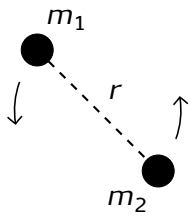
The Quantum Mechanical Two-body Problem

These are lecture notes by Apoorv Potnis of the lecture 'Quantenmechanisches Zweikörperproblem' or 'The Quantum Mechanical Two-body Problem', given by **Prof. Frederic Paul Schuller**, as the seventeenth lecture in the course 'Theoretische Physik 2: Theoretische Quantenmechanik' in 2014/15 at the Friedrich-Alexander-Universität Erlangen-Nürnberg. While the original lecture is in German, these notes are in English and have been prepared using YouTube's automatic subtitle translation tool. The lecture is available at https://www.youtube.com/watch?v=mcM4S3IMMvI&list=PLPO5pgr_frzTeqa_thbltYjyw8F9ehw7v&index=17 and at https://www.fau.tv/clip/id/44891.

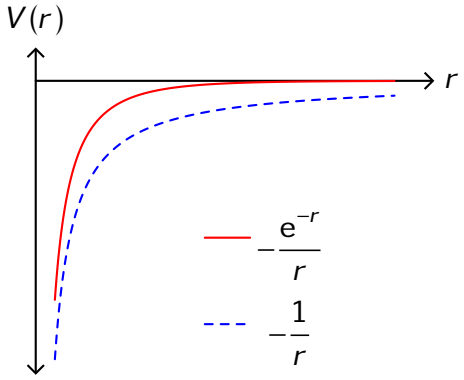
Contents

1 Introduction

Consider a classical system system consisting of two interacting particles of masses m_1 and m_2, such that the interaction is completely determined by the potential $V(r)$, and the potential depends only on the distance r between the particles. If we consider the central force problem, like a planet orbiting the sun, then we know we have bound states corresponding to *all* the negative energy values, and scattering states corresponding to all the positive energy



Classical picture



Yukawa and Coulomb potentials

values. It turns out that if consider the system quantum-mechanically, then bound states cannot admit all the negative energy solutions. Only certain energy levels are allowed. This can be seen experimentally from the discrete lines in the spectra of atoms, demonstrating the quantised nature of energy levels. In this lecture, we shall consider the quantum-mechanical case of the two-body problem.

An example of a potential as described above would be the *Yukawa potential*, defined as

$$V_{\text{Yukawa}}(r) := a\frac{\exp(-kmr)}{r},$$

where k, m and a are constants. $a \in \mathbb{R} \setminus \{0\}$, $m \geq 0$. According to quantum field theory, very roughly speaking, interaction between particles takes place via a 'mediating particle'. If the interaction is mediated by a 'scalar field'[1], then the mass associated to the particle of that scalar field is the mass m appearing in the Yukawa potential. If we plot a graph of the Yukawa potential for a massive scalar field, then we see that the magnitude of the potential becomes very close to zero after a certain distance. Thus, these

[1]Whatever that means

interactions are short-ranged. If instead we have $m = 0$, corresponding to a photon, then we get the familiar long-range Coulomb potential

$$V_{\text{Coulomb}}(r) := a\frac{1}{r}.$$

We also have the finite wall potential $V_{\text{finite wall}}(r) := a\Theta(r - r_0)$ and the isotropic harmonic oscillator $V_{\text{ihc}}(r) := ar^2$.

The Hilbert space of the individual particles is $\mathrm{L}^2(\mathbb{R}^3)$ and the Hilbert space of the composite two-body system is $\mathrm{L}^2(\mathbb{R}^3)\otimes\mathrm{L}^2(\mathbb{R}^3)$, which is naturally isomorphic to $\mathrm{L}^2(\mathbb{R}^6)$. This can be seen from theorem II.10 of the book of Reed and Simon [1, p. 52]. If $f, g \in \mathrm{L}^2(\mathbb{R}^3)$, then we can define an isomorphism $\mathrm{L}^2(\mathbb{R}^3) \otimes \mathrm{L}^2(\mathbb{R}^3) \to \mathrm{L}^2(\mathbb{R}^6)$ by $f \otimes g \mapsto fg \in \mathrm{L}^2(\mathbb{R}^6)$.

The Hamiltonian for our quantum-mechanical two-body system is

$$H := -\frac{\hbar^2}{2m_1}\Delta_{(1)} - \frac{\hbar^2}{2m_2}\Delta_{(2)} + V\left(\|\boldsymbol{x}^{(1)} - \boldsymbol{x}^{(2)}\|\right),$$

where $\Delta_{(i)}$ is the Laplacian operator which acts on the Hilbert space $\mathrm{L}^2(\mathbb{R}^3)$ of the particle i, and $\boldsymbol{x}^{(i)} \in \mathbb{R}^3$ denotes the position vector of the i^{th} particle. Assuming that this Hamiltonian is self-adjoint, we are interested in finding out its spectrum.

