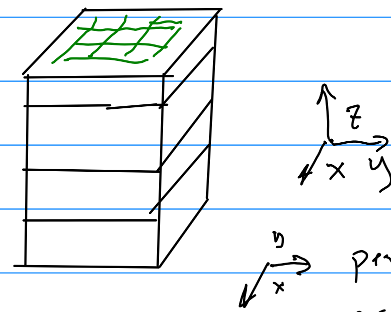
Fields institute mini-course : Lecture 2

"Numerical techniques for simulating collective and coherent quantum states"

Chris Anderson (UCLA Department of Mathematics)

"dimension reduction"



Schroedinger - Poisson.

periodic or infinite. in transverse directions.

(0) Determine ϕ_D such that

$$\Delta_x \phi_D = -\rho_D \qquad \phi_D(z_A) = g_A(x,y) \qquad \phi_D(z_B) = g_B(x,y)$$

(1) Determine $\tilde{\phi}(\vec{x})$, $\rho_e(\vec{x})$ so that

$$\Delta_x \tilde{\phi} = -\rho_e \qquad \tilde{\phi}(z_A) = 0 \qquad \tilde{\phi}(z_B) = 0$$

$$\left[\Delta_m + [\tilde{\phi} + \phi_D + \phi_B] \right] \psi_j = \lambda_j \psi_j$$

$$\rho_e(\vec{x}) = \sum_{|\lambda_j - E_f|} \psi_j^*(\vec{x}) \psi_j(\vec{x})$$

Tasks require solving 3D Poisson problems and 3D eigensystem problems. For some problems - notably those in which the potential applied at the gates is constant, or only depends on one coordinate, e.g. $g_{A,B}(x,y) = \text{constant}$ or $g_{A,B}(x,y) = g_{A,B}(y)$ one can reduce the dimensionality of the tasks to 2D or 1D computational work. With such boundary conditions one can create solutions of the 3D problem by combining analytical solutions with 1D or 2D computational work.

(I) When g_A, g_B are constant and uniform, and $\rho_D(x,y,z) = \rho_D(z)$ (domain periodic)

ϕ_B: only a function of z

ϕ_D: only a function of z and satisfies

$$\frac{d}{dz}\kappa(z)\frac{d}{dz}\phi_D = -\rho_D(z) \qquad \phi(z_A) = g_A \qquad \phi(z_B) = g_B.$$

$\tilde{\phi}$: only a function of z (assume ρ_e is only a function of z) and satisfies

$$\frac{d}{dz}\kappa(z)\frac{d}{dz}\tilde{\phi} = -\rho_e(z) \qquad \tilde{\phi}(z_A) = 0 \qquad \tilde{\phi}(z_B) = 0$$

So 1D Poisson problems.

What about Schroedinger's equation? Assume ϕ only a function of $\vec{z}$.

$$-\frac{\hbar^2}{2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_r(z)}\frac{\partial}{\partial z}\right) + \frac{1}{m_r(z)}\frac{\partial^2}{\partial y^2} + \frac{1}{m_r(z)}\frac{\partial^2}{\partial x^2}\right]\psi_j + \phi(z)\,\psi_j = \lambda_j \psi_j$$

A separable operator $\Rightarrow$ eigenfunctions are given by products of eigenfunctions of x, y, z separately.

$$\psi_j(x,y,z) = \alpha_p(z)\,\beta_q(y)\,\gamma_r(x) \qquad \lambda_j = \lambda_p + \lambda_q + \lambda_r$$

Note: $m_r(z)$ is constant in each layer

(*) $$\left\{ -\frac{\hbar^2}{2m_r(z)}\frac{d^2\beta_q}{dy^2} = \lambda_q\,\beta_q(y) \qquad -\frac{\hbar^2}{2m_r(z)}\frac{d^2\gamma_r}{dx^2} = \lambda_r\gamma_r(x). \right.$$

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_r(z)}\frac{d}{dz}\right) + \phi(z)\right]\alpha_p(z) = \lambda_p\,\alpha_p(z)$$

Why? Plug in formally, factor out $\alpha_p(z)\,\beta_q(y)\,\gamma_r(z)$ to verify eigenfunctions.

Assume periodic with domain size L.

