计算物理第三次作业

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Question 1 ▷ Numerical Solution of 1D Schrödinger Equation

1. $V(x)=\frac{1}{2}m\omega^2x^2$, 对比数值结果与解析结果, 体会误差的来源、大小, 以及误差与 L,N,h 的关系 ($h=L/N$).
2. $V(x)=\frac{1}{2}m\omega^2x^2+A\cos(kx+\theta)$
   (a) 数值求解;
   (b) 微扰计算，MMA算到二阶.

Solution

1.

Schrödinger方程为

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2\right]\psi(x)=E\psi(x)$$
$$\Downarrow \tag{1}$$
$$\left[-\frac{1}{2}\frac{\hbar}{m\omega}\frac{\partial^2}{\partial x^2}+\frac{1}{2}\frac{m\omega}{\hbar}x^2\right]\psi(x)=\frac{E}{\hbar\omega}\psi(x)$$

无量纲化: 令$E=E'\times\hbar\omega$, $x=x'\times\sqrt{\frac{\hbar}{m\omega}}$, x'和E'分别是无量纲长度和无量纲能量. 则无量纲化后的Schrödinger方程为

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial(x')^2}+\frac{1}{2}(x')^2\right]\psi(x')=E'\psi(x'). \tag{2}$$

为求符号上的简洁, 我们接下来用x和E来代替x'和E', 只需记得它们其实是无量纲的即可:

$$\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}x^2\right]\psi(x)=E\psi(x). \tag{3}$$

设求解范围为$\left[-\frac{L}{2},\frac{L}{2}\right]$, 做离散化: $x_i=-\frac{L}{2}+ih$ ($h=L/N, i=0,1,2,\cdots,N$), 则

$$\begin{aligned}\psi(x)\Big|_{x=x_i}&\rightarrow\psi_i=\psi(x_i)\\ \frac{\partial^2}{\partial x^2}\psi(x)\Big|_{x=x_i}&\rightarrow\frac{\psi_{i+1}+\psi_{i-1}-2\psi_i}{h^2}.\end{aligned} \tag{4}$$

因此, 离散化后的Schrödinger方程可写为

$$-\frac{1}{2h^2}(\psi_{i+1}+\psi_{i-1}-2\psi_i)+\frac{1}{2}x_i^2\psi_i=E\psi_i, \tag{5}$$

考虑进端点处的特殊情况后, 可用矩阵的形式写成方程组

$$\left[-\frac{1}{2h^2}\begin{pmatrix}-2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2\end{pmatrix}+\frac{1}{2}\begin{pmatrix}x_0^2 & & & & & \\ & x_1^2 & & & & \\ & & x_2^2 & & & \\ & & & \ddots & & \\ & & & & x_{N-1}^2 & \\ & & & & & x_N^2\end{pmatrix}\right]\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{pmatrix}=E\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{pmatrix}. \tag{6}$$

令

$$H=-\frac{1}{2h^2}\begin{pmatrix}-2 & 1 & & & & \\ 1 & -2 & 1 & & & \\ & 1 & -2 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & -2 & 1 \\ & & & & 1 & -2\end{pmatrix}+\frac{1}{2}\begin{pmatrix}x_0^2 & & & & & \\ & x_1^2 & & & & \\ & & x_2^2 & & & \\ & & & \ddots & & \\ & & & & x_{N-1}^2 & \\ & & & & & x_N^2\end{pmatrix}, \quad \boldsymbol{\psi}=\begin{pmatrix}\psi_0\\ \psi_1\\ \psi_2\\ \vdots\\ \psi_{N-1}\\ \psi_N\end{pmatrix}, \tag{7}$$

则有

$$H\boldsymbol{\psi}=E\boldsymbol{\psi}, \tag{8}$$

问题转化为求解三对角厄米矩阵H的本征值和本征向量.

使用python科学计算包scipy的函数 **scipy.linalg.eig_banded** 可以求解带对角厄米阵的本征值和本征向量.

```python
import numpy as np
from numpy import cos, pi
from scipy.linalg import eig_banded
L = 20; N = 20000; h = L/N;
x = np.array([ -L/2 + i*h for i in range(N+1) ])
V = x**2 / 2
```

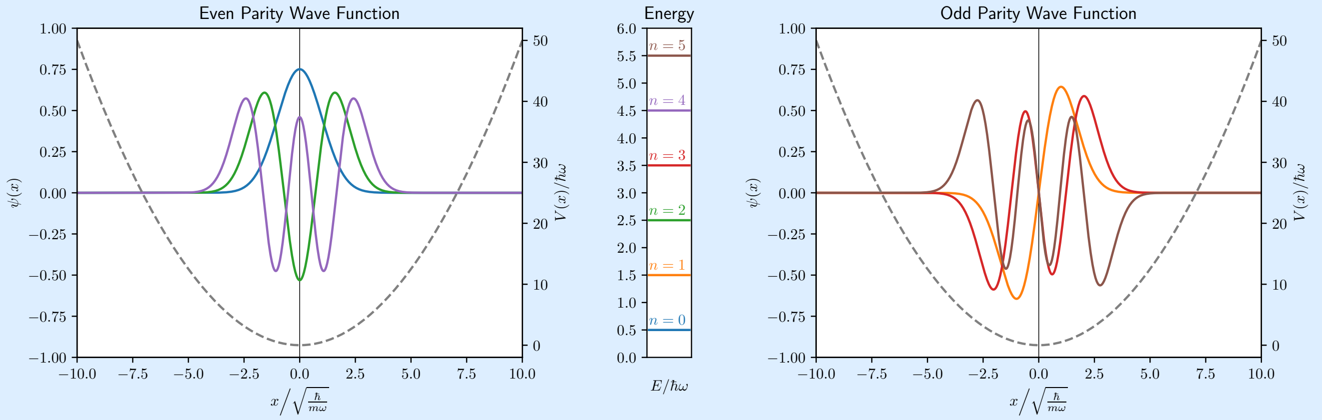
为了针对带对角厄米阵的特点来降低空间复杂度, 函数 **scipy.linalg.eig_banded** 使用带对角厄米阵M对应的"带矩阵"M_b作为输入参数, 例如:

$$M=\begin{pmatrix}-2 & 1 & & \\ 1 & -2 & 1 & \\ & 1 & \ddots & \ddots \\ & & \ddots & -2\end{pmatrix}\to M_b=\begin{pmatrix}0 & 1 & 1 & \cdots & 1\\ -2 & -2 & -2 & \cdots & -2\end{pmatrix}. \tag{9}$$

