2.4.2 The Ehrenfest Theorem

☐ In the following we will need the following important commutators:

$$[\mathbf{r}_k, \mathbf{H}] = i\hbar \frac{\mathbf{p}_k}{m} \tag{2.73}$$

$$[\mathbf{p}_k, f(\vec{\mathbf{r}})] = -i\hbar \nabla f(\vec{\mathbf{r}}) \tag{2.74}$$

for $k = 1, 2, 3$ where $f(\vec{r})$ is any differentiable function on $\mathbb{R}^3$. Proof: For the first identity we find $[\mathbf{r}_k, \mathbf{H}] = [\mathbf{r}_k, \mathbf{p}^2/(2m)] = [\mathbf{r}_k, \mathbf{p}_l]\mathbf{p}_l/m = i\hbar\delta_{k,l}\mathbf{p}_l/m = i\hbar\mathbf{p}_k/m$. The second one is straight forward to show.

☐ Ehrenfest Theorem: Let ψ be a state solving a Schrödinger Equation for particles of mass m in a potential $V(\vec{r})$. Then we find the following equations of motion for the average position and momentum in the state ψ.

$$\boxed{\begin{aligned} m\frac{\langle\vec{\mathbf{r}}\rangle}{dt} &= \langle\vec{\mathbf{p}}\rangle \ , \qquad (2.75) \\ \frac{\langle\vec{\mathbf{p}}\rangle}{dt} &= \langle\mathbf{F}\rangle \ . \qquad (2.76) \end{aligned}}$$

Here $\mathbf{F} = -\nabla V$ is the force associated with the potential energy V. Proof: We have $d\langle\vec{\mathbf{r}}\rangle/dt = \langle[\vec{\mathbf{r}}, \mathbf{H}\rangle/(i\hbar) = \langle\vec{\mathbf{p}}\rangle/m$ and $d\langle\vec{\mathbf{p}}\rangle/dt = \langle[\vec{\mathbf{p}}, \mathbf{H}]\rangle/(i\hbar) = \langle-\nabla V\rangle$.

☐ Recall the canonical equations from classical mechanics,

$$m\frac{\vec{r}}{dt} = \vec{p}, \tag{2.77}$$

$$\frac{\vec{p}}{dt} = -\nabla V(\vec{r}) \ . \tag{2.78}$$

Hence the equations of motion for the expectation values of position and momentum are the same as the equations for their classical counterparts if $\langle\nabla V(\vec{\mathbf{r}})\rangle \approx \nabla V(\langle\vec{\mathbf{r}}\rangle)$.

2.5 Fundamental Properties of Solutions of the Schrödinger Equation

2.5.1 Eigenvalues and Eigenfunctions of Operators

☐ Let $\mathbf{F}$ be a linear operator[11] on a space $\mathcal{S}$ of functions. If there exists a $\psi \in \mathcal{S}$ and a number $\alpha \in \mathbb{C}$ such that

$$\boxed{\mathbf{F}\psi = \alpha\psi} \tag{2.79}$$

we call α an *eigenvalue* of $\mathbf{F}$ and ψ an *eigenfunction* or *eigenvector* (in the vector space of functions).

☐ This is the natural generalization of the concept of eigenvalue and eigenvector from finite-dimensional vector spaces like $\mathbb{R}^n$.

☐ If ψ is eigenfunction for $\mathbf{F}$ with eigenvalue α then $\lambda\psi$ with any $\lambda \in \mathbb{C}$ is also an eigenfunction. The set of vectors $\lambda\psi$ represent a 1-dimensional subspace of $\mathcal{S}$, the *eigenspace* for α.

☐ If an operator $\mathbf{F}$ has more than one linearly independent eigenvector for a given eigenvalue α we call the eigenvalue degenerate with degeneracy k ($\in \mathbb{N}$) if the largest subspace of $\mathcal{S}$ spanned by eigenfunctions for α has dimension k.

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[11] All operators from here on will be linear unless explicitly allowed otherwise.

2.5.2 The Time Evolution Operator

☐ A standard problem of wave mechanics is the following. For a given time-independent Hamilton operator $\mathbf{H}$ find the solution $\psi(\vec{r}, t)$ of the Schrödinger equation $i\hbar\partial\psi/\partial t = \mathbf{H}\,\psi$ such that the initial condition $\psi(\vec{r}, t_0) = \psi_0(\vec{r})$ is satisfied.

☐ If $\mathbf{H}$ were a number instead of an operator the solution to the time-dependent Schrödinger equation were simply an exponential function. Maybe it should come as no surprise that this also holds for operators. We arrive at the following fundamental theorem. The solution

$$\boxed{\psi(\vec{r}, t) = e^{-\frac{i}{\hbar}\mathbf{H}\,(t-t_0)}\psi(\vec{r}, t_0)} \tag{2.80}$$

solves the initial value problem for the time-dependent Schrödinger equation. In other words the *time evolution operator*

$$\boxed{\mathbf{T}\,(t, t_0) = e^{-\frac{i}{\hbar}\mathbf{H}\,(t-t_0)}} \tag{2.81}$$

advances a wave function from time t_0 to time t. Proof: The exponential function if defined via its power series so we have

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi(\vec{r}, t) &= i\hbar\left[\frac{\partial}{\partial t}e^{-\frac{i}{\hbar}\mathbf{H}\,(t-t_0)}\right]\psi(\vec{r}, t_0) = i\hbar\left[\frac{\partial}{\partial t}\,\mathbf{Id} - \frac{i}{\hbar}\mathbf{H}\,\frac{\partial}{\partial t}(t-t_0) + \frac{1}{2!}\left(\frac{i}{\hbar}\right)^2\mathbf{H}^2\frac{\partial^2}{\partial t^2}(t-t_0)^2 + \ldots\right] \\ &= \left[\mathbf{H}\;\mathbf{Id} - \mathbf{H}\,\frac{i}{\hbar}\mathbf{H}\,(t-t_0) + \ldots\right] = \mathbf{H}\,e^{-\frac{i}{\hbar}\mathbf{H}\,(t-t_0)}\psi(\vec{r}, t_0) = \mathbf{H}\psi(\vec{r}, t) \end{aligned} \tag{2.82}$$

☐ The exponential of the operator $\mathbf{H}$ and its application to the initial wave function are usually difficult to evaluate. Therefore, although the time evolution operator offers a compact formal solution, it is by itself not a practical solution.

