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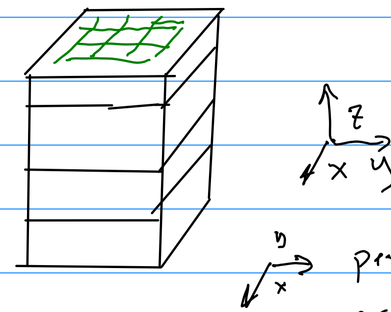
Fields institute mini-course: Lecture 2

"dimension reduction".

Schroedinger - Poisson.



periodic or infinite in transverse directions.

(0) Determine ϕ_D such that

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

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

$$\Delta_K \tilde{\phi} = -\rho_e \qquad \tilde{\phi}(x,y,z_A) = 0 \qquad \tilde{\phi}(x,y,z_B) = 0$$

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

$$\rho_e(\vec{x}) = 2 \sum_{\lambda_j < E_f} \psi_j^*(\vec{x}) \psi_j(x)$$

The tasks required involve solving 3D Poisson equations and for eigenvalues and eigenfunctions of a 3D operator. For some problems, notably those where the potential applied to the gates is uniform, or only depends on one coordinate, e.g. $g_A(x,y) = g_A(x)$ $g_B(x,y) = g_B(x)$, one can reduce the dimensionality of the tasks to only involve 1D or 2D work. For such boundary conditions one can create solutions of the 3D problem by combining analytic solutions with 2D or 1D numerical solutions.

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

ϕ_B : only a function of z

ϕ_D : only a function of z and satisfies

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

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

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

All 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

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

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

Assume periodic with domain size L.

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

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

$\therefore\ \psi_j^*\psi_j = \left(\alpha_p^*(z)\,\alpha_p(z)\right)\underbrace{\left(\beta_q^*(y)\,\beta_q(y)\right)\left(\gamma_r^*(x)\,\gamma_r(x)\right)}_{1}$ = 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

$$\rho_e(z) = 2\sum_{\lambda_p < E_f}{}^{'}\ \alpha_p^*(z)\,\alpha_p(z)\left(\sum_{\lambda_q+\lambda_r < E_f-\lambda_p}{}^{'}\ 1\cdot 1\right)$$

In the limit as the periodic domain size $L \nearrow \infty$, one finds by recognizing the sum as an approximation to an integral, and carrying out the integration that

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

∴ If constant g_A, g_B, ρ_D only a function of z, and the transverse domain is periodic or infinite $\Rightarrow$ 1D Schroedinger equation.

The set of equations for ϕ and ρ_e constitute the 1D Schroedinger-Poisson equations.

(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

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

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

$$\rho_e(z) = 2\sum_{\lambda_p < E_F} \alpha^*_p(z)\alpha_p(z)\cdot W(\lambda_p, E_F)$$

↑ weight factor due to energy contributions of transverse eigenfunctions.

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

The 1D Schroedinger-Poisson is $\underline{\text{not}}$ obtained by averaging over the transverse directions, as is often used in dimension reduction. The dimension reduction occurs because we are using a solution that combines an analytic solution with the numerical solution.

If g_A, g_B are only functions of x (or of y), and $\rho_e(x,y,z) = \rho_e(x,z)$ then one can derive the 2D Schroedinger-Poisson equations by combining a 2D numerical solution with a 1D analytic solution, 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

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

Hartree - Fock. 3D Poisson, 3D Eigensystem

Full Configration Interaction (FCI) using Slater determinant basis.

1D? Useful for many problems

Executes quickly

A good place to start learning about numerical techniques.

2D? 1D → 2D, the numerical methods change a bit.

3D? Typically one uses the same methods as 2D, but is concerned primarily with computational efficiency.