其返回值为 **w,v**, 本征值 **w[i]** 对应的本征向量为 **v[:,i]**. 这里只计算前十个本征态. 得到的本征向量是 $(N+1)$ 维的归一向量, 要再除以因子 $\sqrt{h}$ 以得到一维实空间的连续波函数.

```python
A = np.array([0]+[1]*N)
B = np.array([-2]*(N+1))
Tb = - np.vstack((A, B)) / (2*h**2)
Vb = np.vstack((np.zeros(N+1), V))
Hb = Tb + Vb
E, eigvecs = eig_banded(Hb,select='i',select_range=(0,9))
psi = eigvecs.T / (h**(1/2))
```

计算结果如下:



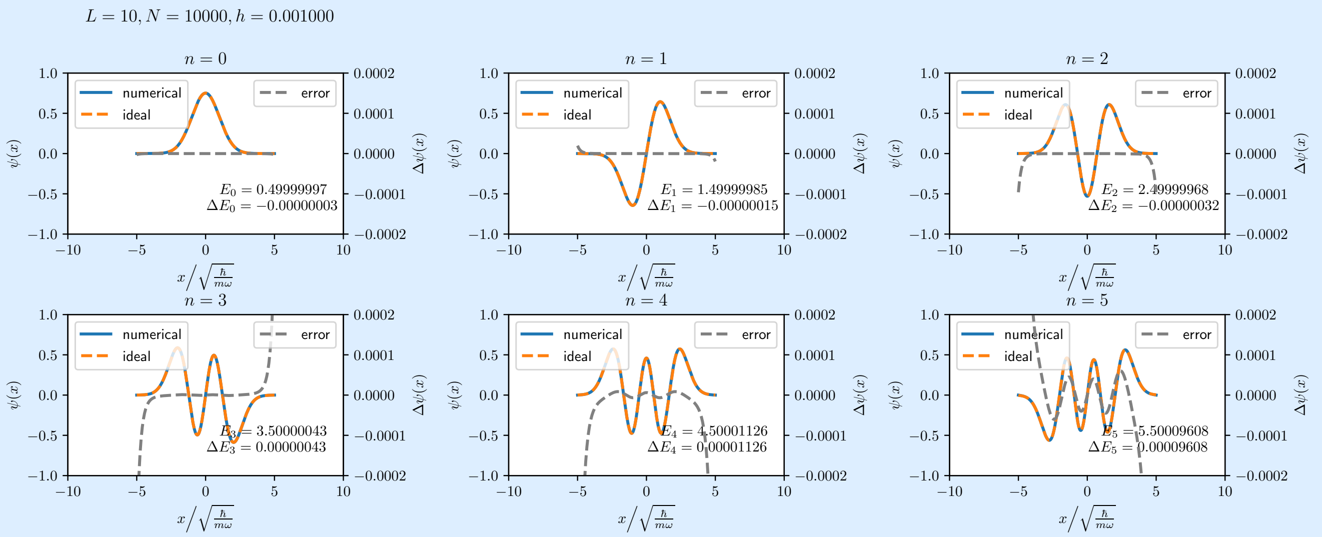
该问题的解析解为:

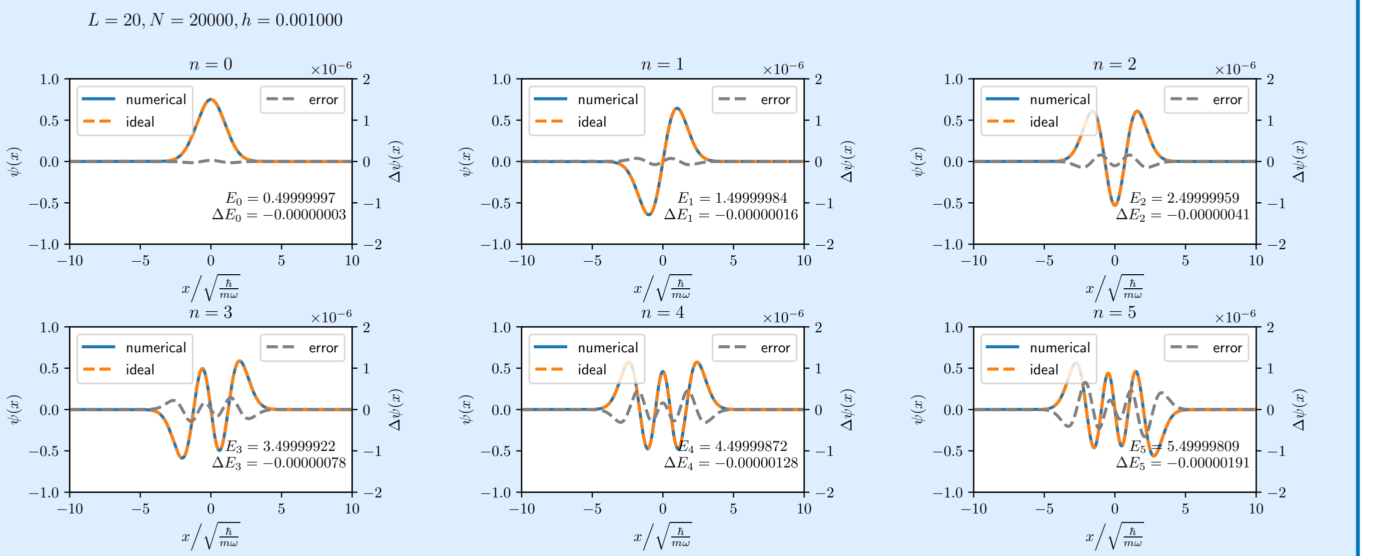
$$E=(n+\frac{1}{2})\hbar\omega,\quad \psi_n(x)=\frac{1}{\sqrt{\pi^{1/2}2^n n!}}H_n(x)\mathrm{e}^{-x^2/2}, \tag{10}$$

