H5: the formalism of quantum mechanics

postulates	1: to an ensemble of physical systems one can associate a wave function or state function which contains all information that can be known about the ensemble > this function is complex and may be multipl. by an arbitrary complex number without altering its physical significance 2: the superposition principle: $\Psi = c_1\Psi_1 + c_2\Psi_2$ 3: with every dynamical variable is associated a linear operator 4: the only result of a precise measurement of the dynamical variable $\mathcal{A}$ is one of the eigenvalues a_n of the linear operator A associated with $\mathcal{A}$ 5: if a series of measurements made of the dynamical variable A on an ensemble of systems, described by the wave function Ψ, the expectation value of A is: $\langle A \rangle = \frac{\langle \Psi | A | \Psi \rangle}{\langle \Psi | \Psi \rangle}.$ 6: A wave function representing any dynamical state can be expressed as a linear combination of the eigenfunctions of A > with A is the operator with a dynamical variable 7: the time evolution of the wave function of a system is determined by the TDSE: $i\hbar \frac{\partial}{\partial t}\Psi(t) = H\Psi(t)$ where H is the Hamiltonian, or total energy operator of the system.
5.1 the state of a system	
dynamical state of a quantum system	In quantum the dynamical state of a system is influenced by measurement > system gets unpredictably altered when measured > according to Heisenberg uncertainty relations ie: sets limit to precision with which complementary dynamical variables can be measured Abandon the classical idea that all dynamical variables of a system have well-defined values at all times > quantum predicts the number n of times a particular result will be obtained in N identical, independent, identically prepared physical systems aka ensembles > ie: quantum predicts the probability n/N
postulate 1)	to an ensemble of physical systems one can associate a wave function or state function which contains all information that can be known about the ensemble > this function is complex and may be multipl. by an arbitrary complex number without altering its physical significance but: 1: some ensembles cannot be described by a single state function > such ensembles aren't considered here 2: its common practice to speak of the wave function associated with a system > it's implied this works on an ensemble
general particle system	consider a particle in given potential V(**r**,t) > particle is structureless ie: no internal degrees of freedom, such as spin this has an associated state function Ψ(**r**,t) which is square integrable if: $I = \int \lvert\Psi(\mathbf{r}, t)\rvert^2 d\mathbf{r}$ is finite for c a complex constant, cΨ describes the same particle > choose this constant such that: $\int \lvert\Psi(\mathbf{r}, t)\rvert^2 d\mathbf{r} = 1.$ with P(**r**,t) = $\lvert\Psi\rvert^2$ the position probability density
postulate 2)	the superposition principle: $\Psi = c_1\Psi_1 + c_2\Psi_2$

5.1.1 momentum space functions	
state of ensemble in momentum space	Use the Fourier transform of Ψ to go to momentum space wave function Φ(**p**,t) > if Ψ is normalised, so is Φ: $$\int |\Phi(\mathbf{p}, t)|^2 \mathrm{d}\mathbf{p} = 1$$ now Π(**p**,t) = $|\Phi|^2$ is the probability density in momentum space > prob. of finding the momentum of a particle in volume d**p** now the FT of Ψ(**r**$_1$,…,**r**$_N$) is: $$\Phi(\mathbf{p}_1, \ldots, \mathbf{p}_N, t) = (2\pi\hbar)^{-3N/2} \int \exp\left[-\frac{\mathrm{i}}{\hbar}(\mathbf{p}_1.\mathbf{r}_1 + \cdots + \mathbf{p}_N.\mathbf{r}_N)\right] \times \Psi(\mathbf{r}_1, \ldots, \mathbf{r}_N, t)\mathrm{d}\mathbf{r}_1 \ldots \mathrm{d}\mathbf{r}_N.$$
5.1.2 Dirac bracket notation	
Dirac bracket notation	define $\langle\Psi_1|\Psi_2\rangle \equiv \int \Psi_1^*(\mathbf{r})\Psi_2(\mathbf{r})\mathrm{d}\mathbf{r}$
properties of Dirac bracket	$\langle\Psi_1|\Psi_2\rangle = \langle\Psi_2|\Psi_1\rangle^*$. **(5.15a)** Moreover, if c is a complex number and Ψ_3 a third function, we also have $\langle\Psi_1|c\Psi_2\rangle = c\langle\Psi_1|\Psi_2\rangle$, **(5.15b)** $\langle c\Psi_1|\Psi_2\rangle = c^*\langle\Psi_1|\Psi_2\rangle$, **(5.15c)** $\langle\Psi_3|\Psi_1 + \Psi_2\rangle = \langle\Psi_3|\Psi_1\rangle + \langle\Psi_3|\Psi_2\rangle$. **(5.15d)** Two functions Ψ_1 and Ψ_2 are said to be orthogonal if their scalar product vanishes: $\langle\Psi_1|\Psi_2\rangle = 0$. **(5.16)** Using the Dirac bracket notation, we see that the normalisation condition (5.5) can be written compactly as $\langle\Psi|\Psi\rangle = 1$. **(5.17)**
5.2 dynamical variables and operators	
postulate 3)	with every dynamical variable is associated a linear operator
associating operators	in configuration space, for a dynamical variable $\mathcal{A} = A(\mathbf{r}_1, \ldots, \mathbf{r}_N, \mathbf{p}_1, \ldots, \mathbf{p}_N, t)$ > associate the linear operator A: $$A(\mathbf{r}_1, \ldots, \mathbf{r}_N, -\mathrm{i}\hbar\nabla_1, \ldots, -\mathrm{i}\hbar\nabla_N, t)$$ on the other hand, in momentum space: $$A(\mathrm{i}\hbar\nabla_{\mathbf{p}_1}, \ldots, \mathrm{i}\hbar\nabla_{\mathbf{p}_N}, \mathbf{p}_1, \ldots, \mathbf{p}_N, t)$$
5.2.1 eigenvalues and eigenfunctions	
postulate 4)	the only result of a precise measurement of the dynamical variable $\mathcal{A}$ is one of the eigenvalues a_n of the linear operator A associated with $\mathcal{A}$
eigenfunction	ψ_n is an eigenfunction of A with eigenvalue a_n if: $$A\psi_n = a_n\psi_n.$$ > totality of eigenvalues of A = spectrum of A
5.2.2 Hermitian operators	
Hermitian operator	An operator is Hermitian if: $\langle X|(A\Psi)\rangle = \langle(AX)|\Psi\rangle$ with Ψ and X square integrable functions However in Dirac notation we usually write $$\langle X|(A\Psi)\rangle \equiv \langle X|A|\Psi\rangle$$

