量子力学笔记

——Griffiths

xtcution

2023 年 1 月 10 日

前言

两年前的笔记，只写了前两章

争取今年都写到微扰

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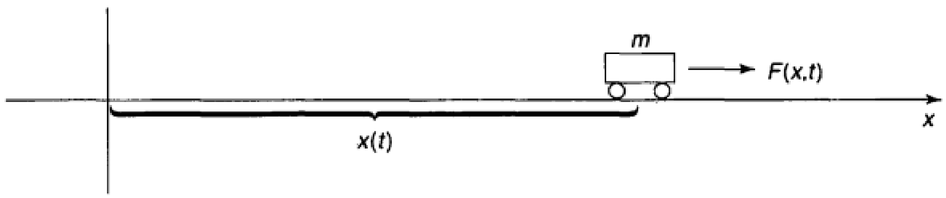
目录

第一章　波函数

1.1　THE schrodinger equation

在牛顿力学中是考虑 $F(x,t)$ 如图



我们可以确定他的　$x(t)$　　$v=\frac{dx}{dt}$　　$p=mv$　　$T=\frac{1}{2}mv^2$

From Newton's scond law:

$$F=ma$$

Under the conservative force Newton's las reads

$$F=-\frac{\partial V}{\partial x} \quad \Rightarrow \quad -\frac{\partial V}{\partial x}=m\frac{d^2x}{dt^2}$$

Quantum Mechanics approaches this same problem quite differently.In this case , we're looking for is the **wave function** $\Psi(x,t)$,and we get it by solving the **Schrodinger equation** :

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V\Psi \qquad \hbar=\frac{h}{2\pi}$$

Schrodinger Equation$\Rightarrow\Psi(x,t)$

1.2 The Statistical Interpretation

What exactly is thes ”wave function”?How can such an object represent the state of a particle?The answer is provided by Born’s **STATISTICAL INTERPRETATION** of the wave function,which says that $|\Psi(x,t)|^2$ gives the probability of finding the particle at point x , at time t on more precisely

$$\int_a^b |\Psi(x,t)|^2 dx = \left\{ \begin{array}{c} \text{probability of finding the particle} \\ \text{between } a \text{ and } b \text{ , at time } t. \end{array} \right\} \tag{1.1}$$

1.3 Probability

1.3.1 引入符号

最概然就是概率最大

平均年龄

$$\langle j\rangle = \frac{\sum jN(j)}{N} = \sum j\frac{N(j)}{N} = \sum jP(j) \tag{1.2}$$

平均的（年龄的平方）

$$\langle j^2\rangle = \sum j^2 P(j) \tag{1.3}$$

j 的函数 $f(j)$

$$\langle f(j)\rangle = \sum f(j)P(j) \tag{1.4}$$

构造 $\langle \Delta j \rangle$

$$\begin{aligned}\langle \Delta j \rangle = \langle j - \langle j \rangle \rangle &= \sum (j - \langle j \rangle) P(j) \\ &= \sum jP(j) - \sum \langle j \rangle P(j) \\ &= \underline{\sum jP(j)^1} - \langle j \rangle \sum P(j) \\ &= \langle j \rangle - \langle j \rangle = 0\end{aligned} \tag{1.5}$$

下划线处为(1.2)代入可得

最后算得 $\langle \Delta j \rangle$ 为 0，结果无意义，取模可以解决，但是由于复数取模是非解析，我们希望得到解析的故此通过平方来解决构造：

$$\begin{aligned}&\sigma^2 \equiv \left\langle (\Delta j)^2 \right\rangle = \langle (j - \langle j \rangle)^2 \rangle = \sum ((j - \langle j \rangle)^2) P(j) \\ &= \sum (j^2 + \langle j \rangle^2 - 2j \langle j \rangle) P(j) = j^2 + \langle j \rangle^2 - 2j - \langle j \rangle P(j) \\ &= j^2 + \langle j \rangle^2 - 2 \langle j \rangle \sum jP(j) = j^2 + \langle j \rangle^2 - 2 \langle j \rangle \langle j \rangle \\ &= j^2 - \langle j \rangle^2\end{aligned} \tag{1.6}$$

我们把 σ 称为标准差，σ^2 为方差

$$\sigma = \sqrt{j^2 - \langle j \rangle^2} \geq 0 \Rightarrow j^2 \langle j \rangle^2 \tag{1.7}$$

and the two are equal only when $\sigma = 0$, which is to say, for distributions with no spread at all (every member having the same value).