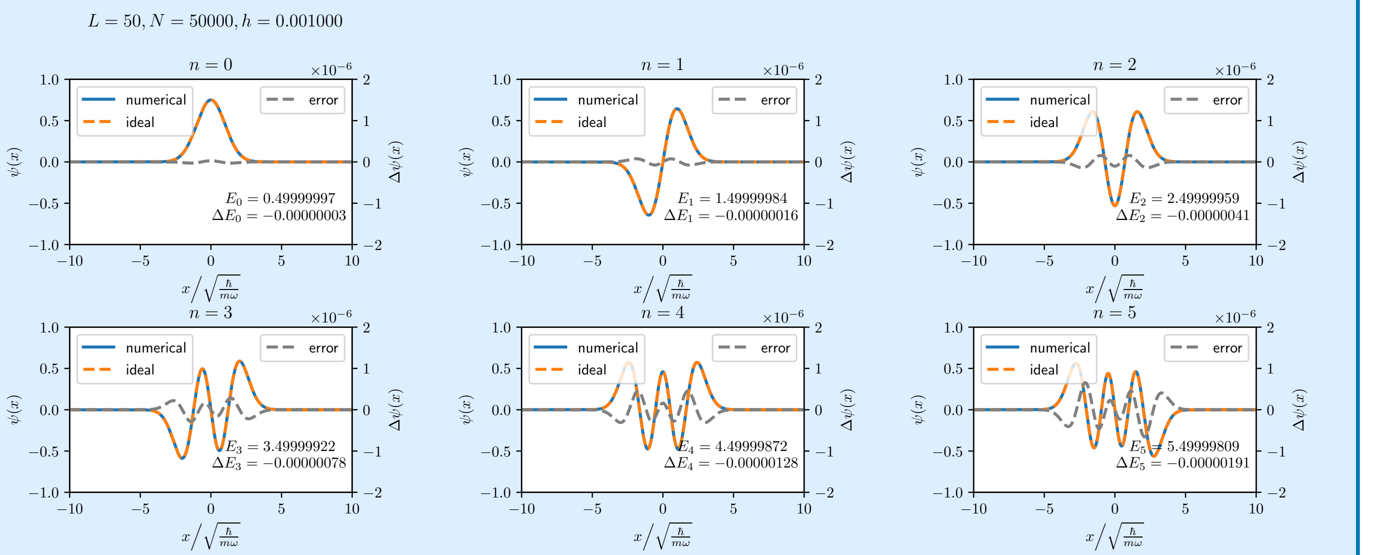
可利用scipy中内置的Hermite函数获得:

```python
from scipy import special
from numpy import math,exp,pi
def sho(n,x):
    return special.hermite(n)(x) * exp(-x**2 / 2) / (pi**(1/2) * 2**n * math.factorial(n))**(1/2)
psi_ideal = [sho(n,x) for n in range(3)]
```

为了确定误差与参数选择的关系, 首先固定 $h=10^{-3}$, 取 $L=10,20,50$.

