Chapter 4

Quantum Mechanics in $\mathcal{L}^2(\mathcal{R}^3)$

According to the considerations in Chapter 1, quantum mechanics is based on self-adjoint operators A, B, ..., which are associated with classical observables, and on Hilbert space vectors $|\psi\rangle, |\varphi\rangle$, ..., which characterize the state of an ensemble. The physical observables are given by the scalar products $\langle \psi \mid A \mid \psi \rangle, \langle \varphi \mid A \mid \varphi \rangle, \cdots$. A specific representation of the abstract vectors and states is given by matrices and column vectors, as shown in the previous chapter. Next we want to show that one can find multiplication and differential operators, as well as functions, such that the commutation relations as well as the algebraic structures are presented. We consider the so-called **coordinate space representation** (or **r-space representation**) of quantum mechanics.

4.1 Position and Momentum Operators

We consider square-integrable functions $\psi(\vec{x})$, depending on vectors $\vec{x} \in \mathbf{R}^3$:

$$\int d^3x \ \psi^*(\vec{x}) \ \psi(\vec{x}) = \int d^3x \ |\psi(\vec{x})|^2 \le \infty \ . \tag{4.1}$$

Together with the scalar product

$$\langle \varphi \mid \varphi \rangle = \int d^3x \ \varphi^*(\vec{x}) \ \psi(\vec{x}) \tag{4.2}$$

those functions are a Hilbert-space, $\mathcal{L}^2(\mathbf{R}^3)$.

The position and momentum operators

$$\vec{X} = \vec{e}_1 X_1 + \vec{e}_2 X_2 + \vec{e}_3 X_3 \tag{4.3}$$

and

$$\vec{P} = \vec{e}_1 P_1 + \vec{e}_2 P_2 + \vec{e}_3 P_3 \tag{4.4}$$

can be represented in $\mathcal{L}^2(\mathbf{R}^3)$ via

$$\vec{X}\psi(\vec{x}) = (\vec{e}_1 x_1 + \vec{e}_2 x_2 + \vec{e}_3 x_3) \psi(\vec{x}) \tag{4.5}$$

and

$$\vec{P} \ \psi(\vec{x}) = \left[\vec{e}_1 \ \frac{\hbar}{i} \frac{\partial}{\partial x_1} + \vec{e}_2 \ \frac{\hbar}{i} \frac{\partial}{\partial x_2} + \vec{e}_3 \ \frac{\hbar}{i} \frac{\partial}{\partial x_3} \right] \psi(\vec{x}) \tag{4.6}$$

i.e., via

$$\vec{X} \ \psi(\vec{x}) = \vec{x} \ \psi(\vec{x}) \tag{4.7}$$

$$\vec{P} \ \psi(\vec{x}) = \frac{\hbar}{i} \ \vec{\nabla}_x \ \psi(\vec{x}) \ . \tag{4.8}$$

With these representations, one has

$$[P_k, X_j] \psi(\vec{x}) = \left[\frac{\hbar}{i} \frac{\partial}{\partial x_k}, x_j\right] \psi(\vec{x})$$

$$= \frac{\hbar}{i} \delta_{kj} \psi(\vec{x}), \qquad (4.9)$$

i.e.,

$$[P_k, X_j] = \frac{\hbar}{i} \delta_{kj} \mathbf{1} \tag{4.10}$$

as previously required for the abstract vectors. The expectation values for the position and momentum operators are then given by

$$\langle \psi \mid \vec{X} \; \psi \rangle = \int d^3x \; \psi^*(\vec{x}) \; \vec{x} \; \psi(\vec{x}) = \int d^3x \; \vec{x} \; |\psi(\vec{x})|^2$$
 (4.11)

and

$$\langle \psi \mid \vec{P} \mid \psi \rangle = \int d^3x \ \psi^*(\vec{x}) \ \frac{\hbar}{i} \ \vec{\nabla} \ \psi(\vec{x})$$
 (4.12)

Hermiticity: From the above relations follows immediately

$$\langle \varphi \mid \vec{X} \psi \rangle = \int d^3x \ \varphi^*(\vec{x}) \ \vec{x} \ \psi(\vec{x}) = \int d^3x \ (\vec{x} \ \varphi(\vec{x} \))^* \ \psi(\vec{x})$$
 (4.13)

and

$$\langle \varphi \mid \vec{P} \; \psi \rangle = \int d^3x \; \varphi^*(\vec{x}) \; \frac{\hbar}{i} \; \vec{\nabla} \; \psi(\vec{x}) = \int d^3x \; \left(\frac{\hbar}{i} \; \vec{\nabla} \; \varphi(\vec{x})\right)^* \; \psi(\vec{x}) \; ,$$
 (4.14)

and thus:

$$\langle \varphi \mid \vec{X} \; \psi \rangle = \langle \vec{X} \; \varphi \mid \psi \rangle$$

$$\langle \varphi \mid \vec{P} \; \psi \rangle = \langle \vec{P} \; \varphi \mid \psi \rangle .$$
(4.15)

Thus, the in (4.7) and (4.8) defined multiplication and differential operators are hermitian, i.e.,

$$\vec{X}^{\dagger} = \vec{X}$$
 $\vec{P}^{\dagger} = \vec{P}$

$$(4.16)$$

on the common range of \vec{X} and \vec{X}^\dagger and \vec{P} and \vec{P}^\dagger , respectively. One can show that the ranges always coincide and thus \vec{X} and \vec{P} are self-adjoint operators.

4.2 Hamiltonian Operator

In $\mathcal{L}^2(\mathbf{R}^3)$ the Hamiltonian

$$H(\vec{P}, \vec{X}) = \frac{\vec{P}^2}{2m} + V(\vec{X}) \tag{4.17}$$

is given as

$$H\left(\frac{\hbar}{i} \vec{\nabla}, \vec{x}\right) = -\frac{\hbar^2}{2m} \Delta + V(\vec{x}) \tag{4.18}$$

with the Laplace-operator being defined as

$$\Delta = \vec{\nabla}^2 = \left(\sum_j \vec{e}_j \frac{\partial}{\partial x_j}\right) \cdot \left(\sum_k \vec{e}_k \frac{\partial}{\partial x_k}\right) = \sum_k \frac{\partial^2}{\partial x_k^2}. \tag{4.19}$$

If the potential is rotationally invariant, i.e.,

$$V = V(r) (4.20)$$

(with $r \equiv |\vec{x}|$), the eigenvalue equation for the energy takes the form

$$H\left(\frac{\hbar}{i} \vec{\nabla}, \vec{x}\right) \psi_{n\ell m}(\vec{x}) = E_{n\ell} \psi_{n\ell m}(\vec{x})$$
$$-\frac{\hbar^2}{2m} \Delta \psi_{n\ell m}(\vec{x}) + V(r) \psi_{n\ell m}(\vec{x}) = E_{n\ell} \psi_{n\ell m}(\vec{x}). \tag{4.21}$$

This is the time-independent Schrödinger equation for rotationally invariant problems.

4.3 Angular Momentum Operators in $\mathcal{L}^2(\mathbf{R}^3)$

The angular momentum operator (given in units of \hbar) (3.15)

$$\vec{L} = \frac{1}{\hbar} \vec{X} \times \vec{P} \tag{4.22}$$

takes in $\mathcal{L}^2(\mathbf{R}^3)$ the form

$$\vec{L} \left(\frac{1}{i} \vec{\nabla}, \vec{x} \right) = \vec{x} \times \frac{1}{i} \vec{\nabla} . \tag{4.23}$$

Its components are given by

$$L_1 = x_2 \frac{1}{i} \frac{\partial}{\partial x_3} - x_3 \frac{1}{i} \frac{\partial}{\partial x_2} \tag{4.24}$$

$$L_2 = x_3 \frac{1}{i} \frac{\partial}{\partial x_1} - x_1 \frac{1}{i} \frac{\partial}{\partial x_3} \tag{4.25}$$

$$L_3 = x_1 \frac{1}{i} \frac{\partial}{\partial x_2} - x_2 \frac{1}{i} \frac{\partial}{\partial x_1} \tag{4.26}$$

As in classical mechanics, spherical coordinates are especially suited for dealing with rotations in \mathbb{R}^3 . When choosing spherical coordinates as basis, the operators for the components of \vec{L} are given as

$$L_1 = i \left(\sin \varphi \frac{\partial}{\partial \theta} + \cot \theta \cos \varphi \frac{\partial}{\partial \varphi} \right)$$
 (4.27)

$$L_2 = i \left(-\cos\varphi \, \frac{\partial}{\partial\theta} + \cot\theta \sin\varphi \, \frac{\partial}{\partial\theta} \right) \tag{4.28}$$

and especially

$$L_3 = \frac{1}{i} \frac{\partial}{\partial \theta} \,. \tag{4.29}$$

From this follows

$$\vec{L}^{2} = -\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) - \frac{1}{\sin^{2} \theta} \frac{\partial^{2}}{\partial^{2} \varphi}. \tag{4.30}$$

It should be noted that the components of L_k and thus $\vec{L} = \sum_{k=1}^3 \vec{e_k} L_k$ depend only on the angles θ and φ and not on the radial coordinate r. This can be expected since \vec{L} is dimensionless. Using (4.29) and (4.30) one verifies that

$$[\vec{L}^{2}, L_{3}] = 0. (4.31)$$

Finally, one has the explicit representation for the ladder operators

$$L_{\pm} = \pm e^{\pm i\varphi} \left(\frac{\partial}{\partial \theta} \pm i \cot \theta \, \frac{\partial}{\partial \varphi} \right) \,. \tag{4.32}$$

Using the definitions, the relations (3.51) and (3.53) can be straightforwardly verified as

$$[L_3, L_{\pm}] = \pm L_{\pm} . ag{4.33}$$

4.4 Eigenfunctions of the Angular Momentum

The abstract eigenfunctions $|Y_{\ell m}\rangle$ fulfill the relation (3.67) and (3.68)

$$\vec{L}^{2} \mid Y_{\ell m} \rangle = \ell(\ell+1) \mid Y_{\ell m} \rangle \tag{4.34}$$

$$L_3 \mid Y_{\ell m} \rangle = m \mid Y_{\ell m} \rangle . \tag{4.35}$$

With (4.29) and (4.30), the same relation read for $\mathcal{L}^2(\mathbf{R}^3)$

$$\left(-\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} - \left(\sin \theta \frac{\partial}{\partial \theta}\right) - \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2}\right) \mathcal{Y}_{\ell m}(\theta, \varphi) = \ell(\ell+1) \mathcal{Y}_{\ell m}(\theta, \varphi)$$
(4.36)

$$\frac{1}{i} \frac{\partial}{\partial \varphi} \mathcal{Y}_{\ell m}(\theta, \varphi) = m \mathcal{Y}_{\ell m}(\theta, \varphi) . \tag{4.37}$$

The functions $\mathcal{Y}_{\ell m}(\theta, \varphi)$ defined through (4.36) and (4.37) are called **spherical harmonics**. They do not depend on the radial variable r, since (4.36) and (4.37) are partial

differential equations in θ and φ . If $\mathcal{Y}_{\ell m}(\theta, \varphi)$ is multiplied by a constant with respect to the differentiation with respect to θ and φ , i.e., in the most general case with a function $\phi_{n\ell}(r)$ depending only on r, then the resulting functions $\phi_{n\ell}(r)$ $\mathcal{Y}_{\ell m}(\theta, \varphi)$ are still solutions of (4.36) and (4.37). This is important for the following considerations.

