中国科学院大学
University of Chinese Academy of Sciences

Simple Harmonic Oscillators

Iridium LINCH-SK

2023.09.23

Syllabus

- Algebra Method
- Analysis Method

Algebra Method

- We know that both position and momentum are operators.
- It's always beneficial to examine the properties the two basic operators.
- Define a commuter: $[A, B] := AB - BA$.

$$\hat{x}|\psi\rangle = x|\psi\rangle,$$

$$\hat{p}|\psi\rangle = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}|\psi\rangle.$$

The Profound Commuter: [*x*, *p*]

- Actually, *x* and *p* operators do not commute.
- *f*(*x*) is an arbitrary differentiable function.

$$
\begin{aligned}
\left[\hat{x},\hat{p}\right]f\left(x\right) &= \hat{x}\hat{p}f\left(x\right)-\hat{p}\hat{x}f\left(x\right) \\
&= -\mathrm{i}\hbar x\cdot\frac{\mathrm{d}}{\mathrm{d}x}f\left(x\right)-\left(-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\left(xf\left(x\right)\right)\right) \\
&= -\mathrm{i}\hbar x\cdot\frac{\mathrm{d}}{\mathrm{d}x}f\left(x\right)+\mathrm{i}\hbar f\left(x\right)+\mathrm{i}\hbar x\cdot\frac{\mathrm{d}}{\mathrm{d}x}f\left(x\right) \\
&= \mathrm{i}\hbar f\left(x\right)
\end{aligned}
$$

The Profound Commuter: [*x*, *p*]

- It's proper to write:

$$\left[\hat{x},\hat{p}\right]=\mathrm{i}\hbar$$

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Simple Harmonic Oscillator

- We have known the Schrödinger equation for SHO:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi+\frac{m\omega^2x^2}{2}\psi=E\psi$$

- It's easy to recognize that:

$$\mathrm{LHS}=\left(\frac{1}{2m}\hat{p}^2+\frac{m\omega^2}{2}\hat{x}^2\right)\psi=\hat{H}x$$

Nondimensionalization

- We are not dealing with more than one particle, and this is not a relativistic problem, so m is an constant.
- $\hbar$ is an universal constant.
- We are dealing with one particular potential, so ω is also a constant.
- It is always awful to have such constants being taken care in every step of calculation, so we are finding a way to get rid of them.

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Nondimensionalization

- E.g. in particle physics, we often say that the rest mass of electron is

$$m_e = 0.511\ \mathrm{MeV}$$

- Rather than

$$m_e = 9.109 \times 10^{-31}\ \mathrm{kg}$$

- In the first expression, MeV is a unit with an energy dimension. However, kg is a unit with mass dimension. How could they be equivalent?

Nondimensionalization

- The Einstein Mass-Energy Relationship:

$$E = mc^2$$

- We known that the speed of light is a constant, this is one of the conjecture of special relativity. We can simply assign c = 1, now E and m are equivalent.

Nondimensionalization

- Caution: You can assign multiple physical quantities as unity, but self-consistency shall always hold.
- E.g.: Fine structure constant is a nondimensional number:

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 \hbar c} \approx \frac{1}{137}$$

- You can always assign e^2 as 1, $4\pi\varepsilon_0$ as 1 simultaneously, but now we can't assign $\hbar c$ as 1.

Nondimensionalization

- Back to the SHO occasion:

	M	L	T
$\hbar$	1	2	−1
m	1	0	0
ω	0	0	−1

- As long as they are linear irrelative, it is well-assigned.
- Calculate the determinant: $$\begin{vmatrix} 1 & 2 & -1 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{vmatrix} = 2 \neq 0$$
- They are linear irrelative.