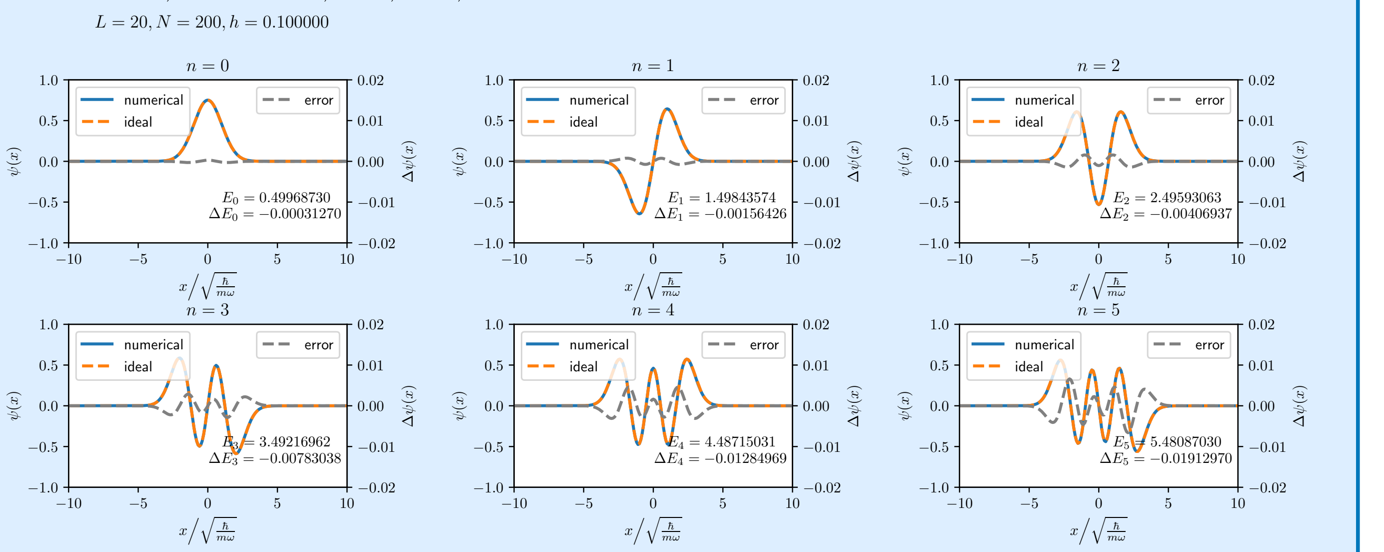


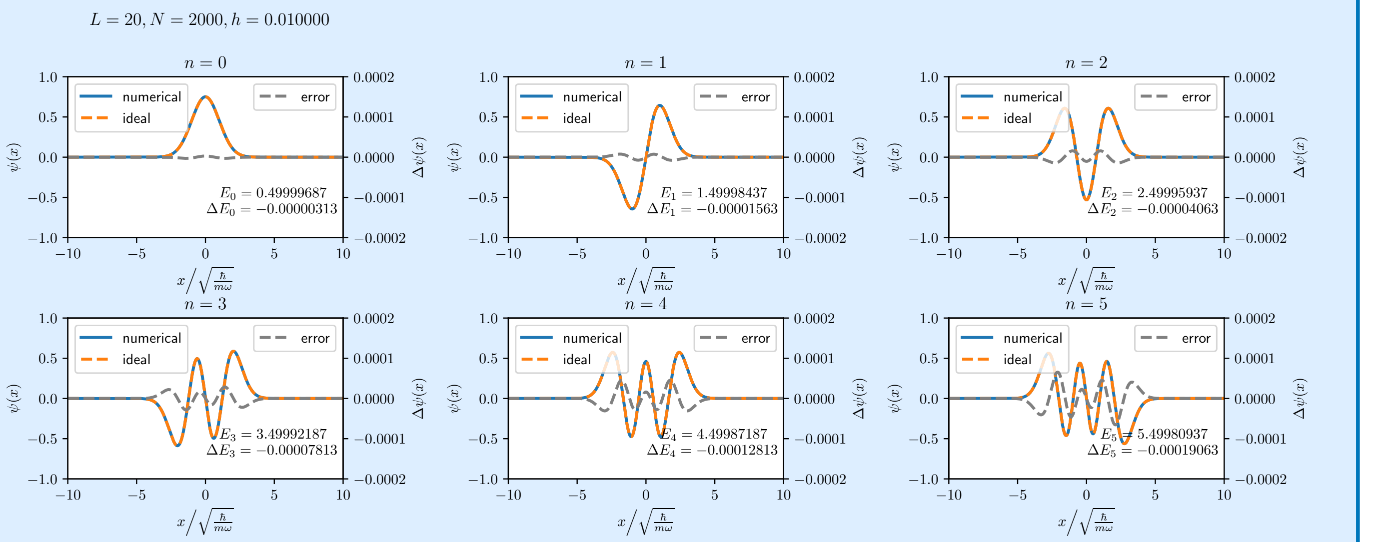


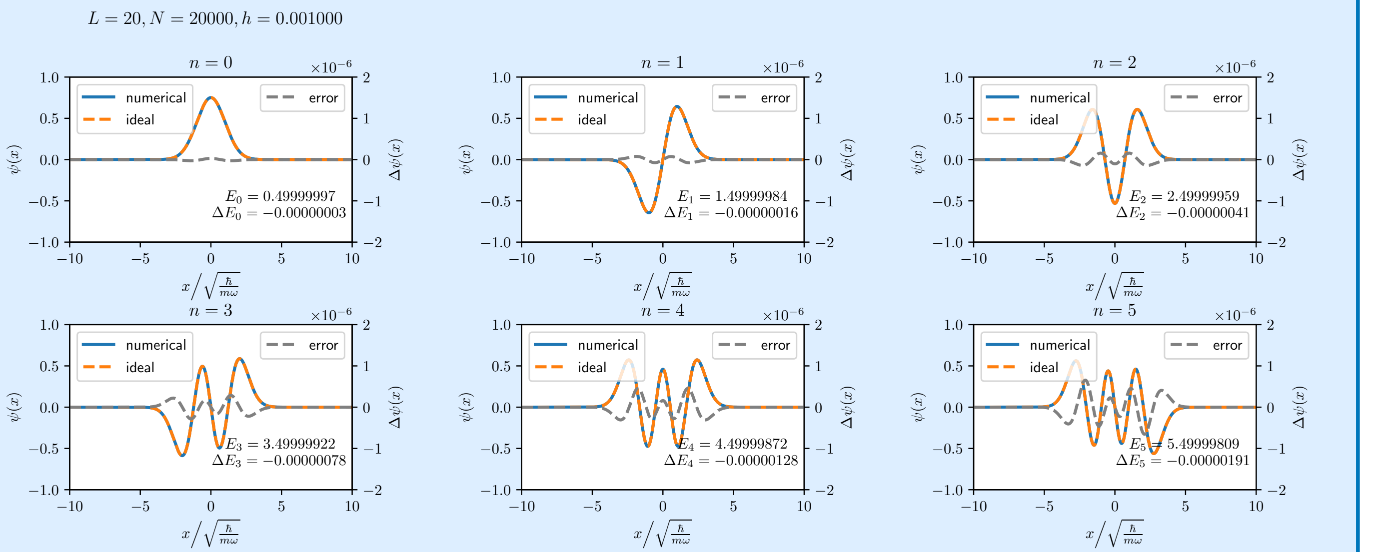


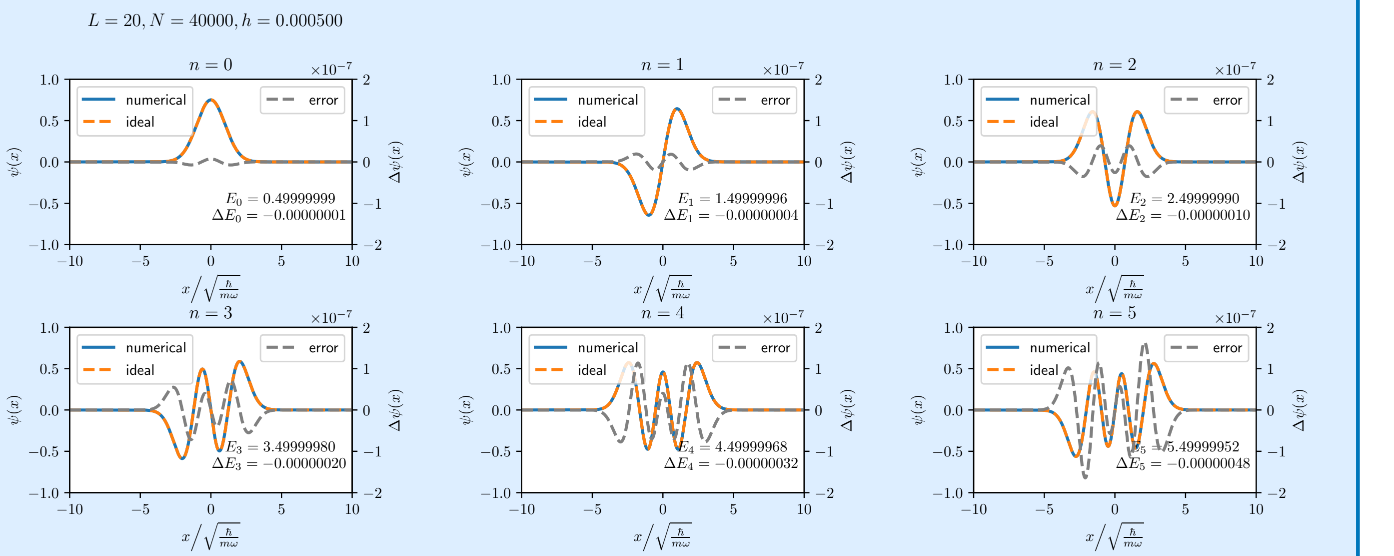
可以看到, 当 $L = 10$ 时, 此范围外仍有明显的波函数分布. 如果只在该范围内求解方程, 会导致边缘处的波函数有很大误差. 而当 $L > 20$ 后, 此时范围之外的波函数已经几乎没有分布, 误差大小与 L 的关系不再显著.

