Finite Differences and Quantum Scars

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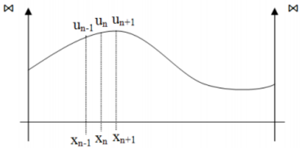
Finite Differences One-Dimensional

Time-independent Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi, \quad \nabla^2 = \frac{d^2}{dx^2}$$

$$V(x) = \begin{cases} 0, & 0 \le x \le 1 \\ \infty, & \text{otherwise} \end{cases}$$

$$-\frac{d^2}{dx^2}\Psi = E\Psi$$

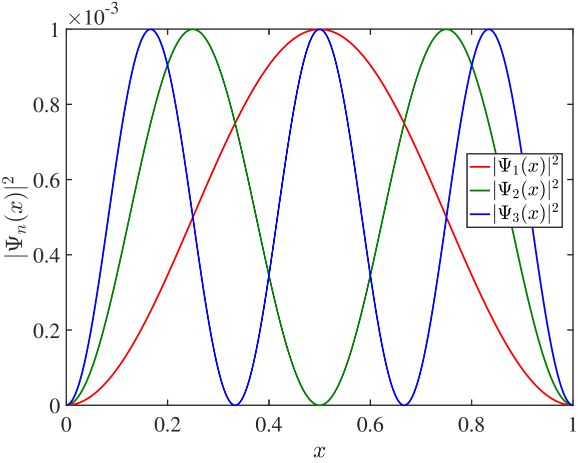


$$\left.\frac{d^2f}{dx^2}\right|_{x_n} \approx \frac{\left.\frac{df}{dx}\right|_{x_{n+1/2}} - \left.\frac{df}{dx}\right|_{x_{n-1/2}}}{h} \approx \frac{\frac{u_{n+1}-u_n}{h} - \frac{u_n - u_{n-1}}{h}}{h} = \frac{u_{n+1} - 2u_n + u_{n-1}}{h^2}$$

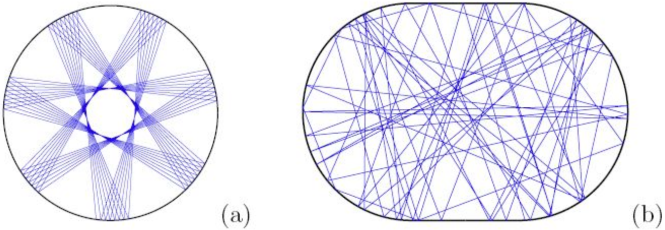
$h = x_n - x_{n-1}$, $u_i = \Psi(x_i)$

$$\nabla^2 \approx A = \begin{bmatrix} -2 & & \cdots & & 0 \\ & \ddots & & & \\ \vdots & 1 & -2 & 1 & \vdots \\ & & & \ddots & \\ 0 & & \cdots & & -2 \end{bmatrix}$$

Finite Differences One-Dimensional



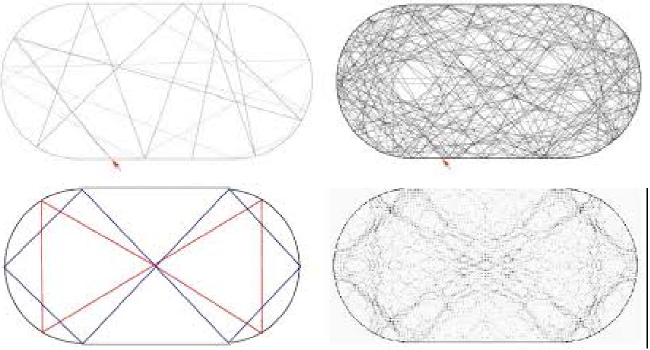
Chaos



- 经典物理：
  (a) 周期轨道
  (b) 混沌轨道

Quantum Scar（量子疤痕）

- Eric J. Heller 1984



- 混沌轨道 → 量子混沌
- 周期轨道 → 量子疤痕 (波函数集中在经典周期轨道)