Nondimensionalization

- We are able to rewrite the Schrödinger equation of SHO in a simpler equation:

$$-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi + \frac{1}{2}x^2\psi = E\psi$$

- In this case, $\omega = \hbar = m = 1$.
- Then the LHS is:

$$\mathrm{LHS} = \frac{1}{2}\left(\hat{x}^2 + \hat{p}^2\right)\psi$$

Commuter

- Some pals may try to represent the LHS Hamiltonian as:

$$\text{LHS?} = \frac{1}{2}\left(\hat{x} + i\hat{p}\right)\left(\hat{x} - i\hat{p}\right)\psi$$

- However now we shall note that *x* and *p* operators are not commutative.
- However, such a “dissolution” inspired us to rewrite the operators in a more symmetric way:

$$\hat{a}_{+} = \frac{1}{\sqrt{2}}\left(\hat{x} - i\hat{p}\right)$$

$$\hat{a}_{-} = \frac{1}{\sqrt{2}}\left(\hat{x} + i\hat{p}\right)$$

Ladder Operator

- Do they commute?

$$
\begin{aligned}
\left[\hat{a}_+,\hat{a}_-\right] &= \hat{a}_+\hat{a}_- - \hat{a}_-\hat{a}_+ \\
&= \frac{1}{2}\left[\left(\hat{x}-\mathrm{i}\hat{p}\right)\left(\hat{x}+\mathrm{i}\hat{p}\right)-\left(\hat{x}+\mathrm{i}\hat{p}\right)\left(\hat{x}-\mathrm{i}\hat{p}\right)\right] \\
&= \frac{1}{2}\left[\left(\hat{x}^2+\mathrm{i}\hat{x}\hat{p}-\mathrm{i}\hat{p}\hat{x}+\hat{p}^2\right)-\left(\hat{x}^2-\mathrm{i}\hat{x}\hat{p}+\mathrm{i}\hat{p}\hat{x}+\hat{p}^2\right)\right] \\
&= \frac{1}{2}\cdot 2\mathrm{i}\left[\hat{x},\hat{p}\right] = \mathrm{i}\left[\hat{x},\hat{p}\right] = -1
\end{aligned}
$$

- The answer is nope.

Ladder Operator

- How to represent Hamiltonian?

$$\hat{H} = \frac{1}{2}\left(\hat{x}^2 + \hat{p}^2\right)$$

$$= \frac{1}{2}\cdot\frac{1}{2}\left[\left(\hat{x}^2 + \mathrm{i}\hat{x}\hat{p} - \mathrm{i}\hat{p}\hat{x} + \hat{p}^2\right) + \left(\hat{x}^2 - \mathrm{i}\hat{x}\hat{p} + \mathrm{i}\hat{p}\hat{x} + \hat{p}^2\right)\right]$$

$$= \frac{1}{2}\left(\hat{a}_+\hat{a}_- + \hat{a}_-\hat{a}_+\right) = \hat{a}_+\hat{a}_- + \frac{1}{2}$$

- Do Hamiltonian commute with ladders?

Ladder Operator

- For ascending operator:

$$\left[\hat{H},\hat{a}_+\right]=\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)\hat{a}_+-\hat{a}_+\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)$$

$$=\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)\hat{a}_+-\hat{a}_+\left(\hat{a}_-\hat{a}_+-\frac{1}{2}\right)$$

$$=\hat{a}_+$$

Ladder Operator

- For descending operator:

$$\left[\hat{H},\hat{a}_-\right]=\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)\hat{a}_- -\hat{a}_-\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)$$

$$=\left(\hat{a}_-\hat{a}_+-\frac{1}{2}\right)\hat{a}_- -\hat{a}_-\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)$$

$$=-\hat{a}_-$$

Ladder Operator

- We are giving the two operators some properties:

$$\hat{a}_+ \left| n \right\rangle = A_n \left| n+1 \right\rangle$$

$$\hat{a}_- \left| n \right\rangle = A_{n-1} \left| n-1 \right\rangle$$

- Every system has a ground state, we are calling it the 0 state. The descending operator should vanish the 0 state:

$$\hat{a}_- \left| 0 \right\rangle = 0$$

Ladder Operator

- Try to operate with Hamiltonian:

$$\hat{H}\left|0\right\rangle = \left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\left|0\right\rangle = \frac{1}{2}\left|0\right\rangle$$

- For a known n^{th} state energy, the next state, i.e., n+1$^{\text{th}}$ has energy:

$$\hat{H}\hat{a}_+\left|n\right\rangle = \hat{a}_+\left|n\right\rangle + \hat{a}_+\hat{H}\left|n\right\rangle = \hat{a}_+\left|n\right\rangle\left(1+E_n\right)$$