As is the case in classical mechanics, we shall move to the center-of-mass co-ordinates. We can move the center-of-mass of the system in any direction by any value, i.e. the spectrum of the 'center-of-mass' position operator is $\mathbb{R}$. The discrete energy levels are due to the angular momentum about the center-of-mass. We thus introduce

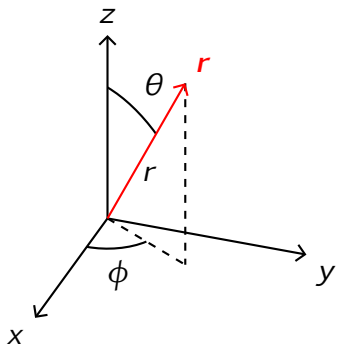
$$\begin{aligned}
\boldsymbol{y} &:= \frac{m_1\boldsymbol{x}^{(1)} + m_2\boldsymbol{x}^{(2)}}{m_1 + m_2}, \\
\boldsymbol{r} &:= \boldsymbol{x}^{(1)} - \boldsymbol{x}^{(2)}, \\
\mu &:= \frac{m_1 m_2}{m_1 + m_2}.
\end{aligned}$$

The Hamiltonian then takes the form

$$H := -\frac{\hbar^2}{2(m_1 + m_2)}\Delta_{\boldsymbol{y}} - \frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{r}} + V(\|\boldsymbol{r}\|).$$

The wave function of the system $\psi\left(\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}\right)$ expressed in the new co-ordinates becomes

$$\phi(\boldsymbol{y}, \boldsymbol{r}) := \psi\left(\boldsymbol{x}^{(1)}(\boldsymbol{y}, \boldsymbol{r}), \boldsymbol{x}^{(2)}(\boldsymbol{y}, \boldsymbol{r})\right).$$



Spherical co-ordinates

The Hamiltonian H can be separated into two parts, H_{free} describing the movement of the center-of-mass and H_{rel}, describing the movement of the particles around the center-of-mass. We have

$$H_{\text{free}} := -\frac{\hbar^2}{2(m_1+m_2)}\Delta_y \qquad \text{and} \qquad H_{\text{rel}} := -\frac{\hbar^2}{2\mu}\Delta_{\boldsymbol{r}} + V(\|\boldsymbol{r}\|).$$

We know that $\text{spec}\,(H_{\text{free}}) = \mathbb{R}_{\geq 0}$, so the task that remains is to find $\text{spec}\,(H_{\text{rel}})$, provided that H_{rel} is self-adjoint, depending on $V(\|\boldsymbol{r}\|)$. We see that H_{rel} is spherically symmetric. Thus, we shall move to the spherical co-ordinates to separate the angular and radial dependencies. This shall reduce our three-dimensional problem to a one-dimensional one.

2 Moving to spherical co-ordinates

We know that the orbital angular momentum operators are self-adjoint and defined on their Stone domains. They were defined as the generators of rotation about an axis. We shall instead consider the restrictions of the these operators on the Schwartz space to avoid running into technical issues. The Schwartz space is dense in the Stone domains and $\mathrm{L}^2(\mathbb{R}^3)$ and the operators are essentially self-adjoint on the Schwartz space. We shall now on not distinguish between the orbital angular momentum operators and their essentially self-adjoint restrictions on the Schwartz space. This machinery has been explained in the twelfth lecture 'Stone's Theorem and Construction of Observables' in the English quantum mechanics series [2, 3]. It was also seen that the spectrum of these operators is contained in the integers.

Let $i \in \{1, 2, 3\}$. We thus have the Cartesian angular momentum operators

$$\begin{aligned} L_i &: \mathcal{S}(\mathbb{R}^3) \to \mathcal{S}(\mathbb{R}^3), \\ L_i &: \psi \mapsto \epsilon_{ijk} Q_j P_k \psi, \end{aligned}$$

where Q_j and P_k denote the j^{th} and k^{th} position and momentum operators respectively. The indices run over 1, 2 and 3. We thus have

$$\begin{aligned} L_1 &= -\mathrm{i}\hbar(y\partial_z - z\partial_y) \\ L_2 &= -\mathrm{i}\hbar(z\partial_x - x\partial_z) \\ L_3 &= -\mathrm{i}\hbar(z\partial_y - y\partial_x). \end{aligned}$$