2.5.3 Stationary Solutions and the Time-Independent Schrödinger Equation

☐ The time evolution operator takes a very simple form in one special case, namely, if the initial condition is an eigenfunction of the Hamilton operator $\mathbf{H}$. In that case the time evolution operator becomes a phase factor. Let $\psi_E(\vec{r})$ be an eigenfunction of H with real eigenvalue E, i.e. $\mathbf{H}\,\psi_E = E\psi_E$. Then if $\psi(\vec{r}, t_0) = \psi_E(\vec{r})$ is the solution to the time-dependent Schrödinger Equation at time t_0, the solution at any other time t is

$$\boxed{\psi(\vec{r}, t) = e^{-\frac{i}{\hbar}E(t-t_0)}\psi(\vec{r}, t_0)\,.} \tag{2.83}$$

Note that the argument of the exponential is now a complex number. Proof:

$$\mathbf{T}(t, t_0)\psi(\vec{r}, t_0) = \sum_k \frac{1}{k!}(t-t_0)^k\mathbf{H}^k\psi_E(\vec{r}) = \sum_k \frac{1}{k!}(t-t_0)^k E^k\psi_E(\vec{r}) = e^{-\frac{i}{\hbar}E(t-t_0)}\psi(\vec{r}, t_0) \tag{2.84}$$

☐ In this case $\psi_E(\vec{r})$ has to satisfy the *time-independent* Schrödinger Equation

$$\boxed{-\frac{\hbar^2}{2m}\triangle\psi_E + V\psi_E = E\psi_E\,.} \tag{2.85}$$

This can be easily seen by plugging the solution (2.83) into the time-dependent Schrödinger Equation. Of course the time-dependent Schrödinger Equation is nothing else than the eigenvalue equation for the eigenvalue E

$$\boxed{\mathbf{H}\,\psi_E = E\psi_E\,.} \tag{2.86}$$

☐ A solution to the time-dependent Schrödinger Equation of the form (2.83) that satisfies (2.85) is called a stationary solution because the $\vec{r}$-dependence of the solution does not change with time except for an overall phase. In particular, for stationary solutions

$$\rho(\vec{r}) = |\psi(\vec{r},t)|^2 = |\psi(\vec{r})|^2 = \text{const.} \tag{2.87}$$

is independent of time. In fact one can easily see that expectation values for any operator $\mathbf{A}$ depending only on position or momentum are constant in a stationary state,

$$\langle \mathbf{A} \rangle = \int \psi(\vec{r},t)^* \mathbf{A}\,\psi(\vec{r},t) d^3r = \int \psi(\vec{r})^* \mathbf{A}\,\psi(\vec{r}) d^3r = \text{const.} \tag{2.88}$$

☐ Since the expectation value of position is constant, according to Ehrenfest $\langle \vec{\mathbf{p}} \rangle = d\langle \vec{\mathbf{r}} \rangle / dt = \vec{0}$. Thus stationary states are not moving. Note that the Ehrenfest Theorem only applies if all the expectation values exist (i.e. the underlying integrals converge). For example, consider plane waves as eigenstates of the free particle Hamiltonian. They have a well defined non-vanishing momentum $\vec{p}$ which coincides with the expectation value of the momentum operator $\langle \vec{\mathbf{p}} \rangle$, but they don't have a well-defined average position $\langle \vec{r}op \rangle$. Thus caution needs to be applied in that case.
☐ Measurements of the energy in a stationary state with energy E have expectation value

$$\langle \mathbf{H} \rangle = E = \text{const.} \tag{2.89}$$

☐ We can go beyond the last statement. The wave function $\psi(\vec{r},t) = e^{-iEt/\hbar}\psi(\vec{r})$ contains only one possible frequency $\omega = E/\hbar$. Therefore it seems reasonable to assume that all measurements of the energy operator $\mathbf{H}$ yield the same value E. This is confirmed by experiment. Thus for a stationary state with energy E not only the expectation value is equal to E, but all individual measurements give the same value E.

2.5.4 Energy Measurement and Energy Spectrum

☐ We have restricted our choice of eigenvalues for $\mathbf{H}$ to real numbers. We now want to see if that makes sense. Suppose $E = \epsilon + i\epsilon'$ is a complex number with ϵ, $\epsilon' \in \mathbb{R}$, and there exists an eigenfunction $\psi(\vec{r})$ such that $\mathbf{H}\,\psi = E\psi$. Then $\psi(\vec{r},t) = e^{-iE(t-t_0)/\hbar}\psi(\vec{r})$ is a solution to the Schrödinger Equation. The probability density $\rho = |\psi(\vec{r},t)|^2 = |\psi(\vec{r})|^2 e^{2\epsilon'(t-t_0)/\hbar}$. For any $\epsilon' \neq 0$ such an exponentially rising or decaying probability density would violate the continuity equation, since also the total probability $\int_{\mathbb{R}^3} \rho d^3r$ would depend exponentially on time. Our conclusion from this argument is that sensible Hamilton operators should indeed only admit real eigenvalues. We will discuss this further below in the context of Hermitian operators.
☐ The set of all (real) eigenvalues of a Hamilton operator $\mathbf{H}$ is called the energy spectrum of the system described by $\mathbf{H}$. The spectrum could be discrete or continuous or have both properties. If there exists a smallest energy eigenvalue, the corresponding eigenstate(s) are called the *ground state(s)*, those with larger energies are summarily called *excited states*.
☐ Examples:

(i) Harmonic oscillator (see Sec. 3.1): Discrete spectrum, ground state energy $E = \frac{1}{2}\hbar\omega$.

(ii) Free particle plane waves: Continuous spectrum with lower bound $E = 0$. $E = 0$ is usually not considered a ground state energy as it is mathematically allowed but physically meaningless.

(iii) Finite potential well (see Sec. 3.3): Discrete spectrum with a finite number of energies and a well defined ground state, followed by a continuous spectrum at higher energies.

☐ Stationary states formally live for an infinite time and allow for infinitely precise measurements of their energies. This might suggest that states with finite lifetime Δt do not allow infinitely sharp energy measurements. Rather they would exhibit a width ΔE around their expectation value $\langle E \rangle$. This is indeed confirmed by experiment. Example: Excited states in an atom which can transition to the ground state on a time scale Δt. Such an excited states has then an experimentally detectable width ΔE.[12]

☐ These results suggest a kind of uncertainty relation between energy E and time t. We can easily confirm this for free wave packets. Let us consider such a wave packet, propagating in the x-direction with width Δp_x. If Δp_x is small we can calculate the energy uncertainty associated with the width in momentum space as

$$\Delta E = \Delta \left(\frac{p_x^2}{2m} \right) = \frac{p_x}{m} \Delta p_x = v_x \Delta p_x \,. \tag{2.90}$$