- Now the mathematical induction proceeds, we have:

$$E_0 = \frac{1}{2}, E_n = n + \frac{1}{2}.$$

Ladder Operator

- As usual we always want such states to be orthonormal:

$$1=\langle n|n\rangle=\frac{1}{A_{n-1}^{2}}\left(\hat{a}_{+}|n-1\rangle\right)^{\dagger}\hat{a}_{+}|n-1\rangle=\frac{1}{A_{n-1}^{2}}\langle n-1|\hat{a}_{-}\hat{a}_{+}|n-1\rangle=\frac{1}{A_{n-1}^{2}}\langle n-1|\left(\hat{H}-\frac{1}{2}\right)|n-1\rangle=\frac{n-1}{A_{n-1}^{2}}$$

- Note that: $\hat{a}_{-}=\hat{a}_{+}^{\dagger}$

- So: $A_{n}=\sqrt{n}$

Analysis Method

- Let’s get back to the SHO Schrödinger equation:

$$\frac{1}{2}\left(x^2 - \frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\psi = E\psi$$

- Examining the asymptotic behavior of this equation will help a lot.

Asymptotic Properties

- At x's infinity, x^2 is a square-divergent term.
- However, the equation still holds. Which means that the 2-order derivative term shall compensate such a divergence.

$$x^2 A(x) \sim \frac{\mathrm{d}^2}{\mathrm{d}x^2} A(x)$$

- Exponential decay is not enough: the product of a polynomial and exp(-x) won't have an increasing order of polynomial after differentiating.
- The Gaussian could work.

Asymptotic Properties

- Gaussian after differentiated twice:

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-x^2} = -2x\mathrm{e}^{-x^2}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\mathrm{e}^{-x^2} = \left(4x^2 - 2\right)\mathrm{e}^{-x^2}$$

- The −2 term doesn't matter, which could contribute to *E*.
- However, such 2-order derivative over-compensated.
- We note that when every time it differentiates, the dominating term is multiplying −2*x*. If the factor is ±*x*, it could be rather good.

Asymptotic Properties

- We are using $-x^2/2$ instead:

$$\frac{\mathrm{d}}{\mathrm{d}x}\mathrm{e}^{-\frac{x^2}{2}} = -x\mathrm{e}^{-\frac{x^2}{2}}$$

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\mathrm{e}^{-\frac{x^2}{2}} = \left(x^2-1\right)\mathrm{e}^{-\frac{x^2}{2}}$$

- That is right now.
- Actually this simplest asymptotic solution gives the exact solution of the original equation:

$$\frac{1}{2}\left(x^2-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\mathrm{e}^{-\frac{x^2}{2}} = \frac{1}{2}\mathrm{e}^{-\frac{x^2}{2}} = E\mathrm{e}^{-\frac{x^2}{2}}$$

$$E = \frac{1}{2}$$

Series Method

- We assume that the solutions can be represented as power series, still having the asymptotic property like exp(−x^2/2).

$$\psi_n(x) = \exp\left(-\frac{x^2}{2}\right)\cdot\sum_{i=0}^{\infty} a_i x^i$$

- Substitute the form into the equation, we have:

$$\mathrm{LHS} = \frac{1}{2}\exp\left(-\frac{x^2}{2}\right)\cdot\left(x^2\sum_{i=0}^{\infty} a_i x^i - \left(\left(x^2-1\right)\sum_{i=0}^{\infty} a_i x^i + 2(-x)\sum_{i=1}^{\infty} i a_i x^{i-1} + \sum_{i=2}^{\infty} i(i-1)a_i x^{i-2}\right)\right)$$

$$= E_n \exp\left(-\frac{x^2}{2}\right)\cdot\sum_{i=0}^{\infty} a_i x^i = \mathrm{RHS}$$