properties of eigenfunctions	for ψ_n an eigenfunction with eigenvalue a_n, it holds: $\langle\psi_n\|A\|\psi_n\rangle = a_n\langle\psi_n\|\psi_n\rangle.$ In addition, since $(A\psi_n)^* = a_n^*\psi_n^*$ we also have $\langle(A\psi_n)\|\psi_n\rangle = a_n^*\langle\psi_n\|\psi_n\rangle.$ Now if A is Hermitian, we have $a_n = a_n^*$ > Hermitian operators always produce *real eigenvalues*
operators for dynamical system $\mathcal{A}$	An operator A for $\mathcal{A}$ must always give real eigenvalues > A must be a Hermitian operator
measurement and probability	if the wave function of a system is one of the eigenfunctions ψ_n of A > then a measurement of $\mathcal{A}$ will certainly produce a result a_n if the wave function of a system is not one of the eigenfunctions ψ_n of A > the a measurement of $\mathcal{A}$ can produce $a_1, a_2, \ldots$ > we can predict the probability of each a_n
postulate 5)	if a series of measurements made of the dynamical variable A on an ensemble of systems, described by the wave function Ψ, the expectation value of A is: $\langle A\rangle = \frac{\langle\Psi\|A\|\Psi\rangle}{\langle\Psi\|\Psi\rangle}.$ if A is Hermitian, then ⟨A⟩ is real if ψ is normalised to unity, ⟨Ψ|Ψ⟩=1, thus $\langle A\rangle = \langle\Psi\|A\|\Psi\rangle.$
5.2.3 adjoint operator	
adjoint operator of A / Hermitian conjugate	the conjugate operator $A^\dagger$ is defined by: $\langle X\|A^\dagger\|\Psi\rangle = \langle(AX)\|\Psi\rangle$ $= \langle\Psi\|A\|X\rangle^*$ with X and Ψ square integrable
self-adjoint operator	is an operator A for which $A^\dagger = A$
consequence of adjoint operator	If we define a bra $\langle\Phi\|$ by the relation $\langle\Phi\| = \langle X\|A^\dagger$ **(5.31)** where the operator $A^\dagger$ acts to the left on the bra $\langle X\|$, then it follows from (5.30) that the kets $\|\Phi\rangle$ and $\|X\rangle$ are related by $\|\Phi\rangle = A\|X\rangle$ **(5.32)**
properties of adjoint operators	$(cA)^\dagger = c^*A^\dagger$ where c is a complex number, $(A+B)^\dagger = A^\dagger + B^\dagger$ and $(AB)^\dagger = B^\dagger A^\dagger.$
5.2.4 functions of operators	
function of an operator	if f(z) can be expanded in a power series $f(z) = \sum_{i=0}^{\infty} c_i z^i$ the f(A) can be defined as: $f(A) = \sum_{i=0}^{\infty} c_i A^i.$
eigenfunctions of f(A)	as a consequence due to the definition we have: $A^i\psi_n = (a_n)^i\psi_n$ and thus $f(A)\psi_n = f(a_n)\psi_n.$

adjoint of f(A)	The adjoint operator to $f(A)$ can be obtained as follows. Using (5.34)–(5.36) and (5.38), we see that $$[f(A)]^\dagger = \sum_{i=0}^{\infty} c_i^* (A^i)^\dagger = \sum_{i=0}^{\infty} c_i^* (A^\dagger)^i$$ $$= f^*(A^\dagger). \quad \textbf{(5.40)}$$ In particular, if A is a self-adjoint operator, we have $$[f(A)]^\dagger = f^*(A). \quad \textbf{(5.41)}$$
5.2.5 inverse and unitary operators	
inverse of A	The unit operator I is the operator that leaves any function Ψ unchanged $I\Psi = \Psi.$ If, given an operator A, there exists another operator B such that $BA = AB = I$ then B is said to be the *inverse* of A and one writes $B = A^{-1}.$
unitary linear operator U	A linear operator U is said to be *unitary* if $U^{-1} = U^\dagger$ or $UU^\dagger = U^\dagger U = I.$ Such an operator can be expressed in the form $U = e^{iA}$ where A is a Hermitian operator. Indeed, using (5.41), we see that $U^\dagger = (e^{iA})^\dagger = e^{-iA}$
5.2.6 projection operators	
idempotent operator	An operator Λ is said to be *idempotent* if $\Lambda^2 = \Lambda.$ If, in addition, Λ is Hermitian, it is called a *projection operator*.
projection operator	Any function Ψ can be expressed in terms of two orthogonal functions Φ and X by means of a projection operator. This can be seen as follows. We first write $$\Psi = \Phi + \mathrm{X} \quad \textbf{(5.49)}$$ with $\Phi = \Lambda\Psi$ and $\mathrm{X} = (I - \Lambda)\Psi$. Now $$\langle \Phi | \mathrm{X} \rangle = \langle \Lambda\Psi | (I - \Lambda)\Psi \rangle$$ $$= \langle \Psi | \Lambda - \Lambda^2 | \Psi \rangle$$ $$= 0 \quad \textbf{(5.50)}$$ where in the second line we have used the fact that Λ is Hermitian and in the third line we have used (5.48). Note that $I - \Lambda$ is also a projection operator, since it is Hermitian, and $$(I - \Lambda)^2 = I - 2\Lambda + \Lambda^2$$ $$= I - \Lambda. \quad \textbf{(5.51)}$$

5.3 expansion in eigenfunctions	
study of eigenfunctions	For an operator A: $A\psi_n = a_n\psi_n$ > assume A is linear and Hermitian representing a dynamical variable > eigenvalues a_n are real >> first look at its properties when ψ_n is square integrable $\langle\psi_n\|\psi_n\rangle = 1.$
5.3.1 orthogonality	
orthogonality of eigenfunctions	for ψ_i ψ_j two different eigenfunctions with eigenvalues a_i, a_j: $A\psi_i = a_i\psi_i$ and $A\psi_j = a_j\psi_j.$ Hence $(a_i - a_j)\langle\psi_i\|\psi_j\rangle = \langle a_i\psi_i\|\psi_j\rangle - \langle\psi_i\|a_j\psi_j\rangle$ $= \langle(A\psi_i)\|\psi_j\rangle - \langle\psi_i\|(A\psi_j)\rangle$ $= 0$ thus we have orthogonality between different eigenfunctions: $\langle\psi_i\|\psi_j\rangle = 0, \qquad i \neq j$
5.3.2 degeneracy	
degeneracy of eigenfunctions	An eigenvalue a_n is degenerate if there are multiple linearly independent eigenfunctions belonging to that eigenvalue > let α be the degree of degeneracy of a certain eigenvalue a_n: $A\psi_{nr} = a_n\psi_{nr}, \qquad r = 1, 2, \ldots, \alpha.$ via Schmidt orthogonalization: make the eigenfunctions ψ_{nr} mutually orthogonal and normalized to unity > since eigenfunctions belonging to different eigenvalues are mutually orthogonal > all eigenfunctions satisfy the orthonormality relations: $\langle\psi_{ir}\|\psi_{js}\rangle = \delta_{ij}\delta_{rs}$ its only necessary to distinguish eigenfunctions belonging to a degenerate eigenvalue explicitly > for the other eigenfunctions, just write: $\langle\psi_m\|\psi_n\rangle = \delta_{mn}.$
postulate 6	A wave function representing any dynamical state can be expressed as a linear combination of the eigenfunctions of A > with A is the operator with a dynamical variable
Now we will study purely discrete eigenvalues for which: $\Psi = \sum_n c_n\psi_n.$ > all wave functions can be expanded in a complete set of eigenfunctions $\{\psi_n\}$	
observables	= Hermitian operator that possesses a complete set of eigenfunctions
finding coefficients c_n	due to orthonormality: $\langle\psi_m\|\Psi\rangle = \sum_n c_n\langle\psi_m\|\psi_n\rangle$ $= \sum_n c_n\delta_{mn}$ $= c_m.$
closure relation	for a one-particle system, we have: $\Psi(\mathbf{r}, t) = \sum_n\left[\int \psi_n^*(\mathbf{r}')\Psi(\mathbf{r}', t)\mathrm{d}\mathbf{r}'\right]\psi_n(\mathbf{r})$ $= \int\left[\sum_n \psi_n^*(\mathbf{r}')\psi_n(\mathbf{r})\right]\Psi(\mathbf{r}', t)\mathrm{d}\mathbf{r}'$ and hence $\sum_n \psi_n^*(\mathbf{r}')\psi_n(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}')$ >> expresses the completeness of the set of functions $\{\psi_n\}$