Let

$$A := [0, +\infty) \times [0, \pi] \times [0, 2\pi).$$

Let T be defined as

$$\begin{aligned} T &: A \to \mathbb{R}^3, \\ T &: (r, \theta, \phi) \mapsto (x, y, z), \end{aligned}$$

where

$$\begin{aligned} x &= r\cos\phi\sin\theta, \\ y &= r\sin\phi\sin\theta, \\ z &= r\cos\theta. \end{aligned}$$

Thus,

$$T(r, \theta, \phi) := (r\cos\phi\sin\theta, \sin\phi\sin\theta, \cos\theta).$$

If $F \in \mathcal{S}(A)$ corresponds to ψ in spherical co-ordinates[2], we have

$$F = \psi \circ T,$$

and the chain rule gives us

$$F'(r, \theta, \phi) = \psi'(x, y, z) \cdot T'(r, \theta, \phi),$$

[2] Note that even though T is only surjective and not injective, $T^{-1}(\psi)$ is a measure zero set for any $\psi \in \mathcal{S}(\mathbb{R}^3)$. Thus, we don't need to make any further identifications in $\mathcal{S}(A)$.

where $(x, y, z) = T(r, \theta, \phi)$. We thus have

$$\partial_\phi = (\partial_\phi x)\partial_x + (\partial_\phi y)\partial_y + (\partial_\phi z)\partial_z.$$

Substituting $x = r\cos\phi\sin\theta$, $y = r\sin\phi\sin\theta$ and $z = r\cos\theta$, we get

$$\begin{aligned}\partial_\phi &= -(r\sin\theta\sin\phi)\partial_x + (r\sin\theta\cos\phi)\partial_y \\ \partial_\phi &= x\partial_2 - y\partial_1.\end{aligned}$$

Thus, as expected on physical grounds, we get

$$\tilde{L}_3 = -\mathrm{i}\hbar\partial_\phi,$$

where $\tilde{L}_3 \colon \mathcal{S}(A) \to \mathcal{S}(A)$ denotes the angular momentum operator in spherical co-ordinates. We now restrict the domain of T suitably such that it becomes injective and T^{-1} becomes a well defined function. More precisely, we take the domain to be $\tilde{A} := (0, +\infty) \times (0, \pi) \times (0, 2\pi)$. This does not cause any problems as we are excluding only measure zero sets which are irrelevant when considering wave-functions. If we define $\tilde{\mathbb{R}^3}$ as $\mathbb{R}^3$ excluding the axes, we have $T^{-1} \colon \tilde{\mathbb{R}^3} \to \tilde{A}$, $T^{-1} \colon (x, y, z) \mapsto (r, \theta, \phi)$ as

$$\begin{aligned}r &= \sqrt{x^2 + y^2 + z^2}, \\ \theta &= \cos^{-1}\left(\frac{z}{\sqrt{x^2 + y^2 + z^2}}\right), \\ \phi &= \cos^{-1}\left(\frac{x}{\sqrt{x^2 + y^2}}\right).\end{aligned}$$

Applying chain rule to $\psi = F \circ T^{-1}$ gives us

$$\partial_i = (\partial_i r)\partial_r + (\partial_i \theta)\partial_\theta + (\partial_i \phi)\partial_\phi.$$

Calculating the partial derivatives and substituting the above in $L_1 = -\mathrm{i}\hbar(y\partial_z - z\partial_y)$ and $L_2 = -\mathrm{i}\hbar(z\partial_x - x\partial_z)$ finally gives us

$$\begin{aligned}\tilde{L}_1 &:= \mathrm{i}\hbar\left(\cos\phi\cot\theta\frac{\partial}{\partial\phi} + \sin\phi\frac{\partial}{\partial\theta}\right), \\ \tilde{L}_2 &:= \mathrm{i}\hbar\left(-\sin\phi\cot\theta\frac{\partial}{\partial\phi} + \cos\phi\frac{\partial}{\partial\theta}\right), \\ \tilde{L}_3 &:= -\mathrm{i}\hbar\frac{\partial}{\partial\phi}.\end{aligned}$$

We also have

$$\tilde{\boldsymbol{L}}^2 F = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}F\right) - \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}F\right),$$

and

$$\tilde{H}_{\text{rel}}F = -\frac{\hbar^2}{2\mu}\left(\frac{1}{r}\left(\frac{\partial}{\partial r}\right)^2 (rF) - \frac{\tilde{\boldsymbol{L}}^2}{r^2}F\right) + V(r)F.$$

We now observe that $\tilde{\boldsymbol{L}}^2 F$ is dependent only on the angular part of F. So, if we multiply F by a function $f(r)$ of r alone, without any dependencies on θ and ϕ, then we have that $\tilde{\boldsymbol{L}}^2(f \cdot F) = f \cdot \tilde{\boldsymbol{L}}^2 F$. Because of this observation, we attempt to decompose the the Hilbert space into radial and angular parts.