Series Method

$$\frac{1}{2}\left(\sum_{i=0}^{\infty} a_i x^i + \sum_{i=1}^{\infty} 2ia_i x^i - \sum_{i=0}^{\infty} (i+2)(i+1) a_{i+2} x^i\right) = E_n \sum_{i=0}^{\infty} a_i x^i$$

$$a_i + 2ia_i - (i+2)(i+1) a_{i+2} = 2E_n a_i$$

$$a_{i+2} = \frac{2i+1-2E_n}{(i+2)(i+1)}$$

- We shall consider the asymptotic behavior of the solution at infinitively high power:

$$i \to \infty, a_{i+2} = \frac{2}{i} a_i.$$

Asymptotic Behavior

- We found that:

$$\exp\left(x^2\right)=\sum_{n=0}^{\infty}\frac{x^{2n}}{n!}=:\sum_{j=0}^{\infty}b_j x^j$$

$$\frac{b_{j+2}}{b_j}=\frac{2}{j}\left(j=2k,k\in\mathbf{N}\right)$$

- Which means that the series has an asymptotic behavior like exp(x^2), multiply it with the factor exp($-x^2/2$), that is exp($x^2/2$), divergent at x's infinity!
- How to solve the problem?
- We shall have the series cut off to a polynomial.

Solution (Analytical)

- At one particular index i, the a_{i+2} vanishes, so do the further terms.

$$a_{i+2} = \frac{2i+1-2E_n}{(i+2)(i+1)} a_i$$

$$E_n \in \left\{ i + \frac{1}{2} \middle| i \in \mathbf{N}. \right\}$$

- There are two sets of recurrence relation for odd or even indices occasions, which originates from a_0 or a_1, respectively.

Symmetry Properties

- Theorem: For an assigned state *n*, the solution is an odd or even function.

$$a_{i+2} = \frac{2i - 2n}{(i+2)(i+1)} a_i$$

$$a_0 = 1, a_1 = 0.$$

$$a_0 = 0, a_1 = 1.$$

Consistency

- How shall we verify the consistency of result of analysis and algebra methods?
- Recall the 0th state:

$$\hat{a}_-|0\rangle \propto (\hat{x}+\mathrm{i}\hat{p})|0\rangle = \left(x+\frac{\mathrm{d}}{\mathrm{d}x}\right)|0\rangle = 0,$$

$$|0\rangle \propto \exp\left(-\frac{x^2}{2}\right).$$

Consistency

- To generate the higher states, apply the explicit form of ascending operator:

$$\left|n\right\rangle \propto \hat{a}_{+}\left|n-1\right\rangle \propto \left(x-\frac{\mathrm{d}}{\mathrm{d}x}\right)\left|n-1\right\rangle$$

- The n^{th} state have form:

$$\left|n\right\rangle \propto \exp\left(-\frac{x^2}{2}\right)\cdot\sum_{i=0}^{n}a_i x^i$$

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Consistency

- In which the coefficients satisfies:

$$a_{i+2} = \frac{2i-2n}{(i+2)(i+1)} a_i$$

- Do the ascending operator:

$$|n+1\rangle \propto \exp\left(-\frac{x^2}{2}\right) \cdot \sum_{i=0}^{n+1} b_i x^i$$

$$b_i = 2a_{i-1} - (i+1)a_{i+1}$$

$$= 2a_{i-1} - \frac{2i-2-2n}{i} a_{i-1}$$

$$= \frac{2n+2}{i} a_{i-1}$$

$$b_{i+2} = \frac{2n+2}{i+2} a_{i+1} = \frac{2n+2}{i+2} \frac{2i-2-2n}{(i+1)i} a_{i-1} = \frac{2i-2(n+1)}{(i+2)(i+1)} b_i$$

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Hermite Polynomials

- Hermite polynomials are defined as the cutoff polynomials in the solution.

$$\psi_n(x) = \exp\left(-\frac{x^2}{2}\right) \cdot \mathrm{H}_n(x)$$

- We have already known some methods to derivatize Hermite polynomials, namely recurrence formulae of coefficients and explicit ascending operator.
- Here we are introducing some other methods.