Since eigenfunctions of $(*)$ are $\beta_q(y) = \dfrac{e^{i\pm\sqrt{\lambda_q \frac{\hbar^2}{2m_r}}\, y}}{\sqrt{L}}$ $\quad \gamma_r(x) = \dfrac{e^{i\pm\sqrt{\lambda_r \frac{\hbar^2}{2m_r}}\, x}}{\sqrt{L}}$

$\Rightarrow \beta_q^*(y)\,\beta_q(y) = 1$ and $\gamma_r^*(x)\,\gamma_r(x) = 1$

$$\therefore \psi_j^*\psi_j = \left(\alpha_p^*(z)\,\alpha_p(z)\right)\underbrace{\left(\beta_q^*(y)\,\beta_q(y)\right)\left(\gamma_r^*(x)\,\gamma_r(x)\right)}_{\text{constant}} = \text{only a function of } z.$$

$\therefore \rho_e$ is only a function of z, e.g. $\rho_e = \rho_e(z)$.

Computation of $\rho_e(z)$?

Compute eigenvalues and eigenvectors of

$$\left[-\frac{\hbar^2}{2}\frac{d}{dz}\left(\frac{1}{m_r(z)}\frac{d}{dz}\right) + \phi(z)\right]\alpha_p(z) = \lambda_p\,\alpha_p(z)$$

$\beta(y)$'s, $\gamma(x)$'s unit L^2 norm

$$\rho_e(z) = \sum_{\lambda_p < E_f} \alpha_p^*(z)\,\alpha_p(z)\left(\sum_{\lambda_q+\lambda_r < E_f-\lambda_p} 1 \cdot 1\right)$$

In the limit as the periodic domain size $\nearrow \infty$ then one gets.

$$\rho_e(z) = \sum_{\lambda_p < E_f} \alpha_p^*(z)\,\alpha_p(z)\cdot \underbrace{\left[\frac{1}{2\pi\hbar^2}\, m_r(z)\right](E_f-\lambda_p)}_{\text{"density of states"}}$$

∴ If uniform g_A, g_B, ρ_D and the transverse domain is periodic or infinite ⇒ 1D Schroedinger - Poisson.

(0) Determine $\phi_D(z)$ so that

$$\frac{d}{dz}\kappa(z)\frac{d}{dz}\phi_D = -\rho_D(z) \qquad \phi_D(z_A) = g_A \quad \phi_D(z_B) = g_B$$

(1) Determine $\tilde{\phi}(z), \rho_e(z)$ so that

$$\frac{d}{dz}\kappa(z)\frac{d}{dz}\tilde{\phi} = -\rho_e(z) \qquad \tilde{\phi}(z_A) = 0 \qquad \tilde{\phi}(z_B) = 0$$

$$-\frac{\hbar^2}{2}\frac{d}{dz}\frac{1}{m_r(z)}\frac{d}{dz}\alpha_p(z) = \lambda_p\,\alpha(z) \qquad \alpha(z_A) = \alpha(z_B) = 0$$

$$\rho_e(z) = \sum_{\lambda_p < E_F} \alpha_p^*(z)\alpha_p(z)\cdot W(\lambda_p, E_F)$$

↑ weight factor due to energy contributions of transverse eigenfunctions.

⇝ 1D tasks for the solution of a $\underline{3D}$ problem.

The dimension reduction is not obtained by 'averaging' over the transverse direction - it's obtained by using an analytic solution in the transverse directions.

Similarly if g_A, g_B only vary in one of the transverse directions then one only needs to compute the electrostatics and eigensystems for $\underline{2D}$ problems.

⇒ 2D Schroedinger - Poisson.

Building up simulation capability.

3D Schroedinger - Poisson & 1D Poisson, 1D Eigensystem (1D Schroedinger Poisson) + 2D analytic solution.

3D Schroedinger - Poisson & 2D Poisson, 2D Eigensystem (2D Schroedinger Poisson) + 1D analytic solution.

3D Schroedinger - Poisson ~ 3D Poisson, 3D Eigensystem

DFT (Density Functional Theory) ~ 3D Poisson, 3D Eigensystem

FCI (Full Configuration Interaction) ~ 3D Poisson, 3D Eigensystem
using Slater determinant wavefunctions.

1D ? Useful for many problems
Executes quickly
A good place to start learning about numerical techniques.

2D ? 1D → 2D, there are things to know about going from 1D->2D eigenproblems.

3D ? You typically focus on computational efficiency.