general closure relation	in multiple dimensions: $$\sum_n \psi_n^*(\mathbf{r}_1', \ldots, \mathbf{r}_N')\psi_n(\mathbf{r}_1, \ldots, \mathbf{r}_N) = \delta(\mathbf{r}_1 - \mathbf{r}_1') \ldots \delta(\mathbf{r}_N - \mathbf{r}_N').$$
scalar product of wave functions	for one-particle case: $$\begin{aligned}\langle X|\Psi\rangle &= \int X^*(\mathbf{r}, t)\Psi(\mathbf{r}, t)\mathrm{d}\mathbf{r} \\ &= \int X^*(\mathbf{r}, t)\delta(\mathbf{r} - \mathbf{r}')\Psi(\mathbf{r}', t)\mathrm{d}\mathbf{r}\mathrm{d}\mathbf{r}' \\ &= \sum_n \int X^*(\mathbf{r}, t)\psi_n(\mathbf{r})\mathrm{d}\mathbf{r} \int \psi_n^*(\mathbf{r}')\Psi(\mathbf{r}', t)\mathrm{d}\mathbf{r}' \\ &= \sum_n \langle X|\psi_n\rangle\langle\psi_n|\Psi\rangle\end{aligned}$$ >> we see that in the Dirac notation the closure relation can be written as: I = unity operator $\sum_n |\psi_n\rangle\langle\psi_n| = I$
5.3.3 probability amplitudes	
expectation value of A	For a wave function Ψ describing a state, normalized to unity > ⟨A⟩ is then: $$\begin{aligned}\langle A\rangle &= \langle\Psi|A|\Psi\rangle \\ &= \sum_m \sum_n c_m^* c_n \langle\psi_m|A|\psi_n\rangle \\ &= \sum_m \sum_n c_m^* c_n a_n \langle\psi_m|\psi_n\rangle \\ &= \sum_n |c_n|^2 a_n\end{aligned}$$ Since Ψ is normalize to unity, we also have: $\langle\Psi|\Psi\rangle = 1$ <=> $\sum_n |c_n|^2 = 1.$
probability of measurement of a_n	- All possible results of measurement of A are the eigenvalues a_n - average value obtained in series of measurements is the expectation value ⟨A⟩ > interpret the quantity P_n as the probability that in a given measurement the particular value a_n will be obtained: $$P_n = |c_n|^2 = |\langle\psi_n|\Psi\rangle|^2$$ >> - $\sum_n |c_n|^2 = 1.$ expresses the fact that the probability of obtaining some result is unity - the coefficients $c_n = \langle\psi_n|\Psi\rangle$ are the *probability amplitudes*
P_n for degenerate eigenvalues	For a a_n that's α times degenerate and ψ_{nr}(r=1,…,α) orthogonal eigenfunctions > we have: $$\Psi = \sum_n \sum_{r=1}^{\alpha} c_{nr}\psi_{nr} \quad (5.69)$$ with $$c_{nr} = \langle\psi_{nr}|\Psi\rangle. \quad (5.70)$$ A simple reworking of (5.66) then yields $$\langle A\rangle = \sum_n \sum_{r=1}^{\alpha} |c_{nr}|^2 a_n \quad (5.71)$$ so that the probability of obtaining upon measurement of A the degenerate eigenvalue a_n is $$P_n = \sum_{r=1}^{\alpha} |c_{nr}|^2 = \sum_{r=1}^{\alpha} |\langle\psi_{nr}|\Psi\rangle|^2. \quad (5.72)$$ After a measurement leading to the value a_n, the system is described by the (unnormalised) wave function $$\Psi_n = \sum_{r=1}^{\alpha} c_{nr}\psi_{nr} \quad (5.73)$$ and if the measurement is immediately repeated the value a_n will be obtained with certainty.

5.3.4 the continuous spectrum

thus far we assumed the observables only posses a spectrum of discrete eigenvalues
> in general they can have a discrete and continuous part
> we need to expand our theory

normalizing continuous spectrum	we have seen that the continuous spectrum cannot be normalised > solution: - enclose the system in a large box > render the system completely discrete > solution independent from size of box, provided its large enough - 'normalise' in terms of Dirac delta functions
⟨A⟩ for continuous spectrum	Consider A with both a discrete and continuous spectrum > discrete eigenvalues a_n with eigenfunctions ψ_n continuous eigenvalues a with eigenfunctions ψ_a $$A\psi_n = a_n\psi_n, \qquad A\psi_a = a\psi_a.$$ - All eigenvalues should be real - discrete eigenvalues are orthonormal > postulate 6: a wave function Ψ is expandable in complete set $\{\psi_n,\psi_a\}$ $$\Psi = \sum_n c_n\psi_n + \int c(a)\psi_a da$$ the integral runs over the whole range of values of a > if Ψ is normalised to unity: $$\begin{aligned}\langle A\rangle &= \langle\Psi|A|\Psi\rangle \\ &= \sum_m\sum_n c_m^* c_n\langle\psi_m|A|\psi_n\rangle + \sum_m\int da\, c_m^* c(a)\langle\psi_m|A|\psi_a\rangle \\ &\quad + \sum_n\int da' c^*(a')c_n\langle\psi_{a'}|A|\psi_n\rangle + \int da\int da' c^*(a')c(a)\langle\psi_{a'}|A|\psi_a\rangle \\ &= \sum_m\sum_n c_m^* c_n a_n\langle\psi_m|\psi_n\rangle + \sum_m\int da\, c_m^* c(a)a\langle\psi_m|\psi_a\rangle \\ &\quad + \sum_n\int da' c^*(a')c_n a_n\langle\psi_{a'}|\psi_n\rangle \\ &\quad + \int da\int da' c^*(a')c(a)a\langle\psi_{a'}|\psi_a\rangle \end{aligned}$$ >> we want to maintain the interpretation of c_n and c(a) as probability amplitudes: $$\langle A\rangle = \sum_n |c_n|^2 a_n + \int |c(a)|^2 a\,da.$$
> closure relation	compare the previous two results and we know $\langle\psi_m|\psi_n\rangle = \delta_{mn}$: - the continuum eigenfunctions are orthogonal to the discrete eigenfunctions $$\langle\psi_m|\psi_a\rangle = 0.$$ - the continuum eigenfunctions satisfy the orthonormalization condition: $$\langle\psi_{a'}|\psi_a\rangle = \delta(a-a').$$ > with these conditions the coefficients are given by: $$c_n = \langle\psi_n|\Psi\rangle, \qquad c(a) = \langle\psi_a|\Psi\rangle.$$ and thus the closure relation: $$\sum_n \psi_n^*(\mathbf{r}')\psi_n(\mathbf{r}) + \int \psi_a^*(\mathbf{r}')\psi_a(\mathbf{r})da = \delta(\mathbf{r}-\mathbf{r}')$$ or thus for N particles $$\begin{aligned}&\sum_n \psi_n^*(\mathbf{r}'_1,\ldots,\mathbf{r}'_N)\psi_n(\mathbf{r}_1,\ldots,\mathbf{r}_N) + \int \psi_a^*(\mathbf{r}'_1,\ldots,\mathbf{r}'_N)\psi_a(\mathbf{r}_1,\ldots,\mathbf{r}_N)da \\ &\quad = \delta(\mathbf{r}_1-\mathbf{r}'_1)\ldots\delta(\mathbf{r}_N-\mathbf{r}'_N). \qquad \textbf{(5.81b)}\end{aligned}$$