Recurrence Formulae in series

- Recall that we need a_0 and a_1 to iterate for one polynomial, which indicates two initial expressions are needed for the recurrence, we are assigning that:

$$\mathrm{H}_0(x)=1,\mathrm{H}_1(x)=2x.$$

$$\left(x-\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_{n-1}(x)\right)=\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_n(x)$$

$$x-\frac{\mathrm{d}}{\mathrm{d}x}=\hat{x}-\mathrm{i}\hat{p}=\sqrt{2}\hat{a}_+$$

$$\hat{a}_-\hat{a}_+\left(\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_{n-1}(x)\right)=n\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_{n-1}(x)$$

$$\frac{1}{2}\left(x+\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(x-\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_{n-1}(x)\right)=n\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_{n-1}(x)$$

$$\left(x+\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_n(x)\right)=2n\exp\left(-\frac{x^2}{2}\right)\cdot\mathrm{H}_{n-1}(x)$$

Recurrence Formulae in series

$$\left(x-\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(x-\frac{\mathrm{d}}{\mathrm{d}x}\right)\left(\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_{n-2}(x)\right)=\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_n(x)$$

$$x\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_{n-1}(x)-\frac{\mathrm{d}}{\mathrm{d}x}\left(\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_{n-1}(x)\right)=\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_n(x)$$

$$2x\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_{n-1}(x)-2(n-1)\left(\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_{n-2}(x)\right)=\exp\left(-\frac{x^2}{2}\right)\cdot \mathrm{H}_n(x)$$

$$\mathrm{H}_n(x)-2x\mathrm{H}_{n-1}(x)+2(n-1)\mathrm{H}_{n-2}(x)=0$$

Hermite Polynomials

- Some low order Hermite polynomials:

$$
\begin{aligned}
&\mathrm{H}_0(x) = 1,\\
&\mathrm{H}_1(x) = 2x,\\
&\mathrm{H}_2(x) = 4x^2 - 2,\\
&\mathrm{H}_3(x) = 8x^3 - 12x,\\
&\mathrm{H}_4(x) = 16x^4 - 48x^2 + 12,\\
&\ldots
\end{aligned}
$$

Orthogonality

- Due to the orthogonality of wave functions, we can easily derive the orthogonality for Hermite polynomials:

$$\int_{-\infty}^{+\infty} \mathrm{d}x \mathrm{H}_m(x) \mathrm{H}_n(x) \exp\left(-x^2\right) = N_n^2 \delta_{mn}$$

- Here, δ_{mn} is called Kronecker delta.
- This orthogonality is not very conventional, in fact, this is a weighted orthogonality with a weight $\exp(-x^2)$.

Normalization

- To obtain orthonormal eigenstates, we have to calculate norm squares of each states:
- But…we have to first calculate integrals of such terms:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, x^{2n} \exp\left(-x^2\right)$$

- There is no need to calculate the odd power terms, because they vanish.

Normalization

- We first calculate the simplest:

$$
\begin{aligned}
&\int_{-\infty}^{+\infty} \mathrm{d}x \exp\left(-\lambda x^2\right) \\
&= \sqrt{\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} \mathrm{d}x\mathrm{d}y \exp\left(-\lambda\left(x^2+y^2\right)\right)} \\
&= \sqrt{\int_0^{2\pi} \mathrm{d}\varphi \int_0^{+\infty} \mathrm{d}r\ r \exp\left(-\lambda r^2\right)} \\
&= \sqrt{\frac{\pi}{\lambda}}
\end{aligned}
$$

Normalization

- Recurrence relationship for higher power:

$$G_{2n} := \int_{-\infty}^{+\infty} \mathrm{d}x\ x^{2n} \exp\left(-\lambda x^2\right)$$

$$= -\frac{\partial}{\partial \lambda} \int_{-\infty}^{+\infty} \mathrm{d}x\ x^{2n-2} \exp\left(-\lambda x^2\right);$$

$$G_0 = \sqrt{\frac{\pi}{\lambda}},$$

$$G_{2n} = \sqrt{\frac{\pi}{\lambda}} \frac{(2n-1)!!}{(2\lambda)^n}$$

Dimension Recovery

- What is the dimension of the desired quantity?
- Simply time it up.

To be continued…

- Rodriguez's formula
- Generating function
- Et cetera