1.3.2 Continuous Variables

$P(x + dx, t) = \rho(x, t) dx$ ，$\rho(x, t)$ 为概率密度

$$1 = \int_{-\infty}^{+\infty} \rho(x) dx \tag{1.8}$$

$$\langle x \rangle = \int_{-\infty}^{+\infty} x\rho(x)dx \tag{1.9}$$

$$\langle f(x) \rangle = \int_{-\infty}^{+\infty} f(x)\rho(x)dx \tag{1.10}$$

$$\sigma^2 \equiv \left\langle (\Delta x)^2 \right\rangle = \left\langle x^2 \right\rangle - \langle x \rangle^2 \tag{1.11}$$

1.4 Normalization

We return now to the statistical interpretation of the wave function (Equation (1.2)), which says that $|\Psi(x,t)|^2$ is the probability density for finding the particle at point x, at time t. It follows (Equation (**??**)) that the integral of $|\Psi|^2$ must be 1 (the particle's got to be some where):

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1 \qquad \text{为什么会为 1?} \tag{1.12}$$

$$\rho(x,t) = |\phi(x,t)|^2 2 \tag{1.13}$$

$$\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \tag{1.14}$$

$\phi(x,t)$ 是基解$\Rightarrow$　A$\phi(x,t)$ 线性组合也是解系数 A 由归一化决定

对于数学上的解:

(1)积分发散　　$\nexists A$　　A 不存在

(2)$\phi \equiv 0$　　$\nexists A$　　这种解不物理，是数学上的解

所以在物理上的解不仅要满足 Schrodinger 方程，还要满足平方可积

$$\boxed{\text{平方可积} \qquad |x| \to \infty\text{时} \qquad \phi(x,t)\sqrt{|x|} \to 0} \tag{1.15}$$

A 是复数可以写成 $Ae^{i\theta}$,下面证明 $\frac{\partial}{\partial x}A = 0$ A 不随时间变化 $\frac{d}{dt}\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx$ 不随时间变化

Proof:

$$\frac{d}{dt}\int_{-\infty}^{+\infty} |\psi(x,t)|^2 dx = \int_{-\infty}^{+\infty} \frac{\partial}{\partial t}|\psi(x,t)|^2 dx \tag{1.16}$$

$$\frac{\partial}{\partial t}|\psi|^2 = \frac{\partial}{\partial t}(\psi^*\psi) = \psi^*\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi \tag{1.17}$$

$$\frac{\partial \psi}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \psi}{\partial x^2} - \frac{i}{\hbar}V\psi \tag{1.18}$$

and hence also

$$\frac{\partial \psi^*}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + \frac{i}{\hbar}V\psi^* \tag{1.19}$$

Equation(1.4)$\cdot\psi^*$ + Equation (1.19)$\cdot\psi$

$$\psi^*\frac{\partial \psi}{\partial t} + \frac{\partial \psi^*}{\partial t}\psi = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi\right) = \frac{i\hbar}{2m}\underline{(\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi)} \tag{1.20}$$

对于划线部分

$$\psi^*\frac{\partial^2 \psi}{\partial x^2} - \frac{\partial^2 \psi^*}{\partial x^2}\psi = \frac{\partial}{\partial x}(\psi^*\frac{\partial \psi}{\partial t} - \frac{\partial \psi^*}{\partial t}\psi) \tag{1.21}$$

The integral in Equation (1.16) can now be evaluated explicitly:

$$\frac{d}{dt}\int_{-\infty}^{+\infty}|\psi(x,t)|^2 dx = \int_{-\infty}^{+\infty}\frac{\partial}{\partial x}(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi) = \frac{i\hbar}{2m}\left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\Bigg|_{-\infty}^{+\infty} \tag{1.22}$$

$$\Rightarrow \left(\psi^*\frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\Bigg|_{-\infty}^{+\infty} \tag{1.23}$$

think about Equation (1.15), when x goes to ∞, $\psi(x,t)\cdot\sqrt{x} \to 0$ S.T $\psi(x,t) \to 0$

$$\boxed{\frac{d}{dt}\int_{-\infty}^{+\infty}|\Psi(x,t)|^2 dx = 0} \tag{1.24}$$

and hence that the integral is constant (independent of time); if Ψ is normalized at $t = 0$, it stays normalized for all future time. QED