box normalization	let ψ_i be the normalised eigenfunction for eigenvalue a_i > large box: eigenvalues a_i for continuum are densely distributed > i can be treated as continuous variable > set i = i(a) and introduce density of states ρ $\rho(a) = \frac{\mathrm{d}i}{\mathrm{d}a}$ **(5.82)** which is equal to the number of discrete states within a unit range of a, we have $\sum_i c_i \psi_i \rightarrow \int c_i \psi_i \mathrm{d}i = \int \rho(a) c_i \psi_i \mathrm{d}a.$ **(5.83)** Requiring that $\int \rho(a) c_i \psi_i \mathrm{d}a = \int c(a) \psi_a \mathrm{d}a$ **(5.84)** and also (from the closure relation and with $\sum_i \rightarrow \int \rho(a)\mathrm{d}a$) $\int \rho(a) \psi_i^*(\mathbf{r}') \psi_i(\mathbf{r}) \mathrm{d}a = \int \psi_a^*(\mathbf{r}') \psi_a(\mathbf{r}) \mathrm{d}a$ **(5.85)** one can make the identifications $\psi_a = [\rho(a)]^{1/2} \psi_i$ **(5.86a)** and $c(a) = [\rho(a)]^{1/2} c_i$ **(5.86b)** which allow one to 'translate' formulae written using the 'box normalisation' into those written using the delta function 'normalisation'.
5.4 commuting observables, compatibility and the Heisenberg uncertainty principles	
commutator [A,B]	define: [A,B] = AB-BA
commutator of x and p_x	The position and momentum operators satisfy: $[x, p_x] = [y, p_y] = [z, p_z] = \mathrm{i}\hbar$ For multiple particles (x_1,y_1,z_1), (x_2,y_2,z_2), … and (p_{1x},p_{1y},p_{1z}), (p_{2x},p_{2y},p_{2z}), … : $[x_i, p_{ix}] = [y_i, p_{iy}] = [z_i, p_{iz}] = \mathrm{i}\hbar \qquad (i = 1, 2, \ldots, N).$ >> all other possible combinations commute (ie: [.,.] = 0)
5.4.1 commuting observables	
compatible observables	two observables A and B are compatible > if there exists a complete set of ψ_n such that ψ_n is both an eigenfunction of A and B $A\psi_n = a_n\psi_n, \qquad B\psi_n = b_n\psi_n.$ example: Cartesian components of **x** and **p** NOT x and p_x
commutation and compatibility	If A and B are compatible, then $AB\psi_n = a_n b_n \psi_n = b_n a_n \psi_n = BA\psi_n.$ thus: $(AB - BA)\Psi = \sum_n c_n (AB - BA)\psi_n = 0$ thus we find [A,B]=0 >> this also works in reverse !! if [A,B]=0 and ψ_n is an eigenfunction of A, this doesn't imply ψ_n is an eigenfunc of B!!
commutator algebra	$[A, B] = -[B, A]$ $[A, B + C] = [A, B] + [A, C]$ $[A, BC] = [A, B]C + B[A, C]$ $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$

5.4.2 Heisenberg uncertainty relations	
uncertainty ΔA	For an operator A define ΔA as: $\Delta A = [\langle (A - \langle A \rangle)^2 \rangle]^{1/2}$ so that $(\Delta A)^2 = \langle (A - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle A \rangle^2$
general Heisenberg uncertainty	For two variables A and B For ⟨Ψ|A|Ψ⟩ and ⟨Ψ|B|Ψ⟩ the expectation values For uncertainties ΔA and ΔB: > it holds: $\Delta A \Delta B \geqslant \frac{1}{2} \lvert \langle [A, B] \rangle \rvert .$
> proof	introduce the linear Hermitian operators: $\bar{A} = A - \langle A \rangle , \qquad \bar{B} = B - \langle B \rangle$ note that: $(\Delta A)^2 = \langle \bar{A}^2 \rangle , \qquad (\Delta B)^2 = \langle \bar{B}^2 \rangle$ and: $[\bar{A}, \bar{B}] = [A - \langle A \rangle , B - \langle B \rangle] = [A, B].$ next introduce the linear operator with real constant λ: $C = \bar{A} + i\lambda \bar{B}$ and its adjoint $C^\dagger = \bar{A} - i\lambda \bar{B}$ where the expectation value of CC† is real and nonnegative: $\langle CC^\dagger \rangle = \langle \Psi \lvert CC^\dagger \rvert \Psi \rangle = \langle C^\dagger \Psi \lvert C^\dagger \Psi \rangle \geqslant 0.$ Now the following expectation value is also real and nonnegative: $\langle (\bar{A} + i\lambda \bar{B})(\bar{A} - i\lambda \bar{B}) \rangle = \langle \bar{A}^2 + \lambda^2 \bar{B}^2 - i\lambda [\bar{A}, \bar{B}] \rangle$ and introduce the real and nonnegative function f(λ): $f(\lambda) = \langle \bar{A}^2 \rangle + \lambda^2 \langle \bar{B}^2 \rangle - i\lambda \langle [\bar{A}, \bar{B}] \rangle$ $= (\Delta A)^2 + \lambda^2 (\Delta B)^2 - i\lambda \langle [A, B] \rangle$ > implies that ⟨[A,B]⟩ is purely imaginary f(λ) has a minimum for $\lambda_0 = \frac{i}{2} \frac{\langle [A, B] \rangle}{(\Delta B)^2}$ for which f(λ_0) is equal to: $f(\lambda_0) = (\Delta A)^2 + \frac{1}{4} \frac{(\langle [A, B] \rangle)^2}{(\Delta B)^2}.$ Since this value is non-negative, we must have $(\Delta A)^2 (\Delta B)^2 \geqslant -\frac{1}{4} (\langle [A, B] \rangle)^2$
Heisenberg for canonical conjugates	For canonical conjugates we have [A,B] = iħ > thus also ⟨[A,B]⟩ = iħ > thus: $\Delta A \Delta B \geqslant \frac{\hbar}{2}.$
Heisenberg for Δx and Δp	for example: $\Delta x \Delta p_x \geqslant \frac{\hbar}{2}, \qquad \Delta y \Delta p_y \geqslant \frac{\hbar}{2}, \qquad \Delta z \Delta p_z \geqslant \frac{\hbar}{2}$ with $\Delta x = [\langle (x - \langle x \rangle)^2 \rangle]^{1/2}, \qquad \Delta p_x = [\langle (p_x - \langle p_x \rangle)^2 \rangle]^{1/2}$

5.4.3 the minimum uncertainty wave packet	
minimum uncertainty wave packet	$\Delta A \Delta B \geqslant \frac{1}{2}\lvert\langle[A, B]\rangle\rvert.$ > there is minimum uncertainty when these two become equal > this is when $\lambda=\lambda_0$ and $C^\dagger\Psi=0$: $$(\bar{A} - i\lambda_0 \bar{B})\Psi = 0.$$ >> use this to find the wave function Ψ such that ΔAΔB is minimal
example: $\Delta x \Delta p_x$	$$\Delta x \Delta p_x = \frac{\hbar}{2}. \quad (5.120)$$ Writing $\psi(x) \equiv \Psi(x, t = 0)$, and using (5.119) with $\bar{A} = x - \langle x\rangle$, $\bar{B} = p_x - \langle p_x\rangle$ and $\lambda_0 = i\langle[x, p_x]\rangle/[2(\Delta p_x)^2] = -\hbar/[2(\Delta p_x)^2]$, we find that $$\left(-i\hbar\frac{d}{dx} - \langle p_x\rangle\right)\psi(x) = \frac{2i(\Delta p_x)^2}{\hbar}(x - \langle x\rangle)\psi(x). \quad (5.121)$$ this gives us: $$\psi(x) = C\exp\left(\frac{i}{\hbar}\langle p_x\rangle x\right)\exp\left[-\frac{(\Delta p_x)^2(x - \langle x\rangle)^2}{\hbar^2}\right]$$ with C normalization constant
5.5 matrix representation of wave functions and operators	
operators as metrices	The action of a linear Hermitian operator A on Ψ creates a new wave function X: $$X = A\Psi.$$ The wave function X can also be expanded in terms of the basis $\{\psi_n\}$ as $$X = \sum_m d_m \psi_m$$ where the coefficients of the expansion are given by $d_m = \langle\psi_m\lvert X\rangle$. $$\begin{aligned} d_m &= \langle\psi_m\lvert X\rangle \\ &= \langle\psi_m\lvert A\rvert\Psi\rangle \\ &= \sum_n \langle\psi_m\lvert A\rvert\psi_n\rangle c_n \end{aligned}$$ define $A_{mn} = \langle\psi_m\lvert A\rvert\psi_n\rangle$ the matrix elements of operator A on basis $\{\psi_n\}$: $$d_m = \sum_n A_{mn} c_n.$$ this can be rewritten as a matrix equation: **d = Ac** thus: $$\begin{pmatrix} d_1 \\ d_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & \dots \\ A_{21} & A_{22} & \dots \\ \vdots & \vdots & \dots \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}$$
$\langle X\rvert\Psi\rangle$ in matrices	Using (5.64) and the fact that $c_n = \langle\psi_n\rvert\Psi\rangle$ and $d_n^* = \langle X\rvert\psi_n\rangle$, the scalar product $\langle X\rvert\Psi\rangle$ can be expressed as $$\langle X\rvert\Psi\rangle = \sum_n d_n^* c_n = \mathbf{d}^\dagger.\mathbf{c} \quad (5.160)$$ where $\mathbf{c}$ is a column vector with elements c_n and $\mathbf{d}^\dagger$ is a row vector with elements d_n^*. Thus (5.160) can be displayed as $$\langle X\rvert\Psi\rangle = (d_1^* \; d_2^* \; \dots)\begin{pmatrix} c_1 \\ c_2 \\ \vdots \end{pmatrix}. \quad (5.161)$$