Finite Differences 2-Dimensional

- 2D

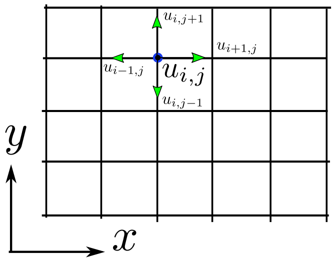
$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V\Psi = E\Psi, \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$$

$$V(x) = \begin{cases} 0, & 0 \le x \le 1, 0 \le x \le 1 \\ \infty, & \text{otherwise} \end{cases}$$

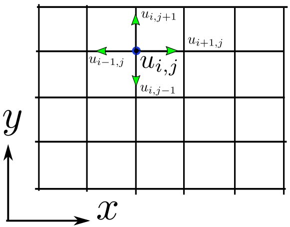
$$-(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2})\Psi = E\Psi$$

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \simeq u_{i+1,j} + u_{i-1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}$$

$$\Psi^\dagger = (u_{11}, u_{21}, ...u_{N1}, u_{12}, ..., u_{N2}, ..., u_{NM})$$



Finite Differences 2-Dimensional



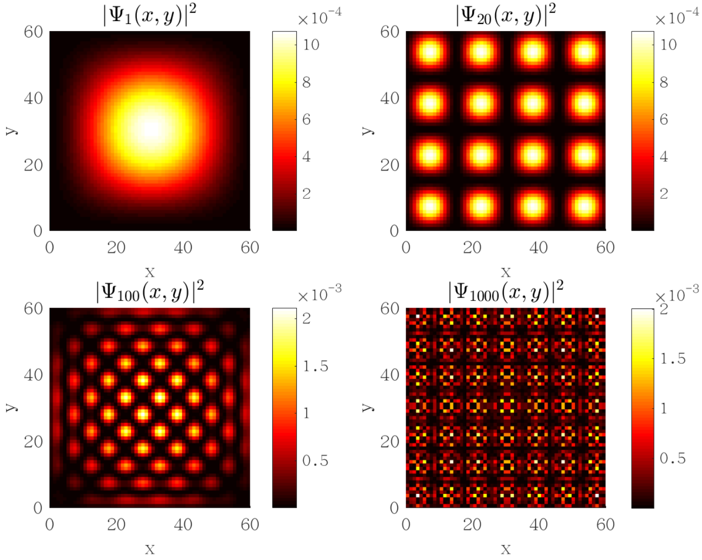
离散化处理，格点记入 $A(x,y) = 1 \rightarrow$ [h,l] $=$ find(A) $\rightarrow$:

```
for i = 1:N*M
    for j = 1:N*M
        if i==j
           H(i,j) = -4;
        else if (abs(h(i)-h(j))==0 && abs(l(i)-l(j))==1)...
                     || (abs(l(i)-l(j))==0 && abs(h(i)-h(j))==1)
                H(i,j) = 1;
            else
                H(i,j) = 0;
            end
        end
    end
end
```

对角化 H 求出本征值和波函数 Ψ, Ψ 对应到 2D 晶格画波函数分布
M(h(i),l(i)) $=$ abs($\Psi(i)$)^2, surf(M)

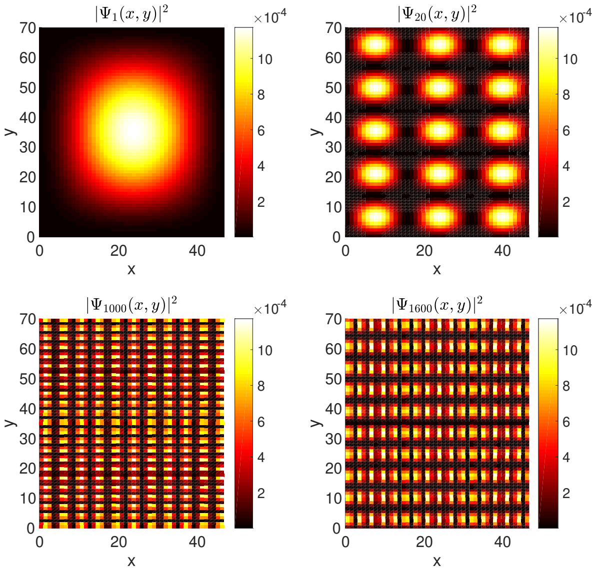
Finite Differences 2-Dimensional

- Square(60×60)



