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

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

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). <u>Proof</u>: If $\mathbf{U}_1, \mathbf{U}_2$ are unitary then

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

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. <u>Proof</u>: Assume eigenvalues and eigenfunctions $\mathbf{U}\psi_1 = \alpha_1\psi_1$, $\mathbf{U}\psi_2 = \alpha_2\psi_2$. Then we have

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

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

2.7.2 Representations and Galilei Group

☐ Symmetry operations usually form groups.

- Translations $t_{\vec{a}} : \vec{r} \to \vec{r} + \vec{a}$ with $\vec{a} \in \mathbb{R}$ form a group with respect to concatenation, i.e. the product $t_{\vec{b}} t_{\vec{a}} : \vec{r} \mapsto (\vec{r} + \vec{a}) + \vec{b} = \vec{r} + (\vec{a} + \vec{b})$ is the same as the translation $t_{\vec{a}+\vec{b}}$. Translations form an abelian group which is isomorphic (i.e. analogous) to $\mathbb{R}^3$ with summations of vectors as the group operation.

- The Galilei group $\mathcal{G}$ of translations, rotations, boosts, and space and time inversions form a group. This is discussed in any good book on classical mechanics. The most general transformation for time t, position $\vec{r}$ and velocity $\vec{v}$ is

$$t \mapsto \lambda t + b \,, \quad \vec{r} \mapsto R\vec{r} + \vec{w}\lambda t + \vec{a} \,, \quad \vec{v} \mapsto \lambda \vec{v} + \vec{w} \,, \tag{2.157}$$

  where $R \in O(3)$ is an orthogonal matrix (rotations and spatial inversions), $\lambda = \pm 1$ (time inversion), $b \in \mathbb{R}$ (time translations), $\vec{a} \in \mathbb{R}^3$ (spatial translations), $\vec{w} \in \mathbb{R}^3$ (boosts). Elements of the Galilei group with $\det R = 1$, $\lambda = 1$ form the proper orthochronous subgroup $\mathcal{G}_+^+$.

☐ In classical mechanics operations of symmetry groups like $\mathcal{G}$ are usually straight forward. In quantum mechanics symmetry operations need to act on states ψ in a Hilbert space $\mathcal{H}$. Hence they need to be respresented by operators on $\mathcal{H}$. For simplicity they should be linear (or anti-linear) operators. Symmetry transformations leave a system invariant thus their operators need to preserve probabilities and therefore scalar products on $\mathcal{H}$. We conclude that operators representing symmetry transformations should by unitary operators.
☐ For any symmetry group G a set of linear (or anti-linear) operators $D(G)$ on a Hilbert space $\mathcal{H}$ is called a representation of G if there is a unique map

$$G \to D(G) \,, \qquad g \mapsto \mathbf{D}_g \,, \tag{2.158}$$

where g is an element of the group and $\mathbf{D}_g$ is an operator representing the action of g on $\mathcal{H}$, and $D(G)$ has the same group structure as G, i.e. $\mathbf{D}_{gh} = \mathbf{D}_g \mathbf{D}_h$. Sometimes we have to relax the latter condition and allow for a (physically unobservable) phase,

$$\mathbf{D}_{gh} = e^{i\phi(g,h)} \mathbf{D}_g \mathbf{D}_h \tag{2.159}$$

where ϕ is real with some additional properties which we will not discuss in detail here[17] If these phases are present the representation is called a projective representation.
☐ Some symmetry transformations are topologically connected to the identity operator **Id**, i.e. they can be continuosly deformed into the identity. For example the proper orthochronous Galilei group $\mathcal{G}_+^+$ is fully connected to **Id**, while the parity transformation $\vec{r} \mapsto -\vec{r}$ can not be deformed into **Id**. Consider translations $t_{\vec{a}}$ as an example of the former. Obviously $t_{\vec{a}} \to$ identity as $\vec{a} \to \vec{0}$.
☐ Just as in the case of translations, generally transformations in the neighborhood of **Id** can be parameterized by sets of real parameters. In that case the operators representing these transformations can be expanded around the indentity operator in the relevant Hilbert space,

$$\mathbf{D}_g = \mathbf{Id} - \frac{i}{\hbar} \epsilon \mathbf{G} + \mathcal{O}(\epsilon^2) \,. \tag{2.160}$$

[17] Projective representations are discussed in many books, e.g. in *Quantum Theory of Fields* by S. Weinberg.