5.5.1 matrix properties and definitions	
transpose	$(A^{\mathrm{T}})_{mn} = A_{nm}$
adjoint	$(A^{\dagger})_{mn} = A^{*}_{nm}.$
Hermitian	$\mathbf{A} = \mathbf{A}^{\dagger}$ thus $A_{mn} = A^{*}_{nm}$
correspondence between operators and metrices	- Hermitian operator represented by Hermitian matrix unitary unitary - A+B operator represented by **A+B** matrix AB **AB**
basis and diagonality	If the basis $\{\psi_n\}$ of eigenfunctions of A is used > than **A** will be a diagonal matrix
5.5.2 change of representation and unitary transforms	
transformation between matrix representations	For $\{\psi_n\}$ and $\{\phi_m\}$ two different orthonormal bases > each member of $\{\psi_n\}$ can be expanded in the basis $\{\phi_m\}$ as: $$\psi_n = \sum_m U_{mn}\phi_m$$ with U_{mn} the scalar product of ϕ_m and ψ_n: $$U_{mn} = \langle\phi_m|\psi_n\rangle.$$ now the matrix of U_{mn} is a unitary matrix: $$\begin{aligned}(UU^{\dagger})_{mn} &= \sum_k U_{mk}(U^{\dagger})_{kn}\\ &= \sum_k U_{mk}U^{*}_{nk}\\ &= \sum_k \langle\phi_m|\psi_k\rangle\langle\psi_k|\phi_n\rangle\\ &= \langle\phi_m|\phi_n\rangle = \delta_{mn}\end{aligned}$$ For basis $\{\psi_n\}$ we have wavefunction Ψ via coefficients c_n $\{\phi_m\}$ c'_m $$\Psi = \sum_n c_n\psi_n = \sum_m c'_m\phi_m$$ met $c_n = \langle\psi_n|\Psi\rangle, \quad c'_m = \langle\phi_m|\Psi\rangle.$ Via the closure relation, we find: $$\begin{aligned}c'_m &= \langle\phi_m|\Psi\rangle\\ &= \sum_n \langle\phi_m|\psi_n\rangle\langle\psi_n|\Psi\rangle\\ &= \sum_n U_{mn}c_n,\end{aligned}$$ or thus: **c' = Uc** For matrix **A** representing operator A in basis $\{\psi_n\}$ **A'** $\{\phi_m\}$ $$\begin{aligned}A'_{mn} &= \langle\phi_m|A|\phi_n\rangle\\ &= \sum_k\sum_l \langle\phi_m|\psi_k\rangle\langle\psi_k|A|\psi_l\rangle\langle\psi_l|\phi_n\rangle\\ &= \sum_k\sum_l U_{mk}A_{kl}(U^{\dagger})_{ln}\end{aligned}$$ thus: $\mathbf{A}' = \mathbf{U}\mathbf{A}\mathbf{U}^{\dagger}$ and $\mathbf{A} = \mathbf{U}^{\dagger}\mathbf{A}'\mathbf{U}.$ >> for transformations between different matrix representations, the transforming operators are unitary matrices

trace property of unitary matrices	if **A** and **A'** are connected via **A'** = **UAU†** we have: $$\begin{aligned}\mathrm{Tr}\,\mathbf{A}' &= \sum_m A'_{mm} \\ &= \sum_k \sum_l \sum_m U_{mk} A_{kl} (U^\dagger)_{lm} \\ &= \sum_k \sum_l \sum_m [(U^\dagger)_{lm} U_{mk}] A_{kl} \\ &= \sum_k \sum_l \delta_{lk} A_{kl} \\ &= \sum_k A_{kk} = \mathrm{Tr}\,\mathbf{A}.\end{aligned}$$ >> trace of Hermitian matrix is equal to the sum of its eigenvalues
eigenvalues of **A**	any Hermitian matrix can be diagonalised by a unitary transformation >> if you want to find the eigenfunction of **A**: 1: diagonalise **A** via **A'** = **UAU†** 2: eigenfunctions are on the diagonal
5.5.3 the state vector	
state vector	= $\|\Psi\rangle$
Dirac quantum representation	for each state vector there's an associated conjugate bra $\langle\Psi\|$ > $\langle\Psi\|\Psi\rangle$ is a real quantity representing the square of the norm of $\|\Psi\rangle$
5.5.4 the linear harmonic oscillator revisited	
1D linear harmonic oscillator	with $\omega = (k/m)^{1/2}$ the Hamiltonian for a 1D oscillator is: $$H = \frac{p_x^2}{2m} + \frac{1}{2}kx^2 = \frac{p_x^2}{2m} + \frac{1}{2}m\omega^2 x^2$$ introduce the operators a_{+-} $$a_\pm = \frac{1}{\sqrt{2}}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x \mp \mathrm{i}\frac{p_x}{(m\hbar\omega)^{1/2}}\right]$$ since x and p_x are Hermitian, a_+ and a_- are adjoint: $a_+ = a_-^\dagger$ > we can find: $[a_+, a_-] = 1$ > the Hamiltonian can be rewritten as, with $N = a_+a_-$: $$H = \frac{\hbar\omega}{2}(a_-a_+ + a_+a_-) = \hbar\omega\left(a_-a_+ - \tfrac{1}{2}\right) = \hbar\omega\left(a_+a_- + \tfrac{1}{2}\right) = \hbar\omega\left(N + \tfrac{1}{2}\right)$$ (5.1) furthermore $$[H, a_\pm] = \pm\hbar\omega a_\pm.$$ If $\|E\rangle$ is an eigenvector of H with eigenvalue E, so that $H\|E\rangle = E\|E\rangle$ we have: $$\begin{aligned}Ha_\pm|E\rangle &= (a_\pm H \pm \hbar\omega a_\pm)|E\rangle \\ &= (E \pm \hbar\omega)a_\pm|E\rangle.\end{aligned}$$ ie: $a_{+-}\|E\rangle$ are eigenvectors of H with eigenvalues E+-ħω > a_+ raises & a_- lowers the value of E, thus they are resp. *raising* and *lowering* operators now: H only contains squares of p_x and x > expectation value of H cannot be negative > eigenvalues of H must be non-negative Let E be the smallest eigenvalue > then $a_-\|E_0\rangle = 0$, for otherwise $a_-\|E_0\rangle$ would be an eigenket with eigenvalue E_0-ħω which cannot be since E_0 is the smallest eigenvalue > we can find: $$\hbar\omega a_+a_-|E_0\rangle = \hbar\omega N|E_0\rangle = \left(H - \tfrac{1}{2}\hbar\omega\right)|E_0\rangle = 0$$ thus $E_0 = \hbar\omega/2$ > we find the other eigenkets by working a_+ on $\|E_0\rangle$ $$|E_0\rangle, a_+|E_0\rangle, a_+^2|E_0\rangle, \ldots,$$ thus the eigenvalue corresponding to an eigenket $a_+^n\|E_0\rangle$ is: $$E_n = \left(n + \tfrac{1}{2}\right)\hbar\omega, \qquad n = 0, 1, 2, \ldots$$