Suppose the wave packet is passing a detector. The width of the wave packet Δx in space implies that the time of detection is smeared out by the time Δt it takes the wave packet to pass the detector,

$$\Delta t = \frac{\Delta x}{v_x} \geq \frac{\hbar}{2} \frac{1}{v_x \Delta p_x} = \frac{\hbar}{2} \frac{1}{\Delta E} \,, \tag{2.91}$$

where we have used the uncertainty principle between Δx and Δp_x in the second step. Thus we arrive at the uncertainly relation between energy and time

$$\boxed{\Delta E \Delta t \geq \frac{\hbar}{2} \,.} \tag{2.92}$$

2.5.5 Solutions in Momentum Space

☐ If $\psi(\vec{r})$ is a solution of the time-independent Schrödinger Equation

$$\left[-\frac{\hbar^2}{2m} \triangle + V(\vec{r}) \right] \psi(\vec{r}) = E \psi(\vec{r}) \tag{2.93}$$

then the Fourier transformed wave function $\phi(\vec{p})$, if it exists, is a solution to the *time-independent Schrödinger Equation in momentum space*

$$\boxed{\left[\frac{p^2}{2m} + V\left(i\hbar \nabla_p \right) \right] \phi(\vec{p}) \,,} \tag{2.94}$$

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[12] More generally, the picture of states with width usually consists of a Hamiltonian H_0 which defines those states as belonging to eigenvalues E_i of H_0, i.e. those states would be stationary states for H_0. The full Hamiltonian is $H = H_0 + h$ where h is a "small correction" (in ways we will quantify later on). The eigenstates of H_0 are no longer stationary states for the full Hamiltonian. But if h is a small perturbation a description of the system in terms of eigenstates to H_0, now with a finite life time, is very convenient.

i.e. E and $\phi(\vec{p})$ are also eigenvalue and eigenfunction of the Hamilton operator in momentum space. Proof: Clear.

☐ Such an energy eigenfunction $\phi(\vec{p})$ also represents a stationary state and its time evolution, which satisfies the time-dependent Schrödinger Equation is given by

$$\boxed{\phi(\vec{p},t) = e^{-\frac{i}{\hbar}Et}\phi(\vec{p})\,.} \tag{2.95}$$

☐ Plane waves are stationary states. They satisfy at any time the relevant time-independent Schrödinger Equation[13]:

$$\psi_{\vec{p}_0} = \frac{1}{(2\pi\hbar)^{3/2}}e^{\frac{i}{\hbar}\vec{p}_0\cdot\vec{r}} \qquad \text{and} \qquad -\frac{\hbar^2}{2m}\triangle\psi_{\vec{p}_0}(\vec{r}) = E\psi_{\vec{p}_0}(\vec{r}) \qquad \text{with} \qquad E = \frac{p_0^2}{2m}\,. \tag{2.96}$$

The corresponding momentum space wave function is

$$\phi_{\vec{p}_0} = \delta^{(3)}\left(\vec{p}-\vec{p}_0\right) \qquad \text{with} \qquad \frac{p^2}{2m}\phi_{\vec{p}_0}(\vec{p}) = E\phi_{\vec{p}_0}(\vec{p}) \qquad \text{and} \qquad E = \frac{p_0^2}{2m}\,. \tag{2.97}$$

The energy spectrum is continuous and is equal to the positive real line. There is a continuous degeneracy to each allowed eigenvalue $E > 0$. All $\vec{p}$ to one value of E lie on a sphere with radius $|\vec{p}| = \sqrt{2mE}$.

2.5.6 General Solutions

☐ We can build more general solutions of the time-dependent Schrödinger Equation from linear combinations of stationary solutions. In particular, suppose the initial wave function $\psi(\vec{r},t_0)$ at some time t_0 can be decomposed as[14]

$$\psi(\vec{r},t_0) = \sum_E\sum_{j=1}^{k_E} c_{E,j}\psi_{E,j}(\vec{r}) \tag{2.98}$$

for a system with a discrete energy spectrum where k_E is the degeneracy of eigenvalue E and the $\psi_{E,j}$, $j = 1,\ldots,k_E$ span the eigenspace of E. The $c_{E,j} \in \mathbb{C}$ are complex coefficients. Then the wave function

$$\boxed{\psi(\vec{r},t) = \sum_E\sum_{j=1}^{k_E} c_{E,j}e^{-\frac{i}{\hbar}E(t-t_0)}\psi_{E,j}(\vec{r})} \tag{2.99}$$

is a solution to the time-dependent Schrödinger Equation which satisfies the initial condition.

☐ We will often encounter sums over eigenvalue spectra which include sums over degeneracies. In such a case we will often simply write $\sum_E$ (in the case of energy eigenvalues) and assume that all degeneracies of eigenvalues are summed over implicitly. In the case of a continuous energy spectrum the decomposition would lead to continuous coefficients $c(E)$ and the sum itself would become an integral,

$$\psi(\vec{r}) = \int_{\text{spec}} c(E)\psi_E(\vec{r})dE\,. \tag{2.100}$$

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[13] The choice of normalizaton factor of the plane wave will be dealt with in the next section.

[14] More on the existence of such a decomposition later.

For a mixture of discrete and continuous parts in the spectrum sometimes you find the symbol

$$\psi(\vec{r}) = \sum\!\!\!\!\!\!\int_{\text{spec}} c(E)\psi_E(\vec{r})dE \tag{2.101}$$

in the literature. In both cases we again assume that degeneracies are implicitly summed or integrated over. Recall that degeneracies can by themselves be discrete or continuous (as in the case of plane waves). Eq. (2.99) generalizes in a straight forward manner to spectra with continuous parts.

2.6 Hilbert Spaces and Hermitian Operators

2.6.1 Hilbert Spaces

☐ Let $\mathcal{S}$ be a complex vector space of functions on $\mathbb{R}^n$. If the integral of the function $g^*(\vec{r})f(\vec{r})$ over all of $\mathbb{R}^n$ exists for all f, $g \in \mathcal{S}$ then this integral defines a scalar product (or inner product) on $\mathcal{S}$. We write

$$\boxed{\langle g|f\rangle = \int_{\mathbb{R}^n} g^*(\vec{r})f(\vec{r})d^n r\,.} \tag{2.102}$$

It is called the L^2-scalar product. One can check that this definition satisfies all the properties expected for a scalar product that results in complex numbers. In particular we can see the symmetry property, bi-linearity and positive definiteness, i.e.

$$\begin{aligned}\langle g|f\rangle &= \langle f|g\rangle^* \\ \langle \alpha g + h|f\rangle &= \alpha^*\langle g|f\rangle + \langle h|f\rangle \\ \langle f|\alpha g + h\rangle &= \alpha\langle f|g\rangle + \langle f|h\rangle \\ \langle f|f\rangle &\geq 0\end{aligned} \tag{2.103}$$

for arbitrary $f, g, h \in \mathcal{S}$, $\alpha \in \mathbb{C}$.