Here ϵ is a real parameter and the operator $\mathbf{G}$ is called the generator of the transformation.
☐ The operator $\mathbf{D}_g$ is unitary exactly if the generating operator *gop* is Hermitian. Proof: We have

$$\mathbf{D}_g^\dagger \mathbf{D}_g = \left(\mathbf{Id} - \frac{i}{\hbar}\epsilon \mathbf{G}\right)^\dagger \left(\mathbf{Id} - \frac{i}{\hbar}\epsilon \mathbf{G}\right) + \mathcal{O}(\epsilon^2) = \mathbf{Id} + \frac{i}{\hbar}\epsilon(\mathbf{G}^\dagger - \mathbf{G}) + \mathcal{O}(\epsilon^2) \tag{2.161}$$

and so $\mathbf{D}_g^\dagger \mathbf{D}_g = \mathbf{Id} \Longleftrightarrow \mathbf{G}^\dagger = \mathbf{G}$.

2.7.3 Translations

☐ The time translation operator

$$\mathbf{D}_b = \mathbf{T}(b) = e^{-\frac{i}{\hbar}\mathbf{H}b} \tag{2.162}$$

is a unitary operator and represents time translations $t \mapsto t+b$ for a system with Hamilton operator $\mathbf{H}$. In particular, $-\mathbf{H}$ is the generator of time translations. Proof: Obviously $\mathbf{D}_b \psi(\vec{r}, t) = \psi(\vec{r}, t+b)$ for all wave functions ψ in the Hilbert space. Furthermore the group stucture is carried by the time evolution operators, $\mathbf{D}_{b_2}\mathbf{D}_{b_2} = e^{-i/\hbar \mathbf{H}(b_1+b_2)} = \mathbf{D}_{b_2+b_1}$. Lastly we note that $\mathbf{D}_b^\dagger \mathbf{D}_b = \mathbf{Id}$ so the operators are unitary.
☐ The effect of a spatial translation by $\vec{a}$ on a wave function is $\psi(\vec{r}, t) \mapsto \psi(\vec{r} - \vec{a}, t)$. What is the operator that maps the original wave function onto the shifted one? A Taylor expansion gives

$$\psi(\vec{r} - \vec{a}, t) = \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\vec{a} \cdot \nabla_r\right)^n \psi(\vec{r}) = e^{\vec{a}\cdot\nabla_r}\psi(\vec{r}) = e^{-\frac{i}{\hbar}\vec{a}\cdot\vec{\mathbf{p}}}\psi(\vec{r}) \,, \tag{2.163}$$

where $\vec{\mathbf{p}}$ is the momentum operator. Therefore the generators of translations in x, y, z are the momentum operators $\mathbf{p}_x$, $\mathbf{p}_y$, $\mathbf{p}_z$, respectively.
☐ Commutators of the generators of symmetry operations are rather important:

- $[\mathbf{p}_i, \mathbf{p}_j] = 0$ for any $i, j = 1, 2, 3$, hence translations in arbitary directions commute.
- $[\mathbf{p}_i, \mathbf{H}] \neq 0$ in general, hence translations in time and space are not expected to commute.

2.7.4 Galilei Boosts

☐ Consider a change to another frame of reference moving with velocity $-\vec{w}$ with respect to the original one,

$$\vec{r} \mapsto \vec{r} + \vec{w}t \,, \quad \vec{v} \mapsto \vec{v} + \vec{w} \,, \tag{2.164}$$

where $\vec{r}$ and t are position and time and $\vec{v}$ is the velocity of a particle in the original frame. We note that a because of the change in position a wave function would be shifted as $\psi(\vec{r}, t) \mapsto \psi(\vec{r} - \vec{w}t)$. But we expect that the boost should change the shape of the wave function as well.
☐ Let us therefore consider the changes in momentum $\vec{p}$ and energy E of a particle of mass m

$$\vec{p} \mapsto \vec{p} + m\vec{w} \,, \quad E \mapsto E + \vec{p}\cdot\vec{w} + \frac{m}{2}w^2 \,. \tag{2.165}$$