The eigenvalue equation (4.37) can be solved immediately, and one obtains

$$\mathcal{Y}_{\ell m}(\theta, \varphi) = Y_{\ell m}(\theta) e^{im\varphi} . \tag{4.38}$$

From the general considerations in Section 3.7, we know that $|Y_{\ell m}\rangle$ can be obtained from $|Y_{\ell\ell}\rangle$ via (3.84), such that

$$\mathcal{Y}_{\ell m}(\theta,\varphi) = \frac{\sqrt{(\ell+m)!}}{\sqrt{(2\ell)!(\ell-m)!}} (L_{-})^{(\ell-m)} \mathcal{Y}_{\ell \ell}(\theta,\varphi) . \tag{4.39}$$

Here L_{-} is given as differential operator through (4.32). Therefore, it is sufficient to find the spherical harmonic corresponding to the general vector $|Y_{\ell\ell}\rangle$

$$\mathcal{Y}_{\ell\ell}(\theta,\varphi) = Y_{\ell\ell}(\theta) e^{i\ell\varphi} , \qquad (4.40)$$

and determine the function $\mathcal{Y}_{\ell m}(\theta, \varphi)$ by $(\ell - m)$ -fold application of L_- . One has the general relation (3.70)

$$L_{+} \mid \mathcal{Y}_{\ell\ell} \rangle = \mid 0 \rangle , \qquad (4.41)$$

and thus using (4.32)

$$e^{i\varphi} \left(\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \theta} \right) Y_{\ell\ell}(\theta) e^{i\ell\varphi} = 0,$$
 (4.42)

i.e.,

$$\left(\frac{\partial}{\partial \theta} - \ell \cot \theta\right) Y_{\ell\ell}(\theta) = 0. \tag{4.43}$$

The solution of (4.43) is given by

$$Y_{\ell\ell} = c_{\ell} \sin^{\ell} \theta , \qquad (4.44)$$

i.e., one has

$$Y_{\ell\ell}(\theta,\varphi) = c_{\ell} \sin^{\ell} \theta \ e^{i\ell\varphi} \ . \tag{4.45}$$

The constant c_{ℓ} is fixed through the normalization

$$\mathbf{1} = \langle Y_{\ell\ell} | Y_{\ell\ell} \rangle = \int_0^{2\pi} d\varphi \int_0^{\pi} \sin \theta \, d\theta \, | \, \mathcal{Y}_{\ell\ell}(\theta, \varphi) \, |^2
= 2\pi \, | \, c_{\ell} \, |^2 \int_{-1}^{-1} d\cos \theta \sin^{2\ell} \theta
= 2\pi \, | \, c_{\ell} \, |^2 \int_{-1}^{1} d\xi (1 - \xi^2)^{\ell}
= 2\pi \, | \, c_{\ell} \, |^2 \, 2 \, \frac{(2^{\ell} \ell!)^2}{(2\ell + 1)!} \, .$$
(4.46)

The normalization condition fixes the state up to a phase factor. If one chooses the phase factor according to the general convention, one obtains

$$\mathcal{Y}_{\ell\ell}(\theta,\varphi) = (-1)^{\ell} \frac{1}{2^{\ell}\ell!} \sqrt{\frac{(2\ell+1)!}{4\pi}} \sin^{\ell}\theta \ e^{i\ell\varphi} \ . \tag{4.47}$$

Application of $(L_{-})^{\ell-m}$ gives the spherical harmonics $\mathcal{Y}_{\ell m}(\theta,\varphi)$ according to (4.39). If one uses

$$(L_{-})^{\ell-m}e^{i\ell\varphi}\sin^{-\ell}\theta = \left\{-e^{-i\varphi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\,\frac{\partial}{\partial\varphi}\right)\right\}^{\ell-m}e^{i\ell\varphi}\sin^{\ell}\theta$$
$$= e^{em\varphi}\sin^{-m}\theta\,\left(\frac{d}{d\cos\theta}\right)^{\ell-m}\sin^{2\ell}\theta$$
(4.48)

then the spherical harmonics can be written in a particular simple form

$$\mathcal{Y}_{\ell m}(\theta,\varphi) = \frac{(-1)^{\ell}}{2^{\ell}\ell!} \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell+m)!}{(\ell-m)!}} e^{im\varphi} \sin^{-m}\theta \frac{d^{\ell-m}}{d\xi^{\ell-m}} (1-\xi^{2})^{\ell}$$
(4.49)

with $\xi = \cos \theta$. With this result our task to find an explicit representation of the abstract eigenvectors of \vec{L}^2 and L_3 in $\mathcal{L}^2(\mathbf{R}^3)$ is finished.

4.5 Special Cases

Here a special, very simple, but important application should be discussed; the case m = 0. This case is e.g., important in scattering problems. For m = 0, one has

$$\mathcal{Y}_{\ell 0}(\theta,\varphi) = \sqrt{\frac{2\ell+1}{4\pi}} \, \frac{(-1)^{\ell}}{2^{\ell}\ell!} \, \frac{d^{\ell}}{d\xi^{\ell}} \, (1-\xi^2)^{\ell}$$

$$= \sqrt{\frac{2\ell+1}{4\pi}} P_{\ell}(\xi) . \tag{4.50}$$

Here

$$P_{\ell}(\xi) = \frac{(-1)^{\ell}}{2^{\ell}\ell!} \frac{d^{\ell}}{d\xi^{\ell}} (1 - \xi^{2})^{\ell}$$
(4.51)

is the Legendre polynomial of degree ℓ in $\xi = \cos \theta$. Obviously the spherical harmonics are for m = 0 independent of φ .

For $\ell = 0$ one has

$$P_0(\xi) = 1 (4.52)$$

for all ξ , and thus

$$\mathcal{Y}_{00}(\theta,\varphi) = \frac{1}{\sqrt{4\pi}} \tag{4.53}$$

is not only independent of φ , but also of θ . The different values of the constant, 1 and $\frac{1}{\sqrt{4\pi}}$, result from the fact that $P_{\ell}(\xi)$ is fixed by choosing the value for $\xi = 1$,

$$P_{\ell}(\xi = 1) = 1 , \qquad (4.54)$$

whereas the normalization of $Y_{\ell m}(\theta, \varphi)$ is given by

$$\langle Y_{\ell m} \mid Y_{\ell m} \rangle = \int d\cos\theta \, d\varphi \mid \mathcal{Y}_{\ell m}(\theta, \varphi) \mid^2 = 1.$$
 (4.55)

This gives the general relation (4.52) and especially for \mathcal{Y}_{00} :

$$|\mathcal{Y}_{00}|^2 4\pi = 1$$
 (4.56)

corresponding to (4.53). This difference in fixing the normalization constant (either through fixing the value of the function at $\theta = 0$ or through the integral of the absolute square of the function) leads to different constants, which is in principal trivial, but extremely important in applications.

Legendre Functions: The Legendre polynomials P_{ℓ} are defined via (4.51). The connection to the spherical harmonics is given for m = 0 in (4.50). Using the P_{ℓ} , one defines the "associated Legendre functions" via

$$P_{\ell}^{m}(\xi) = (1 - \xi^{2})^{m/2} \frac{d^{m} P_{\ell}(\xi)}{d\xi^{m}}. \tag{4.57}$$

The associated Legendre functions allow the representation of the $\mathcal{Y}_{\ell m}(\theta,\varphi)$ via

$$\mathcal{Y}_{\ell m}(\theta,\varphi) = (-1)^m \sqrt{\frac{2\ell+1}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} e^{im\varphi} P_{\ell}^m(\cos\theta) . \tag{4.58}$$

Details can be looked up in Edmonds: Angular Momentum in Quantum Mechanics, a text which is very useful for working with angular momentum. It should be noted that the spatial distribution of the probability with respect to the angles θ and φ is given through $|\mathcal{Y}_{\ell m}(\theta,\varphi)|^2$. Obviously, the φ -dependence vanishes when taking the absolute value of the square. For $\ell = 0$, there is in addition no θ -dependence. For a graphical representation of the $\mathcal{Y}_{\ell m}(\theta,\varphi)$, see the corresponding section of the CUPS program package on quantum mechanics.

4.6 Bound State Problem for Rotational Symmetric Potentials

As demonstrated in Section 3.11, the Hamiltonian

$$H = \frac{\vec{P}^{\ 2}}{2m} + V \tag{4.59}$$

can be written as

$$H = \frac{P_r^2}{2m} + \frac{\hbar^2 \vec{L}^2}{2m |\vec{X}|^2} + V \tag{4.60}$$

with

$$P_r^2 = \frac{1}{\vec{X}^2} \left\{ (\vec{X} \cdot \vec{P})^2 - \hbar i \vec{X} \cdot \vec{P} \right\} . \tag{4.61}$$

In the coordinate representation, one has

$$\vec{X} \cdot \vec{P} = \frac{\hbar}{i} \vec{x} \cdot \vec{\nabla} = \frac{\hbar}{i} r \frac{\partial}{\partial r}$$
 (4.62)

and thus

$$P_r^2 = -\hbar^2 \frac{1}{r^2} \left[r \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + r \frac{\partial}{\partial r} \right]$$
$$= -\hbar^2 \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} . \tag{4.63}$$

One can show immediately that the square of

$$P_r = \frac{\hbar}{i} \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \tag{4.64}$$

gives the expression (4.63).