再固定 $L = 20$, 取 $h = 10^{-1}, 10^{-2}, 10^{-3}, 5 \times 10^{-4}$.









可以看到随着h变小, 能量本征值和波函数的误差逐渐降低. 且每当h减小一个量级, 误差大约随之减小两个量级, 即误差以$O(h^2)$的关系下降.

2.

Schrödinger方程为

$$
\begin{aligned}
&\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}m\omega^2x^2+A\cos(kx+\theta)\right]\psi(x)=E\psi(x)\\
&\Downarrow \\
&\left[-\frac{1}{2}\frac{\hbar}{m\omega}\frac{\partial^2}{\partial x^2}+\frac{1}{2}\frac{m\omega}{\hbar}x^2+\frac{A}{\hbar\omega}\cos\left(\sqrt{\frac{\hbar}{m\omega}}k\sqrt{\frac{m\omega}{\hbar}}x+\theta\right)\right]\psi(x)=\frac{E}{\hbar\omega}\psi(x)
\end{aligned}
\tag{11}
$$

令$E=E'\times\hbar\omega$, $x=x'\times\sqrt{\frac{\hbar}{m\omega}}$, $k=k'\times\sqrt{\frac{m\omega}{\hbar}}$, $W=\frac{A}{\hbar\omega}$. 则无量纲化后的Schrödinger方程为

$$
\left[-\frac{1}{2}\frac{\partial^2}{\partial(x')^2}+\frac{1}{2}(x')^2+W\cos(k'x'+\theta)\right]\psi(x')=E'\psi(x'). \tag{12}
$$

为简便, 仍然用不带撇号的物理量表示:

$$
\left[-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\frac{1}{2}x^2+W\cos(kx+\theta)\right]\psi(x)=E\psi(x). \tag{13}
$$

i.e.

$$
-\frac{1}{2h^2}(\psi_{i+1}+\psi_{i-1}-2\psi_i)+\left[\frac{1}{2}x_i^2+W\cos(kx_i+\theta)\right]\psi_i=E\psi_i, \tag{14}
$$

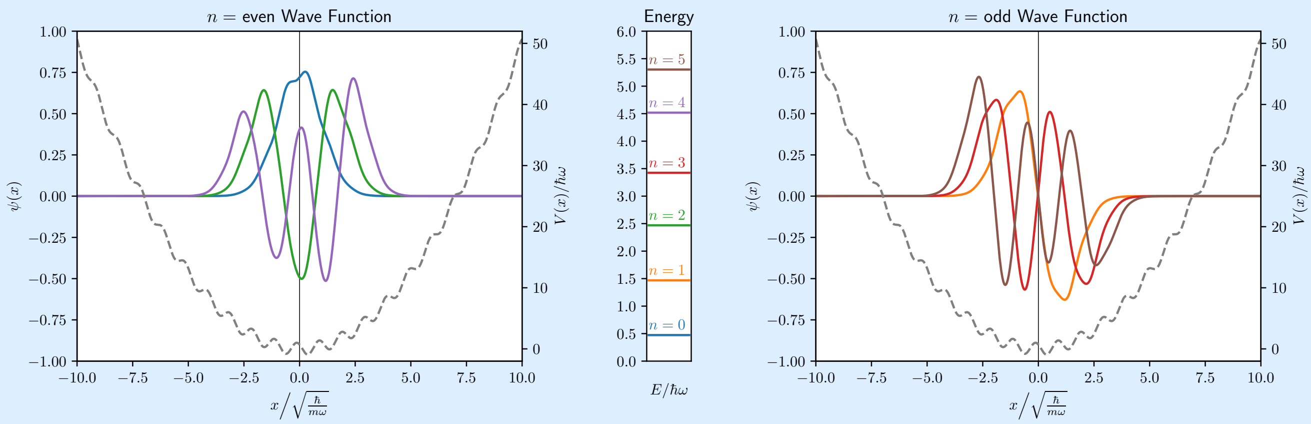
令

$$
H=-\frac{1}{2h^2}\begin{pmatrix}-2&1&&&\\1&-2&1&&\\&1&-2&\ddots&\\&&\ddots&\ddots&1\\&&&1&-2\end{pmatrix}+\frac{1}{2}\begin{pmatrix}x_0^2&&&&\\&x_1^2&&&\\&&x_2^2&&\\&&&\ddots&\\&&&&x_N^2\end{pmatrix}+W\begin{pmatrix}\cos(kx_0+\theta)&&&&\\&\cos(kx_1+\theta)&&&\\&&\cos(kx_2+\theta)&&\\&&&\ddots&\\&&&&\cos(kx_N+\theta)\end{pmatrix} \tag{15}
$$

则有

$$
H\boldsymbol{\psi}=E\boldsymbol{\psi}. \tag{16}
$$

取 $W=1,k=2\pi,\theta=\frac{\pi}{4}$; 使用python数值求解结果如下:



使用Mathematica进行微扰论求解:

```
In[30]:= ψ[n_, x_] := HermiteH[n, x] e^(-x^2/2) / Sqrt[Sqrt[π] 2^n n !]

         E0[n_] := n + 1/2

In[32]:= W = 1; k = 2 π; θ = π/4;

         V[x_] := W Cos[k x + θ]
                    余弦

In[34]:= E1[n_] := NIntegrate[V[x] × ψ[n, x]^2, {x, -100, 100}]
                   数值积分

In[35]:= E2[n_] := -Sum[NIntegrate[ψ[m, x] × V[x] × ψ[n, x], {x, -100, 100}]^2 / (E0[m] - E0[n]),
                    求和 数值积分
            {m, Range[0, 100] ~DeleteCases~ n}]
                范围              删除匹配元素

In[36]:= Table[E0[n] + E1[n] + E2[n], {n, 0, 5}]
         表格

Out[36]= {0.473268, 1.46882, 2.46911, 3.42417, 4.50312, 5.25073}
```

能量本征值对比如下:

Method	E_0	E_1	E_2	E_3	E_4	E_5
Perturbation	0.473268	1.46882	2.46911	3.42417	4.50312	5.25073
Numerical	0.473302	1.46885	2.46939	3.42453	4.51798	5.30224

Question 2 ▷ Numerical Solution of 2D Schrödinger Equation

1. 操场(一个长方形加两个半圆), 内部 $V=0$, 外部 $V=\infty$.
2. 心形线, 内部 $V=0$, 外部 $V=\infty$.