1D linear harmonic oscillator	for $\|E_n\rangle$ now a normalised eigenket with eigenvalue E_n > we have, with C_{n+1} the normalization coefficient: $$\|E_{n+1}\rangle = C_{n+1}a_+\|E_n\rangle$$ since $\langle E_{n+1}\|E_{n+1}\rangle$=1 and a_+=$a_-^\dagger$, we find that: $$\|C_{n+1}\|^2\langle E_n\|a_-a_+\|E_n\rangle = 1.$$ since $a_-a_+ = (H/\hbar\omega)+1/2$ and $H\|E_n\rangle=E_n\|E_n\rangle$ and $E_n = (n+1/2)\hbar\omega$ and $\langle E_n\|E_n\rangle$: $$C_{n+1} = (n+1)^{-1/2}$$ and thus we find: $$a_+\|E_n\rangle = (n+1)^{1/2}\|E_{n+1}\rangle.$$ or starting from E_0: $$\|E_n\rangle = (n!)^{-1/2}a_+^n\|E_0\rangle$$ We also have $\|E_n\rangle = C_n a_+\|E_{n-1}\rangle$ with $C_n = n^{-1/2}$ > operator both sides with a_-: $$a_-\|E_n\rangle = n^{-1/2}a_-a_+\|E_{n-1}\rangle$$ now: $a_-a_+ = (H/\hbar\omega) + 1/2$ and $H\|E_{n-1}\rangle = (n-1/2)\hbar\omega\|E_{n-1}\rangle$ $$a_-\|E_n\rangle = n^{1/2}\|E_{n-1}\rangle$$
5.5.5 matrix representation in the $\{\|E_n\rangle\}$ basis	
matrix representation of **H** and **N**	in terms of $\{\|E_n\rangle\}$ with n=0,1,2,… we find H via its eigenvalues $E_n = (n+1/2)\hbar\omega$ > N is just the diagonal matrix with elements n: $$\mathbf{H} = \hbar\omega\begin{pmatrix}\frac{1}{2} & 0 & 0 & \dots\\ 0 & \frac{3}{2} & 0 & \dots\\ 0 & 0 & \frac{5}{2} & \\ \vdots & \vdots & \vdots & \vdots\end{pmatrix}, \qquad \mathbf{N} = \begin{pmatrix}0 & 0 & 0 & \dots\\ 0 & 1 & 0 & \dots\\ 0 & 0 & 2 & \\ \vdots & & & \vdots\end{pmatrix}$$
matrix $\mathbf{a}_+$ and $\mathbf{a}_-$	from the orthogonality of eigenvectors we have: $$\langle E_k\|E_{n+1}\rangle = C_{n+1}\langle E_k\|a_+\|E_n\rangle = \delta_{k,n+1}$$ hence, the matrix elements of a_+ in $\{\|E_n\rangle\}$: $$(a_+)_{kn} = (n+1)^{1/2}\delta_{k,n+1}$$ thus $\mathbf{a}_+$ is a real matrix whose elements are directly below the main diagonal from a_+=$a_-^\dagger$ we find: $$(a_-)_{kn} = (k+1)^{1/2}\delta_{k+1,n}$$ thus: $$\mathbf{a}_+ = \begin{pmatrix}0 & 0 & 0 & \dots\\ \sqrt{1} & 0 & 0 & \dots\\ 0 & \sqrt{2} & 0 & \dots\\ 0 & 0 & \sqrt{3} & \\ \vdots & \vdots & \vdots & \ddots\end{pmatrix}, \quad \mathbf{a}_- = \begin{pmatrix}0 & \sqrt{1} & 0 & 0 & \dots\\ 0 & 0 & \sqrt{2} & 0 & \dots\\ 0 & 0 & 0 & \sqrt{3} & \dots\\ \vdots & \vdots & \vdots & & \ddots\end{pmatrix}$$

5.5.6 transition form the {|E_n⟩} to the position representation	
transition to position	since x = x and p_x = -iħd/dx: $$a_{\pm} = \frac{1}{\sqrt{2}}\left[\left(\frac{m\omega}{\hbar}\right)^{1/2} x \mp \frac{1}{(m\hbar\omega)^{1/2}}\frac{\mathrm{d}}{\mathrm{d}x}\right]$$ or, in terms of the variable $\xi = (m\omega/\hbar)^{1/2}x = \alpha x$ $$a_{\pm} = \frac{1}{\sqrt{2}}\left(\xi \mp \frac{\mathrm{d}}{\mathrm{d}\xi}\right).$$ We can rewrite $a_-\|E_0\rangle = 0$ in position representation as: $$\left(\xi + \frac{\mathrm{d}}{\mathrm{d}\xi}\right)\psi_0(\xi) = 0.$$ This equation has the solution $$\psi_0(\xi) = N_0 e^{-\xi^2/2}$$ where N_0 is a constant. Hence $$\psi_0(x) = N_0 e^{-\alpha^2 x^2/2}.$$ If N_0 is chosen to be real and such that $\psi_0(x)$ is normalised to unity, we have $$N_0 = \left(\frac{\alpha}{\sqrt{\pi}}\right)^{1/2}.$$ all other eigenfunctions can be found using $\|E_n\rangle = (n!)^{-1/2}a_+^n\|E_0\rangle$: $$\psi_n(\xi) = (n!)^{-1/2}\left[\frac{1}{\sqrt{2}}\left(\xi - \frac{\mathrm{d}}{\mathrm{d}\xi}\right)\right]^n \psi_0(\xi)$$ and thus: $$\psi_n(\xi) = \left(\frac{\alpha}{\sqrt{\pi}2^n n!}\right)^{1/2} e^{-\xi^2/2} H_n(\xi)$$ where $H_n(\xi)$ is the Hermite polynomial of order n.
5.7 the Schrödinger equation and the time evolution of a system	
postulate 7	the time evolution of the wave function of a system is determined by the TDSE: $$i\hbar\frac{\partial}{\partial t}\Psi(t) = H\Psi(t)$$ where H is the Hamiltonian, or total energy operator of the system.
obtaining the Hamiltonian	we can find H via substitution rule > examples: see p231
5.7.1 the evolution operator	
evolution operator	TDSE is a first-order diff.eq in time > state vector Ψ(t) is defined at all t once its specified for any t_0 > introduce an evolution operator $U(t_0,t)$ such that: $$\Psi(t) = U(t, t_0)\Psi(t_0)$$ with $$U(t_0, t_0) = I.$$ Applying twice the definition (5.232), we also have $$U(t, t_0) = U(t, t')U(t', t_0)$$ and $$U^{-1}(t, t_0) = U(t_0, t)$$ substituting in the TDSE we see U satisfies the equation: $$i\hbar\frac{\partial}{\partial t}U(t, t_0) = HU(t, t_0)$$ remark that we can rewrite this as: $$U(t, t_0) = I - \frac{\mathrm{i}}{\hbar}\int_{t_0}^{t} HU(t', t_0)\mathrm{d}t'.$$

