Chapter 7

Discretized Grid Space in Higher Dimension

Poisson equation $\nabla^2\Phi(\vec{r}) = -S(\vec{r})$ or time independent Schrödinger equation

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r}) \;=\; E\psi(\vec{r})$$

in 2-dimensional space is an Elliptic differential equation

$$\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\Phi(x,y) \;=\; -k^2(x,y)\Phi(x,y) - S(x,y). \tag{7.1}$$

Wave equation

$$\frac{\partial^2}{\partial t^2}\Psi(\vec{r},t) \;=\; v^2\nabla^2\Psi(\vec{r},t)$$

in 1-dimensional spatial space is a Parabolic differential equation

$$\left[\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2}\right]\Phi(x,y) \;=\; -k^2(x,y)\Phi(x,y) - S(x,y). \tag{7.2}$$

Both the elliptic and parabolic differential equations have second order differential in all variables x and y and the same numerical method can be used. Time dependent Schrödinger equation or diffusion equation,

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}\psi(\vec{r},t) &= \left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right]\psi(\vec{r},t), \\ \frac{\partial}{\partial t}\Phi(\vec{r},t) &= \vec{\nabla}\cdot\left[D(\vec{r})\vec{\nabla}\Phi(\vec{r},t)\right] + S(\vec{r},t), \end{aligned}$$

in 1-dimensional spatial space is a Hyperbolic differential equation

$$\frac{\partial}{\partial t}\phi(x,t) = D(x,t)\frac{\partial^2}{\partial x^2}\phi(x,t) - K(x,t)\phi(x,t) + S(x,t). \qquad (7.3)$$

The hyperbolic differential equation has first order differential for one variable and second order differential for other variables. Numerical methods for 3-dimension are simple extension of numerical methods in 2-dimensional space.

7.1 Discretization and Variational Principle

There are some ambiguity in discretizing spatial space. This can be clarified with variational principle. The equation $\vec{\nabla}\cdot[D\vec{\nabla}\phi] = -S$ can be derived from the corresponding functional

$$E = \int d^3r \left[\frac{1}{2}D(\vec{\nabla}\phi)^2 - S\phi\right] \qquad (7.4)$$

by using variational method with respect to the function ϕ. To find $\phi(\vec{r})$ which minimizes the value of the functional E, vary E with respect to the function ϕ by using $\phi + \delta\phi$. The first order in $\delta\phi(\vec{r})$ is

$$\int_V d^3r \left[\frac{1}{2}D(\vec{r})\nabla\phi(\vec{r})\cdot\vec{\nabla}\delta\phi(\vec{r}) - S(\vec{r})\delta\phi(\vec{r})\right]$$
$$= \int_V d^3r \left[-\vec{\nabla}\cdot D(\vec{r})\nabla\phi(\vec{r}) - S(\vec{r})\right]\delta\phi(\vec{r}) = 0 \qquad (7.5)$$

for arbitrary variation $\delta\phi(\vec{r})$ with $\delta\phi = 0$ at the boundary surface due to the boundary condition of the differential equation. Thus we finally get the differential equation $\vec{\nabla}\cdot\left[D\vec{\nabla}\phi(\vec{r})\right] = -S(\vec{r})$. Actually this equation is the condition for the extremum of E.

In 2-dimensional space,

$$\frac{\partial}{\partial x}\left(D\frac{\partial\phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(D\frac{\partial\phi}{\partial y}\right) = -S(x,y), \qquad (7.6)$$

$$\frac{1}{2}\int dx\int dy\frac{\partial\phi}{\partial x}D\frac{\partial\phi}{\partial x} + \frac{1}{2}\int dx\int dy\frac{\partial\phi}{\partial y}D\frac{\partial\phi}{\partial y} - \int dx\int dy S(x,y)\phi(x,y) = 0. \qquad (7.7)$$

In Eq.(7.6), every terms should be evaluated at a same point while in Eq.(7.7) each term can be integrated separately independent to the other terms. Thus convert Eq.(7.4) into discretized space by evaluating each term separately independent of other terms and then use variational method to obtain the difference equation for ϕ_{ij} in the grid space.

7.2 Boundary Value Problem

Consider boundary condition for a difference equation in 2-dimensional grid space such as discretized elliptic equation

$$\frac{\phi_{i+1j} - 2\phi_{ij} + \phi_{i-1j}}{\Delta x^2} + \frac{\phi_{ij+1} - 2\phi_{ij} + \phi_{ij-1}}{\Delta y^2} = -S_{ij}$$

for the grid sizes of Δx and Δy. This is simplified as

$$4\phi_{ij} - \phi_{i+1j} - \phi_{i-1j} - \phi_{ij+1} - \phi_{ij-1} = h^2 S_{ij}$$

for the case of $\Delta x = \Delta y = h$.

