

1 Quantum Mechanics - The Harmonic Oscillator

1.1 Quantum mechanics

1.1.1 The postulates of quantum mechanics

- The state of a quantum mechanical system is completely specified by a wavefunction $\Psi(x, t)$
- The observables are selfadjoint operators
- The wavefunction of a system solves the time-dependent Schrödinger equation

$$H\Psi(x, t) = -i\hbar \frac{\partial \Psi}{\partial t}$$

where H is the Hamilton operator.

- In any measurement of an observable, the only values that will ever be observed are the eigenvalues.

1.1.2 The understanding of quantum mechanics

1.1.3 Physical Problem

In physics the problem of quantum mechanics is more or less to solve the eigenvalue equation for a given Hamilton. Because you work with physical known systems you just assume that the Hamilton you are working with is indeed a physical observable, because it has to be!

This does not work in mathematics. So the goal for these notes is to prove that the Hamilton for the system of the Harmonical Oscillator is indeed an observable

1.1.4 The physics of the Harmonical Oscillator

This example is chosen because it is by far the most interesting of the typical examples, because of its usefulness.

A particle moving according to the Hamilton of the Harmonic Oscillator is vibrating back and forth in one dimension.

The Hamilton looks like this

$$H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m \omega^2 x^2$$

This can be written in terms of two other operators

$$A_+ = -\frac{\hbar}{2m\omega} \frac{d}{dx} + cx$$

$$A_- = \frac{d}{dx} + cx$$

such that

$$H = \frac{\hbar^2}{2m}(A_+A_- + c)$$

where $c = \frac{m\omega}{\hbar}$

1.2 Some necessary math

1.2.1 Essentially selfadjoint operators

Definition 1 An essentially self-adjoint operator $(D(T); T)$ is a symmetric operator such that the closure of T , \overline{T} is self-adjoint.

Corrolary 1 If $(D(T), T)$ is essentially selfadjoint, then there exist an unic extenstion of T , that is selfadjoint.

1.2.2 Lemma 1

Let H be a separable Hilbert space and $(D(T), T)$ a positive, symetric unbounded operator

Assume there is an orthonormal basis (e_j) of H such that $\forall j : e_j \in D(T)$ and that they, e_j , are eigenfunctions of T with eigenvalues $\lambda_j \geq 0$

Then T is essentially selfadjoint.

The proof is the proof of lemma 5.10 in the sugested notes for my presentation topic.

1.2.3 Scharwtzspace for \mathbb{R}

The definition of the Schwartzspace of \mathbb{R} is

$$S(\mathbb{R}) = \{f \in C^\infty(\mathbb{R}) \mid \|f\|_{\alpha, \beta} < \infty \forall \alpha, \beta\}$$

where

$$\|f\| = \sup_{x \in \mathbb{R}} |x^\alpha D^\beta f(x)|$$

1.2.4 Eigenspace

The eigenspace is defined as

$$Ker(\lambda - T) = \{v \in D(T) \mid Tv = \lambda v\}$$

1.2.5 Hermitian Polynomials

The Hermitian polynomials are the polynomials on the form

$$H_n = (-1)^n e^{\frac{x^2}{2}} \frac{d^n}{dx^n} e^{-\frac{x^2}{2}}$$

They obey the following recursion formula

$$H_{n+1}(x) = xH_n(x) - H'_n(x)$$

1.3 The Harmonic Oscillator

1.4 Theorem 2

Let $(D(T), T)$ be the operator $H = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$ acting on $D(T) = S(\mathbb{R})$. Then T is essentially selfadjoint (and can therefore be extended to a selfadjoint operator). Its eigenvalues are

$$\lambda_n = \hbar\omega \left(\frac{1}{2} + n \right)$$

where $n \geq 0$ and the eigenspaces are 1 dimensional.

Specifically are the eigenvectors

$$\psi_n = \frac{1}{\sqrt{2^n n!}} \frac{m\omega^{\frac{1}{4}}}{\hbar\pi} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right) e^{-\frac{m\omega}{2\hbar} x^2}$$

and span the eigenspace for n

Proof

To prove that T is essentially selfadjoint we have from Lemma 1 that all we need to show is that 1) that (ψ_n) is an orthonormal basis of $L^2(H)$ and 2) that ψ_n is an eigenvector.

1.4.1 Proof of (ψ_n) is an orthonormal basis of $L^2(H)$

To prove this we start by checking that $\forall m, n \in \mathbb{N} : n > m : \psi_n, \psi_m$ is orthonormal.

