t|^2$ with $R + T = 1$ (flux).

Bound vs. Scattering
Bound: $E < V(\pm\infty)$, $\psi \to 0$ as $|x| \to \infty$.
Scattering: $E > V(\pm\infty)$, plane-wave asymptotics.

Infinite Square Well
$V = 0$ for $0 < x < a$, $V = \infty$ else.
$\psi_n = \sqrt{\frac{2}{a}}\sin\frac{n\pi x}{a}$, $E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}$.
$\psi(x, t) = \sum_n c_n \psi_n(x)\mathrm{e}^{-\mathrm{i}E_n t/\hbar}$,
$c_n = \int_0^a \psi_n^*(x)\psi(x, 0)\mathrm{d}x = \langle n|\psi(0)\rangle$.

Quantum Harmonic Oscillator
$V = \frac{1}{2}m\omega^2 x^2$, $\omega = \sqrt{k/m}$.
$a = \sqrt{\frac{m\omega}{2\hbar}}x + \frac{\mathrm{i}}{\sqrt{2m\omega\hbar}}p$, $[a, a^\dagger] = 1$.
$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$, $E_n = \hbar\omega\left(n + \frac{1}{2}\right)$.
$a^\dagger |n\rangle = \sqrt{n+1}\,|n+1\rangle$, $a|n\rangle = \sqrt{n}\,|n-1\rangle$.
$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$, $p = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(a^\dagger - a)$.
$\psi_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\mathrm{e}^{-m\omega x^2/2\hbar}$.
$\psi_n = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}H_n(\xi)\mathrm{e}^{-\xi^2/2}$, $\xi = \sqrt{\frac{m\omega}{\hbar}}x$.
$H_n(\xi) = (-1)^n \mathrm{e}^{\xi^2}\frac{\mathrm{d}^n}{\mathrm{d}\xi^n}\mathrm{e}^{-\xi^2}$.

Linear Algebra (Dirac)
$A^\dagger = (A^*)^T$. Hermitian: $A = A^\dagger$ (real eigenvalues).
Unitary: $U^\dagger U = I$. Orthogonal: $O^T O = I$.
Orthonormal basis: $\sum_n |n\rangle\langle n| = I$, $\langle m|n\rangle = \delta_{mn}$.
$|\psi\rangle = \sum_n c_n |n\rangle$, $c_n = \langle n|\psi\rangle$.

Angular Momentum
$[L_i, L_j] = \mathrm{i}\hbar\,\varepsilon_{ijk}L_k$, $[L^2, L_i] = 0$.
$L^2|lm\rangle = \hbar^2 l(l+1)|lm\rangle$, $L_z|lm\rangle = \hbar m|lm\rangle$.
$L_\pm = L_x \pm \mathrm{i}L_y$, $L_\pm|lm\rangle = \hbar\sqrt{l(l+1) - m(m\pm 1)}\,|l, m\pm 1\rangle$.

3D Central Potentials
$\psi(\boldsymbol{r}) = R_{nl}(r)Y_l^m(\theta, \phi)$, $n = 1, 2, \ldots$, $l = 0, \ldots, n-1$.
$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{L^2}{\hbar^2 r^2}$.
$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\partial_\theta(\sin\theta\,\partial_\theta) + \frac{1}{\sin^2\theta}\partial_\phi^2\right]$.
$Y_l^m = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\,P_l^m(\cos\theta)\mathrm{e}^{\mathrm{i}m\phi}$.
$P_l^m(x) = (1 - x^2)^{m/2}\frac{\mathrm{d}^m}{\mathrm{d}x^m}P_l(x)$,
$P_l(x) = \frac{1}{2^l l!}\frac{\mathrm{d}^l}{\mathrm{d}x^l}(x^2 - 1)^l$.

Hydrogen Atom
$V(r) = -\frac{e^2}{4\pi\varepsilon_0 r}$, $a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2}$.
$E_n = -\frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2}\frac{1}{n^2} = -\frac{13.6\text{ eV}}{n^2}$.
$\rho = \frac{2r}{na_0}$,
$R_{nl} = \left(\frac{2}{na_0}\right)^{3/2}\sqrt{\frac{(n-l-1)!}{2n[(n+l)!]}}\,\mathrm{e}^{-\rho/2}\rho^l L_{n-l-1}^{2l+1}(\rho)$.