1.4.1 Momentum

For a particle in stateΨ,the expectation value of x is

$$\langle x \rangle = \int_{-\infty}^{+\infty} x|\Psi(x,t)|^2 dx \tag{1.25}$$

$$\frac{d\langle x\rangle}{dt}=\int x\frac{\partial}{\partial t}|\Psi|^2dx=\frac{i\hbar}{2m}\int x\underline{\frac{\partial}{\partial x}\left(\Psi^*\frac{\partial\Psi}{\partial x}-\frac{\partial\Psi^*}{\partial x}\Psi\right)}dx \tag{1.26}$$

下划线的部分是根据 Equation(1.20)，之后凑出下划线的部分。随后再进行分部积分，把 $\frac{\partial\Psi^*}{\partial x}$ 拿到 dx 中

$$\int\frac{i\hbar}{2m}\psi\frac{\partial\psi^*}{\partial x}dx=-\int\frac{i\hbar}{2m}\psi^*\frac{\partial\psi}{\partial x}dx \tag{1.27}$$

$$\frac{d\langle x\rangle}{dt}=-\frac{i\hbar}{m}\int\Psi^*\frac{\partial\Psi}{\partial x}dx\quad\text{类比于}\quad\langle v\rangle=\frac{d\langle x\rangle}{dt} \tag{1.28}$$

所以写出

$$\langle p\rangle=m\frac{d\langle x\rangle}{dt}=-i\hbar\int\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)dx \tag{1.29}$$

Let me write the expressions for $\langle x\rangle$and $\langle p\rangle$ in a more suggestive way:

$$\langle x\rangle=\int\psi^*(x)\psi dx \tag{1.30}$$

$$\langle p\rangle=\int\psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\psi dx \tag{1.31}$$

$\hat{x}$ $\hat{p}$ 称为算符 (Operator)

$$\hat{p}=-i\hbar\frac{\partial}{\partial x}\quad\text{且算符作用在 }\psi\text{ 上，读出本征值} \tag{1.32}$$

看到动量想到动能

$$T=\frac{1}{2}mv^2=\frac{p^2}{2m} \tag{1.33}$$

所有经典力学量都可以表示为坐标和动量的函数 $\hat{Q}=\langle x,p\rangle$

$$\langle Q(x,p)\rangle=\int\psi^*Q\left(x,-i\hbar\frac{\partial}{\partial x}\right)\psi dx \tag{1.34}$$

第二章　定态 Schrodinger Equation

2.1　稳定态

如何求解 Schrodinger Equation?

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}+V\psi=i\hbar\frac{\partial\Psi}{\partial t} \tag{2.1}$$

设 $\psi=\psi(x)f(t)$ 代入到方程中

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2}f(t)+V\psi f(t)=i\hbar\psi\frac{\partial f(t)}{\partial t}\quad \text{(同除以 f 和 }\psi\text{)} \tag{2.2}$$

$$\underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2}+V}_{thefunctionofX}=\underbrace{i\hbar\frac{1}{f}\frac{\mathrm{d}f}{\mathrm{d}t}}_{thefunctionoft} \tag{2.3}$$

这两个式子相等且是对不同变量的倒数，则一定等于一个常数记为 E（注：$f\psi$ 不会为 0，因为波函数为 0 则粒子不可能出现在该点，无意义要去掉）

$$\text{记作}\qquad i\hbar\frac{1}{f}\frac{\mathrm{d}f}{\mathrm{d}t}=E \tag{2.4}$$

所以定态薛定谔方程（time independent schrodinger equation）可以写成

$$\boxed{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\partial^2\psi}{\partial x^2}+V=E} \tag{2.5}$$

随后可以解一下

$$i\hbar\frac{1}{f(t)}\frac{\mathrm{d}f(t)}{\mathrm{d}t}=E(E\text{ 是一个常实数}) \tag{2.6}$$

$$\frac{1}{f(t)}\frac{\mathrm{d}f}{\mathrm{d}t}=-\frac{i}{\hbar}E \quad \Rightarrow \quad f(t)=e^{\frac{-iEt}{\hbar}} \tag{2.7}$$