$U(t,t_0)$ a unitary operator	conservation of probability requires: $\langle\Psi(t)\|\Psi(t)\rangle = \langle\Psi(t_0)\|\Psi(t_0)\rangle.$ however, from $\Psi(t) = U\Psi(t_0)$ we find: $\langle\Psi(t)\|\Psi(t)\rangle = \langle U(t,t_0)\Psi(t_0)\|U(t,t_0)\Psi(t_0)\rangle$ $= \langle\Psi(t_0)\|U^\dagger(t,t_0)U(t,t_0)\|\Psi(t_0)\rangle$ from which: $U^\dagger(t,t_0)U(t,t_0) = I.$ in same fashion we find, starting from $\langle\Psi(t_0)\|\Psi(t_0)\rangle$: $U(t,t_0)U^\dagger(t,t_0) = I$ >> U is a unitary transformation
infinitesimal unitary transformation	The change in evolution operator induced after a small time δt: $i\hbar[U(t_0+\delta t,t_0) - U(t_0,t_0)] = HU(t_0+\delta t,t_0)\delta t.$ Hence, to first order in δt, and using the initial condition (5.233), we have $U(t_0+\delta t,t_0) = I - \frac{i}{\hbar}H\delta t.$ > H is the generator of an infinitesimal unitary transformation described by the evolution operator $U(t_0+\delta t, t_0)$
U in time-independent H	consider the case for which H is time-independent > a solution of U is: $U(t,t_0) = \exp\left[-\frac{i}{\hbar}H(t-t_0)\right]$ thus a solution of the TDSE for time-ind. H is given by: $\Psi(t) = \exp\left[-\frac{i}{\hbar}H(t-t_0)\right]\Psi(t_0).$
U in time-independent H and V	suppose the potential V is also time-independent: V(**r**) > we can rewrite the wave function as: $\Psi(\vec{r},t) = \exp\left[-\frac{i}{\hbar}H(t-t_0)\right]\Psi(\vec{r},t_0)$ $= \int d\vec{r}\,'\exp\left[-\frac{i}{\hbar}H(t-t_0)\right]\delta(\vec{r}-\vec{r}\,')\Psi(\vec{r}\,',t_0)$ $= \int d\vec{r}\,'K(\vec{r},t;\vec{r}\,',t_0)\Psi(\vec{r}\,',t_0)$ (PROPAGATOR) Now, according to the closure relation satisfied by the energy eigenfunctions, we have $\sum_E \psi_E^*(\mathbf{r}')\psi_E(\mathbf{r}) = \delta(\mathbf{r}-\mathbf{r}')$ **(5.247)** so that we can recast (5.246) in the form $\Psi(\mathbf{r},t) = \sum_E \int \exp\left[-\frac{i}{\hbar}H(t-t_0)\right]\psi_E^*(\mathbf{r}')\psi_E(\mathbf{r})\Psi(\mathbf{r}',t_0)d\mathbf{r}'.$ **(5.248)** Since $H\psi_E = E\psi_E$, it follows that $\Psi(\mathbf{r},t) = \sum_E\left[\int \psi_E^*(\mathbf{r}')\Psi(\mathbf{r}',t_0)d\mathbf{r}'\right]\exp[-iE(t-t_0)/\hbar]\psi_E(\mathbf{r})$ **(5.249)** in agreement with the result (3.155) obtained in Chapter 3.

5.7.2 time variation of expectation values	
A as a constant of motion	consider an observable A > expectation value ⟨A⟩ in state Ψ, normalised to unity is ⟨Ψ|A|Ψ⟩ > rate of change of ⟨A⟩ is therefore: $\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = \frac{\mathrm{d}}{\mathrm{d}t}\langle\Psi\|A\|\Psi\rangle$ $= \left\langle\frac{\partial\Psi}{\partial t}\|A\|\Psi\right\rangle + \left\langle\Psi\left\|\frac{\partial A}{\partial t}\right\|\Psi\right\rangle + \left\langle\Psi\|A\|\frac{\partial\Psi}{\partial t}\right\rangle$ $= -(\mathrm{i}\hbar)^{-1}\langle H\Psi\|A\|\Psi\rangle + \left\langle\Psi\left\|\frac{\partial A}{\partial t}\right\|\Psi\right\rangle + (\mathrm{i}\hbar)^{-1}\langle\Psi\|AH\|\Psi\rangle$ since H is Hermitian, rewrite the fist matrix element on the right as ⟨Ψ|HA|Ψ⟩, so that: $\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = (\mathrm{i}\hbar)^{-1}\langle[A, H]\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle$ where $\langle[A, H]\rangle = \langle\Psi\|[A, H]\|\Psi\rangle = \langle\Psi\|AH - HA\|\Psi\rangle$ and $\left\langle\frac{\partial A}{\partial t}\right\rangle = \left\langle\Psi\left\|\frac{\partial A}{\partial t}\right\|\Psi\right\rangle.$ if A doesn't depend explicitly on time (∂A/∂t = 0), then this reduces to: $\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = (\mathrm{i}\hbar)^{-1}\langle[A, H]\rangle.$ >> does not vary in time > A is constant of motion
5.7.3 time-independent Hamiltonian	
energy conservation	If H is time-independent, consider the case A=H: $\frac{\mathrm{d}}{\mathrm{d}t}\langle H\rangle = (\mathrm{i}\hbar)^{-1}\langle[H, H]\rangle = 0$ total energy is constant of motion
expectation value of A	for ψ_E an eigenfunction of the time-ind. H with eigenenergy E > for a stationary state $\Psi_E = \psi_E\exp(-\mathrm{i}Et/\hbar)$ and time-ind. A its clear that: $\langle\Psi_E\|A\|\Psi_E\rangle = \langle\psi_E\|A\|\psi_E\rangle$ does not depend on the time. thus we find: $\langle\psi_E\|[A, H]\|\psi_E\rangle = 0.$
5.7.4 virial theorem	
virial theorem	consider a particle with mass m in potential V(**r**) with above particular case: $H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}).$ choose A = **r.p** time independent: $\langle\psi_E\|[\mathbf{r}.\mathbf{p}, H]\|\psi_E\rangle = 0.$ we can find that: $[\mathbf{r}.\mathbf{p}, H] = \left[(xp_x + yp_y + zp_z), \frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(x, y, z)\right]$ $= \frac{\mathrm{i}\hbar}{m}(p_x^2 + p_y^2 + p_z^2) - \mathrm{i}\hbar\left(x\frac{\partial V}{\partial x} + y\frac{\partial V}{\partial y} + z\frac{\partial V}{\partial z}\right)$ $= 2\mathrm{i}\hbar T - \mathrm{i}\hbar(\mathbf{r}.\nabla V)$ with $T = \mathbf{p}^2/2m = -(\hbar^2/2m)\nabla^2$ is the kinetic energy operator. >> thus for a stationary state!!: $2\langle T\rangle = \langle\mathbf{r}.\nabla V\rangle$

5.7.5 the Schrödinger equation for a two-body system

example: interacting masses

Consider two particles with mass m_1, m_2 interacting via time-indep. potential $V(\mathbf{r_1}-\mathbf{r_2})$
> only depends on relative position $\mathbf{r_1}-\mathbf{r_2}$

The classical Hamiltonian of the system is given by:

$$H = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + V(\mathbf{r}_1 - \mathbf{r}_2).$$

now make the substitutions $p=-i\hbar\nabla$
> we can than formulate the TDSE in configuration space:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r}_1, \mathbf{r}_2, t) = \left[-\frac{\hbar^2}{2m_1}\nabla_{\mathbf{r}_1}^2 - \frac{\hbar^2}{2m_2}\nabla_{\mathbf{r}_2}^2 + V(\mathbf{r}_1 - \mathbf{r}_2)\right]\Psi(\mathbf{r}_1, \mathbf{r}_2, t).$$

which is a seven-dimensional partial-differential equation
> simplify: introduce **r** and **R** which determine the centre of mass CM of the system