For rotationally invariant potentials $V=V(|\vec{X}|)$, the Hamiltonian takes the following form in coordinate space:

$$H = -\frac{\hbar^2}{2m} \frac{1}{r^2} r^2 \frac{\partial}{\partial r} + \frac{\hbar^2 \vec{L}^2}{2mr^2} + V(r) . \tag{4.65}$$

As shown in Chapter 3, one can choose a set of simultaneous eigenvectors to H, \vec{L}^2 , and L_3 , namely

$$H\psi_{n\ell m} = E_{n\ell} \psi_{n\ell m}$$

$$\vec{L}^{2}\psi_{n\ell m} = \ell(\ell+1)\psi_{n\ell m}$$

$$L_{3}\psi_{n\ell m} = m \psi_{n\ell m}$$

$$(4.66)$$

Using (4.65) one obtained the eigenvalue equation for the energy in coordinate space

$$\left\{ -\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r) \right\} \psi_{n\ell m}(r,\theta,\varphi) = E_{n\ell} \psi_{n\ell m}(r,\theta,\varphi) , (4.67)$$

which is called the **radial Schrödinger equation**. The solutions of this equation are fixed up to constants with respect to differentiation with respect to r, i.e., up to functions of θ and φ . Therefore, the solutions are of the form

$$\psi_{n\ell m}(r,\theta,\varphi) = \psi_{n\ell}(r) c_{n\ell m}(\theta,\varphi) . \tag{4.68}$$

On the other hand, the solutions with respect to the angular momentum eigenvalue equations are given by the spherical harmonics. Thus, the general solution of the eigenvalue equations (4.66) is of the form

$$\psi_{n\ell m}(r,\theta,\varphi) = \phi_{n\ell}(r) \mathcal{Y}_{\ell m}(\theta,\varphi)m. \qquad (4.69)$$

A remaining constant, independent of r, θ and φ , is fixed up to phase factor through the normalization of $\psi_{n\ell m}(r, \theta, \varphi)$. Since the normalization of $\mathcal{Y}_{\ell m}(\theta, \varphi)$ is already fixed, it follows for $\phi_{n\ell}(r)$

$$\int r^{2} dr d\cos\theta d\varphi | \psi_{n\ell m}(r,\theta,\varphi) |^{2}$$

$$= \int r^{2} dr | \phi_{n\ell}(r) |^{2} \int d\cos\theta d\varphi | \mathcal{Y}_{\ell m}(\theta,\varphi) |^{2} = 1.$$
(4.70)

If one chooses $\phi_{n\ell}$ real (and positive)

$$\int r^2 dr \, \phi_{n\ell}^2(r) = 1 . \tag{4.71}$$

When inserting (4.69) into (4.67), one can omit the spherical harmonics $\mathcal{Y}_{\ell m}(\theta, \varphi)$, since they are constants for a differentiation with respect to r. Thus one obtains the ordinary differential equation

$$\left[-\frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} \phi_{n\ell}(r) + \frac{\hbar^2 \ell(\ell+1)}{2mr^2} + V(r) \right] \phi_{n\ell}(r) = E_{n\ell} \phi_{n\ell}(r) . \quad (4.72)$$

With

$$\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d\phi}{dr} = \frac{1}{r} \frac{d^2}{dr^2} (r\phi)$$
 (4.73)

this leads to

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}(r\phi_{n\ell}) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}\phi_{n\ell}(r) + V(r)\phi_{n\ell}(r) = E_{n\ell}\phi_{n\ell}(r)$$
(4.74)

which is the usual radial Schrödinger equation. If one multiplies this equation with r, one obtains in all terms the function

$$u_{n\ell}(r) = r\phi_{n\ell}(r) . (4.75)$$

With this the radial Schrödinger equation takes the simple form

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u_{n\ell}(r) + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2}u_{n\ell}(r) + V(r)u_{n\ell}(r) = E_{n\ell}u_{n\ell}(r), \qquad (4.76)$$

and the normalization condition (4.71) becomes

$$\int dr \ u_{n\ell}^2(r) = 1 \ . \tag{4.77}$$

4.7 Solution of the Radial Schrödinger Equation

If one considers (4.74) as differential equation, then this equation has in principle solution for all values $E_{n\ell}$. However, (4.74) was derived from the eigenvalue problem (4.66) in the Hilbert space, here $\mathcal{L}^2(\mathbf{R}^3)$. We are looking, therefore, for solutions which fulfill the normalization condition (4.77). Since eigenvectors to different eigenvalues are orthogonal, but on the other hand because of the separability of $\mathcal{L}^2(\mathbf{R}^3)$ only countable orthonormal systems occur, the spectrum of eigenvalues in (4.74) for normalizable solutions can only have a countable amount of eigenvalues $E_{n\ell}$. One has to take into account that the normalization requirement restricts the solutions in two ways, namely with respect to the behavior of the functions at r = 0 and at $r \to \infty$.

Case r=0: The equation (4.76) is a second-order linear differential equation and thus has two linearly independent solutions for each $E_{n\ell}$. On the other hand, a general theorem about spectral decomposition of self-adjoint operator in a Hilbert space guarantees the uniqueness of the normalizable solutions $\psi_{n\ell m}$ (if there is no further degeneracy). One may expect, therefore, that the normalization condition excludes one of the linear independent solutions. Let us consider the behavior of (4.76) at the origin. In the following we assume that V(r) for $r \to 0$ becomes singular weaker than $\frac{1}{r^2}$, i.e., weaker than the centrifugal term. In the vicinity of the origin one can approximate (4.76) by

$$-\frac{d^2u_{\ell}}{dr^2} + \frac{\ell(\ell+1)}{r^2} u_{\ell} \stackrel{r\to 0}{\sim} 0.$$
 (4.78)

Two linearly independent solutions of this asymptotic equation are given by $r^{\ell+1}$ and $r^{-\ell}$. The latter has to be excluded, at least for $\ell \neq 0$ since

$$\int_0^\varepsilon dr \ u_\ell^2(r) \sim \int_0^\varepsilon \frac{1}{r^{-2\ell}} dr = \infty . \tag{4.79}$$

For $\ell = 0$ there is none such restriction since both solutions are square integrable at the origin. For the wave function, however, the solution $u_{n\ell} \sim r^{-\ell}$ would lead because of (4.75) to

$$\psi_{n00}(\vec{x}) \stackrel{r \to 0}{\sim} \frac{1}{r} . \tag{4.80}$$

The application of the Laplace operator in $\vec{P}^2=-\hbar^2\Delta$ onto this function would then because of

$$\Delta \frac{1}{r} = -4\pi \delta(\vec{x}) \tag{4.81}$$

lead to an additional δ -function in the three-dimensional Schrödinger equation, which cannot be compensated by any other term. Therefore, we allow for **all** ℓ only the so-called **regular solution** with

$$u_{\ell}(r) \stackrel{r \to 0}{\sim} r^{\ell+1}$$
 (4.82)

This, in turn, means that the eigenfunctions $u_{n\ell}(r)$ for each $E_{n\ell}$ are **uniquely** fixed through the requirement (4.82) at the origin.

Case $r \to \infty$: Through the considerations about the behavior of $u_{n\ell}(r)$ at the origin, one has for each $E_{n\ell}$ a unique solution of (4.76). Now we only have to determine those values of $E_{n\ell}$ for which the corresponding $u_{n\ell}^2$ stays finite when integrating over the **entire** space. In order to do this, we have to consider the behavior of the solution for $r \to \infty$. We assume that for large r the potential V(r) falls of at least like the Coulomb potential. We also consider that the centrifugal term $-\frac{\hbar^2}{2m} \frac{\ell(\ell+1)}{r^2}$ because negligible for large r. Thus for arbitrary E we have the asymptotic equation

$$-\frac{\hbar^2}{2m}\frac{d^2u_\ell}{dr^2} - Eu_\ell \stackrel{r\to\infty}{\sim} 0. \tag{4.83}$$

If $E \leq 0$, then two linearly independent solutions are given by

$$u_{\ell}(r) \sim_{r \to \infty} e^{\pm i\sqrt{\frac{2m}{\hbar^2}E}} r , \qquad (4.84)$$

which do not disappear for $r \to \infty$ and thus are not square integrable.

For E < 0, one has in general a superposition of the form

$$u_{\ell}(r) \sim_{r \to \infty} a(E)e^{-\sqrt{\frac{2m}{\hbar^2}|E|}} r + b(E) e^{\sqrt{\frac{2m}{\hbar^2}|E|}} r.$$
 (4.85)

Since the solution is already fixed up to a constant through the behavior at r=0, it cannot be avoided in general that the non-square integrable term $e^{\sqrt{\frac{2m}{\hbar^2}|E|}}$ appears, unless for specific energies there is

$$b(E_{n\ell}) = 0. (4.86)$$

Then only the square integrable term

$$u_{n\ell}(r) \stackrel{r \to \infty}{\sim} a(E_{n\ell}) e^{-\sqrt{\frac{2m}{\hbar^2} |E_{n\ell}|}} r$$
 (4.87)

remains. The values $E_{n\ell}$, for which the condition (4.86) occurs, are obviously the energy eigenvalues of (4.76).

Remark: Strictly speaking, the above conditions are not 100% conclusive since the asymptotic behavior of the solution of correct equation (4.76) does not have to be the same as the solution of the asymptotic equation (4.85). For a true proof one has to either give the solution explicitly (like the Coulomb problem) or represent the equation in a suitable form, e.g., as integral equation, and then study the asymptotic behavior of the solution.