We know that

$$\mathbb{R}^3 = \mathbb{S}^2 \times [0, +\infty)$$

as sets. The standard Lebesgue measure on $\mathbb{R}^3$ can be seen as the tensor product of the measures on $\mathbb{S}^2$ and $[0, \infty)$. Let $\mathcal{B}(\mathbb{S}^2)$ be the Borel σ-algebra on $\mathbb{S}^2$, generated by the standard induced subset topology on $\mathbb{S}^2$, and let $\mathcal{B}([0, +\infty))$ be the Borel σ-algebra on $[0, +\infty)$ generated by the standard induced subset topology on $[0, +\infty)$. We know that $\mathbb{S}^2 = [0, \pi] \times [0, 2\pi)$, as sets. Every element of $\mathcal{B}(\mathbb{S}^2)$, i.e. every measurable set of $\mathbb{S}^2$, can be expressed as a countable union of sets $\Theta \times \Phi$, where $\Theta := (\theta_1, \theta_2)$ and $\Phi := (\phi_1, \phi_2)$ are open sets in $[0, \pi]$ and $[0, 2\pi)$. Let

$$\nu \colon \mathcal{B}(\mathbb{S}^2) \to \mathbb{R}$$

be the measure defined on $\mathbb{S}^2$ by

$$\nu((\Theta, \Phi)) := (\phi_2 - \phi_1) \int_{\theta_1}^{\theta_2} \sin\theta \, \mathrm{d}\theta.$$

ν is known as the standard spherical measure on $\mathbb{S}^2$. It can be easily seen that $\nu((\Theta, \Phi))$ is nothing but the area of a surface element on the sphere which subtends the angles Θ and Φ at the origin in the polar and azimuthal directions respectively. We define the measure

$$\xi \colon \mathcal{B}([0, +\infty)) \to \mathbb{R}$$

on $[0, +\infty)$ by

$$\xi((a, b)) := \int_a^b r^2 \mathrm{d}r,$$

with $a, b \in (0, +\infty)$. Note that in both the cases, we have defined the measure on open sets. Every element of the Borel σ-algebra can be expressed as a countable union or a countable intersection of the open sets. The standard Lebesgue measure μ on $\mathbb{R}^3$ can be expressed as

$$\mu = \nu \otimes \xi.$$

Applying theorem II.10 of the book of Reed and Simon [1, p. 52] again, we see that

$$\mathrm{L}^2(\mathbb{R}^3, \mu) = \mathrm{L}^2(\mathbb{S}^2, \nu) \otimes \mathrm{L}^2([0, +\infty), \xi). \tag{1}$$

We define the operators $\tilde{\boldsymbol{L}}^2_{\mathbb{S}^2} : C^\infty(\mathbb{S}^2, \nu) \to C^\infty(\mathbb{S}^2, \nu)$ and $\tilde{L}_{3,\mathbb{S}^2} : C^\infty(\mathbb{S}^2, \nu) \to C^\infty(\mathbb{S}^2, \nu)$. These are simply the angular parts of the $\tilde{\boldsymbol{L}}^2$ and $\tilde{L}_3$ operators, which anyway act on $C^\infty(\mathbb{S}^2, \nu)$ since they did not have any radial dependence.

$$\begin{aligned}
\tilde{\boldsymbol{L}}^2_{\mathbb{S}^2} &= -\mathrm{i}\hbar\partial_\phi, \\
\tilde{L}_{3,\mathbb{S}^2} &= -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) - \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\right).
\end{aligned}$$

We use the fact that $C^\infty(\mathbb{S}^2, \nu)$ is dense in $\mathrm{L}^2(\mathbb{S}^2, \nu)$. It can be seen that these operators are symmetric.

We need the fact that $\tilde{\boldsymbol{L}}^2$ is essentially self-adjoint on $\mathrm{C}^\infty(\mathbb{S}^2)$ [4]. In order to fully determine $\mathrm{spec}(H_{\mathrm{rel}})$, along with the continuous spectrum, i.e. the part containing the generalised eigenvalues, we would need to lift the eigenvalue equation to the distribution space and solve it.[3] However, we already know from experiments that the hydrogen atom has discrete lines in its observed spectrum. Thus, we shall first solve for the point spectrum

$$\mathrm{spec}_{\mathrm{p}}(H_{\mathrm{rel}}) = \{E \in \mathbb{R} \mid H_{\mathrm{rel}}F = EF\},$$

which was historically a major validation for the quantum theory.