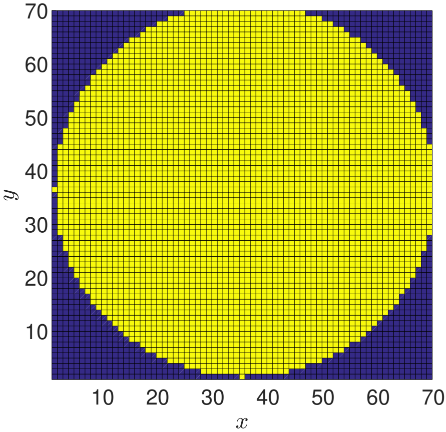
Finite Differences 2-Dimensional

- Rectangle(47×70)



Finite Differences 2-Dimensional

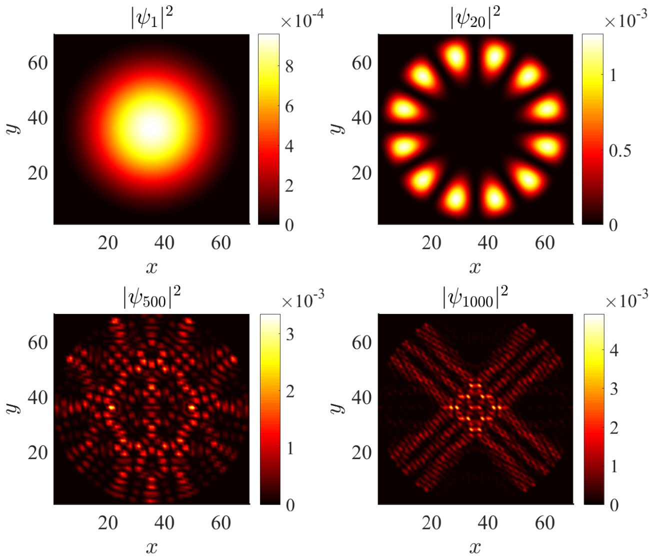
- Circle(70×70)



- 圆心 (c_x, c_y)，则 $(x - c_x)^2 + (y - c_y)^2 \leq R^2$ 在圆内标记 $A(x, y) = 1$ 否则不在圆内标记 $A(x, y) = 0 \rightarrow$ [h,l] = find(A) $\rightarrow$ If (abs(h(i)-h(j))==0 && abs(l(i)-l(j))==1) || (abs(l(i)-l(j))==0 && abs(h(i)-h(j))==1), $H(i, j) = 1$.
  If i==j, $H(i, j) = -4$, Else $H(i, j) = 0$

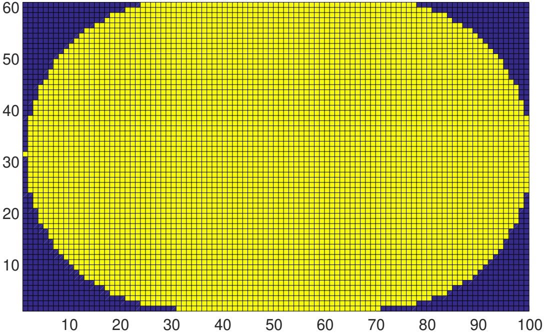
Finite Differences 2-Dimensional

- Circle(70×70)



