Quantum Computing +X HW4 房伯文 2024010794

【1】

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x) \qquad |\psi\rangle = Ae^{-\lambda x^2}$$

$$\langle\psi|H|\psi\rangle = \int_{-\infty}^{+\infty} A^2 e^{-\lambda x^2}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \alpha x^4\right)e^{-\lambda x^2}dx$$

$$= \int_{-\infty}^{+\infty} A^2 e^{-2\lambda x^2}\left[\alpha x^4 - \frac{\hbar^2}{2m}\cancel{(-2\lambda)(x+1)}\,(4\lambda^2x^2 - 2\lambda)\right] dx$$

$$= A^2\int_{-\infty}^{+\infty} e^{-2\lambda x^2}\left[\alpha x^4 - \frac{2\hbar^2\lambda^2}{m}x^2 + \frac{\hbar^2\lambda}{m}\right] dx$$

We know that

$$\int_{-\infty}^{+\infty} e^{-x^2}dx = \sqrt{\pi}, \quad \int_{-\infty}^{+\infty} e^{-ax^2}dx = \sqrt{\frac{\pi}{a}}, \quad a>0$$

$$\int_{-\infty}^{+\infty} e^{-ax^2}x^2 dx = \frac{1}{2a}\int_{-\infty}^{+\infty} e^{-ax^2}x\, d(ax^2)$$

$$= \frac{1}{2a}(-1)\left[e^{-ax^2}x\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} e^{-ax^2}dx\right]$$

$$= \frac{1}{2a}\sqrt{\frac{\pi}{a}}$$

$$\int_{-\infty}^{+\infty} e^{-ax^2}x^4 dx = \frac{1}{2a}\int_{-\infty}^{+\infty} e^{-ax^2}x^3\, d(ax^2)$$

$$= \frac{1}{2a}(-1)\left[e^{-ax^2}x^3\Big|_{-\infty}^{+\infty} - \int_{-\infty}^{+\infty} e^{-ax^2}dx^3\right]$$

$$= \frac{3}{2a}\int_{-\infty}^{+\infty} e^{-ax^2}x^2 dx$$

$$= \frac{3}{4a^2}\sqrt{\frac{\pi}{a}}$$

$$\therefore \langle\psi|H|\psi\rangle = A^2\left[\alpha\frac{3}{16\lambda^2}\sqrt{\frac{\pi}{2\lambda}} - \frac{2\hbar^2\lambda^2}{m}\frac{1}{4\lambda}\sqrt{\frac{\pi}{2\lambda}} + \frac{\hbar^2\lambda}{m}\sqrt{\frac{\pi}{2\lambda}}\right]$$

$$= A^2 \cancel{\alpha\frac{3\sqrt{\pi}}{16}\lambda^{-\frac{5}{2}} - \frac{2\hbar\sqrt{\pi}}{m}}$$
$$\sqrt{\frac{\pi}{2\lambda}}\left[\frac{3}{16}\alpha\frac{1}{\lambda^2} + \frac{\hbar^2}{2m}\lambda\right]$$

$$\langle\psi|\psi\rangle = A^2\int_{-\infty}^{+\infty} e^{-2\lambda x^2}dx$$

$$= A^2\sqrt{\frac{\pi}{2\lambda}}$$

$$E(\lambda) = \left[\frac{3}{16}\alpha\frac{1}{\lambda^2} + \frac{\hbar^2}{2m}\lambda\right]$$

$$= \left[\frac{3}{16}\alpha\frac{1}{\lambda^2} + \frac{\hbar^2}{4m}\lambda + \frac{\hbar^2}{4m}\lambda\right]$$

$$\geq 3\sqrt[3]{\frac{3}{16}\alpha\left(\frac{\hbar^2}{4m}\right)^2}$$

$$= \frac{3}{4}\sqrt[3]{\frac{3\alpha\hbar^4}{4m^2}}$$

The equations holds when

$$\frac{3}{16}\alpha\frac{1}{\lambda^2} = \frac{\hbar^2}{4m}\lambda$$

$$\Rightarrow \lambda^3 = \frac{3m\alpha}{4\hbar^2} \qquad \lambda = \sqrt[3]{\frac{3m\alpha}{4\hbar^2}}$$