☐ The scalar product defines a metric and a norm on the vector space $\mathcal{S}$. The norm $\|f\|$ of a vector f is akin to its length or distance from the origin,

$$\|f\| = \sqrt{\langle f|f\rangle} = \left(\int_{\mathbb{R}^n} |f|^2 d^n r\right)^{\frac{1}{2}} . \tag{2.104}$$

The metric $d(f,g)$ tells us how to measure a distance between two elements f, g in $\mathcal{S}$

$$d(f,g) = \|f-g\| = \left(\int_{\mathbb{R}^n} |f-g|^2 d^n r\right)^{\frac{1}{2}} . \tag{2.105}$$

We demand that a proper metric also satisfies the following *triangle inequality*

$$d(f,g) \leq d(f,h) + d(h,g)\,. \tag{2.106}$$

We assume that this is always the case for spaces we consider. For a space with the L^2-scalar product the triangle inequality follows directly from the Schwartz Inequality we have used previously to prove the uncertainty relation. We skip the details of the proof.

☐ In mathematics we call a space with such a metric a metric space, and it also implies that this is a topological space. This is important because metric and topological spaces allow the notion of convergence. A series of functions f_n in $\mathcal{S}$, $n \in \mathbb{N}$, is said to converge to the limit $g \in \mathcal{S}$ (i.e. $f_n \to g$), if

$$\lim_{n\to\infty} d(f_n, g) = 0 \tag{2.107}$$

or more explicitly

$$\lim_{n\to\infty} \int_{\mathbb{R}^n} |f_n - g|^2 d^n r = 0\,. \tag{2.108}$$

Thus the scalar product helps us rephrase the question of convergence in $\mathcal{S}$ into a question of convergence of real numbers. Note that this L^2-*convergence* is a much weaker convergence criterion than a *pointwise convergence* where we would demand $f_n(\vec{r}) \to g(\vec{r})$ for all points $\vec{r}$ individually. In a sense an L^2-convergence only means that the series of functions f_n needs to converge towards g "on average".

☐ Even though we started this section looking specifically at vector spaces of functions we now state a very general definition. *Any* vector space with a scalar product that satisfies conditions (2.103) and (2.106) is called a *pre-Hilbert space*. It is further called a *Hilbert space* $\mathcal{H}$ if the following additional separability criterion is satisfied: For any series f_n, $n \in \mathbb{N}$ for which the norms can be summed, i.e. $\sum_{n\in\mathbb{N}} \|f_n\| < \infty$, there exists a g in the space $\mathcal{H}$ which corresponds to the sum of the f_n, i.e. $\sum_{n\in\mathbb{N}} f_n = g$. More explicitly we have

$$\lim_{n\to\infty} \int \left| \sum_{n\in\mathbb{N}} f_n - g \right|^2 d^n r = 0\,. \tag{2.109}$$

☐ Separability is a rather technical but mathematically important condition. We will not often make explicit use of it but it is cited here for completeness. We will simply state without further proof here that the space of square-integrable functions with the L^2-scalar product is separable and hence it is a Hilbert space. Generally, we will always assume from here forth that spaces of states we consider in quantum mechanics are Hilbert spaces, and this is in fact part of the Axiom (Q1) we introduced earlier.

2.6.2 Hermitian Operators

☐ Let $\mathbf{F}$ be a (linear) operator on a Hilbert space $\mathcal{H}$. The operator $\mathbf{F}^\dagger$ is called the *adjoint* operator to $\mathbf{F}$ if for all f, $g \in \mathcal{H}$ the condition

$$\boxed{\langle \mathbf{F} f | g \rangle = \langle f | \mathbf{F}^\dagger g \rangle} \tag{2.110}$$

holds. Specifically if $\mathcal{H}$ is a space of functions with the L^2-scalar product for any functions f, g the condition reads

$$\int (\mathbf{F} f)^*\, g\, d^n r = \int f^* \mathbf{F}^\dagger g\, d^n r\,. \tag{2.111}$$

☐ An operator is called *self-adjoint* or *Hermitian* if $\mathbf{F} = \mathbf{F}^\dagger$. In other words for a Hermitian operator

$$\boxed{\langle \mathbf{F} f | g \rangle = \langle f | \mathbf{F} g \rangle,} \tag{2.112}$$

and for the L^2-scalar product in particular

$$\int (\mathbf{F} f)^* \, g \, d^n r = \int f^* \mathbf{F} \, g \, d^n r \, . \tag{2.113}$$

☐ The adjoining operation has a few important basic properties. For operators **F**, **G** and $\lambda \in \mathbb{C}$ we have

$$\begin{aligned} \left(\mathbf{F}^\dagger\right)^\dagger &= \mathbf{F} \\ (\lambda \mathbf{F} + \mathbf{G})^\dagger &= \lambda^* \mathbf{F}^\dagger + \mathbf{G}^\dagger \qquad (2.114) \\ \mathbf{Id}^\dagger &= \mathbf{Id} \\ (\mathbf{F}\mathbf{G})^\dagger &= \mathbf{G}^\dagger \mathbf{F}^\dagger \, . \qquad (2.115) \end{aligned}$$

Proof: This is straight forward to check.
☐ Multiplication operators with real numbers, for example $\vec{r}$ or any function $f(\vec{r})$ in coordinate space, $\vec{p}$ and any function $g(\vec{p})$ in momentum space, are Hermition operators. The operators $-i\hbar\nabla_r = \vec{p}_r$ in coordinate space and $i\hbar\nabla_p = \vec{r}_p$ in momentum space are Hermitian, since

$$\int f^*(\vec{r}) \, (-i\hbar\nabla) \, g(\vec{r}) d^3 r = \int \left(-i\hbar\nabla f(\vec{r})\right)^* g(\vec{r}) d^3 r \tag{2.116}$$

through partial integration for sufficiently fast falling functions f, g (similar for the position operator in $\vec{p}$-space). Generally, it is straight forward to check that if an operator $\mathbf{F}_r$ is Hermitian in coordinate space then its corresponding operator $\mathbf{F}_p$ in momentum space is Hermitian and vice versa. Thus we can just say the "abstract" operator **F** that $\mathbf{F}_r$ and $\mathbf{F}_p$ represent is Hermitian. All important operators mentioned in Sec. 2.3.1 are Hermitian.
☐ Let **F** be an operator representing a physical observable. Obviously we demand that the expectation value $\langle \mathbf{F} \rangle$ of measurements be real for any wave function ψ in which the expectation value is taken. Thus

$$\langle \mathbf{F} \rangle^* = \left(\int \psi^* \mathbf{F} \, \psi d^3 \right)^* = \int (\mathbf{F} \, \psi)^* \psi d^3 r \tag{2.117}$$

and it should equal

$$\langle \mathbf{F} \rangle = \int \psi^* \mathbf{F} \, \psi d^3 r \tag{2.118}$$

which, if demanded to hold for any ψ, means that **F** has to be Hermitian. Thus operators representing physical observables must be Hermitian!
☐ Recall that measurements of the Hamilton operator **H** in an eigenstate ψ_E of **H** with eigenvalue E yield only the value E. Here is the generalization of this important statement.