4.8 Solution of the Radial Schrödinger Equation for the Hydrogen Atom

The potential energy of the hydrogen atom is given as

$$V(r) = -\frac{e^2}{r} \,. {4.88}$$

The radial Schrödinger equation takes then the form

$$\left[\frac{d^2}{dr^2} - \frac{\ell(\ell+1)}{r^2} + \frac{2m}{\hbar^2} \frac{e^2}{r} + \frac{2m}{\hbar^2} E_{n\ell} \right] u_{n\ell}(r) = 0.$$
 (4.89)

By convention, one relates the variable r as well as the energy $E_{n\ell}$ to 'atomic units,' i.e., defines

$$r_1 = \frac{\hbar^2}{me^2} = 0.529 \cdot 10^{-8} \ cm \ (\equiv \text{ first Bohr orbit})$$
 (4.90)

and

$$E_1 = -\frac{me^4}{2\hbar^2} = 13.53 \ eV \ (\equiv \text{ energy of lowest level in the hydrogen spectrum}) \ . (4.91)$$

These are characteristic units of magnitudes valid for atomic systems. In addition, heuristic considerations based on the Bohr model for the atom are particularly simple. With

$$\xi = \frac{r}{r_1} = \frac{r}{\hbar^2 m e^2} \tag{4.92}$$

and

$$-\lambda_{n\ell} = r^2 \frac{2m}{\hbar^2} E_{n\ell} = \frac{E_{n\ell}}{|E_1|} = \frac{2\hbar^2}{me^4} E_{n\ell}$$
 (4.93)

equation (4.89) takes the form

$$\left(\frac{d^2}{d\xi^2} - \frac{\ell(\ell+1)}{\xi^2} + \frac{2}{\xi} - \lambda_{n\ell}\right) u_{n\ell}(r_1\xi) = 0.$$
 (4.94)

The asymptotic behavior of $u_{n\ell}(r)$ for $r \to \infty$, as discussed in the previous section, suggest that the ansatz

$$u_{n\ell}(r) = u_{n\ell}(r_1\xi) = h_{n\ell}(\xi) e^{-\sqrt{\lambda_{n\ell}} \xi}$$
 (4.95)

for a square integrable solution of (4.94). Substituting (4.95) into (4.94) gives

$$h_{n\ell}'' - 2\sqrt{\lambda_{n\ell}} h_{n\ell}' - \frac{\ell(\ell+1)}{\xi^2} h_{n\ell} + \frac{2}{\xi} h_{n\ell} = 0.$$
 (4.96)

This is an ordinary differential equation with non-constant coefficients, which depend on the variable ξ in an **analytic** fashion. We make the ansatz as polynomial

$$h_{n\ell}(\xi) = \xi^{\ell+1} \sum_{\nu=0}^{\infty} a_{\nu} \xi^{\nu} .$$
 (4.97)

Here the factor $\xi^{\ell+1}$ has been taken out to account for the considerations in the previous chapter about the behavior of the solution at r=0. Taking the factor out guarantees that the series starts with order $\chi_{\ell+1}$. Inserting (4.97) into (4.96) leads to

$$\sum_{v=0}^{\infty} \quad [(\ell+\nu+1)(\ell+\nu) \, \xi^{\ell+\nu-1} - 2\sqrt{\lambda_{n\ell}} \, (\ell+\nu+1) \, \xi^{\ell+\nu} - \ell(\ell+1) \, \xi^{\ell+\nu-1}$$

$$+ 2\xi^{\ell+\nu}] \, a_v = 0 \, . \tag{4.98}$$

Renaming the summation indices in such a way that all terms create the same order in ξ (i.e., replacing in the first and third term ν by $\nu + 1$) gives

$$\sum_{\nu=0}^{\infty} \left[(\ell + \nu + 2)(\ell + \nu + 1) - \ell(\ell + 1) \right] \xi^{\ell+\nu} a_{\nu+1} = \sum_{\nu=0}^{\infty} \left[2\sqrt{\lambda_{n\ell}} (\ell + \nu + 1) \right] \xi^{\ell+\nu} a_{\nu} (4.99)$$

A comparison of the coefficients leads to the recursion relation for the constants in (4.97)

$$a_{\nu+1} = \frac{2\sqrt{\lambda_{n\ell}}(\ell+1+\nu) - 2}{(\ell+2+\nu)(\ell+1+\nu) - \ell(\ell+1)} a_{\nu} . \tag{4.100}$$

If one calculates the coefficient a_{ν} according to (4.100), then (4.97) is a solution to (4.96). However, the solution $u_{n\ell}$ found by the ansatz (4.97) is then and only then square integrable, if the summation in (4.97) is finite. Again, this can only happen for specific values of $\lambda_{n\ell}$, namely if for $\nu - n_r$ holds

$$2\sqrt{\lambda_{n\ell}} \ (\ell+1+n_r) - 2 = 0 \ . \tag{4.101}$$

With this solution, $\lambda_{n\ell}$ and thus $E_{n\ell}$ is fixed. One has

$$\lambda_{n\ell} = \frac{1}{(\ell + 1 + n_r)^2} \tag{4.102}$$

or with (4.93)

$$E_n = -\frac{me^4}{2\hbar^2} \frac{1}{(\ell+1+n_r)^2} . (4.103)$$

Here the energy eigenvalues are not characterized as $E_{n\ell}$, since different combinations of ℓ and n_r can lead to the same energy

$$E_n = -\frac{me^4}{2\hbar^2} \frac{1}{n^2} (4.104)$$

as long as

$$n = \ell + 1 + n_r . (4.105)$$

Since the 'radial quantum number' (historical term) represents a special value of the index ν , i.e., can be $0, 1, 2, \cdots$ the value of ℓ is restricted via

$$0 \le \ell \le n - 1. \tag{4.106}$$

This result shows that the Coulomb problem has a special place among the bound state problems with rotationally invariant potentials. According to (4.106) states with different values of ℓ can lead to the same energy E_n . Since to each ℓ one has the $(2\ell + 1)$ -fold m-degeneracy, which is valid for **all** rotational invariant problems, this additional ℓ -degeneracy leads to a degeneracy of

$$\sum_{\ell=0}^{n-1} (2\ell+1) = n^2. (4.107)$$

We have already understood the underlying reason for this high degeneracy as consequence of the special dynamic symmetry of the Coulomb problem.

4.9 The Radial Solution

From (4.95) and (4.97) follows with (4.102), i.e., with $\lambda_{n\ell} = \frac{1}{n^2}$ for the solution of the radial Schrödinger equation for the hydrogen atom

$$u_{n\ell}(r) = e^{-\frac{r}{nr_1}} \left(\frac{r}{r_1}\right)^{\ell+1} \sum_{n=0}^{\infty} a_{\nu}^{(n,\ell)} \left(\frac{r}{r_1}\right)^{\nu} .$$
 (4.108)

The coefficients $a_{\nu}^{(n,\ell)}$ are given through the recursion relation (4.100) which reads with (4.102)

$$a_{\nu+1}^{(n,\ell)} = 2 \frac{\frac{1}{n} (\ell+1+\nu) - 1}{(\ell+2+\nu)(\ell+1+\nu) - \ell(\ell+1)} a_{\nu}^{(n,\ell)}. \tag{4.109}$$

Especially simple is the behavior of $u_{n\ell}(r)$ for the maximum ℓ . According to (4.106) the maximum value of ℓ is n-1, i.e., we have to consider $u_{n,n-1}(r)$. Here applying (4.109) shows that already

$$a_1^{(n,n-1)} = 2 \frac{\frac{1}{n} n - 1}{(n+1)n - (n-1)n} a_0^{(n,n-1)} = 0.$$
 (4.110)

Thus for $\ell = n - 1$ the solution of the radial Schrödinger equation is given by

$$u_{n,n-1}(r) = e^{-\frac{1}{n} \frac{r}{r_1}} \left(\frac{r}{r_1}\right)^2 a_0^{(n,n-1)}. \tag{4.111}$$

With the normalization condition (4.77), this result is completely fixed up to a phase factor. For r = 0 the function $u_{n,n-1}(r = 0)$ is zero, as it has be to according to the considerations in the previous section. The function has a maximum, which is determined from

$$\frac{d}{dr} u_{n,n-1}(r) = \left[-\frac{1}{nr_1} + \left(\frac{u}{r_1}\right) \left(\frac{r}{r_1}\right)^{-1} \right] e^{-\frac{1}{n} \frac{r}{r_1}} \left(\frac{r}{r_1}\right)^n a_0^{(n,n-1)} = 0 \qquad (4.112)$$

to be

$$r_n = n^2 r_1 . (4.113)$$

Thus the maximum of $u_{n,n-1}(r)$ is located at the radius of the *n*-th Bohr-orbit. One can understand this result that one obtains for the maximum allowed ℓ , a result resembling the Bohr-orbits, by the following plausibility argument. In the classical case, one has

$$E = \frac{m}{2} \dot{r}^2 + \frac{\ell^2}{2mr^2} + V(r) \tag{4.114}$$

from which follows that for a fixed energy the angular momentum is maximized for $\dot{r} = 0$, which is the case for circular orbits.

Small Angular Momenta:

As example, let us consider

$$u_{2,0} = \frac{1}{\sqrt{2r_1}} e^{-\frac{r}{2r_1}} \left[\frac{r}{r_1} - \frac{1}{2} \left(\frac{r}{r_1} \right)^2 \right] . \tag{4.115}$$

This function has two maxima, one (the larger one) at $r=5.24~r_1$ and another at $r=0.76~r_1$. There is a finite probability to find the electron even at small distances r. This is in agreement with the fact that for small ℓ the repulsive centrifugal term $\ell(\ell+1)/2mr^2$ is small.

In general, the function $u_{n,n-1}(r)$ has a maximum at the value of the corresponding 'Bohr-radius,' $r_n = n^2 r_1$, whereas $u_{n,n-k}(r)$ has K maxima, consistent with the fact that the polynomial expansion on which $u_{n,n-k}(r)$ is based has k terms. Thus, only for the maximum value ℓ one has the simple picture, where the wave function has a probability distribution resembling a "Bohr-orbit." A visualization of the different radial wave functions, the $\mathcal{Y}_{\ell m}(\theta, \varphi)$ and the probability distribution of the total wave function can be made with the CUPS program in the volume Quantum Mechanics.