【2】

Please See the code loaded up to the github repo

【3】 $m(x,y) = 8x + 12y + x^2 - 2y^2$

(a) Since the function is analytic

$$\begin{cases} \frac{\partial m}{\partial x} = 0 \Rightarrow x = -4 \\ \frac{\partial m}{\partial y} = 0 \Rightarrow y = 3 \end{cases}$$

At this point,

$$m(x,y) = (x+4)^2 - 2(y-3)^2 + 2$$

It's obvious that on x direction. $(-4,3)$ is a minimum point, while on y direction. $(-4,3)$ is a maximum point

$\Rightarrow (-4,3)$ is a saddle point

(b) ~~We have already know~~
We know that $(-4,3)$ is not the best point

let

$g(x,y) = 8x+12y+x^2-2y^2+\lambda(x^2+y^2-25)$

$$\begin{cases} \frac{\partial g}{\partial x} = 8+2x+2\lambda x = 0 \\ \frac{\partial g}{\partial y} = 12-4y+2\lambda y = 0 \\ \frac{\partial g}{\partial \lambda} = x^2+y^2-25 = 0 \end{cases}$$

$\Rightarrow x = -\frac{4}{\lambda+1} \quad y = \frac{-6}{\lambda-2}$

$\left(\frac{4}{\lambda+1}\right)^2 + \left(\frac{6}{\lambda-2}\right)^2 = 25$

$16(\lambda^2-4\lambda+4)+36(\lambda^2+2\lambda+1) = 25(\lambda^2+2\lambda+1)\cdot(\lambda^2-4\lambda+4)$

$\cancel{\Rightarrow 25\lambda^4-50\lambda^3-127\lambda^2}$

solving the problem using computer

$\lambda \approx 3.222$

$(x,y) \approx (-0.947, -4.909)$

The direction of gradient descent method is given by

$\cancel{\frac{\partial m}{\partial x}(0,0) = 8 \quad \frac{\partial m}{\partial y}(0,0)}$

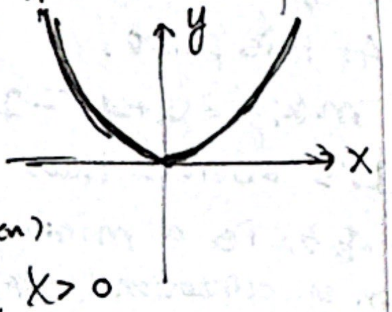
$\nabla m(0,0) = (8, 12)$

$\therefore$ the gradient direction is

$-\nabla m(0,0) = (-2,-3)$

these two are different

[4] $f(x) = |x|^{3/2}$



$x_{n+1} = x_n - \alpha f'(x_n)$

$$f'(x) = \begin{cases} \frac{3}{2}\sqrt{x}, & x>0 \\ \cancel{\frac{3}{2}\sqrt{|x|}}\ -\frac{3}{2}\sqrt{-x}, & x<0 \end{cases}$$

If $x_n > 0$

$x_{n+1} = x_n - \alpha \frac{3}{2}\sqrt{x_n}$

we just let x_{n+1} & x_n to be symmetric regarding y axis

$\cancel{-t = t - \alpha \frac{3}{2}\sqrt{t}}$

$-x^* = x^* - \alpha \frac{3}{2}\sqrt{x^*}$

$\Rightarrow x^* = \left(\frac{3}{4}\alpha\right)^2$, this is a pair of stationary points that will generate the sequence

$x^* \to -x^* \to x^* \to -x^* \to \cdots$

and will not converge

[5] & [6]

Please refer to the code