For Dirichlet boundary condition, the values of function at the boundary are given; ϕ_{1j}, ϕ_{Nj}, ϕ_{i1}, and ϕ_{iN}. The boundary condition incorporates with the difference equation as

$$4\phi_{iN-1} - \phi_{i+1N-1} - \phi_{i-1N-1} - \phi_{iN-2} = h^2 S_{iN-1} + \phi_{iN} \qquad (7.8)$$

for ϕ_{iN} as an example. The values on the right hand side are known from the value of the source and the Dirichlet boundary condition of the function. The values on the left side should be determined by numerical method.

For Neumann boundary condition, the normal component of gradient at the boundary are given; for example $\partial\phi/\partial y = g(x)$ are given at the boundary of $y = y_N$ which becomes

$$\phi_{iN} - \phi_{iN-1} = hg_i \qquad (7.9)$$

in the grid space. Then the difference equation becomes

$$3\phi_{iN-1} - \phi_{i+1N-1} - \phi_{i-1N-1}\phi_{iN-2} = h^2 S_{iN-1} + hg_i \qquad (7.10)$$

at the boundary (x_i, y_N). The values on the right hand side are known from the value of the source and the Neumann boundary condition Eq.(7.9) of the function. The values on the left side should be determined by numerical method.

7.3 Iterative Gauss-Seidel Method

For an elliptic or parabolic difference equation, iterative Gauss-Seidel method can be used. For $\nabla^2\phi = -S$, the difference equation in 1-dimensional grid space is

$$\phi_{i+1} - 2\phi_i + \phi_{i-1} = -h^2 S_i$$

for ϕ_i which is the solution of the differential equation. The Gauss-Seidel iteration Method for this case is

$$\phi_i' = (1-\omega)\phi_i + \frac{\omega}{2}[\phi_{i+1} + \phi_{i-1} + h^2 S_i]. \tag{7.11}$$

Use old values ϕ_i to evaluate the value of ϕ_i' and renew the value of ϕ_i with the value of ϕ_i' for every grid points i except for the boundary points. For 2-dimensional difference equation

$$4\phi_{ij} - \phi_{i+1j} - \phi_{i-1j} - \phi_{ij+1} - \phi_{ij-1} = h^2 S_{ij}$$

the iterative Gauss-Seidel method is

$$\phi_{ij}' = (1-\omega)\phi_{ij} + \frac{\omega}{4}[\phi_{i+1j} + \phi_{i-1j}\phi_{ij+1} + \phi_{ij-1} + h^2 S_{ij}]. \tag{7.12}$$

Choose the relaxation parameter ω to be some value between $0 < \omega < 1$ for the faster convergence. To use iterative Gauss-Seidel method we should assume some function for ϕ to start the iteration steps. Properly guessed values of ϕ on the grid points as a starting value reduces iteration step number very much.

7.4 Gaussian Elimination

Diffusion equation and time dependent Schrödinger equation are examples of hyperbolic differential equation;

$$\begin{aligned} \frac{\partial \phi(\vec{r},t)}{\partial t} &= \vec{\nabla}\cdot\left[D(\vec{r},t)\vec{\nabla}\phi(\vec{r},t)\right] - K(\vec{r},t)\phi(\vec{r},t) + S(\vec{r},t) \\ &= -H\phi(\vec{r},t) + S(\vec{r},t). \end{aligned} \tag{7.13}$$

A hyperbolic differential equation has first order differential for one variable t while second order differential for other variables $\vec{r}$. The discretization of H in grid space is the same as for the case of elliptic or parabolic differential equation.

At a discretized time step $t_n = n\Delta t$ for one spatial dimension

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} = -(H\phi)_i + S_i^n. \tag{7.14}$$

Evaluating ϕ in the right hand side of Eq.(7.14) on the spatial grid point x_i at time t_n, explicit differencing scheme becomes

$$\phi^{n+1} = (1 - H\Delta t)\phi^n + S^n \Delta t. \quad (7.15)$$

The right hand side is evaluated at time t_n.

In implicit scheme, by evaluating ϕ in the right hand side of Eq.(7.14) at time t_{n+1},

$$\begin{aligned} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} &= -(H\phi^{n+1})_i + S_i^n, \\ \phi^{n+1} &= \frac{1}{1 + H\Delta t}[\phi^n + S^n \Delta t], \end{aligned} \quad (7.16)$$

or by evaluating ϕ in the right hand side of Eq.(7.14) as the average of ϕ^{n+1} and ϕ^n,

$$\begin{aligned} \frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} &= -\left(H\left[\frac{\phi^{n+1} + \phi^n}{2}\right]\right)_i + S_i^n, \\ \phi^{n+1} &= \frac{1}{1 + \frac{1}{2}H\Delta t}\left[\left(1 - \frac{1}{2}H\Delta t\right)\phi^n + S^n \Delta t\right]. \end{aligned} \quad (7.17)$$

The right hand side are all known quantity at time t_n. However matrix inversion appears as $\phi^{n+1} = \mathsf{A}^{-1}\mathsf{b}^n$ in implicit scheme.