If a system is in an eigenstate ψ_α with (real) eigenvalue α of an Hermitian operator A representing the physical quantity A, then measurements of A yield only the value of the eigenvalue α.

Proof: On average the measurements yield $\langle \mathbf{A} \rangle = \langle \psi_\alpha | \mathbf{A} \, \psi_\alpha \rangle = \langle \psi_\alpha | \alpha \psi_\alpha \rangle = \alpha$. For the spread around the mean we calculate

$$(\Delta A)^2 = \left\langle (\mathbf{A} - \langle \mathbf{A} \rangle)^2 \right\rangle = \langle \psi_\alpha | (\mathbf{A} - \alpha)^2 \psi_\alpha \rangle = 0 \, . \tag{2.119}$$

☐ Recall that in a finite-dimensional Hilbert space of dimension n (e.g. $\mathbb{R}^n$) any Hermitian operator (matrix) **A** has n real eigenvalues and their eigenvectors can be chosen to form an orthonormal basis of the entire space. Here is the generalization of this statement for arbitary Hilbert spaces.

For a Hermitian operator $\mathbf{A}$ on a Hilbert space $\mathcal{H}$ (i) all eigenvalues are real, (ii) its eigenvectors for different eigenvalues are orthogonal, and (iii) for a large class of operators the space spanned by all the eigenvectors is equal to the entire space $\mathcal{H}$ (completeness property). We will always assume completeness to hold for any operators and spaces relevant for Quantum Mechanics.[15]

Proof: For eigenvectors ψ_1 and ψ_2 of $\mathbf{A}$ with eigenvalues α_1 and α_2, respectively, we have $\alpha_1 = \langle\psi_1|\mathbf{A}\,\psi_1\rangle = \langle\mathbf{A}\,\psi_1|\psi_1\rangle = \alpha_1^*$, i.e. eigenvalues are real. Furthermore $0 = \langle\psi_2|\mathbf{A}\,\psi_1\rangle - \langle\mathbf{A}\,\psi_2|\psi_1\rangle = (\alpha_1 - \alpha_2^*)\,\langle\psi_2|\psi_1\rangle$ and thus for different eigenvalues, $\alpha_1 \neq \alpha_2$, the two eigenvectors ψ_1 and ψ_2 are orthogonal. The completeness property is easy to show in the finite dimensional case but more difficult to deal with in the inifite dimensional case, as indicated in the footnote. We take it as an assumption here an explore its consequences in the next subsection.

☐ **We conclude that in quantum mechanics the eigenvectors of a Hermitian operator form an orthogonal basis of the underlying Hilbert space.**

Proof: This follows directly from the last statement and the fact that within the eigenspace of any degenerate eigenvalue we can always find an orthogonal basis for that subspace, and each such all such basis vectors will automatically be eigenvectors.

☐ **Simultaneous Diagonalizability.** This is another very important property of Hermitian operators. Let $\mathbf{A}$ and $\mathbf{B}$ be two commuting Hermitian operators on a Hilbert space $\mathcal{H}$, i.e. $[\mathbf{A},\mathbf{B}] = 0$. **Then there exists a common set of eigenstates ψ_i for $\mathbf{A}$ and $\mathbf{B}$, i.e. if $\mathbf{A}\,\psi_i = \alpha_i\psi_i$ then $\mathbf{B}\,\psi_i = \beta_i\psi_i$ and vice versa with eigenvalues $\alpha_i, \beta_i \in \mathbb{R}$.** Proof: Again this is a standard theorem for finite dimensional Hilbert spaces. We skip the proof of the general case here.

2.6.3 Completeness

Let us explore the consequences of the completeness property in more detail.

☐ Recall that general solutions to the time-dependent Schrödinger Equation can be built from eigenfunctions of the Hamilton operator $\mathbf{H}$. On the other hand those eigenfunctions form a complete, orthogonal basis of the Hilbert space $\mathcal{H}$. In the following we distinguish two cases:

(A) The spectrum of $\mathbf{H}$ is discrete. Then the dimension of $\mathcal{H}$ is either finite (if the spectrum has a finite number of points) or infinite but countable.

(B) The spectrum of $\mathbf{H}$ is continuous or has at least one continuous section. Then the dimension of $\mathcal{H}$ is infinite and uncountable.[16]

Case A

☐ We consider a Hermitian operator $\mathbf{A}$ on $\mathcal{H}$ with orthogonal eigenstates ψ_α, where α is from an index set I which can be chosen to be $\mathbb{N}$ or a subset thereof. The eigenstates form a complete

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[15] This touches a subtle mathematical point that many operators can actually not be properly defined on all of a Hilbert space but only on "almost" all of the Hilberts space. We will not dwell on this details further but take the pragmatic stance here that completeness holds for all the cases we are interested in.

[16] Without invoking two much mathematics we take the set of natural numbers $\mathbb{N}$ and the set of real numbers $\mathbb{R}$ as examples of countable and uncountable infinite sets.

set of functions of $\mathcal{H}$ which means that for any wave function ϕ in $\mathcal{H}$ we can find a set of complex coefficients c_α, $\alpha \in I$ such that

$$\boxed{\phi(\vec{r}) = \sum_{\alpha \in I} c_\alpha \psi_\alpha(\vec{r})\,.} \tag{2.120}$$

Note that degeneracies are implicitly included in this sum, i.e. I counts eigenvalues including their degeneracies.

☐ Note that if this is a Hilbert space of wave functions with L^2 scalar product the scalar product of any two wave functions yields a finite complex number, and thus all wave functions in $\mathcal{H}$ are square integrable, $\mathcal{H} \subset L^2(\mathbb{R}^n)$. We can choose our eigenfunctions be an *orthonormal* basis, i.e.

$$\boxed{\langle \psi_\alpha | \psi_\beta \rangle = \int \psi_\alpha^* \psi_\beta d^3r = \delta_{\alpha\beta}\,.} \tag{2.121}$$

☐ The coefficients c_α in the expansion of an arbitrary wave function $\phi(\vec{r})$ can be obtained from a projection

$$\boxed{c_\alpha = \langle \psi_\alpha | \phi \rangle = \int \psi_\alpha^* \phi d^3r\,.} \tag{2.122}$$

Proof: It is easily checked that

$$\int \psi_\alpha^* \phi d^3r = \sum_{\beta \in I} c_\beta \int \psi_\alpha^*(\vec{r}) \psi_\beta(\vec{r})\, d^3r = c_\alpha\,. \tag{2.123}$$

We have explicitly referred here to integrals over coordinate space wave functions, but we could have formulated everything in terms of the abstract scalar product notation $\langle .|. \rangle$. We will increasingly do so in the future. That would have made it even more obvious that all of these statements are true in any representation of the quantum system.