为什么要分离变量？

1. 稳定态，其中只看 ψ 来说没有意义，要看 $|\psi|^2$

$$\Psi(x,t)=\psi(x)=e^{-\frac{iEt}{\hbar}} \tag{2.8}$$

$$|\Psi(x,t)|^2=\psi(x)\psi(x)*=\psi(x)^2e^{-\frac{iEt}{\hbar}}e^{\frac{iEt}{\hbar}}=|\Psi(x)|^2 \tag{2.9}$$

取完模平方后，时间 t 消失，取模平方后不随时间变化，稳定的 $|\psi|^2$

我们还喜欢另一个量 本征值

$$\langle Q(x,p)\rangle=\int\psi^*Q\left(x,\frac{\hbar}{i}\frac{d}{dx}\right)\psi dx \tag{2.10}$$

也进行分离变量（分离变量 Equation(2.7)）

$$=\int\psi^*e^{\frac{iEt}{\hbar}}Q\left(x,\frac{\hbar}{i}\frac{d}{dx}\right)\psi e^{\frac{-iEt}{\hbar}}dx=\int\psi^*\hat{Q}(x,\frac{h\partial}{i\partial x})\psi e^{\frac{-iEt}{\hbar}}dx \tag{2.11}$$

$$=\int\psi*\hat{Q}(x,\frac{h\partial}{i\partial x})\psi dx \tag{2.12}$$

称 $\psi(x)$ 为波函数定态波函数 | 不含时波函数

总能量在 Classical mechanics Hamiltonian：

$$H(x,p)=\frac{p^2}{2m}+V(x) \tag{2.13}$$

$$\hat{H}(x,p)=-\frac{\hbar}{2m}\frac{\partial^2}{\partial x^2}+V(x) \qquad (\hat{H}\text{ 作用到 }\psi\text{ 上}) \tag{2.14}$$

$$\hat{H}(x,p)\psi=\underline{-\frac{\hbar}{2m}\frac{\partial^2\psi}{\partial x^2}+V(x)\psi}=i\hbar\frac{\partial\psi}{\partial t}(\text{刚好为 Eq(2.1)}) \tag{2.15}$$

$$f(t)=e^{\frac{-iEt}{\hbar}}\Rightarrow\frac{df}{dt}=-\frac{iE}{\hbar}e^{\frac{-iEt}{\hbar}}=-\frac{iE}{\hbar}f(t) \tag{2.16}$$

我们期望得到 $i\hbar\frac{\partial\psi}{\partial t}$ 所以

$$i\hbar\frac{\partial\Psi}{\partial t}=i\hbar\psi\frac{df(t)}{d}t=i\hbar\psi f(-\frac{iE}{\hbar})=E \tag{2.17}$$

$$i\hbar\frac{\partial\Psi}{\partial t}=E\psi \tag{2.18}$$

$$\hat{H}\psi=E\psi \tag{2.19}$$

$\hat{H}$ 读出了本征值 E，再看 $\hat{H}$ 平均数

$$\langle H\rangle=\int\psi^*\hat{H}\psi dx=E\int|\psi|^2dx=E\int|\Psi|^2dx=E \tag{2.20}$$

(Notice that the normalization of Ψ entails the nomalization of ψ)Moreover

$$\hat{H}^2\psi=\hat{H}(\hat{H}\psi)=\hat{H}(E\psi)=E(\hat{H}\psi)=E^2\psi \tag{2.21}$$

$$\langle H\rangle=\int\psi^*\hat{H}\psi dx=E\int|\psi|^2dx=E\int|\Psi|^2dx=E\left\langle H^2\right\rangle=\int\psi^* \tag{2.22}$$

and hence

$$\hat{H}^2\psi dx=E^2\int|\psi|^2dx=E^2 \tag{2.23}$$

So the variance of H is

$$\sigma_H^2=\left\langle H^2\right\rangle-\langle H\rangle^2=E^2-E^2=0 \tag{2.24}$$

Dirac required that all operators corresponding to mechanical quantities should be Hermitian operators, and the eigenvalues of a Hermitian operator must be real numbers （见田老师讲义定理 3.2 定理 3.3）

3.The general solution is a linear combination of separable solutions. As we're about to discover, the time-independent Schrodinger equation (Equation (2.1))yields an infinite collection of solutions $(\psi_1 x,\psi_2 x,\psi_3 x,..)$each withits associated value of the separation constant $(E1,E2,E3,...)$; thus there is a different wave function for each allowed energy:

$$\Psi_1(x,t)=\psi_1(x)e^{-iE_1t/\hbar},\quad \Psi_2(x,t)=\psi_2(x)e^{-iE_2t/\hbar},\ldots \tag{2.25}$$