Spin-1/2
$S^2|sm\rangle = \hbar^2 s(s+1)|sm\rangle$, $S_z|sm\rangle = \hbar m|sm\rangle$.
$s = \frac{1}{2}$, $m = \pm\frac{1}{2}$. $S_\pm = S_x \pm \mathrm{i}S_y$.
$S_i = \frac{\hbar}{2}\sigma_i$,
$\sigma_x = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$, $\sigma_y = \begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}$, $\sigma_z = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$.
$|+z\rangle = \begin{pmatrix}1\\ 0\end{pmatrix}$, $|-z\rangle = \begin{pmatrix}0\\ 1\end{pmatrix}$.

Perturbation Theory
$H = H_0 + \lambda H'$, $|n\rangle = |n^0\rangle + \lambda|n^1\rangle + \cdots$.
$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots$.
$E_n^1 = \langle n^0|H'|n^0\rangle$.
$|n^1\rangle = \sum_{m\neq n}\frac{\langle m^0|H'|n^0\rangle}{E_n^0 - E_m^0}|m^0\rangle$.
$E_n^2 = \sum_{m\neq n}\frac{|\langle m^0|H'|n^0\rangle|^2}{E_n^0 - E_m^0}$.
Degenerate: diagonalize H' within degenerate subspace.
TDPT: $c_f^{(1)}(t) = \frac{1}{\mathrm{i}\hbar}\int_0^t \langle f|H'(t')|i\rangle\,\mathrm{e}^{\mathrm{i}\omega_{fi}t'}\mathrm{d}t'$,
$\omega_{fi} = (E_f - E_i)/\hbar$, $w_{i\to f} = \frac{2\pi}{\hbar}|\langle f|H'|i\rangle|^2\rho(E_f)$.

WKB Approximation
$p(x) = \sqrt{2m[E - V(x)]}$.
Allowed region: $\psi \approx \frac{C}{\sqrt{p(x)}} \cos\left(\frac{1}{\hbar}\int^x p(x')\mathrm{d}x' - \frac{\pi}{4}\right)$.
Quantization (two soft turning points): $\int_{x_1}^{x_2} p(x)\mathrm{d}x = \left(n + \frac{1}{2}\right)\pi\hbar$.
Two hard walls: $\int_{x_1}^{x_2} p(x)\mathrm{d}x = n\pi\hbar$.
One hard wall + one soft turning point: $\int_{x_1}^{x_2} p(x)\mathrm{d}x = \left(n + \frac{3}{4}\right)\pi\hbar$.

Gram–Schmidt
$|e_1\rangle = |a_1\rangle / \| |a_1\rangle \|$.
$|u_2\rangle = |a_2\rangle - \langle e_1|a_2\rangle |e_1\rangle$, $|e_2\rangle = |u_2\rangle / \| |u_2\rangle \|$.
$|u_3\rangle = |a_3\rangle - \langle e_1|a_3\rangle |e_1\rangle - \langle e_2|a_3\rangle |e_2\rangle$,
$|e_3\rangle = |u_3\rangle / \| |u_3\rangle \|$.

Taylor Series
$f(a+h) = \sum_{n=0}^{\infty} \frac{f^{(n)}(a)}{n!} h^n$.
$\sin^2\theta = \frac{1}{2}(1 - \cos 2\theta)$, $\cos^2\theta = \frac{1}{2}(1 + \cos 2\theta)$.

Gaussian Integrals
$\int_{-\infty}^{\infty} \mathrm{e}^{-\alpha x^2}\mathrm{d}x = \sqrt{\frac{\pi}{\alpha}}$.
$\int_0^{\infty} x^{2n}\mathrm{e}^{-x^2/a^2}\mathrm{d}x = \sqrt{\pi}\,\frac{(2n)!}{n!\,2^{2n+1}}\,a^{2n+1}$.