Let us now consider specifically a free particle desribed by a plane wave. The boost would act as

$$\psi(\vec{r}, t) = (2\pi\hbar)^{-\frac{3}{2}} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{r} - Et)} \mapsto (2\pi\hbar)^{-\frac{3}{2}} e^{\frac{i}{\hbar}\left((\vec{p}+m\vec{w})\cdot\vec{r} - \left(E + \vec{p}\cdot\vec{w} + \frac{m}{2}w^2\right)t\right)} \,. \tag{2.166}$$

Note that the coordinates on the right hand side are in the new coordinate system. A comparison with the shifted wave function tells us that in the new reference frame the wave function is shifted and multplied with an additonal phase factor

$$\psi(\vec{r},t) \mapsto e^{\frac{i}{\hbar}\left(m\vec{w}\cdot\vec{r}-\frac{m}{2}w^2 t\right)}\psi(\vec{r}-\vec{w}t,t)\,. \tag{2.167}$$

Note that the phase factor does not depend on p or E, so for any wave function that can be expanded in plane waves Eq. (2.167) would hold for each mode. We conclude that Eq. (2.167) describes a Galilei boost for any wave function.

☐ We have now established the action of the boost operator by finding the new wave function that a given wave function in the old frame is mapped to. However, we would still like to find a representation of this operator as an exponential of known Hermitian operators: The unitary operator

$$\mathbf{D}_{\vec{w}} = e^{\frac{i}{\hbar}\vec{\omega}\cdot\vec{\mathbf{K}}} \tag{2.168}$$

represents Galilei boosts by a velocity $\vec{w}$ on the Hilbert space $\mathcal{H}$ as given by (2.167). The operator

$$\boxed{\vec{\mathbf{K}} = m\vec{\mathbf{r}} - \vec{\mathbf{p}}t\,,} \tag{2.169}$$

where $\vec{\mathbf{r}}$ and $\vec{\mathbf{p}}$ are the usual position and momentum operators, is the (Hermitian) generator of boosts.

☐ The representation of $\mathcal{G}_+^\uparrow$ discussed here is projective, i.e. phases can appear upon concatenation of symmetry operators. Details will be discussed in the homework. We discuss representations of rotations and the complete set of commutation relations of the Galilei group in a later chapter.

2.8 The Schrödinger Equation with Electromagnetic Fields

☐ Recall that magnetic fields generally can not be described by a scalar potential energy. Rather they require a vector potential $\vec{A}(\vec{r},t)$. The physical fields $\vec{B}$ and $\vec{E}$ are related to $\vec{A}$ and the scalar potential Φ as

$$\vec{E} = -\nabla\Phi - \frac{\partial\vec{A}}{\partial t}\,, \quad \vec{B} = \nabla\times\vec{A}\,. \tag{2.170}$$

How can the vector potential be incorporated into the Schrödinger Equation?

☐ Recall: The Hamilton function for a classical particle of mass m and electric charge q subject to potentials $\Phi(\vec{r},t)$, $\vec{A}(\vec{r},t)$ is

$$H = \frac{1}{2m}\left(\vec{p}-q\vec{A}\right)^2 + q\Phi\,. \tag{2.171}$$

We find that the Schrödinger Equationwith electromagnetic potentials

$$\boxed{i\hbar\frac{\partial\psi}{\partial t} = \frac{1}{2m}\left(-i\hbar\nabla - q\vec{A}\right)^2\psi + q\Phi\psi} \tag{2.172}$$

reduces to the classical Hamilton-Jacobi equation with electromagnetic potential and the classical continuity equation in the limit $\hbar\to 0$. <u>Proof</u>: Analogous to the derivation in the case without a vector potential.