The (time-dependent) Schrodingerequation(Equation 2.1) has the property that any linear combination of solutions is itself a solution.Once we have found the separable solutions,then，we can immediately construct a much more general solution, of the form

$$\boxed{\Psi(x,t)=\sum_{n=1}^{\infty}c_n\psi_n(x)e^{-iE_nt/\hbar}} \qquad \text{(定态薛定谔方程的通解)} \tag{2.26}$$

2.2　无限深方势阱

Suppose

$$V(x)=\begin{cases}0 & ,0\le x\le a\\ \infty & ,\text{otherwise.}\end{cases} \tag{2.27}$$

在 Classical Mechanics 是匀速周期运动

在 Quantum Mechanics :Outside the well,$\psi(x=0)$the probability of finding the particle here is zero.Inside the well

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \quad (E\text{ 取何值}E>0E<0E=0?) \tag{2.28}$$

其中 E<0 没有意义，因为总能量 < 势能最低点，根本不存在

$$\psi(x)=A\sin kx+B\cos kx \tag{2.29}$$

$$\psi(x=0)=A+B=0 \qquad \psi(x=a)=Ae^{\sqrt{2mEa/\hbar}}+Be^{-2mEa/\hbar}=0 \tag{2.30}$$

a 处也在井外概率为 0, 除一个 $e^{-2mEa/\hbar}$

$$A(e^{2\sqrt{2mEa/\hbar}}-1)=0 \tag{2.31}$$

所以只能 A=0 ，若 A=0 且 $A+B=0$ 则 B 为 0 ψ=0 不存在。同理若 E=0，则 $\psi=Ax+B$ 且 x,a 处有两个零点，则也恒为 0，A=0，B 为 0。所以 E 必须 >0 正且为常实数

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi \quad\Rightarrow\frac{d^2\psi}{dx^2}=-\frac{2mE}{\hbar^2}\psi=-k^2\psi,\quad \text{where } k\equiv\frac{\sqrt{2mE}}{\hbar} \tag{2.32}$$

$$\psi(x) = A\sin kx + B\cos kx \tag{2.33}$$

边界条件 $\psi(a) = 0$,$\psi(0) = 0$

$$\psi(0) = 0 + B = 0 \Rightarrow \psi(a) = Asinka = 0 \quad (A \neq 0) \quad \therefore sinka = 0$$

$sinka = 0 \quad \Rightarrow ka = n\pi \quad n = \emptyset, 1, 2, ...(n = 0$又是恒为零，所以不要)

根据 Equation(2.32)

$$k^2 = \frac{2mE}{\hbar} \Rightarrow k = \frac{\sqrt{2m}}{\hbar} \Rightarrow E = \frac{n^2\pi^2\hbar^2}{2ma^2}$$

我们本来想通过边界条件确定 A, B，结果确定的 E 且能量不是任意的，$E \propto n^2$ 才呈现量子效应。所以如何确定 A? 归一化

$$1 = \int_0^a |\psi(x)|^2 dx = \int_0^a |A|^2 \sin^2 \frac{n\pi k}{a} dx \tag{2.34}$$

$$= |A|^2 \int_0^a \frac{1 - \cos\frac{2n\pi x}{a}}{2} dx = \frac{a}{2}A^2 \Rightarrow A = \sqrt{\frac{2}{a}} \tag{2.35}$$

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right), \quad E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{2.36}$$

当 $n = 1$ 时

$$\psi_1 = \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a}, \quad E_1 = \frac{\pi^2\hbar^2}{2ma^2}$$

$n = 1$ 的态称为基态，$n > 1$ 的态成为激发态

总结 $\Psi_n(x)$ 的性质：

1. 她们对势阱中心（$x = a/2$）对称：ψ_1 偶,ψ_2 奇,ψ_3 偶,...

