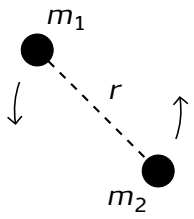
The Quantum Mechanical Two-body Problem

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.

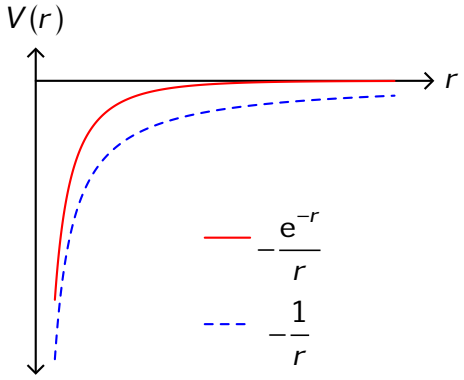
Contents

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



Classical picture



Yukawa and Coulomb potentials

sun, then we know we have bound states corresponding to *all* the negative energy values, and scattering states corresponding to all the positive energy 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

[1]Whatever that means

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 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. We are interested in finding out the spectrum of this Hamiltonian.

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

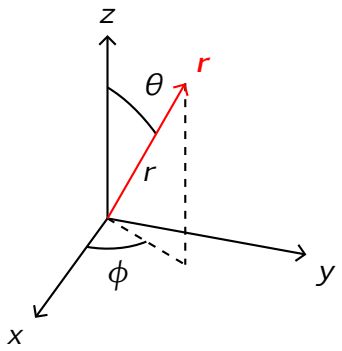
$$\begin{aligned}
\boldsymbol{y} &:= \frac{m_1\boldsymbol{x}^{(1)} + m_2\boldsymbol{x}^{(2)}}{m_1 + m_2}, \\
\boldsymbol{r} &:= \boldsymbol{x}^{(1)} - \boldsymbol{x}^{(2)}, \\
\mu &:= \frac{m_1 m_2}{m_1 + m_2}.
\end{aligned}$$

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

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

We know that $\operatorname{spec}(H_{\text{free}}) = \mathbb{R}_{\geq 0}$, so the task that remains is to find $\operatorname{spec}(H_{\text{rel}})$. 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

Now we know that the angular momentum operators are self-adjoint and defined on their Stone domains. We shall instead consider the restrictions of the angular momentum operators on the Schwartz space to avoid running into technical issues. The Schwartz space is dense in the Stone domains and $\mathrm{L}^2(\mathbb{R}^3)$. These restrictions are essentially self-adjoint. We shall now on not distinguish between the angular momentum operators and their essentially self-adjoint restrictions on the Schwartz space. Let $i \in \{1,2,3\}$. We thus have the Cartesian angular momentum operators

$$L_i \colon \mathcal{S}(\mathbb{R}^3) \to \mathcal{S}(\mathbb{R}^3),$$
$$L_i \colon \psi \mapsto \epsilon_{ijk} Q_j P_k \psi,$$

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

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

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

$$F = \psi \cdot T,$$

and the chain rule gives us

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

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

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

[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 $\mathcal{S}(A)$.

Thus, as expected on physical grounds, we get

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

where $\tilde{L}_3 : \mathcal{S}(A) \to \mathcal{S}(A)$ denotes the angular momentum operator in spherical co-ordinates. We now restrict the domain of T suitably[3] such that it becomes injective and T^{-1} becomes a well defined function. Thus, applying chain rule to $\psi = FT^{-1}$ gives us

$$\begin{aligned}
\partial_x &= (\partial_x r)\partial_r + (\partial_x \theta)\partial_\theta + (\partial_x \phi)\partial_\phi, \\
\partial_y &= (\partial_y r)\partial_r + (\partial_y \theta)\partial_\theta + (\partial_y \phi)\partial_\phi, \\
\partial_z &= (\partial_z r)\partial_r + (\partial_z \theta)\partial_\theta + (\partial_z \phi)\partial_\phi.
\end{aligned}$$

Substituting the above in $L_1 = -\mathrm{i}\hbar(y\partial_z - z\partial_y)$ and $L_2 = -\mathrm{i}\hbar(z\partial_x - x\partial_z)$ and calculating the partial derivatives 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

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

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.[4] However, we

[3] 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.

[4] This can 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.

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 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 $\mathcal{S}(\mathbb{R}^3)$ and $\mathcal{S}(\tilde{A})$ are isomorphic to each other.

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. Also recall the raising and lowering operators $\tilde{L}_+ := \tilde{L}_1 + i\tilde{L}_2$ and $\tilde{L}_- := \tilde{L}_1 - i\tilde{L}_2$. We have

$$\tilde{L}_\pm\psi_l^m = \sqrt{l(l+1) - m(m\pm 1)}\,\psi_l^m.$$

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 $\tilde{\boldsymbol{x}} = T(\boldsymbol{x})$. 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 [2, p. 200].

4 Spectrum of the Hamiltonian operator

References

[1] Michael Reed and Barry Simon. *Methods of Modern Mathematical Analysis I: Functional Analysis*. Revised and Enlarged editon. Vol. 1. Academic Press, Inc. London, 1980. ISBN: 978-0-080-57048-8.

[2] Philip Bowers. *Lectures on Quantum Mechanics*. Cambridge University Press, Cambridge, 2020. ISBN: 978-1-108-42976-4.

[3] Frederic Schuller, Simon Rea, and Richie Dadhley. 'Lectures on Quantum Theory'. Lecturer: Prof. Frederic Paul Schuller. 2019. URL: https://docs.wixstatic.com/ugd/6b203f_a94140db21404ae69fd8b367d9fcd360.pdf.

[4] Frederic Schuller. *Lectures on Quantum Theory*. 2015. URL: https://youtube.com/playlist?list=PLPH7f_7ZlzxQVx5jRjbfRGEzWY_upS5K6.

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.