Finite Differences 2-Dimensional

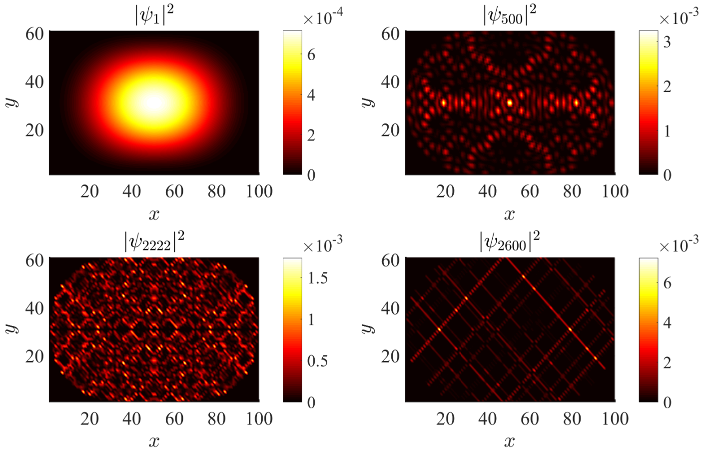
- Billiard(61×100)



- 矩形两边接半圆构造，离散化生成矩阵 $A \to$ [h,l] = find$(A) \to$
  If (abs(h(i)-h(j))==0 $\&\&$ abs(l(i)-l(j))==1) $||$ (abs(l(i)-l(j))==0 $\&\&$ abs(h(i)-h(j))==1), $H(i,j) = 1$.
  If i==j, $H(i,j) = -4$, Else $H(i,j) = 0$

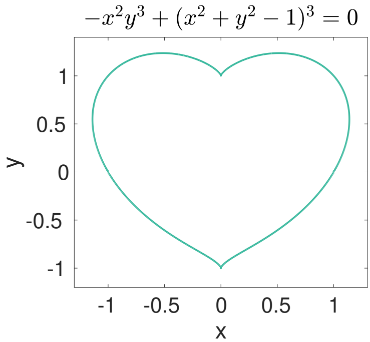
Finite Differences 2-Dimensional

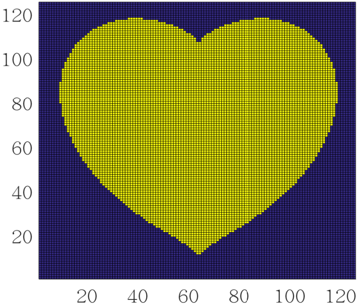
- Billiard(61×100)



Finite Differences 2-Dimensional

- Heart-shaped





- 离散化生成矩阵 $A \to$ [h,l] = find(A) $\to$
  If (abs(h(i)-h(j))==0 && abs(l(i)-l(j))==1) || (abs(l(i)-l(j))==0 && abs(h(i)-h(j))==1), $H(i,j)=1$.
  If i==j, $H(i,j)=-4$, Else $H(i,j)=0$

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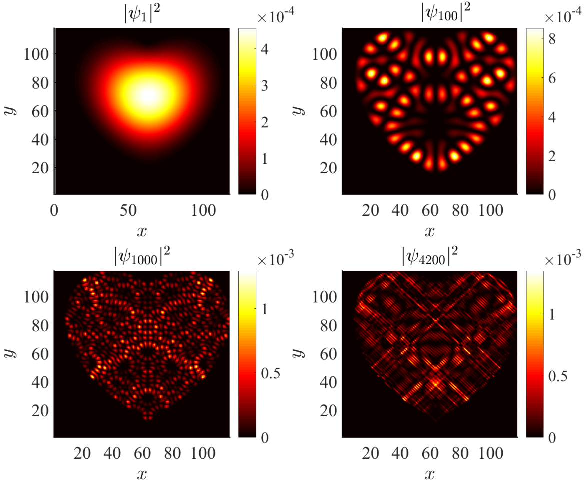

Summary

- 具体的二维图形离散化：在图形里面的格点标记为 $A(x,y)=1$，在图形外面的格点标记为 $A(x,y)=0$.
- 得到非零格点位置：$[h,l]=find(A)$
- 生成哈密顿量矩阵形式：
  If (abs(h(i)-h(j))==0 && abs(l(i)-l(j))==1) || (abs(l(i)-l(j))==0 && abs(h(i)-h(j))==1), $H(i,j)=1$.
  If i==j, $H(i,j)=-4$
  Else $H(i,j)=0$
- 对角化 H 求出本征值 E_n 和波函数 Ψ_n
- 波函数分布：$M(h(i),l(i))=|\Psi_n(i)|^2$, surf(M)