Solution

Schrödinger方程为

$$\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\psi(x,y)=E\psi(x,y) \tag{17}$$

令$x=x'\times l$, $y=y'\times l$, $E=E'\times\dfrac{\hbar^2}{ml^2}$, $V=V'\times\dfrac{\hbar^2}{ml^2}$, x'和E'分别是无量纲长度和无量纲能量. 则无量纲化后的Schrödinger方程为

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial (x')^2}+\frac{\partial^2}{\partial (y')^2}\right)+V'(x',y')\right]\psi(x',y')=E'(x',y'). \tag{18}$$

使用不带撇号的记号:

$$\left[-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)+V(x,y)\right]\psi(x,y)=E\psi(x,y). \tag{19}$$

设求解范围为 $\left[-\dfrac{L_x}{2},\dfrac{L_x}{2}\right]\times\left[-\dfrac{L_y}{2},\dfrac{L_y}{2}\right]$, 做离散化:

$$\begin{aligned} x_i&=-\frac{L_x}{2}+ih_x \quad (h_x=L_x/N_x, i=0,1,2,\cdots,N_x),\\ y_j&=-\frac{L_y}{2}+jh_y \quad (h_y=L_y/N_y, j=0,1,2,\cdots,N_y), \end{aligned} \tag{20}$$

则

$$
\begin{aligned}
\psi(x,y)\Big|_{(x_i,y_j)} &\to \psi_{ij} = \psi(x_i, y_j), \\
V(x,y)\Big|_{(x_i,y_j)} &\to V_{ij} = V(x_i, y_j), \\
\frac{\partial^2}{\partial x^2}\psi(x,y)\Big|_{(x_i,y_j)} &\to \frac{\psi_{i+1,j} + \psi_{i-1,j} - 2\psi_{ij}}{h_x^2}, \\
\frac{\partial^2}{\partial y^2}\psi(x,y)\Big|_{(x_i,y_j)} &\to \frac{\psi_{i,j+1} + \psi_{i,j-1} - 2\psi_{ij}}{h_y^2}.
\end{aligned}
\tag{21}
$$

令

$$
\begin{aligned}
\boldsymbol{\psi} = \Big(&\underbrace{\psi_{00}, \psi_{01}, \psi_{02}, \cdots, \psi_{0N_y}}_{x=x_0}, \underbrace{\psi_{10}, \psi_{11}, \psi_{12}, \cdots, \psi_{1N_y}}_{x=x_1}, \underbrace{\psi_{20}, \psi_{21}, \psi_{22}, \cdots, \psi_{2N_y}}_{x=x_2}, \\
&\cdots, \underbrace{\psi_{N_x0}, \psi_{N_x1}, \psi_{N_x2}, \cdots, \psi_{N_xN_y}}_{x=x_{N_x}} \Big)^\top,
\end{aligned}
\tag{22}
$$

$$
\begin{aligned}
\frac{\partial^2}{\partial x^2} \to (\partial_x^2 \otimes I_y) &= \frac{1}{h_x^2}
\begin{pmatrix}
-2 & 1 & & \\
1 & -2 & \ddots & \\
 & \ddots & \ddots & 1 \\
 & & 1 & -2
\end{pmatrix}_{N_x \times N_x}
\otimes
\begin{pmatrix}
1 & & & \\
 & 1 & & \\
 & & \ddots & \\
 & & & 1
\end{pmatrix}_{N_y \times N_y} \\
&= \frac{1}{h_x^2}
\begin{pmatrix}
\begin{matrix} -2 & & & \\ & -2 & & \\ & & \ddots & \\ & & & -2 \end{matrix} & \begin{matrix} +1 & & & \\ & +1 & & \\ & & \ddots & \\ & & & +1 \end{matrix} & & \\
\begin{matrix} +1 & & & \\ & +1 & & \\ & & \ddots & \\ & & & +1 \end{matrix} & \begin{matrix} -2 & & & \\ & -2 & & \\ & & \ddots & \\ & & & -2 \end{matrix} & \ddots & \\
 & \ddots & \ddots & \begin{matrix} +1 & & & \\ & +1 & & \\ & & \ddots & \\ & & & +1 \end{matrix} \\
 & & \begin{matrix} +1 & & & \\ & +1 & & \\ & & \ddots & \\ & & & +1 \end{matrix} & \begin{matrix} -2 & & & \\ & -2 & & \\ & & \ddots & \\ & & & -2 \end{matrix}
\end{pmatrix},
\end{aligned}
\tag{23}
$$

$$
\begin{aligned}
\frac{\partial^2}{\partial y^2}\to(I_x\otimes\partial_y^2)&=\frac{1}{h_y^2}\begin{pmatrix}1&&&\\&1&&\\&&\ddots&\\&&&1\end{pmatrix}_{N_x\times N_x}\otimes\begin{pmatrix}-2&1&&\\1&-2&\ddots&\\&\ddots&\ddots&1\\&&1&-2\end{pmatrix}_{N_y\times N_y}\\
&=\frac{1}{h_y^2}\begin{pmatrix}
\begin{matrix}-2&+1&&\\+1&-2&\ddots&\\&\ddots&\ddots&+1\\&&+1&-2\end{matrix}&&&&&\\
&\begin{matrix}-2&+1&&\\+1&-2&\ddots&\\&\ddots&\ddots&+1\\&&+1&-2\end{matrix}&&&&\\
&&\ddots&&&\\
&&&\ddots&&\\
&&&&\ddots&\\
&&&&&\begin{matrix}-2&+1&&\\+1&-2&\ddots&\\&\ddots&\ddots&+1\\&&+1&-2\end{matrix}
\end{pmatrix},
\end{aligned}
\tag{24}
$$

则

$$\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\to(\partial_x^2\otimes I_y)+(I_x\otimes\partial_y^2)=\partial_x^2\oplus\partial_y^2 \tag{25}$$