[3] This can be in principle be achieved using Gelfand's rigged Hilbert space formalism, which was introduced in an earlier lecture. The lecture itself can be found on this link: https://www.youtube.com/watch?v=FNJOyxOp3Ik&list=PLPO5pgr_frzTeqa_thbltYjyw8F9ehw7v&index=8. The notes for this lecture can be found here: https://github.com/apoorvpotnis/schuller_rigged_hilbert_spaces/blob/main/schuller_rigged_hilbert_spaces.pdf.

3 Spherical Harmonics

In the previous lectures, we have already discussed the simultaneous eigenvectors and eigenvalues of $\boldsymbol{L}^2$ and L_a, as they commute with each other. We thus consider the simultaneous eigenvalues of H_{rel}, $\boldsymbol{L}^2$ and L_3 in the hope that this will give us more equations to work with and make the job easier. It can be seen that all three operators commute with each other pairwise. Up to isomorphism, the eigenvectors and eigenvalues of an operator are not affected by co-ordinate changes, as $\mathcal{S}(\mathbb{R}^3)$, $\mathcal{S}(\tilde{\mathbb{R}^3})$, $\mathcal{S}(A)$ and $\mathcal{S}(\tilde{A})$ are all isomorphic to each other. The self-adjointness is unaffected by the co-ordinate changes as well.

We know that the common eigenvectors of $\tilde{\boldsymbol{L}}^2$ and $\tilde{L}_3$ come as families $\psi_l^m \in \mathcal{S}(\tilde{A})$, where $m = -l, -l+1, \dots, l-1, l$ and $l \in \mathbb{N}_0$. We have

$$\begin{aligned}\tilde{\boldsymbol{L}}^2 \psi_l^m &= l(l+1)\psi_l^m, \\ \tilde{L}_3 \psi_l^m &= m\psi_l^m.\end{aligned}$$

Note that l can take only integer values, not half-integer values as we are dealing with the orbital angular momentum operator. In spherical co-ordinates, it turns out that the solutions ψ_l^m are given by

$$\psi_l^m(\tilde{\boldsymbol{x}}(r,\theta,\phi)) = k \cdot Y_l^m(\theta,\phi) \cdot f(r),$$

where

$$Y_l^m(\theta,\phi) := \frac{(-1)^m}{2^l l!}\left(\frac{(2l+1)(l-m)!}{4\pi(l+m)!}\right)^{\frac{1}{2}} \cdot \mathrm{e}^{\mathrm{i}m\phi} \cdot (\sin\theta)^m \left(\frac{\partial}{\partial \cos\theta}\right)^{l+m} (\cos^2\theta - 1)^l$$

and $\tilde{\boldsymbol{x}} = T^{-1}(\boldsymbol{x})$. These Y_l^m's are called as *spherical harmonic functions*. Since the operators $\tilde{\boldsymbol{L}}^2$ and $\tilde{L}_3$ act only on the angular components and not the radial components when expressed in spherical co-ordinates, we have that

$$\begin{aligned}\tilde{\boldsymbol{L}}^2 Y_l^m &= l(l+1)Y_l^m, \\ \tilde{L}_3 Y_l^m &= mY_l^m,\end{aligned}$$

i.e. the spherical harmonic functions are eigenvectors of $\tilde{\boldsymbol{L}}^2$ and $\tilde{L}_3$. These functions actually form an orthonormal basis of the Hilbert space $\mathrm{L}^2(\mathbb{S}^2)$ consisting of complex square-integrable functions defined on the 2-sphere.

$$\langle Y_l^m, Y_{l'}^{m'} \rangle = \delta_{l,l'} \cdot \delta_{m,m'}.$$

We request that the reader consult section 14.2 of the book of Bowers for a derivation of these spherical harmonic functions [5, p. 200].

4 Spectrum of the Hamiltonian operator

Since $\tilde{\boldsymbol{L}}^2$, $\tilde{L}_3$ and H_{rel} are self-adjoint operators which commute pair-wise, and $\tilde{\boldsymbol{L}}^2$ and $\tilde{L}_3$ have a pure point spectrum, there exists a family of simultaneous eigenbasis of the Hilbert space.

References

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The source code, updates and corrections to this document can be found on this GitHub repository: https://github.com/apoorvpotnis/schuller_two-body_problem. The source code, along with the `.bib` file is embedded in this PDF. Comments and corrections can be mailed at apoorvpotnis@gmail.com.