☐ In particular, the Hamilton operator with electromagnetic potentials corresponding to the classical Hamilton function is

$$\boxed{\mathbf{H} = \frac{1}{2m}\left(\vec{\mathbf{p}}-q\vec{A}\right)^2 + q\Phi\,.} \tag{2.173}$$

where $\vec{A}$ and Φ are now also operators (multiplicative in coordinate space representation).

☐ The important concept of gauge invariance also translates to quantum mechanics. Interestingly, it also involves the phase of the wave function. The Schrödinger Equationis invariant under simultaneous transformations

$$\vec{A} \mapsto \vec{A} + \nabla f \quad \Phi \mapsto \Phi - \frac{\partial \Phi}{\partial t}, \quad \psi \mapsto e^{\frac{i}{\hbar} q f} \psi, \tag{2.174}$$

of the potentials and the wave function. Here $f(\vec{r}, t)$ is an arbitary function. Proof: Homework

☐ The expectation value of the generalized velocity operator

$$\vec{\mathbf{v}} = \frac{1}{m} \left(\vec{\mathbf{p}} - q\vec{A} \right) \tag{2.175}$$

moves according to

$$m \frac{d \langle \vec{\mathbf{v}} \rangle}{dt} = \frac{q}{2} \left\langle \vec{\mathbf{v}} \times \vec{B} - \vec{B} \times \vec{\mathbf{v}} \right\rangle + q \langle \vec{E} \rangle \,. \tag{2.176}$$

2.9 The Virial Theorem

☐ For system with time-independent Hamilton operator $\mathbf{H}$ and position and momentum operators $\vec{\mathbf{r}}$ and $\vec{\mathbf{p}}$ we find the commutator

$$[\vec{\mathbf{r}} \cdot \vec{\mathbf{p}}, \mathbf{H}] = i\hbar \left(\mathbf{T} - \vec{\mathbf{r}} \cdot \nabla \mathbf{V} \right) = [\mathbf{H}, \vec{\mathbf{r}} \cdot \vec{\mathbf{p}}] \tag{2.177}$$

where $\mathbf{T}$ and $\mathbf{V}$ are the kinetic and potential energy operators of the system. Proof: Homework. We conclude that

$$\frac{d}{dt} \langle \vec{\mathbf{r}} \cdot \vec{\mathbf{p}} \rangle = 2\langle \mathbf{T} \rangle - \langle \vec{\mathbf{r}} \cdot \nabla \mathbf{V} \rangle = 2\langle \mathbf{T} \rangle + \langle \vec{\mathbf{r}} \cdot \nabla \mathbf{F} \rangle \,. \tag{2.178}$$

☐ We define the time average of a time-dependent quantity $A(t)$ as usual as

$$\overline{A} = \lim_{T \to \infty} \frac{1}{T} \int_0^T A(t) dt \,. \tag{2.179}$$

W call a quantum mechanical system bound if the average position and momentum are not exceeding upper bounds as functions of time, i.e. $|\langle \vec{\mathbf{r}} \rangle| < c_r$, $|\langle \vec{\mathbf{p}} \rangle| < c_p$ for all times where c_r and c_p are finite real numbers.

☐ Virial Theorem of Quantum Mechanics: For a bound system

$$\boxed{2\overline{\langle \mathbf{T} \rangle} = \overline{\langle \vec{\mathbf{r}} \cdot \nabla \mathbf{V} \rangle} \,.} \tag{2.180}$$

Thus the time averages of expectation values of kinetic and potential energy are related just as in classical mechanics. Recall that in the classical case directly $2\overline{T} = \overline{\vec{r} \cdot \nabla V}$ for the classical kinetic and potential energies T and V. Proof: The Virial Theorem follows immediately from

$$\overline{\frac{d}{dt} \langle \vec{\mathbf{r}} \cdot \vec{\mathbf{p}} \rangle} = 0 \tag{2.181}$$

which is true since the time average is taken of a total time derivative.

☐ For averages taken for stationary states a stronger version of the virial theorem holds. Since expectation values are independent of time we find

$$2\langle \mathbf{T} \rangle = \langle \vec{\mathbf{r}} \cdot \nabla \mathbf{V} \rangle \,. \tag{2.182}$$

2.10 Wigner Function Formalism