其中 $\otimes,\oplus$ 表示Kronecker积和Kronecker和, 有

$$
\begin{aligned}
&(A\otimes B)_{p(r-1)+v,q(s-1)+w}=a_{rs}b_{vw},\\
&A\oplus B=A\otimes I+I\otimes B.
\end{aligned}
\tag{26}
$$

取 $h_x=h_y=h$, Schrödinger方程可用矩阵写为

$$H\boldsymbol{\psi}=E\boldsymbol{\psi},\quad \text{with } H=T+V, \tag{27}$$

其中

$$
\begin{aligned}
&T=-\frac{1}{2}\partial_x^2\oplus\partial_y^2,\\
&V=\mathrm{diag}\Big\{\underbrace{V_{00},V_{01},V_{02},\cdots,V_{0N_y}}_{x=x_0},\underbrace{V_{10},V_{11},V_{12},\cdots,V_{1N_y}}_{x=x_1},\underbrace{V_{20},V_{21},V_{22},\cdots,V_{2N_y}}_{x=x_2},\\
&\qquad\qquad\cdots,\underbrace{V_{N_x0},V_{N_x1},V_{N_x2},\cdots,V_{N_xN_y}}_{x=x_{N_x}}\Big\}.
\end{aligned}
\tag{28}
$$

注意到 $H=T+V$ 是一个非常稀疏的矩阵, 使用python科学计算包scipy的 **scipy.sparse** 包来进行稀疏矩阵运算.

```python
import numpy as np
from numpy import cos,pi
from scipy import sparse
from scipy.sparse import linalg

```

```python
L = 40; N = 200; h = L / N;
Y,X = np.meshgrid(np.linspace(-L/2,L/2,N+1),np.linspace(-L/2,L/2,N+1) )


@np.vectorize
def get_potential(x,y):
    ...

diags = np.array([[1]*(N+1),[-2]*(N+1),[1]*(N+1)])
D = sparse.spdiags(diags, np.array([-1,0,1]), N+1, N+1)
U = get_potential(X,Y)
```

上面的代码中，取x和y方向的范围和步长均相等, `D` 是一维的二阶导数对应矩阵,， 还需要求Kronecker和才是二维情况下的矩阵; `U` 是一个对应 x、y 网格的二维数组, 用 `reshape` 函数可以将其变成列向量, 再用 `scipy.sparse.diags` 可得到我们需要的对角矩阵. 这样得到 $H = T + V$ 后, 便可使用 `scipy.sparse.linalg.eigsh` 函数求其本征值和本征向量.

```python
T = -1/2 * sparse.kronsum(D,D)
V = sparse.diags(U.reshape((N+1)**2))
H = T + V

E, eigvecs = linalg.eigsh(H, 10, which='SM')
print(E)
```

其返回值为 `E,v`, 本征值 `E[n]` 对应的本征向量为 `E[:,n]`, 这里只计算前十个本征态. 得到的本征向量是 $(N+1)^2$ 维的归一向量, 要再除以因子 h, 并重新整形成 $(N+1)\times(N+1)$ 维的数组, 以得到二维实空间的连续波函数. 该过程由函数 `get_psi` 实现:

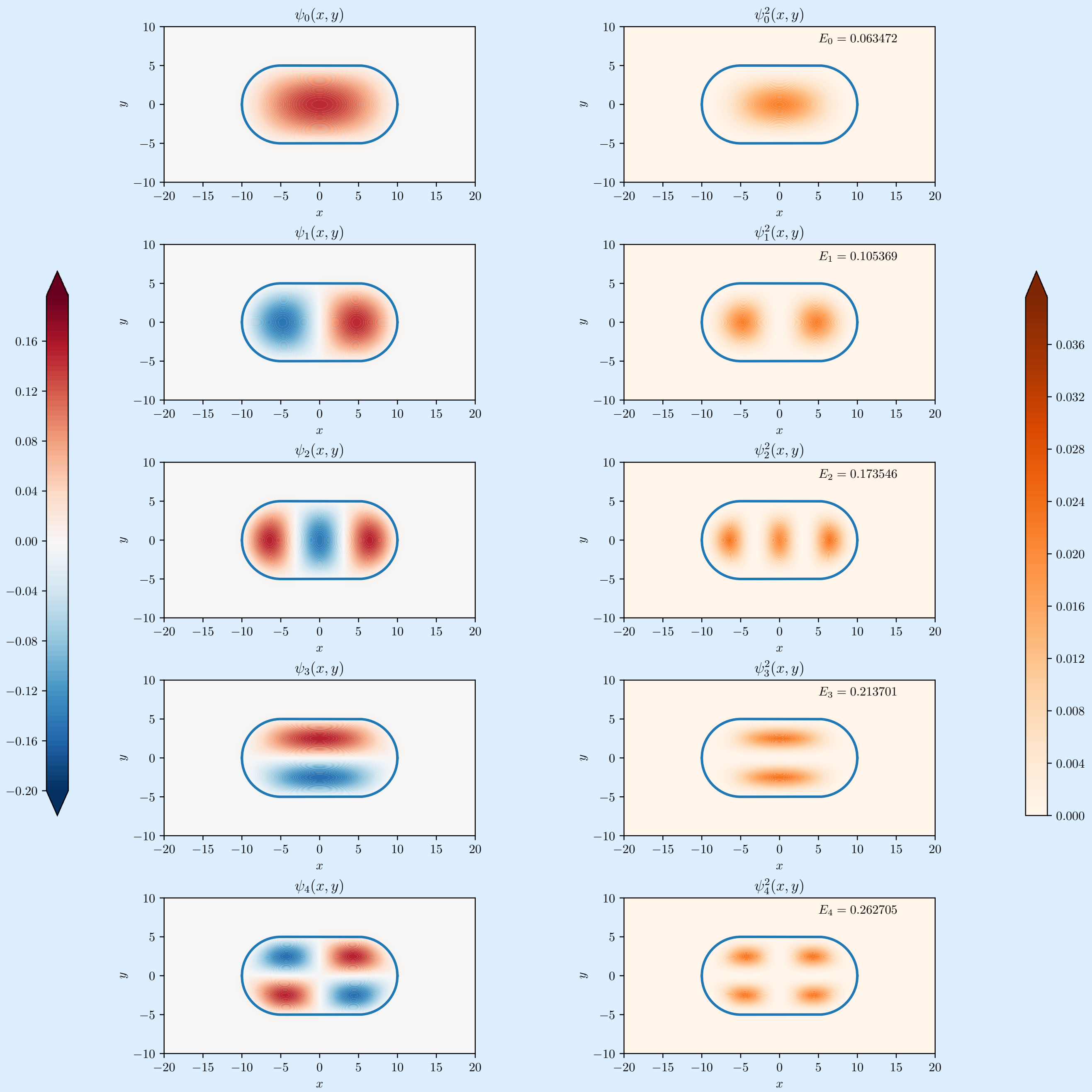
```python
def get_psi(n):
    return eigvecs.T[n].reshape((N+1,N+1)) / h
```