Let

$$\begin{aligned} \phi_n &= K * \psi_n = H_n e^{-\frac{1}{2}y^2} \\ &= (yH_{n-1}(y) - H'_n(y))e^{-\frac{1}{2}y^2} \\ &= A_+ \phi_{n-1} \end{aligned}$$

So $\phi_n = a_n A_+^n \phi_0$ and hence $\psi_n = a_n A_+^n \psi_0$. So for all $n, m \geq 0, n > m$ we have

$$\langle \psi_n, \psi_m \rangle = \langle A_+^n \psi_0, \psi_m \rangle = \langle \psi_0, A_-^n \psi_m \rangle$$

But since $A_- \phi_n = (\frac{d}{dy} + cy)e^{-\frac{1}{2}y^2} = H'_n e^{-\frac{1}{2}y^2}$, and then $\deg(A_- \phi_n) < \deg(\phi_n)$ and hence $\deg(A_- \psi_n) < \deg(\psi_n)$ and then it follows that since $n > m$ then

$$\langle \psi_0, A_-^n \psi_m \rangle = \langle \psi_0, 0 \rangle = 0$$

The proof that $(\psi_n)_{n \geq 0}$ is a basis for $L^2(\mathbb{R})$ is done by showing that the $\text{span}((\psi_n)_{n \geq 0})^\perp = \{0\}$ in the following two steps.

1. $\forall p \in \mathbb{R} : \phi \in \overline{\text{span}} \{ \psi_n \mid \forall n \geq 0 \in \mathbb{N} \}, \phi = e^{ixp} \psi_0, x \in \mathbb{R}$
2. $\{ \phi_p \mid p \in \mathbb{R} \}^\perp = \{0\}$

To prove 1 notice that $\forall n \psi_n$ is on the form $P_n(x)e^{\frac{-x^2}{2}}$ where $P_n(x)$ is a polynomial of order n . So $\text{span}(\psi_n) = \{Q(x)\psi_0\}$ where $Q(x)$ is a polynomial. So in order to show

$$\forall p \in \mathbb{R} \phi_p \in \text{span} \{\psi_n\}$$

we need to show that there exists a polynomial $Q(x)$ such that ϕ_p converges towards $Q(x)\psi_0$ but that is the same as showing that e^{ixp} converges towards $Q(x)$. Choose $Q(x) = \sum_k \frac{(ix)^k}{k!}$, this is the Taylor expansion of e^{ixp} , and hence e^{ixp} converges towards it. So $\forall p \in \mathbb{R} : \phi_p \in \overline{\text{span}} \{\psi_n \mid \forall n \geq 0 \in \mathbb{N}\}$

To prove 2 assume that $f \in \mathbb{R} \text{ and } f \perp \phi_p$ then

$$\int_{\mathbb{R}} f \phi_p = f \psi_0 e^{ixp} = 0$$

The last part we recognize as the fourier transformation of f and ψ_0 so we have that $F(\cdot \psi_0) = 0$, but since the fourier transformation is an isometry the $f \cdot \psi_0 = 0$ and since $\forall x \psi_0 > 0$ then $f = 0$. Hence it follows that $\{\phi_p \mid p \in \mathbb{R}\}^\perp = \{0\}$.

And since

$$\{\psi_p \mid p \in \mathbb{R}\} \subseteq \overline{\text{span}} \{\psi_n\}$$

then

$$\overline{\text{span}} \{\psi_n\}^\perp \subseteq \{\psi_p \mid p \in \mathbb{R}\}^\perp = \{0\}$$

so $\overline{\text{span}} \{\psi_n\}^\perp = \{0\}$ and hence $(\psi_n)_{n \geq 0}$ is a basis for $L^2(\mathbb{R})$.