Spectroscopic Notation:

The quantization of the energy levels if the bound state problem causes because of $E_n - E_m = \hbar w_{nm}$ a discrete frequency spectrum for the transition of electrons between the different levels. Without understanding the underlying physics, there were very early attempts to organize the spectra. From this period the notation of the different levels originates and has never been changed. One calls states with $\ell = 0, 1, 2, 3, 4, 5$ S, P, D, F, G, H-states. The pairs (n, ℓ) of quantum numbers originating from the $0 \le \ell \le n-1$ possibilities for ℓ are often characterized according to the following scheme:

4.10 Laguerre Polynomials

With (4.69) and (4.75), one has for the total wave function of the hydrogen atom

$$\psi_{n\ell m}(r,\theta,\varphi) = \frac{u_{n\ell}(r)}{r} \mathcal{Y}_{\ell m}(\theta,\varphi) . \tag{4.116}$$

For the Coulomb problem, this solution is explicitly given in form of the power series (4.108), where the coefficients are given by (4.109). Only the first coefficient $a_0^{(n,\ell)}$ can be chosen arbitrarily. It is, however, restricted through the normalization condition (4.77). Only a phase factor remains undetermined.

The power series can be brought into closed form. Without proof, the result is given as

$$\psi_{n\ell m}(r,\theta,\varphi) = \sqrt{\frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} \sqrt[3]{\frac{2}{nr_1}} e^{-\frac{r}{nr_1}} \times \left(\frac{2r}{nr_1}\right) L_{n+1}^{(2\ell+1)} \left(\frac{2r}{nr_1}\right) \mathcal{Y}_{\ell m}(\theta,\varphi) .$$

$$(4.117)$$

Here

$$L_{n+1}^{(2\ell+1)}(\xi) = \frac{d^{2\ell+1}}{d\xi^{2\ell+1}} L_{n\ell}(\xi)$$
 (4.118)

is the $(2\ell+1)$ -th derivative of the Laguerre polynomial, which is defined via

$$L_k(\xi) = e^{\xi} \frac{d^k}{d\xi^k} (\xi^k e^{-\xi}) . {(4.119)}$$

See, e.g., Section 13.2 (Laguerre Functions) in *Mathematical Methods for Physicists* by G.B. Arfken and H.J. Weber.

4.11 Ionized Atoms with One Electron

An atom with a nuclear charge Z has in its neutron stage Z electrons. If one strips all electrons but one, i.e., ionizes the atom (Z-1) fold, then one has again a problem of the kind treated in Sections 4.8 and 4.9. However, in (4.88) e^2 has to be replaced by Ze^2 , and instead of (4.103) one obtains for the energy eigenvalues

$$E_n(z) = -\frac{mZ^2e^4}{2\hbar^2} \frac{1}{n^2} . (4.120)$$

Furthermore, the radius of the lowest Bohr-orbit is given by

$$r_1(Z) = \frac{\hbar^2}{mZe^2} = \frac{r_1}{Z},$$
 (4.121)

i.e., the lowest Bohr-orbit is reduced by $\frac{1}{Z}$ compared to the hydrogen atom. Correspondingly, the wave functions are given as

$$\psi_{n\ell m}(r,\theta,\varphi) = \sqrt{\frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} \sqrt[3]{\frac{2Z}{rn_1}} e^{-\frac{rZ}{rn_1}} \times \left(\frac{2Zr}{nr_1}\right)^{\ell} L_{n+1}^{(2\ell+1)} \left(\frac{2Zr}{nr_1}\right) \mathcal{Y}_{\ell m}(\theta,\varphi) . \tag{4.122}$$

As an aside, the maximum of $\psi_{n,n-1,m}$ is located at

$$r_{n,Z} = n^2 \frac{r_1}{Z} = \frac{r_n}{Z},$$
 (4.123)

which corresponds to the radius of the Bohr-orbit.

4.12 More General: Eigenvectors of the Position Operators in \mathbb{R}^3

In (4.1) the components of the vector operators

$$\vec{X} = \sum_{j=1}^{3} \vec{e}_{j} X_{j} \tag{4.124}$$

and

$$\vec{P} = \sum_{j=1}^{3} \vec{e_j} P_j \tag{4.125}$$

were introduced with the commutation relations

$$[X_j, X_k] = 0$$

$$[P_j, P_k] = 0$$

$$[P_j, X_k] = \frac{\hbar}{i} \delta_{jk} \mathbf{1} .$$

$$(4.126)$$

Since the operators X_1, X_2 and X_3 commute, one can expect that according to the theorem (3.27) there are simultaneous eigenvectors $|\varphi_{x_1,x_2,x_3}\rangle$ of these operators with

$$X_{1} \mid \varphi_{x_{1},x_{2},x_{3}} \rangle = x_{1} \mid \varphi_{x_{1},x_{2},x_{3}} \rangle$$

$$X_{2} \mid \varphi_{x_{1},x_{2},x_{3}} \rangle = x_{2} \mid \varphi_{x_{1},x_{2},x_{3}} \rangle$$

$$X_{3} \mid \varphi_{x_{1},x_{2},x_{3}} \rangle = x_{3} \mid \varphi_{x_{1},x_{2},x_{3}} \rangle.$$

$$(4.127)$$

Multiplying these equations with \vec{e}_1 , \vec{e}_2 and \vec{e}_3 , respectively, and adding all equations gives

$$(\vec{e}_1 X_1 + \vec{e}_2 X_2 + \vec{e}_3 X_3) \mid \varphi_{x_1, x_2, x_3} \rangle = (\vec{e}_1 X_1 + \vec{e}_2 X_2 + \vec{e}_3 X_3) \mid \varphi_{x_1, x_2, x_3} \rangle$$
(4.128)

and

$$\vec{X} \mid \varphi_{\vec{x}} \rangle = \vec{x} \mid \varphi_{\vec{x}} \rangle. \tag{4.129}$$

Let us consider the operator

$$e^{-\frac{i}{\hbar} a_{i} P_{i}} = 1 + \left(-\frac{i}{\hbar}\right) a_{i} P_{i} + \frac{1}{2!} \left(-\frac{i}{\hbar}\right)^{2} (a_{i} P_{i})^{2} + \cdots$$

$$= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^{n} (a_{i} P_{i})^{n}.$$
(4.130)

From the commutation relations (4.127) follows

$$[P_i^n, X_i] = \frac{\hbar}{i} n P_i^{n-1} = \frac{\hbar}{i} \frac{d}{dP_i} P_i^n, \qquad (4.131)$$

i.e., the commutator with X_i acts (with the factor $\frac{\hbar}{i}$) like a differentiation with respect to P_i . Thus one obtains

$$\left[e^{-\frac{i}{\hbar} \ a_i P_i}, X_i\right] = \frac{\hbar}{i} \frac{d}{dP} e^{-\frac{i}{\hbar} \ a_i P_i} = -a_i e^{-\frac{i}{\hbar} \ a_i P_i}. \tag{4.132}$$

As proof one only has to explicitly apply (4.130)

$$\begin{aligned}
\left[e^{-\frac{i}{\hbar} a_{i} P_{i}}, X_{i}\right] &= \sum_{n=0}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar}\right)^{n} \left[(a_{i} P_{i})^{n}, X_{i}\right] \\
&= \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left(-1\right) \left(-\frac{i}{\hbar}\right)^{n-1} a_{i}^{n} P_{i}^{n-1} \\
&= -a_{i} e^{-\frac{i}{\hbar} a_{i} P_{i}} .
\end{aligned} \tag{4.133}$$

Thus for a specific component, one has

$$e^{-\frac{i}{\hbar} a_i P_i} X_i \mid \varphi_{x_1} \rangle = x_i e^{-\frac{i}{\hbar} a_i P_i} \mid \varphi_{x_1} \rangle \tag{4.134}$$

or with (4.132)

$$(X_i - a_i \mathbf{1}) e^{-\frac{i}{\hbar} a_i P_i} | \varphi_{x_i} \rangle = x_i e^{-\frac{i}{\hbar} a_i P_i} | \varphi_{x_i} \rangle$$
 (4.135)

and thus

$$X_i e^{-\frac{i}{\hbar} a_i P_i} | \varphi_{x_i} \rangle = (x_i + a_i) e^{-\frac{i}{\hbar} a_i P_i} | \varphi_{x_i} \rangle. \tag{4.136}$$

This result derived for one specific component i generalizes immediately to

$$\vec{X} e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{P}} | \varphi_{\vec{x}} \rangle = (\vec{x} + \vec{a}) e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{P}} | \varphi_{\vec{x}} \rangle. \tag{4.137}$$

Starting from (4.132) and generalizing to three components, one obtains

$$e^{\frac{i}{\hbar} \ \vec{a} \cdot \vec{P}} \ \vec{X} \ e^{-\frac{i}{\hbar} \ \vec{a} \cdot \vec{P}} = \vec{X} + \vec{a} \ \mathbf{1}$$
 (4.138)

where \vec{a} is an **arbitrary** vector $\in \mathbb{R}^3$. Applying (4.138) on $|\varphi_{\vec{x}}\rangle$ yields

$$\vec{X} e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{P}} | \varphi_{\vec{x}} \rangle = (\vec{x} + \vec{a}) e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{P}} | \varphi_{\vec{x}} \rangle. \tag{4.139}$$

If $|\varphi_{\vec{x}}\rangle$ is an eigenvector of $\vec{X} |\varphi_{\vec{x}}\rangle = \vec{x} |\varphi_{\vec{x}}\rangle$, i.e., to the eigenvalue \vec{x}_1 , then $e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{P}} |\varphi_{\vec{x}}\rangle$ is also eigenvector to the \vec{X} operator, but with eigenvalue $(\vec{x} + \vec{a})$, i.e., one has

$$e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{P}} \mid \varphi_{\vec{x}} \rangle = \mid \varphi_{\vec{x} + \vec{a}} \rangle . \tag{4.140}$$

This means \vec{X} can take all possible values, and its components obey

$$-\infty \le x_i \le \infty . \tag{4.141}$$

This means, in particular, that each eigenvalue x_1, x_2 and x_3 in (4.127) has an infinite degeneracy. If x_1 is fixed, e.g., then one has infinitely many choices of fixing x_2 and x_3 in order to characterize the state $|\varphi_{x_1,x_2,x_3}\rangle$.

In Section 1.7 we have shown that due to the uncertainty principle

$$(\Delta X)_{\psi} \neq 0 , \qquad (4.142)$$

which means that eigenvectors to X can **not** exist.