Gaussian elimination method to find ϕ of $\mathsf{A}\phi = \mathsf{b}$ for tri-diagonal matrix;

$$A_i^- \phi_{i-1}^{n+1} + A_i^0 \phi_i^{n+1} + A_i^+ \phi_{i+1}^{n+1} = b_i^n, \quad (7.18)$$

which is a three point recurrence relation for ϕ^{n+1} with the known functions A_i and b_i. As an example,

$$\begin{aligned} b_i^n &= \phi_i^n + S_i^n \Delta t, \\ A_i^0 &= 1 + \frac{2}{h^2}\Delta t, \\ A_i^\pm &= -\frac{\Delta t}{h^2} \end{aligned} \quad (7.19)$$

for Eq.(7.16) with $H = -\frac{d^2}{dx^2}$ and the grid size h. Using a forward two point recurrence relation for ϕ^{n+1},

$$\phi_{i+1}^{n+1} = \alpha_i \phi_i^{n+1} + \beta_i, \quad (7.20)$$

Eq.(7.18) becomes

$$
\begin{aligned}
A_i^- \phi_{i-1} + A_i^0 \phi_i + A_i^+(\alpha_i \phi_i + \beta_i) &= b_i, \\
\phi_i &= \gamma_i A_i^- \phi_{i-1} + \gamma_i (A_i^+ \beta_i - b_i),
\end{aligned}
$$

which gives backward two point recurrence relations

$$
\begin{aligned}
\alpha_{i-1} &= \gamma_i A_i^-, \\
\beta_{i-1} &= \gamma_i (A_i^+ \beta_i - b_i), \\
\gamma_i &= -\frac{1}{A_i^0 + A_i^+ \alpha_i}.
\end{aligned} \tag{7.21}
$$

The boundary condition for α and β at x_{N-1} are

$$
\begin{aligned}
\alpha_{N-1} &= 0, \\
\beta_{N-1} &= \phi_N,
\end{aligned} \tag{7.22}
$$

which come from the boundary condition ϕ_N at x_N

$$
\phi_N = \alpha_{N-1} \phi_{N-1} + \beta_{N-1}.
$$

The Gaussian elimination method is composed with a forward two point recursion relation Eq.(7.20) starting with boundary condition ϕ_1 and backward two point recurrence relations Eq.(7.21) starting with boundary condition ϕ_N through Eq.(7.22).

In 2-d H is not tridiagonal such as

$$
\begin{aligned}
(H\phi)_{ij} &= -(\nabla^2 \phi)_{ij} \\
&= -\frac{1}{h^2} \left(\phi_{i+1j} - 2\phi_{ij} + \phi_{i-1j} + \phi_{ij+1} - 2\phi_{ij} + \phi_{ij-1} \right).
\end{aligned} \tag{7.23}
$$

If we separate as

$$
H = H_x + H_y \tag{7.24}
$$

for each coordinate, then

$$
[1 + H_x \Delta t + H_y \Delta t] \phi^{n+1} \approx [1 + H_x \Delta t][1 + H_y \Delta t] \phi^{n+1} = \phi^n + S^n \Delta t \tag{7.25}
$$

for implicit scheme. Thus

$$
\phi^{n+1} = \left[\frac{1}{1 + H_x \Delta t} \right] \left[\frac{1}{1 + H_y \Delta t} \right] [\phi^n + S^n \Delta t],
$$

which is

$$\begin{aligned} \phi^{n+1/2} &= \frac{1}{[1+H_y\Delta t]}[\phi^n + S^n\Delta t], \\ \phi^{n+1} &= \frac{1}{[1+H_x\Delta t]}\phi^{n+1/2}. \end{aligned} \tag{7.26}$$

The matrix H_i in each of these equation is now tridiagonal.

Gaussian elimination method can also be used for an elliptical differential equation with source term such as

$$(H_x + H_y)\phi = S \tag{7.27}$$

in 2-d. Using acceleration parameter ω

$$(H_x + H_y + \omega)\phi = S + \omega\phi,$$

which becomes

$$\begin{aligned} \phi^{n+1/2} &= \frac{1}{(\omega + H_x)}[S - (H_y - \omega)\phi^n], \\ \phi^{n+1} &= \frac{1}{(\omega + H_y)}[S - (H_x - \omega)\phi^{n+1/2}]. \end{aligned} \tag{7.28}$$

Iterate these equation starting with a guessed function ϕ^1. The matrices H_i for each component are tridiagonal and thus the Gaussian elimination method can be used for matrix inversion.