☐ We find the following sum rule for the expansion coefficients

$$\langle \phi | \phi \rangle = \sum_{\alpha \in I} |c_\alpha|^2\,. \tag{2.124}$$

The proof is straight forward. For wave functions normalized to unity this implies

$$\sum_{\alpha \in I} |c_\alpha|^2 = 1\,. \tag{2.125}$$

Note that if the set of basis wave functions is agreed upon the set of coefficients $(c_\alpha)_{\alpha \in I}$ contains all the information about the wave function ϕ.

☐ Consider a Hermitian operator $\mathbf{A}$ with an orthonormal basis set of eigenfunctions ψ_α, $\alpha \in I$, and eigenvalue a_α for each eigenfunction ψ_α. The expectation value of $\mathbf{A}$ with respect to a wave function ϕ with expansion coefficients c_α in that basis we find

$$\boxed{\langle \mathbf{A} \rangle = \sum_{\alpha \in I} a_\alpha |c_\alpha|^2\,.} \tag{2.126}$$

Generally, for any function $f(\mathbf{A})$ we have

$$\boxed{\langle f(\mathbf{A}) \rangle = \sum_{\alpha \in I} f(a_\alpha) |c_\alpha|^2\,.} \tag{2.127}$$

Proof: This is easy to check.

☐ This suggests the following interpretation.

(a) If α corresponds to a non-degenerate eigenvalue a_α then the number $|c_\alpha|^2$, with $0 \leq |c_\alpha|^2 \leq 1$ for properly normalized wave functions ϕ is the probability to measure the value a_α for the observable $\mathbf{A}$ in the state ϕ, i.e.

$$\boxed{P(a_\alpha) = |c_\alpha|^2 = |\langle \psi_\alpha | \phi \rangle|^2 \,.} \tag{2.128}$$

(b) **The eigenvalues of A are the only allowed outcomes of a measurement of the observable A.**

(c) If the eigenvalue a is degenerate, $a = a_\alpha$ for a subset of I, then the probability to measure a requires a sum over the degeneracy.

$$\boxed{P(a) = \sum_{\alpha \,\text{with}\, a_\alpha = a} |c_\alpha|^2 \,.} \tag{2.129}$$

Even though these ideas are suggested by our results so far they nevertheless do not follow strictly from our wave mechanics. They need to be confirmed by experiment which has indeed been the case.

☐ Sometimes it is useful to rewrite the completeness property in terms of the so called *closure relation.* For any orthonormal basis $\psi_\alpha(\vec{r})$, $\alpha \in I$ we find

$$\boxed{\sum_{\alpha \in I} \psi^*_\alpha(\vec{r}\,')\psi_\alpha(\vec{r}) = \delta^{(3)}(\vec{r} - \vec{r}\,') \,.} \tag{2.130}$$

Proof: To check if the left hand side is a δ-function we need to integrate with a test function ϕ,

$$\int \phi(\vec{r}\,') \left(\sum_\alpha \psi^*_\alpha(\vec{r}\,')\psi_\alpha(\vec{r}) \right) d^3r' = \sum_\alpha \psi_\alpha(\vec{r}) \int \psi^*_\alpha(\vec{r}\,')\phi(\vec{r}\,')\, d^3r' = \sum_\alpha c_\alpha \psi_\alpha(\vec{r}) = \phi(\vec{r}) \,, \tag{2.131}$$

which is the same result that we would get if this integral were taken over the right hand side.

Case B

☐ In the case of a completely continuous spectrum for a Hermitian operator $\mathbf{A}$ on $\mathcal{H}$ with orthogonal eigenstates ψ_α there exists a decomposition

$$\boxed{\phi(\vec{r}) = \int b_\alpha \psi_\alpha(\vec{r}) d\alpha} \tag{2.132}$$

for any state ϕ in $\mathcal{H}$. Note that the notation $\int d\alpha$ is symbolic and needs to be carried out over all eigenvalues and their degeneracies. This might be an integration over a space with more than one dimension. E.g. the eigenvalues of the free momentum operators consist of the entire space of momentum vectors $\sim \mathbb{R}^3$. As usual degeneracies are implicitly included. $b_\alpha = b(\alpha)$ is a function of α. If the spectrum has continuous and discrete parts the decomposition could be explicitly written as

$$\phi(\vec{r}) = \sum_{\text{discr.}\, \alpha} c_\alpha \psi_\alpha(\vec{r}) + \int_{\text{cont.}\, \alpha} b_\alpha \psi_\alpha(\vec{r}) d\alpha \,. \tag{2.133}$$

☐ Each eigenfunction in the expansion above has an infinitely small weight and this opens a way for us to incorporate wave functions into the Hilbert space with L^2-scalar product for which the integral that defines the scalar product formally diverges. We can demand the following condition for orthonormality:

$$\boxed{\langle\psi_{\alpha'}|\psi_\alpha\rangle = \int \psi^*_{\alpha'}(\vec{r})\psi_\alpha(\vec{r})d^3r = \delta(\alpha-\alpha')\,.} \tag{2.134}$$

This is often referred to as the **A**-normalization since the δ-function is in terms of eigenvalues of the operator **A**. Note that this definition formally allows an L^2-norm of inifinity, but it turns out that the condition (2.134) leads to mathematically well defined results. As a practical matter one can arrive at it by taking continuous spectra as a limit of the case of discrete spectra, e.g. by considering wave functions in a finite volume of size L and then taking the limit $L\to\infty$ (cf. [1], p. 61f).

☐ One can check that all basic properties discussed in case (A) generalize appropriately to case (B). In particular coeffecients can be obtained by projection

$$\boxed{b_\alpha = \langle\psi_\alpha|\phi\rangle = \int \psi^*_\alpha(\vec{r})\phi(\vec{r})\,d^3r\,,} \tag{2.135}$$

expectation values of functions of the operator **A** can be calculated from the knowledge of the coefficient functions

$$\boxed{\langle f(\mathbf{A})\rangle = \int f(a_\alpha)|b_\alpha|^2 d\alpha\,,} \tag{2.136}$$

and there is a completeness relation

$$\boxed{\int_\alpha \psi^*_\alpha(\vec{r}\,')\psi_\alpha(\vec{r})\,d\alpha = \delta^{(3)}(\vec{r}-\vec{r}\,')\,.} \tag{2.137}$$

2.6.4 Two Simple Examples

We briefly discuss two typical examples for cases (A) and (B) from the previous subsection.