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$$

and the vector

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2}$$

change the variables:

$$-\frac{\hbar^2}{2m_1}\nabla_{\mathbf{r}_1}^2 - \frac{\hbar^2}{2m_2}\nabla_{\mathbf{r}_2}^2 = -\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2$$

with $M = m_1+m_2$ the total mass and μ the reduced mass of the system

$$\mu = \frac{m_1 m_2}{m_1 + m_2}$$

the TDSE therefore becomes:

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{R}, \mathbf{r}, t) = \left[-\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2 - \frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 + V(\mathbf{r})\right]\Psi(\mathbf{R}, \mathbf{r}, t).$$

we can separate this equation
ie: 1: time dependence can be separated like in 3.5
> because the potential $V(\mathbf{r})$ is time-independent

2: spatial part of wave function $\Psi(\mathbf{R}, \mathbf{r}, t)$ separated in product of functions of centre of mass coordinate **R** and relative coordinate **r**

> TDSE has a solution of the form:

$$\Psi(\mathbf{R}, \mathbf{r}, t) = \Phi(\mathbf{R})\psi(\mathbf{r})\exp[-i(E_{CM} + E)t/\hbar]$$

where $\Phi(\mathbf{R})$ and $\psi(\mathbf{r})$ satisfy respectively:

$$-\frac{\hbar^2}{2M}\nabla_{\mathbf{R}}^2\Phi(\mathbf{R}) = E_{CM}\Phi(\mathbf{R}) \qquad \text{and} \qquad \left[-\frac{\hbar^2}{2\mu}\nabla_{\mathbf{r}}^2 + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}).$$

the first eq. is a TISE describing the centre of mass as a free particle of mass M
the 2nd eq. is a TISE describing the relative motion of the two particles
> is same as the Schrodinger eq. of a particle with mass μ in $V(\mathbf{r})$

total energy of the system $E_{tot} = E_{CM} + E$

>> we have separated the problem into two one-body problems

5.8 The Schrödinger and Heisenberg pictures	
Schrödinger picture	- Operators A are time-independent - wave function Ψ is time-dependent > represents time evolution of the system The wave function Ψ is related to its value at t_0 by performing unitary transformation: $$\Psi(t) = U(t, t_0)\Psi(t_0)$$ with $U(t,t_0)$ the evolution operator The time dependence of the expectation value of an operator is given by: $$\frac{\mathrm{d}}{\mathrm{d}t}\langle A\rangle = (\mathrm{i}\hbar)^{-1}\langle [A, H]\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle$$ >> this is the picture we have used thus far
Heisenberg picture	- Operators A_H are time-dependent - wave function Ψ_H is time-independent The Heisenberg wave function is defined by its value at t_0: > or thus for unitary operator $U(t,t_0)$ this is compared to the Schrödinger picture: $$\Psi_H = U^\dagger(t, t_0)\Psi(t) = U(t_0, t)\Psi(t) = \Psi(t_0)$$ the corresponding Heisenberg operators are time-dependent > they can be found from the Schrödinger picture via: $$\begin{aligned} A_H(t) &= U^\dagger(t, t_0)AU(t, t_0) \\ &= U(t_0, t)AU^\dagger(t_0, t) \end{aligned}$$
> time dependence of A_H	We find via the definition: $$\frac{\mathrm{d}}{\mathrm{d}t}A_H(t) = \frac{\partial U}{\partial t}AU^\dagger + U\frac{\partial A}{\partial t}U^\dagger + UA\frac{\partial U^\dagger}{\partial t}. \quad \textbf{(5.281)}$$ Using (5.236) and the facts that H is Hermitian and U is unitary, we then find that $$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}A_H(t) &= (\mathrm{i}\hbar)^{-1}(-UHAU^\dagger + UAHU^\dagger) + U\frac{\partial A}{\partial t}U^\dagger \\ &= (\mathrm{i}\hbar)^{-1}(-UHU^\dagger UAU^\dagger + UAU^\dagger UHU^\dagger) + U\frac{\partial A}{\partial t}U^\dagger. \quad \textbf{(5.282)} \end{aligned}$$ Defining the Heisenberg operators $$H_H = UHU^\dagger \quad \textbf{(5.283)}$$ and $$\left(\frac{\partial A}{\partial t}\right)_H = U\frac{\partial A}{\partial t}U^\dagger \quad \textbf{(5.284)}$$ we obtain $$\frac{\mathrm{d}}{\mathrm{d}t}A_H(t) = (\mathrm{i}\hbar)^{-1}[A_H, H_H] + \left(\frac{\partial A}{\partial t}\right)_H \quad \textbf{(5.285)}$$
> Hamiltonian in Schrödinger vs Heisenberg	In the Schrödinger picture, H is time-independent > the evolution operator in that picture is given by: $$U(t, t_0) = \exp\left[-\frac{\mathrm{i}}{\hbar}H(t - t_0)\right]$$ The Heisenberg wave function is then related to the Schrödinger one via: $$\Psi_H \equiv \Psi(t_0) = \exp\left[\frac{\mathrm{i}}{\hbar}H(t - t_0)\right]\Psi(t)$$ thus we find $H_H = H$

5.11 the classical limit

5.11.1 the Ehrenfest theorem

First Ehrenfest relation

for a particle of mass m moving in a potential V(**r**,t):

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t)$$

and we know for ⟨x⟩ that:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = (\mathrm{i}\hbar)^{-1}\langle [x, H]\rangle$$

$$= (\mathrm{i}\hbar)^{-1}\left\langle \left[x, \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t)\right]\right\rangle$$

since x commutes with V(**r**,t), p_y and p_z, we have:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{1}{2m\mathrm{i}\hbar}\langle [x, p_x^2]\rangle$$

$$= \frac{1}{2m\mathrm{i}\hbar}\langle [x, p_x]p_x + p_x[x, p_x]\rangle$$

and $[x,p_x] = \mathrm{i}\hbar$, thus:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle x\rangle = \frac{\langle p_x\rangle}{m}$$

so in 3D we have:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{r}\rangle = \frac{\langle \mathbf{p}\rangle}{m}$$ The first Ehrenfest relation

Second Ehrenfest relation

we do the same for the momentum p_x:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle = (\mathrm{i}\hbar)^{-1}\langle [p_x, H]\rangle$$

$$= (\mathrm{i}\hbar)^{-1}\left\langle \left[p_x, \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}, t)\right]\right\rangle$$

$$= -\left\langle \frac{\partial V}{\partial x}\right\rangle$$

where we have used the fact that $[p_x, \mathbf{p}^2] = 0$ together with the equation

$$[p_x, V] = -\mathrm{i}\hbar\frac{\partial V}{\partial x}$$

We thus find for 3D:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathbf{p}\rangle = -\langle \nabla V(\mathbf{r}, t)\rangle$$

> quantum becomes classical in the limit

For 1D motion in a potential V(x)

> expand dV/dx = V'(x) about the expectation value ⟨x⟩:

$$V'(x) = V'(\langle x\rangle) + (x - \langle x\rangle)V''(\langle x\rangle) + \frac{1}{2}(x - \langle x\rangle)^2 V'''(\langle x\rangle) + \cdots$$

or thus:

$$\langle V'(x)\rangle = V'(\langle x\rangle) + \frac{1}{2}\langle (x - \langle x\rangle)^2\rangle V'''(\langle x\rangle) + \cdots$$

where we've used ⟨x-⟨x⟩⟩ = 0

> the quantity -V'(⟨x⟩) is the classical force at point ⟨x⟩

> thus, if only the first term is retained, we have=

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle p_x\rangle = -V'(\langle x\rangle),$$

>> the expectation values ⟨x⟩ and ⟨p_x⟩ obey Newton's law