Remark: The characteristic property of finite dimensional hermitian matrices consists of the fact that they have complete system of eigenvectors. In infinite dimensional spaces, this is normally not fulfilled (exception: harmonic oscillator). The position operator illustrates this clearly. \vec{X} is a self-adjoint operator in an infinite dimensional space for which **no** eigenvectors exist.

This means there is **no** vector $|\varphi_{\vec{x}}\rangle$, which is element of the Hilbert space (i.e., has a finite norm) and which fulfills $\vec{X} | \varphi_{\vec{x}'}\rangle = \vec{x}' | \varphi_{\vec{x}'}\rangle$. The question is if the eigenvalue equation can be fulfilled if one does not require that $|\varphi_{\vec{x}'}\rangle$ is normalizable, i.e., if one allows eigenvectors, which are **not** elements of the Hilbert space. Consider the space $\mathcal{L}^2(\mathbf{R}^3)$ of square integrable functions. Here \vec{X} acts as a multiplication with the variable \vec{x} . The eigenvalue equation reads

$$\vec{X} \varphi_{\vec{x}'}(\vec{x}) = \vec{x}' \varphi_{\vec{x}'}(\vec{x}) . \tag{4.143}$$

If one writes this equation in the form

$$(\vec{x} - \vec{x}') \varphi_{\vec{x}'}(\vec{x}) = 0$$
 (4.144)

then it is obvious that the solution is proportional to the δ -function. If one chooses the proportionality constant to be 1, then

$$\varphi_{\vec{x}'}(\vec{x}) = \delta(\vec{x} - \vec{x}') . \tag{4.145}$$

Remember, that the main property of the δ -function is to set in the product $\varphi(\vec{x})$ $\delta(\vec{x})$ the argument of the function ψ to $\vec{x} = \vec{0}$. Especially $\vec{x}\delta(\vec{x}) = \vec{0}\delta(\vec{x}) = 0$. With this, (4.145) obviously solves (4.143).

Of course, the solution (4.145) is not normalizable, i.e., is not in $\mathcal{L}^2(\mathbf{R}^3)$. Building the scalar product gives the non-existing quantity

$$\langle \varphi_{\vec{x}'} \mid \varphi_{\vec{x}'} \rangle = \int d^3x \; \varphi_{\vec{x}'}^*(\vec{x}) \; \varphi_{\vec{x}}(\vec{x}) = \int d^3x \; \delta(\vec{x}' - \vec{x}) \; \delta(\vec{x}' - \vec{x}) = \delta(0) \; .$$
 (4.146)

Building the scalar product of two solutions (4.145) with different eigenvalues \vec{x}' and \vec{x}'' gives

$$\langle \varphi_{\vec{x}''} \mid \varphi_{\vec{x}'} \rangle = \int d^3x \ \delta(\vec{x}'' - \vec{x}) \ \delta(\vec{x} - \vec{x}') = \delta(\vec{x}'' - \vec{x}') \ .$$
 (4.147)

The δ -function is a generalized function (more precisely a functional), which vanishes for $\vec{x}'' \neq \vec{x}'$ and gives a contribution for $\vec{x}'' = \vec{x}'$. It then acts like a Kronecker δ_{ij} with respect to eigenfunctions belonging to the self-adjoint operator \vec{X} . In this sense the solution (4.145) of (4.143) are an orthonormal system. They are 'normalized to a δ -function'.

If an observable A depends only on operators \vec{P} and \vec{X} , i.e., $A = A(\vec{P}, \vec{X})$, then the position operators X_1, X_2, X_3 form complete set of operators, and $|\varphi_{\vec{x}}\rangle$ is completely characterized when fixing \vec{x} . This implies the completeness relation

$$\mathbf{1} = \int d^3x |\varphi_{\vec{x}}\rangle\langle\varphi_{\vec{x}}| . \tag{4.148}$$

The momentum operator \vec{P} acts as

$$\vec{P} \mid \varphi_{x_1, x_2, x_3} \rangle = \left[\vec{e}_1 \frac{\hbar}{i} \frac{\partial}{\partial x_1} + \vec{e}_2 \frac{\hbar}{i} \frac{\partial}{\partial x_2} + \vec{e}_3 \frac{\hbar}{i} \frac{\partial}{\partial x_3} \right] \mid \varphi_{x_1, x_2, x_3} \rangle$$

$$= -\frac{\hbar}{i} \vec{\nabla}_x \mid \varphi_{\vec{x}} \rangle . \tag{4.149}$$

Proof in the One-Dimensional Case:

According to (4.140) we have

$$e^{-\frac{i}{\hbar} aP} \mid \varphi_x \rangle = \mid \varphi_{x+a} \rangle . \tag{4.150}$$

Differentiation with respect to a yield

$$-\frac{i}{\hbar} P \mid \varphi_{x+a} \rangle = \frac{d}{da} \mid \varphi_{x+a} \rangle , \qquad (4.151)$$

where we used that the differentiation with respect to the real variable is derived from (4.130) and gives the same result as differentiating real functions.

If one further considers that

$$\frac{d}{da} \mid \varphi_{x+a} \rangle = \frac{d}{d(a+x)} \mid \varphi_{x+a} \rangle = \frac{d}{dx} \mid \varphi_{x+a} \rangle \tag{4.152}$$

and sets the arbitrary parameter a to zero in (4.151), one obtains

$$P \mid \varphi_x \rangle = -\frac{\hbar}{i} \frac{d}{dx} \mid \varphi_x \rangle \tag{4.153}$$

which is the result (here derived) postulated in Section 4.1.

4.13 Coordinate Space Representation of One-Particle Problems in \mathbb{R}^3

Using the completeness relation (4.148), an arbitrary state $|\psi\rangle$ can be represented as

$$|\psi\rangle = \mathbf{1} |\psi\rangle = \int d^3x |\varphi_{\vec{x}}\rangle\langle\varphi_{\vec{x}}|\psi\rangle = \int d^3x |\varphi_{\vec{x}}\rangle \psi(\vec{x}), \qquad (4.154)$$

as long as $|\psi\rangle$ characterizes problems in which the observables only depend on \vec{X} and \vec{P} . A general state $|\psi\rangle$ is thus associated in the coordinate space representation with the "wave function" $\psi(\vec{x})$

$$|\psi\rangle \longrightarrow \psi(\vec{x}) . \tag{4.155}$$

The absolute square of this component is obviously a measure for the probability to find the vector $|\varphi_{\vec{x}}\rangle$ in $|\psi\rangle$. Thus one defines the probability for the position

$$w_{\psi}(\vec{x}) = |\langle \varphi_{\vec{x}} | \psi \rangle|^2 = |\psi(\vec{x})|^2, \qquad (4.156)$$

where

$$\|\psi\|^2 = \int d^3x \langle \psi \mid \varphi_{\vec{x}} \rangle \langle \varphi_{\vec{x}} \mid \psi \rangle = \int d^3x \mid \psi(\vec{x}) \mid^2 = 1$$
 (4.157)

was assumed. Then the total probability is

$$\int d^3x \ w_{\psi}(\vec{x}) = 1 \ . \tag{4.158}$$

as it should be for a meaningful definition of probability. In the coordinate representation, one has

$$|\psi\rangle \longrightarrow \psi(\vec{x})$$

$$\vec{X} |\psi\rangle \longrightarrow \vec{x} \psi(\vec{x})$$

$$\vec{P} |\psi\rangle \longrightarrow \frac{\hbar}{i} \vec{\nabla}_x \psi(x)$$

$$(4.159)$$

and

$$\langle \varphi_{\vec{x}} \mid \vec{X} \mid \varphi_{\vec{x}'} \rangle = \vec{x} \, \delta(\vec{x} - \vec{x}')$$

$$\langle \varphi_{\vec{x}} \mid \vec{P} \mid \varphi_{\vec{x}'} \rangle = -\frac{\hbar}{i} \, \vec{\nabla}_x \, \delta(\vec{x} - \vec{x}') . \tag{4.160}$$

A Hamiltonian of the form

$$H = \frac{P^2}{2m} + V {(4.161)}$$

has thus in coordinate representation the following form

$$\langle \varphi_{\vec{x}} \mid H \mid \varphi_{\vec{x} \, \prime} \rangle = -\frac{\hbar^2}{2m} \, \Delta_x \, \delta(\vec{x} - \vec{x}') + \langle \varphi_{\vec{x}} \mid V \mid \varphi_{\vec{x} \, \prime} \rangle , \qquad (4.162)$$

or if one applies H on an arbitrary state $|\psi\rangle$

$$\langle \varphi_{\vec{x}} \mid H \mid \psi \rangle = \int d^3x' \langle \varphi_{\vec{x}'} \mid H \mid \varphi_{\vec{x}'} \rangle \langle \varphi_{\vec{x}'} \mid \psi \rangle$$

$$= \int d^3x' \left[-\frac{\hbar 2}{2m} \Delta_x \delta(\vec{x} - \vec{x}') \right] = \langle \varphi_{\vec{x}} \mid V \mid \varphi_{\vec{x}'} \rangle \langle \varphi_{\vec{x}'} \mid \psi \rangle$$

$$= -\frac{\hbar 2}{2m} \Delta_x \psi(\vec{x}) + \int d^3x' \langle \varphi_{\vec{x}} \mid V \mid \varphi_{\vec{x}'} \rangle \psi(\vec{x}') . \tag{4.163}$$

The energy eigenvalue equation $H\mid\psi\rangle=E\mid\psi\rangle$ takes the form

$$\langle \varphi_{\vec{x}} \mid H \mid \psi \rangle = \int d^3x' \langle \varphi_{\vec{x}} \mid H \mid \varphi_{\vec{x}'} \rangle \langle \varphi_{\vec{x}'} \mid \varphi \rangle = E \langle \varphi_{\vec{x}} \mid \psi \rangle \tag{4.164}$$

and thus

$$-\frac{\hbar^2}{2m} \Delta_x \psi(\vec{x}) + \int d^3x' \langle \varphi_{\vec{x}} | V | \varphi_{\vec{x}'} \rangle \psi(\vec{x}') = E \psi(\vec{x}). \qquad (4.165)$$

If one has a **local** potential, i.e., $\langle \varphi_{\vec{x}} | V | \varphi_{\vec{x}'} \rangle = V(\vec{x}) \delta(\vec{x} - \vec{x}')$, then (4.165) reduces to the previously considered equation

$$\left[-\frac{\hbar^2}{2m} \Delta_x + V(\vec{x}) \right] \psi(\vec{x}) = E \psi(\vec{x}). \tag{4.166}$$

Thus the eigenvalue equation solved in Sections 4.6-4.8 is the eigenvalue equation in a special representation, namely the coordinate space representation.