---

1. 操场形状的二维无限深势阱, `get_potential` 函数定义为:

```python
x0 = 5
@np.vectorize
def get_potential(x,y):
    region1 = ( (x-x0)**2 + y**2 < x0**2 )
    region2 = ( (x+x0)**2 + y**2 < x0**2 )
    region3 = ( abs(x) < x0 and abs(y) < x0 )
    return 10000 * float(not(region1 or region2 or region3))
```

`@np.vectorize` 修饰器的作用是让此函数可以作用在数组上. 计算结果如下:



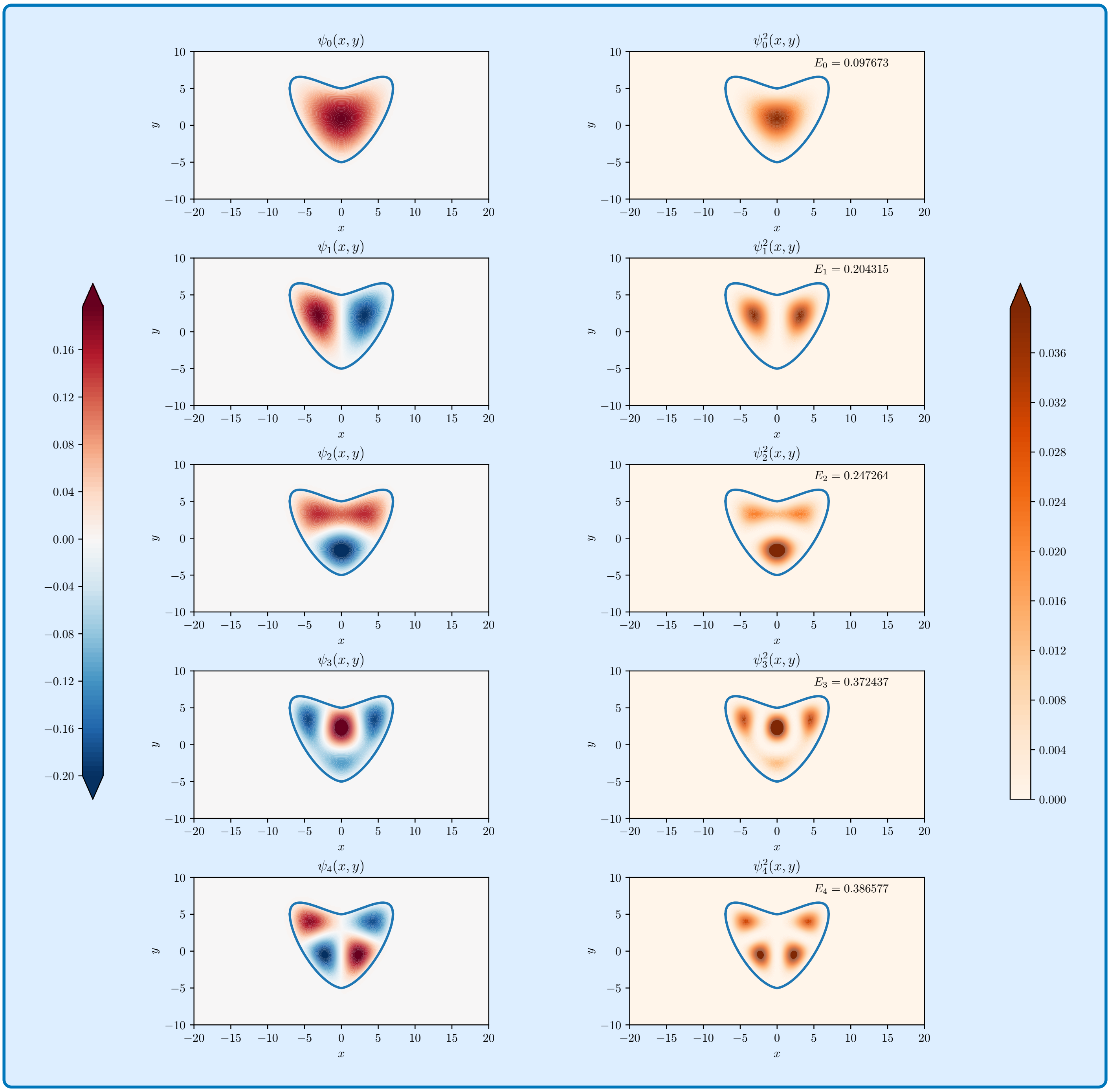
2. 心形的二维无限深势阱, 区域为

$$\left(\frac{x}{x_0}\right)^2 + \left[\frac{y}{y_0} - \left(\frac{x}{x_0}\right)^{3/2}\right]^2 < 1 \tag{29}$$

get_potential 函数定义为:

```python
x0 = 7; y0 = 5
@np.vectorize
def get_potential(x,y):
    region = ( (x/x0)**2 + ( y/y0 -abs(x/x0)**(3/2) )**2 < 1 )
    return 10000 * float(not(region))
```

计算结果如下:


$\psi_0(x,y)$
$\psi_0^2(x,y)$
$E_0 = 0.097673$
$\psi_1(x,y)$
$\psi_1^2(x,y)$
$E_1 = 0.204315$
$\psi_2(x,y)$
$\psi_2^2(x,y)$
$E_2 = 0.247264$
$\psi_3(x,y)$
$\psi_3^2(x,y)$
$E_3 = 0.372437$
$\psi_4(x,y)$
$\psi_4^2(x,y)$
$E_4 = 0.386577$
x
y