Case A: Infinite Square Well

☐ Consider a particle of mass m in a potential $V(\vec{r}) = V(x,y,z)$ for which

$$V(\vec{r}) = 0 \qquad \text{for} \quad 0<x<L,\ 0<y<L,\ 0<z<L \tag{2.138}$$

$$V(\vec{r}) = \infty \qquad \text{elsewhere} \tag{2.139}$$

We would like to solve the time-independent Schrödinger Equation

$$-\frac{\hbar^2}{2m}\triangle\psi(x,y,z) = E\psi(x,y,z)\,. \tag{2.140}$$

It is immediately clear that $\psi = 0$ outside of the cube L^3 in which the potential vanishes, or otherwise the energy $\langle\mathbf{V}\rangle$ of the particle would diverge. At the walls of the well, the continuity equation tells us that the particle current $\vec{j}$ of the Schrödinger field is continuous and thus it has to approach zero on the inside of the wall since it vanishes on the outside. Hence $\psi = 0$ on the walls of the cube.

☐ Since the problem is symmetric under interchange of the x-, y- and z-directions we try a separation ansatz

$$\psi(x, y, z) = X(x)Y(y)Z(z) \tag{2.141}$$

and it follows that the factors have to obey the individual equations

$$\frac{d^2X}{dx^2} = -k_x^2 X \quad , \quad \frac{d^2Y}{dy^2} = -k_y^2 Y \quad , \quad \frac{d^2Z}{dz^2} = -k_z^2 Z \tag{2.142}$$

where the wave number squares have to add up to deliver the correct energy

$$E = \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right) . \tag{2.143}$$

These are very simple wave equations and the solutions, taking into account that $\psi = 0$ on the boundaries, are sine functions with wave numbers given by multiples of $\frac{\pi}{L}$. Hence the wave function inside the well is

$$\boxed{\psi_{n_x,n_y,n_z}(x, y, z) = C \sin\left(n_x \frac{\pi}{L} x\right) \sin\left(n_y \frac{\pi}{L} y\right) \sin\left(n_z \frac{\pi}{L} z\right)} \tag{2.144}$$

with strictly positive integer numbers $n_x, n_y, n_z \in \mathbb{N}$. and the energy eigenvalues are given by

$$\boxed{E = E_0\left(n_x^2 + n_y^2 + n_z^2\right) = \frac{\hbar^2\pi^2}{2mL^2}\left(n_x^2 + n_y^2 + n_z^2\right)} \tag{2.145}$$

where E_0 sets the energy scale. $C = \sqrt{8/L^3}$ is a normalization factor that can be determined from the normalization condition for ψ.

☐ The formula for E determines the energy spectrum, i.e. the allowed energies of particles in the well, and their degeneracies. In 3 dimensions, as discussed here, many eigenvalues are degenerate. We can summarize the lowest eigenvalues in the spectrum in the following table. Even this simple quantum problem has a surprisingly rich energy spectrum.

E	$3E_0$	$6E_0$	$9E_0$	$11E_0$	$12E_0$	$14E_0$
d_E	1	3	3	3	1	6
(n_x, n_y, n_z)	$(1,1,1)$	$(1,1,2)$ $(1,2,1)$ $(2,1,1)$	$(1,2,2)$ $(2,1,2)$ $(2,2,1)$	$(1,1,3)$ $(1,3,1)$ $(3,1,1)$	$(2,2,2)$	$(1,2,3)$ $(1,3,2)$ $(2,1,3)$ $(2,3,1)$ $(3,1,2)$ $(3,2,1)$

Table 2.1: The lowest energy eigenvalues E, their degeneracies d_E, and the modes that describe the d_E eigenfunctions to this energy for the infinite 3-dimensional square well.

☐ According to our assumptions the eigenfunctions $\psi_{n_x,n_y,n_z}(\vec{r})$ should form a complete orthonormal basis of square-integrable functions on the cube L^3 with vanishing values on the boundary. We can confirm that this is indeed the case in this particular situation. The completeness statement turns out to be a special case of Fourier's Theorem that states that every function on a compact interval of the real line can be decomposed into a series of trigonometric functions (Fourier series!).

☐ Let us visualize the lowest lying eigenstates in the 1-D case. Obviously in 1-D the eigenfunctions are

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(n\frac{\pi}{L}x\right) \quad , \quad E = \frac{\hbar^2\pi^2}{2mL}n^2 \tag{2.146}$$

with one integer index $n > 0$, i.e. the eigenstates are not degenerate.