4.14 Momentum Space Representation

Instead of (4.127) and (4.128), one can equally extract from the commutation relations (4.126) eigenvalue equations for the momentum operator \vec{P}

$$\vec{P} \mid \chi_{\vec{p}} \rangle = \vec{p} \mid \chi_{\vec{p}} \rangle \tag{4.167}$$

with

$$\vec{P} = \sum_{j=1}^{3} \vec{e_j} P_j . {(4.168)}$$

Similarly to (4.138), one has

$$e^{\frac{i}{x} - \vec{a} \cdot \vec{X}} \vec{P} e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{X}} = \vec{P} - \vec{a} \mathbf{1}$$
 (4.169)

a result which already has to hold, since the exchange of \vec{P} and \vec{X} in the last relation of (4.126) only leads to a change of sign. Applying (4.169) on $|\chi_{\vec{p}}\rangle$ allows a conclusion analogous to (4.140), namely that starting from a specific $|\chi_{\vec{p}}\rangle$, one can always find momentum eigenstates

$$|\chi_{\vec{p}-\vec{a}}\rangle = e^{-\frac{i}{\hbar} \vec{a} \cdot \vec{X}} |\chi_{\vec{p}}\rangle \tag{4.170}$$

which belong to an **arbitrary** momentum $\vec{p}' = \vec{p} - \vec{a}$. Here \vec{a} is to be considered as arbitrary parameter. Thus the components P_j of \vec{P} can take all values $-\infty \leq p_j \leq \infty$. Further, from (4.170) follows

$$\vec{X} \mid \chi_{\vec{p}} \rangle = \frac{\hbar}{i} \vec{\nabla}_p \mid \chi_{\vec{p}} \rangle . \tag{4.171}$$

A comparison with (4.149) shows again the change of sign typical for the interchange of the operators \vec{X} and \vec{P} .

Assuming again that observables only depend on \vec{X} and \vec{P} , i.e., $A(\vec{X}, \vec{P})$, one sees that $|\chi_{\vec{p}}\rangle$ is also a complete set of states with the normalization condition

$$\langle \chi_{\vec{p}'} \mid \chi_{\vec{p}} \rangle = \delta(\vec{p}' - \vec{p}) \tag{4.172}$$

and the completeness relation

$$\mathbf{1} = \int d^3p \mid \chi_{\vec{p}} \rangle \langle \chi_{\vec{p}} \mid . \tag{4.173}$$

Expanding an arbitrary state according to momentum eigenvectors leads to the **momentum space representation**

$$|\psi\rangle = \int d^{3}p |\chi_{\vec{p}}\rangle\langle\chi_{\vec{p}}|\psi\rangle = \int d^{3}p |\chi_{\vec{p}}\rangle\tilde{\psi}(\vec{p})$$

$$P|\psi\rangle = \int d^{3}pP |\chi_{\vec{p}}\rangle\langle\chi_{\vec{p}}|\psi\rangle = \int d^{3}p |\chi_{\vec{p}}\rangle\tilde{p}\,\tilde{\psi}(\vec{p})$$

$$\vec{X}|\psi\rangle = \int d^{3}p\vec{X} |\chi_{\vec{p}}\rangle\langle\chi_{\vec{p}}|\psi\rangle = \int d^{3}p\,\frac{\hbar}{i}\,\vec{\nabla}_{p} |\chi_{\vec{p}}\rangle\,\tilde{\psi}(\vec{p})$$

$$= \int d^{3}p |\chi_{\vec{p}}\rangle\frac{-\hbar}{i}\,\vec{\nabla}_{p}\,\tilde{\psi}(\vec{p}).$$

$$(4.174)$$

In this representation \vec{P} acts as multiplicative operator and \vec{X} as differential operator. Analogously to (4.160), one has

$$\langle \chi_{\vec{p}} \mid \vec{X} \mid \chi_{\vec{p}'} \rangle = \vec{p} \, \delta(\vec{p} - \vec{p}') , \qquad (4.175)$$

i.e., the momentum operator is diagonal, and

$$\langle \chi_{\vec{p}} \mid \vec{X} \mid \chi_{\vec{p}'} \rangle = -\frac{\hbar}{i} \vec{\nabla}_{p} \delta(\vec{p} - \vec{p}') . \tag{4.176}$$

The expectation values of the momentum operator are simple

$$\langle \vec{P} \rangle_{\psi} = \langle \psi \mid \vec{P} \mid \psi \rangle$$

$$= \int d^{3}p \, \langle \psi \mid \vec{P} \mid \chi_{\vec{p}} \rangle \langle \chi_{\vec{p}} \mid \psi \rangle$$

$$= \int d^{3}p \, \vec{p} \, \langle \psi \mid \chi_{\vec{p}} \rangle \langle \chi_{\vec{p}} \mid \psi \rangle$$

$$= \int d^{3}p \, \vec{p} \mid \langle \chi_{\vec{p}} \mid \psi \rangle \mid^{2}$$

$$= \int d^{3}p \, \vec{p} \mid \tilde{\psi}(\vec{p}) \mid^{2} . \tag{4.177}$$

The absolute square

$$\tilde{w}_{\psi}(\vec{p}) = |\langle \chi_{\vec{p}} | \psi \rangle|^2 = |\tilde{\psi}(\vec{p})|^2 \tag{4.178}$$

is the probability to find the momentum eigenstate $|\chi_{\vec{p}}\rangle$ in the state $|\psi\rangle$. Already in (4.177), it was assumed that $|\psi| = 1$, so that

$$\int d^3 p \ \tilde{w}(\vec{p} \) = \int d^3 p \ \langle \psi \mid \chi_{\vec{p}} \rangle \langle \chi_{\vec{p}} \mid \psi \rangle$$

$$= \langle \psi \mid \psi \rangle = 1$$
(4.179)

which confirms that (4.178) is the momentum probability with respect to a total probability 1.

The position expectation value is in the momentum space representation more complicated

$$\langle \psi \mid \vec{X} \mid \psi \rangle = \int d^3p \ \langle \psi \mid \chi_{\vec{p}} \rangle \langle \chi_{\vec{p}} \mid \vec{X} \mid \psi \rangle = \int d^3p \ \tilde{\psi}^*(\vec{p}) - \frac{\hbar}{i} \ \vec{\nabla}_p \ \tilde{\psi}(\vec{p}) \ . \tag{4.180}$$

The Hamiltonian is in momentum space representation given as

$$\langle \chi_{\vec{p}} \mid H \mid \chi_{\vec{p}'} \rangle = \langle \chi_{\vec{p}} \mid \frac{P^2}{2m} + V \mid \chi_{\vec{p}'} \rangle = \frac{p^2}{2m} \delta(\vec{p} - \vec{p}') + \langle \chi_{\vec{p}} \mid V \mid \chi_{\vec{p}'} \rangle, (4.181)$$

and eigenvalue equation for the energy

$$\langle \chi_{\vec{p}} \mid H \mid \psi \rangle = E \langle \chi_{\vec{p}} \mid \psi \rangle$$
 (4.182)

takes the form

$$\frac{p^2}{2m} \tilde{\psi}(\vec{p}) + \int d^3p' \langle \chi_{\vec{p}} | V | \chi_{\vec{p}'} \rangle \tilde{\psi}(\vec{p}') = E \tilde{\psi}(\vec{p}). \tag{4.183}$$

In general, one cannot extract a δ -function from $\langle \chi_{\vec{p}} \mid V \mid \chi_{\vec{p}'} \rangle$ for a **local** potential, as it was the case in the coordinate space representation. For a **local** potential, one has

$$\langle \chi_{\vec{p}} \mid V \mid \chi_{\vec{p}'} \rangle = \tilde{V}(\vec{p} - \vec{p}') , \qquad (4.184)$$

so that (4.183) stays in the form of an integro-differential equation. Thus for local potentials the coordinate space representation is more suitable for solving the energy eigenvalue equation, as explicitly demonstrated for the Coulomb potential.

4.15 Separable Potentials

In this insert, a specific class of potentials shall be considered, which historically have played a major role in the development of few-body physics. For simplicity we consider only the one-dimensional case and have in mind that when separating off the angular momentum part for a rotationally invariant problem, then the energy eigenvalue equation is one-dimensional. In practice, separable potentials have been defined for each ℓ -state.

A separable potential is given by

$$V^s = |g\rangle \lambda \langle g|, \qquad (4.185)$$

where λ is a parameter. Precisely, V^s is a so-called rank-1 separable potential.