2.n→n+1　1　1

3.x_x 彼此正交（归一化）

$$\int \psi_{\mathrm{m}}^*(\mathrm{x})\psi_{\mathrm{n}}(\mathrm{x})dx = 0\begin{cases} \mathrm{n=m} & ,1 \\ \mathrm{n\neq m} & ,0. \end{cases} \tag{2.37}$$

Proof:

$$\begin{aligned} &\int \psi_{\mathrm{m}}^*(x)\psi_{\mathrm{n}}(x)dx = \tfrac{2}{a}\int_0^a \sin\left(\tfrac{m\pi}{a}x\right)\sin\left(\tfrac{\mathrm{n}\pi}{a}x\right)dx \\ &= \tfrac{1}{a}\int_0^a \left[\cos\left(\tfrac{m-n}{a}\pi x\right) - \cos\left(\tfrac{m+n}{a}\pi x\right)\right]dx \\ &= \left\{\tfrac{1}{(m-n)\pi}\sin\left(\tfrac{m-n}{a}\pi x\right) - \tfrac{1}{(m+n)\pi}\sin\left(\tfrac{m+n}{a}\pi x\right)\right\}\Big|_0^1 \\ &= \tfrac{1}{\pi}\left\{\tfrac{\sin[(m-n)\pi]}{(m-n)} - \tfrac{\sin[(m-n)\pi]}{(m-n)}\right\} = 0 \end{aligned} \tag{2.38}$$

由归一性可得积分等于 1，可将归一化和正交性写在一起：

$$\int \psi_m^*(x)\psi_n(x)dx = \delta_{mn} \tag{2.39}$$

4. 它们是完备的，任意一个函数 $f(x)$，可以用它们的线性叠加表示：

$$f(x) = \sum_{n=1}^{\infty} c_n\psi_n(x) = \sqrt{\frac{2}{a}}\sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a}x\right) \quad \text{（傅里叶级数完备）} \tag{2.40}$$

The coefficients c_n can be evaluated - for a given $f(x)$- by a method I call Fourier's trick, which beautifully exploits the orthonormality of $\{\psi_n\}$: Multiply both sides of Equation 2.38 by $\psi_m(x)^*$, and integrate.

$$\int \psi_m^*(x)f(x)dx = \sum^{\infty} c_n \int \psi_m^*(x)\psi_n(x)dx = \sum^{\infty} c_n\delta_{mn} = c_m \tag{2.41}$$

Kroneckerδ 只留下 $n=m$

$$c_n=\int \psi_{\mathrm{n}}^*(\mathrm{x}) f(x) d x \tag{2.42}$$

随时间演化:

$$\Psi(x, t)=\sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{a}} \sin \left(\frac{n \pi}{a} x\right) e^{-i\left(n^2 \pi^2 \hbar / 2 m a^2\right) t} . \tag{2.43}$$

记得补上

2.3 Harmonic Oscillaton 简谐振子

Hooke's Low ，解为

$$F=-k x=m \frac{d^2 x}{d t^2}\ x(t)=A \sin (\omega t)+B \cos (\omega t)$$

简谐振子势能为

$$V=\frac{1}{2} k x^2,(x \rightarrow \infty, V \rightarrow \infty)$$

但物理都会在平衡位置附近被破坏，实际中可以将 $V(x)$, 在极小值附近做泰勒展开

$$V(x)=V\left(x_0\right)+V^{\prime}\left(x_0\right)\left(x-x_0\right)+\frac{1}{2} V^{\prime \prime}\left(x_0\right)\left(x-x_0\right)^2+\cdots$$

$$V(x) \cong \frac{1}{2} V^{\prime \prime}\left(x_0\right)\left(x-x_0\right)^2$$

The quantum problem is to solve the Schrodinger equaton for the potential

$$V(x)=\frac{1}{2} \omega^2 x^2$$

As we have seen,it suffices to solve the time-independent Schrodinger equaiton:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi \tag{2.44}$$

2.3.1 Algebraic Method

$$\frac{1}{2m}\left[\hat{p}^2+(m\omega x)^2\right]\psi=E\psi,(\hat{p}=\frac{\hbar}{i}\frac{d}{dx}) \tag{2.45}$$

$$u^2+v^2=(u+iv))(u-iv)\quad(\text{暗含 } uv=vu)$$

The basic ieda is to $Factor$ the Hamiltonian

强制性写作 $u=\frac{\hbar}{i}\frac{d}{dx}$, $v=m\omega x$

$$a_\pm\equiv\frac{1}{\sqrt{2\hbar m\omega}}(\mp ip+m\omega x)\quad(a+=a\dagger,a-=a)$$

$$=\frac{1}{2m}(\frac{\hbar}{i}\frac{d}{dx}-im\omega x)(\frac{\hbar}{i}\frac{d}{dx}+im\omega x) \tag{2.46}$$