1.4.2 ψ_n an eigenvector of T for all n

We prove that $\forall n \geq 0 \in \mathbb{N} \psi_n$ is an eigenvector by induction.

i=0

$$\begin{aligned} T\psi_0 &= \frac{\hbar^2}{2m} \left(\frac{-d^2}{dx^2} + \frac{(m\omega)^2}{\hbar^2} x^2 \right) \psi_0 \\ &= \frac{\hbar \cdot \omega}{2} \psi_0 \end{aligned}$$

i=n+1

Assume that ψ_n is an eigenvector then

$$\begin{aligned} T\psi_{n+1} &= aH(A_+\psi_n) \\ &= a \frac{\hbar^2}{2m} (A_+A_- + c) A_+\psi_n \\ &= a \frac{\hbar^2}{2m} (A_+A_-A_+ + cA_+) \psi_n \end{aligned}$$

$$\begin{aligned}
&= a \frac{\hbar^2}{2m} (A_+(A_-A_+ + c) \psi_n \\
&= a \frac{\hbar^2}{2m} (A_+(H + 2c) \psi_n \\
&= (\lambda_n + 2c) \psi_{n+1} = \hbar\omega \left(n + \frac{1}{2} \right) \psi_{n+1}
\end{aligned}$$

And hence it is proven that $\forall n \in \mathbb{N}$ ψ_n is an eigenvector.

Hence it is proven that T is an essentially self adjoint operator. To finish the proof of the theorem we know only need to show that the eigenspaces are 1-dimensional. This follows from the definition of the eigenspaces. Assume namely that $\psi_n, \psi_m \in \text{Ker}(\lambda - T)$. Then $\lambda_m = \lambda_n$ but then $\hbar\omega \left(\frac{1}{2} + m \right) = \hbar\omega \left(\frac{1}{2} + n \right) \Leftrightarrow m = n$ hence there is only 1 eigenvector in every eigenspace, and hence the eigenspaces are 1 dimensional.

1.5 Plot of the first couples of eigenfunctions for the Harmonic Oscillator

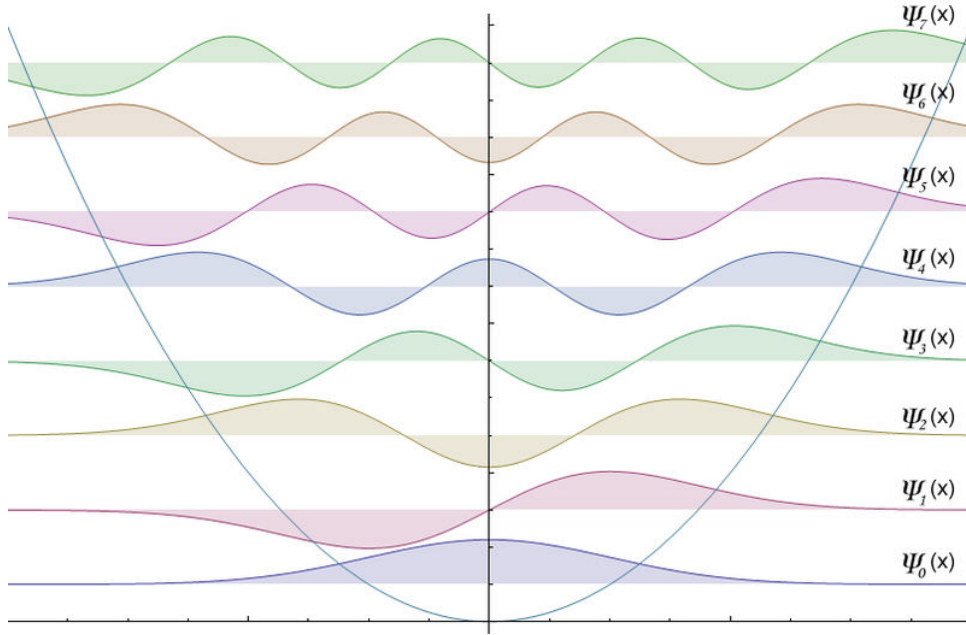


Figure 1: Plot of the first 8 unnormalized eigenfunctions. Each of the eigenfunctions oscillate around the.. eigenvalue. The blue line marks the potential

In figure 1 is showed a plot of the first 8 eigenvectors for the Harmonic Oscillator. This plots ilustrats perfectly some of the biggest difference between a classical system and a quantum mechanical system.

In the clasiscal system, a particle moving according to a harmonic oscillator, can only

move in the area inside of the parable.

This is not the case in the quantum mechanical system. There the particle is aloud to be on either side of the parable, even though it is much more likely that it is found to be in the clasical area.

If you measure the energy of the paricle in a clasical system, the value you get, could in theory, be any positiv number. Again, this is not the case in the quantum mechanical system, there the energy is quantisized, such that you will have a discret set of possible energy values. This is not

1.6 References

For the proof: <http://www.math.ethz.ch/~kowalski/spectral-theory.pdf>)

For the plot: http://en.wikipedia.org/wiki/Quantum_harmonic_oscillator