In coordinate space representation, one has

$$\langle \varphi_x \mid V^s \mid \varphi_{x'} \rangle = \langle \varphi_x \mid g \rangle \lambda \langle g \mid \varphi_{x'} \rangle = g(x) \lambda g^*(x')$$
 (4.186)

and in momentum space representation

$$\langle \chi_p \mid V^s \mid \chi_{p'} \rangle = \langle \chi_p \mid g \rangle \lambda \langle g \mid \chi_{p'} \rangle = \tilde{g}(p) \lambda \tilde{g}^*(p') . \tag{4.187}$$

Thus, in both representations V^s has the same form. The functions g(x) and $\tilde{g}(p)$ are sometimes called "form factors," which should not be confused with the form factors introduced to describe the charge distribution of an atom or the electromagnetic properties of nucleons. (4.186) and (4.187) give no preference in which representation the eigenvalue equation for the energy should be solved. Comparing (4.183) with (4.166) shows that now (4.183) is simpler due to the simpler kinetic energy term:

$$\frac{p^2}{2m} \,\tilde{\psi}(p) + \tilde{g}(p) \,\lambda \,\int dp' \,\tilde{g}^*(p') \,\tilde{\psi}(p') = E \,\tilde{\psi}(p') \,. \tag{4.188}$$

From this follows

$$\tilde{g}(p) \lambda \int dp' \, \tilde{g}^*(p') \, \tilde{\psi}(p') = \left(E - \frac{p^2}{2m}\right) \, \tilde{\psi}(p)$$
 (4.189)

or

$$\frac{1}{E - \frac{p^2}{2m}} \tilde{g}(p) \lambda \int dp' \, \tilde{g}^*(p') \, \tilde{\psi}(p') = \tilde{\psi}(p) . \tag{4.190}$$

Multiplication of (4.190) with $\tilde{g}^*(p)$ and integration over p results in

$$\int dp \ \tilde{g}^*(p) \ \frac{1}{E - \frac{p^2}{2m}} \tilde{g}(p) \int dp' \ \tilde{g}^*(p') \ \tilde{\psi}(p') = \lambda^{-1} \int dp \ \tilde{g}^*(p) \ \tilde{\psi}(p)$$
(4.191)

from which the dependence on $\tilde{\psi}(p)$ can be completely eliminated

$$\int dp \ \tilde{g}^*(p) \ \frac{1}{E - \frac{p^2}{2m}} \ \tilde{g}(p) = \lambda^{-1} \ . \tag{4.192}$$

This is an equation which completely determines the energy eigenvalue E and only contains potential parameters. Thus in the momentum space representation separable potentials lead to a closed form equation for E, which can be easily treated with standard numerical methods. This made separable potentials quite appealing.

It is quite instructive to consider the above derivation again, but now without a specific representation. The eigenvalue equation (4.188) reads then

$$\left(\frac{p^2}{2m} + \mid g \rangle \lambda \langle g \mid \right) \mid \psi \rangle = E \mid \psi \rangle \tag{4.193}$$

which can also be written as

$$\mid g \rangle \lambda \langle g \mid \psi \rangle = \left(E - \frac{p^2}{2m} \right) \mid \psi \rangle$$
 (4.194)

or

$$\frac{1}{E - \frac{p^2}{2m}} \mid g \rangle \lambda \langle g \mid \psi \rangle = \mid \psi \rangle . \tag{4.195}$$

Multiplication with $\langle g \mid \text{gives} \rangle$

$$\langle g \mid \frac{1}{E - \frac{p^2}{2m}} \mid g \rangle \lambda \langle g \mid \psi \rangle = \langle g \mid \psi \rangle$$
 (4.196)

from which $\langle g \mid \psi \rangle$ can be eliminated

$$\langle g \mid \frac{1}{E - \frac{p^2}{2m}} \mid g \rangle = \lambda^{-1} . \tag{4.197}$$

The only operator present in this equation is the momentum operator. It is thus most reasonable to use the momentum space representation, since here P is diagonal

$$\int dp \langle g \mid \frac{1}{E - \frac{p^2}{2m}} \mid \chi_p \rangle \langle \chi_p \mid g \rangle = \lambda^{-1}$$
(4.198)

from which (4.192) directly follows:

$$\int dp \, \frac{|g(p)|^2}{E - \frac{p^2}{2m}} = \lambda^{-1} . \tag{4.199}$$

Thus different from local potentials, for separable potentials the momentum space representation is much more suited. For the so-far considered cases, the harmonic oscillator and the Coulomb potential, the discussion in this section appears quite academic, since both potentials are not separable. Even the, in principle, very complex nuclear force seems to be approximately local, at least for larger distances. There the nucleon-nucleon force is of Yukawa-type

$$\langle \varphi_{\vec{x}} \mid V_{NN} \mid \varphi_{\vec{x}} \rangle = \lambda \frac{e^{-\mu r}}{r} \delta(\vec{x} - \vec{x}') . \tag{4.200}$$

On the other hand, one often has to rely on approximative methods for solving complicated problems. However, perturbative methods are often not accurate enough or do not converge. A different method consists of the expansion of local potentials in terms of separable potentials. Then the above considerations are of central importance, and in this case it is definitely easier to work in momentum space.

Literature on the use of separable potentials:

- Y. Yamaguchi: Two-Nucleon Problem when the potential is nonlocal but separable I, Physical Review **95**, 1628 (1954)
- Y. Yamaguchi: Two-Nucleon Problem when the potential is nonlocal but separable II, Physical Review **95**, 1653 (1954)
- D. J. Ernst and C. M. Shakin and R. M. Thaler: Separable representation of two-body interactions, Physical Review C8, 46 (1973)
- D. J. Ernst and C. M. Shakin and R. M. Thaler: Separable representation of T matrices valid in the vicinity of off-shell points, Physical Review C9, 1780 (1974)
- J. Haidenbauer and W. Plessas: Separable representation of the Paris nucleon-nucleon potential, Physical Review C30, 1822 (1984)
- J. Haidenbauer and Y. Koike and W. Plessas: Separable representation of the Bonn nucleon-nucleon potential, Physical Review C33, 439 (1986)

4.16 Transition from Coordinate Space to Momentum Space Representation

The abstract state $| \psi \rangle$ can be represented either as superposition of coordinate space eigenvectors

$$|\psi\rangle = \int d^3x |\varphi_{\vec{x}}\rangle \langle \psi_{\vec{x}} |\psi\rangle = \int d^3x |\varphi_{\vec{x}}\rangle \psi(\vec{x})$$
 (4.201)

or of momentum eigenvectors

$$|\psi\rangle = \int d^3p |\chi_{\vec{p}}\rangle \langle \chi_{\vec{p}} |\psi\rangle = \int d^3p |\chi_{\vec{p}}\rangle \tilde{\psi}(\vec{p}). \qquad (4.202)$$

Here the expansion coefficients ("wave functions") are either $\psi(\vec{x}) = \langle \varphi_{\vec{x}} \mid \psi \rangle$ or $\tilde{\psi}(\vec{p}) = \langle \chi_{\vec{p}} \mid \psi \rangle$, and represent the **same** state $|\psi\rangle$. Going from one representation to another simply means a change of basis. We have

$$\psi(\vec{x}) = \langle \varphi_{\vec{x}} \mid \psi \rangle = \int d^3p \, \langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle \langle \chi_{\vec{p}} \mid \psi \rangle = \int d^3p \, \langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle \, \tilde{\psi}(\vec{p}) \qquad (4.203)$$

and

$$\tilde{\psi}(\vec{p}) = \langle \chi_{\vec{p}} \mid \psi \rangle = \int d^3x \, \langle \chi_{\vec{p}} \mid \varphi_{\vec{x}} \, \rangle \, \langle \varphi_{\vec{x}} \mid \psi \rangle = \int d^3x \, \langle \chi_{\vec{p}} \mid \varphi_{\vec{x}} \rangle \, \psi(\vec{x}) . \quad (4.204)$$

As always when performing a change of basis, we have to determine the new basis in terms of the old basis and vice verse, i.e., we have to determine the coefficients $\langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle$ and $\langle \chi_{\vec{p}} \mid \varphi_{\vec{x}} \rangle$. For this, let us consider

$$\langle \varphi_{\vec{x}} \mid \vec{P} \mid \chi_{\vec{p}} \rangle = \vec{p} \langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle \tag{4.205}$$

and

$$\langle \varphi_{\vec{x}} \mid \vec{P} \mid \chi_{\vec{p}} \rangle = \frac{\hbar}{i} \vec{\nabla}_x \langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle. \tag{4.206}$$

Thus the coefficients $\langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle$ have to obey the differential equation

$$\frac{\hbar}{i} \vec{\nabla}_x \langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle = \vec{p} \langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle. \tag{4.207}$$

The solution is given by

$$\langle \varphi_{\vec{x}} \mid \chi_{\vec{p}} \rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{x}}$$

$$(4.208)$$

if one takes into account the normalization conditions

$$\langle \varphi_{\vec{x}} \mid \varphi_{\vec{x}'} \rangle = \delta(\vec{x} - \vec{x}') \quad \text{and} \quad \langle \chi_{\vec{p}} \mid \chi_{\vec{p}'} \rangle = \delta(\vec{p} - \vec{p}')$$
 (4.209)

and appropriate choice of the arbitrary phase factor. Inserting (4.208) into (4.203) and (4.204) gives

$$\psi(\vec{x}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3p \ e^{\frac{i}{\hbar} \ \vec{p} \cdot \vec{x}} \ \tilde{\psi}(\vec{p})
\tilde{\psi}(\vec{p}) = \frac{1}{(2\pi\hbar)^{3/2}} \int d^3x \ e^{-\frac{i}{\hbar} \ \vec{p} \cdot \vec{x}} \ \psi(\vec{x})$$
(4.210)

which is the expected result that coordinate space and momentum space representation of a state $|\psi\rangle$ transform into each other via **Fourier transformation**.

Finally, it should be derived that the momentum space representation of **local potentials**, i.e., of potentials that are diagonal in coordinate space representation $\langle \varphi_{\vec{x}} \mid V \mid \varphi_{\vec{x}'} \rangle = V(\vec{x}) \delta(\vec{x} - \vec{x}')$ is indeed of the form (4.184). On has in general

$$\langle \chi_{\vec{p}} \mid V \mid \chi_{\vec{p}'} \rangle = \int d^3x \int d^3x' \langle \chi_{\vec{p}} \mid \varphi_{\vec{x}} \rangle \langle \varphi_{\vec{x}} \mid V \mid \varphi_{\vec{x}'} \rangle \langle \varphi_{\vec{x}'} \mid \chi_{\vec{p}'} \rangle$$

$$= \int d^3x \int d^3x' \frac{1}{(2\pi\hbar)^3} e^{\frac{i}{\hbar} \vec{p} \cdot \vec{x}} \langle \varphi_{\vec{x}} \mid V \mid \varphi_{\vec{x}'} \rangle e^{\frac{i}{\hbar} \vec{p}' \cdot \vec{x}'}$$

$$(4.211)$$

which becomes for local potentials

$$\langle \chi_{\vec{p}} | V | \chi_{\vec{p}'} \rangle = \frac{1}{(2\pi\hbar)^3} \int d^3x \ e^{-\frac{i}{\hbar} (\vec{p} - \vec{p}') \cdot \vec{x}} V(\vec{x}) \equiv \tilde{V}(\vec{p} - \vec{p}') \ .$$
 (4.212)