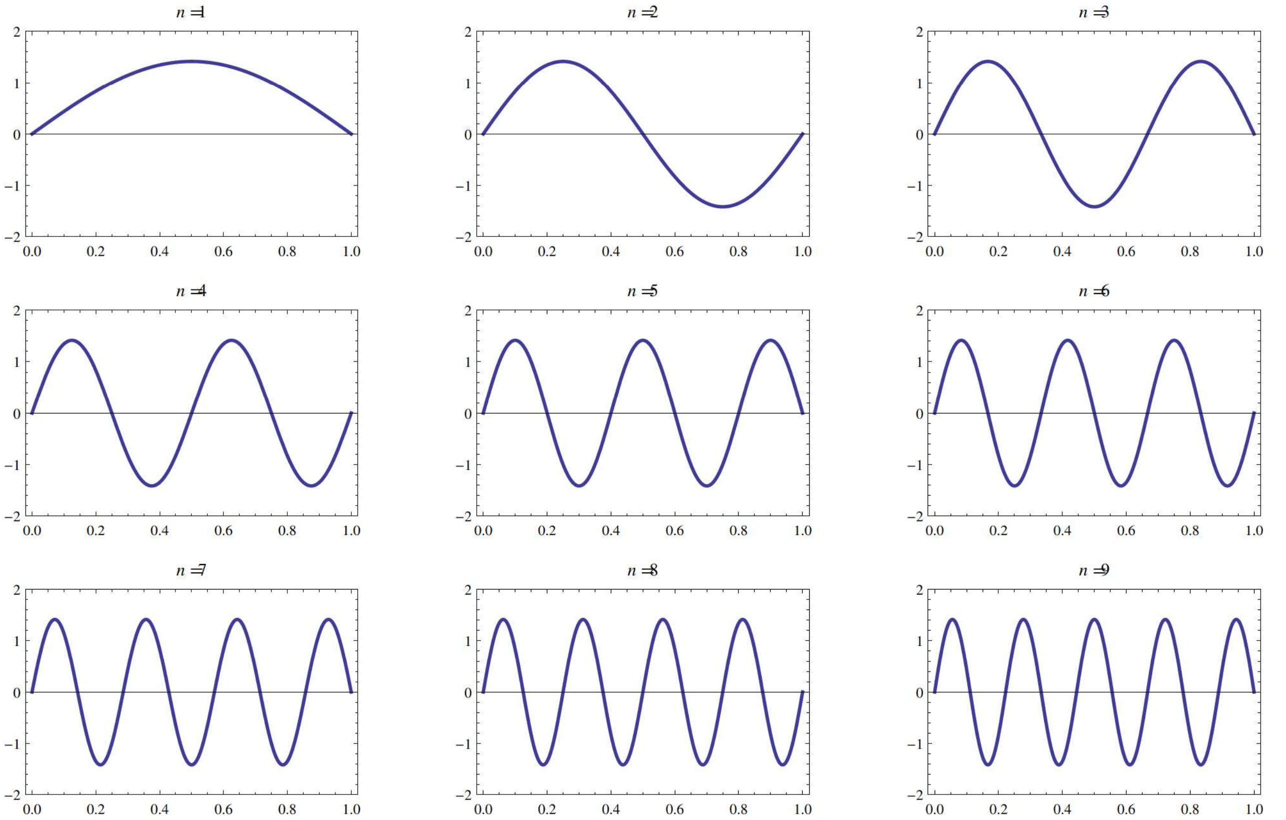

Figure 2.1: The nine lowest energy eigenfunctions for the infinite 1-D potential well ($n = 1, \ldots, 9$).

Case B: Free Particles

☐ We know the solution to the free Schrödinger Equation are linear combinations of plane waves. Thus the solutions to the corresponding time-independent Schrödinger Equation are

$$\psi_{\vec{p}}(\vec{r}) = Ce^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} . \tag{2.147}$$

for all momentum vectors $\vec{p} \in \mathbb{R}^3$, $\vec{p} \neq \vec{0}$. These wave functions are eigenstates to both the momentum operator $\vec{\mathbf{p}} = -i\hbar\nabla_r$ and the Hamiltonian $\mathbf{H} = p^2/(2m)$, i.e.

$$\vec{\mathbf{p}}\,\psi_{\vec{p}}(\vec{r}) = \vec{p}\psi_{\vec{p}}(\vec{r}) , \tag{2.148}$$

$$\mathbf{H}\,\psi_{\vec{p}}(\vec{r}) = \frac{\vec{p}^2}{2m}\psi_{\vec{p}}(\vec{r}) . \tag{2.149}$$

We should specify what we precisely mean with the first equation: $\psi_{\vec{p}}$ is a simultaneous eigenstate for the three operators $\mathbf{p}_x, \mathbf{p}_y, \mathbf{p}_z$. We will prefer to label these eigenstates with their eigenvalues $\vec{p}$ with respect to the momentum operator since there is no degeneracy for $\vec{p}$ while for energy eigenvalues E there is the continuous degeneracy that can be parameterized by the points $\hat{n}$ on the unit sphere. So alternatively we can label $\psi_{\vec{p}} \equiv \psi_{E,\hat{n}}$ where $\hat{n} = \vec{p}/p$.

☐ Using the normalization condition for continuous spectra

$$\langle \psi_{\vec{p}'} | \psi_{\vec{p}} \rangle = |C|^2 \int e^{\frac{i}{\hbar}(\vec{p}' - \vec{p})\cdot\vec{r}} d^3r = |C|^2 \left(2\pi\hbar\right)^3 \delta^{(3)}(\vec{p}' - \vec{p}) \tag{2.150}$$

we find $C = (2\pi\hbar)^{-3/2}$ as a suitable normalization factor, as already used in Sec. 2.5.5.

☐ The expansion of arbitrary functions

$$\psi(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} \int b_{\vec{p}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} d^3p \tag{2.151}$$

in terms of eigenstates of free particles is just the known Fourier integral. In particular, the expansion coefficients $b_{\vec{p}} \equiv \phi(\vec{p})$ just give the Fourier transform of ψ.

☐ It is easy to check that the closure relation holds in this example,

$$\int \psi^*_{\vec{p}}(\vec{r}')\psi_{\vec{p}}(\vec{r}) d^3p = \frac{1}{(2\pi\hbar)^3} \int e^{\frac{i}{\hbar}\vec{p}\cdot(\vec{r}' - \vec{r})} d^3p = \delta^{(3)}(\vec{r}' - \vec{r}) \,, \tag{2.152}$$

as expected.

2.7 Unitary Operators and Representations

2.7.1 Unitary Operators

☐ Let $\mathcal{H}$ be a Hilbert space. A linear operator $\mathbf{U}$ on $\mathcal{H}$ is called unitary, if

$$\boxed{\mathbf{U}^\dagger \mathbf{U} = \mathbf{U}\mathbf{U}^\dagger = \mathbf{Id}\,.} \tag{2.153}$$

This is equivalent to the condition

$$\boxed{\langle \mathbf{U}f | \mathbf{U}g \rangle = \langle f | g \rangle} \tag{2.154}$$

for all $f, g \in \mathcal{H}$, because $\langle \mathbf{U}f | \mathbf{U}g \rangle = \langle f | \mathbf{U}^\dagger \mathbf{U} g \rangle = \langle f | g \rangle$. In other words, unitary operators are the ones who preserve scalar produces and norms.

☐ Recall: In $\mathbb{R}^n$ unitary operators (matrices) are rotations and inversions. They form a group of matrices called $O(n)$, the *orthogonal group*. We can generalize: the unitary operators on $\mathcal{H}$ form a (usually non-abelian) group with respect to their product (concatenation). Proof: If $\mathbf{U}_1, \mathbf{U}_2$ are unitary then

$$\left(\mathbf{U}_1\mathbf{U}_2\right)^\dagger \left(\mathbf{U}_1\mathbf{U}_2\right) = \mathbf{U}_2^\dagger \mathbf{U}_1^\dagger \mathbf{U}_1 \mathbf{U}_2 = \mathbf{Id} \tag{2.155}$$

and $\mathbf{U}_1\mathbf{U}_2$ is a unitary operator. $\mathbf{Id}$ is the unit element of the group and the inverse $\mathbf{U}^{-1} = \mathbf{U}^\dagger$ is unitary.

☐ Eigenvalues of unitary operators have modulus 1, i.e. they can be written as $e^{i\phi}$ with some phase $\phi \in \mathbb{R}$, and eigenfunctions for different eigenvalues are orthogonal. Proof: Assume eigenvalues and eigenfunctions $\mathbf{U}\psi_1 = \alpha_1\psi_1$, $\mathbf{U}\psi_2 = \alpha_2\psi_2$. Then we have

$$0 = \langle \psi_2 | \psi_1 - \langle \mathbf{U}\psi_2 | \mathbf{U}\psi_1 \rangle = \left(1 - \alpha_2^*\alpha_1\right) \langle \psi_2 | \psi_1 \rangle \,. \tag{2.156}$$

If $\alpha_1 \neq \alpha_2$ the states are orthogonal. If the eigenvalues are the same then $|\alpha_1|^2 = 1$.