aa†$aa\dagger f(x)=\frac{1}{2m}(\frac{\hbar}{i}\frac{d}{dx}-im\omega x)(\frac{\hbar}{i}\frac{d}{dx}+im\omega x)f(x)$

$$aa\dagger f(x)=\frac{1}{2m}(-\hbar^2\frac{d^2f(x)}{dx^2}+m^2\omega^2x^2f(x)-m^2\omega^2x^2f(x)+m^2\omega x^2f(x)f(x))$$

$$=\frac{1}{2m}(-\hbar^2\frac{d^2f(x)}{dx^2}+m\omega^2\hbar xf(x)-m\omega^2\hbar xf(x)+m^2\omega^2x^2f(x)f(x))$$

$$=\frac{1}{2m}(-\hbar^2\frac{d^2f(x)}{dx^2}+m^2\omega x^2f(x)f(x)i-im\omega(\hat{x}\hat{p}-\hat{p}\hat{x}))\quad(\hat{x}\hat{p}\psi-\hat{p}\hat{x}\psi=i\hbar\psi)$$

$$=\frac{1}{2m}-\hbar^2\frac{d^2f(x)}{dx^2}+\frac{1}{2}m\omega x^2f(x)f(x)i+\frac{1}{2}\omega\hbar f(x)=E+\frac{1}{2}\hbar\omega$$

故此 Equation (2.46)可以写成

$$a\dagger a = E - \frac{1}{2}\hbar\omega, \qquad aa\dagger = E + \frac{1}{2}\hbar\omega$$

$$a\dagger a - aa\dagger = -\hbar\omega$$

$$(a\dagger a + \frac{1}{2}\hbar\omega\psi) = E\psi$$

Proof:Now, here comes the crucial step: I claim that if ψ satisfies the Schrödinger equation with energy E , (that is: $H\psi = E\psi$) , then $a_+\psi$ satisfies the Schrödinger equation with energy $(E + \hbar\omega)$: $H\left(a_+\psi\right) = \left(E + \hbar\omega\right)\left(a_+\psi\right)$.

设 $E' = E + \hbar\omega$,$a\dagger\psi = \psi'$

$$\begin{aligned} H\left(a\dagger\psi\right) &= \hbar\omega\dagger a(a + \frac{1}{2})\left(a\dagger\psi\right) = \hbar\omega\left(a\dagger aa\dagger + \frac{1}{2}a\dagger\right)\psi \\ &= \hbar\omega a\dagger\left(aa\dagger + \frac{1}{2}\right)\psi = a\dagger\left[\hbar\omega\left(a\dagger a + 1 + \frac{1}{2}\right)\psi\right] \\ &= a\dagger(H + \hbar\omega)\psi = a\dagger(E + \hbar\omega)\psi = (E + \hbar\omega)\left(a\dagger\psi\right) \end{aligned}$$

所以 $a\dagger\psi = \psi'$ 也是解，且 $E' = E + \hbar\omega$ $a\dagger$ 是升算符，a 是减算符，指定最低态，$a\psi_0 = 0$

$$\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0, \psi_0 = A_0e^{-m\omega x^2/2\hbar} \quad \text{代入薛定谔方程}$$

得 $E_0 = \frac{1}{2}\hbar\omega, \psi_n(x) = A_n a\dagger^n\psi_0, E_n = (n+1)\hbar\omega$

例题

$$\begin{aligned} \psi_1(x) = A_1 a\dagger\psi_0 &= \frac{A_1}{\sqrt{2\hbar m\omega}}\left(-\hbar\frac{d}{dx} + m\omega x\right)\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2} \\ &= A_1\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\sqrt{\frac{2m\omega}{\hbar}}xe^{-\frac{m\omega}{2\hbar}x^2} \end{aligned} \tag{2.47}$$

2.3.2 Analytic Method

做几个变量代换

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2 x^{a2}\psi=E\psi$$

令 $\xi\equiv\sqrt{\frac{m\omega}{\hbar}}x$ 得

$$\frac{d^2\psi}{d\xi^2}=\left(\xi^2-K\right)\psi,\quad K=\frac{2E}{\hbar\omega} \tag{2.48}$$

用幂级数解常微分方程，先讨论极限条件:

1.ξ 很大时，

$$\frac{d^2\psi}{d\xi^2}=\xi^2\psi,\psi()=Ae^{\frac{-\xi^2}{2}}+Be^{\frac{\xi^2}{2}}$$

因为归一化，B 项消掉，不然为无穷大,$\psi(x)$ 改为

$$\psi(x)=h(\xi)e^{-\frac{\xi^2}{2}}\quad ,\text{使用常数变易法} \tag{2.49}$$

$$\psi(x)=(\frac{dh(\xi)}{d\xi}-h(\xi)\xi)e^{-\frac{\xi^2}{2}}$$

$$\psi(x)=(\frac{d^2h(\xi)}{d\xi^2}-2\xi\frac{dh(\xi)}{d\xi}+(\xi^2-1)h)e^{-\frac{\xi^2}{2}}(\text{带回薛定谔})$$

$$\frac{d^2h}{d\xi^2}-2\xi\frac{dh}{d\xi}+(K-1)h=0 \tag{2.50}$$

上式一定可以用级数进行求解，设

$$h(\xi)=a_0+a_1\xi+a_2\xi^2+\cdots=\sum_{j=0}^{\infty}a_j\xi^j$$

and

$$\frac{dh}{d\xi}=a_1+2a_2\xi+3a_3\xi^2+\cdots=\sum_{j=0}^{\infty}ja_i\xi^{j-1}$$

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2\cdot 3a_3\xi + 3\cdot 4a_4\xi^2 + \cdots = \sum_{j=0}^{\infty}(j+1)(j+2)a_{j+2}\xi^j$$

$$\sum_{j=0}^{\infty} = \left[(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j\right]\xi^j = 0$$

代入得

$$\sum_{j=0}^{\infty} = [(j+1)(j+2)a_{j+2} - 2ja_j + (K-1)a_j]\xi^j = 0$$

$$aj_{j+2} = \frac{2j+1-K}{(j+1)(j+2)}a_j = 0$$

This fecursion formula is entirely equivalent to the Schrodinger equation. 接下来用 a^j 推出 a^{j+2}

$$h^{even} = a^0 + a^2\xi^2 + a^4\xi^4 + ...$$

$$h^{even} = a^1 + a^3\xi^3 + a^5\xi^5 + ...$$

当 j 很大时，公式可以近似写成

$$a^{j+2} \approx \frac{2}{j}a^j \qquad a^j \approx \frac{c}{(j/2)!}$$

则

$$h(\xi) \approx C\sum_{j\in even}\frac{1}{(j/2)!}\xi^j \tag{2.51}$$

用 k 代替 $j/2$(因为 j 是偶数)

$$h(\xi) \approx C\sum_{k=0}\frac{1}{(k)!)}\xi^{2k} \tag{2.52}$$

由 Equantion (2.49)和 2.52 可知

$$\psi = Ce^{\xi^2/2} \tag{2.53}$$

因为发散, 所以截断, 不然无法归一化。所以 $\exists j_{max} = n, a_{n+2} = 0, E_n$ 代入, 且 Equation (2.48)要求 $K = 2n+1$, 能量为

$$E_n = (n+1/2)\hbar\omega$$

对允许得 K，递归公式为

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)}a_j = 0 \tag{2.54}$$

$n = 0, a_1 = 0, j = 0$ 时

$$h_0(\xi) = a_0$$

$$\psi_0(\xi) = a_0 e^{-\xi^2/2}$$

$n = 1, a_0 = 0, j = 1$ 时

$$h_1(\xi) = a_1\xi$$

$$\psi_1(\xi) = a_1 e^{-\xi^2/2}$$

称其为 Hermite polynomial $h_n(\xi) = a_{01}\,\xi = H_n(\psi)$ 所以归一化因子为

$$\psi_n(x) = (\frac{m\omega}{\pi\hbar}^{1/4})\frac{1}{\sqrt{2^n n!}}H_n(\xi)e^(-\xi^2/2) \tag{2.55}$$

前提是如下

$$
\begin{aligned}
H_0 &= 1 \\
H_1 &= 2\xi \\
H_2 &= 4\xi^2 - 1 \\
H_3 &= 8\xi^3 - 12\xi \\
H_4 &= 16\xi^4 - 48\xi^2 + 12, \\
H_5 &= 32\xi^5 - 160\xi^3 + 120\xi.
\end{aligned}
\tag{2.56}
$$