Fields institute mini-course : Lecture 1 April 16, 2018

"Numerical techniques for simulating collective and coherent quantum states"

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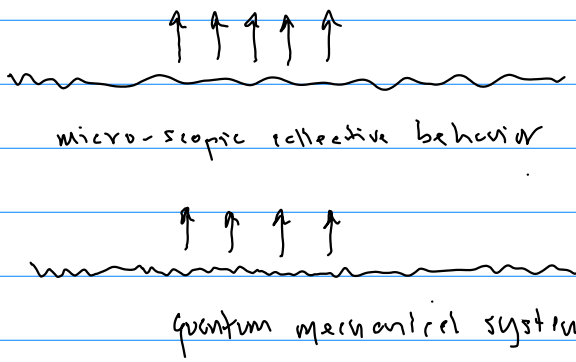
Today

- Why?
- Overview
  - 3D problem (General, then specific to Schroedinger-Poisson)
  - Task dimension reduction (separation of variables / density of states
  - 1D, 2D, 3D. Schroedinger-Poisson

Why



Development/Exploration/Use of ODE and PDE mathematical models at all scales requires simulation

Fortunately, at every scale there is great commonality of the computational tasks that must be done within a simulation based on the models. Specifically

charged particles — electrostic problems — Poisson's equation

$$\Delta \phi = -\rho$$

$$\text{div}(\kappa \nabla \phi) = -\rho$$

$\Rightarrow$ need to solve Poisson's equation.

Wavefunctions ~ time-independent Schroedinger equation ~ Eigenfunction/Eigenvalue computation
"quantum states" (or dynamics projected onto eigenfunctions of time independent Schroedinger operator)

⇒ need to solve eigensystem problems, for example the time independent single particle Schroedinger equation

$$[-\beta\Delta + V(\vec{x})]\psi = \lambda\psi \quad \vec{x} \in \mathbb{R}^3$$

or ∇^2 if you prefer.

$$-\text{div}(\beta\nabla\psi) + V(\vec{x})\psi = \lambda\psi \quad \vec{x} \in \mathbb{R}^3$$

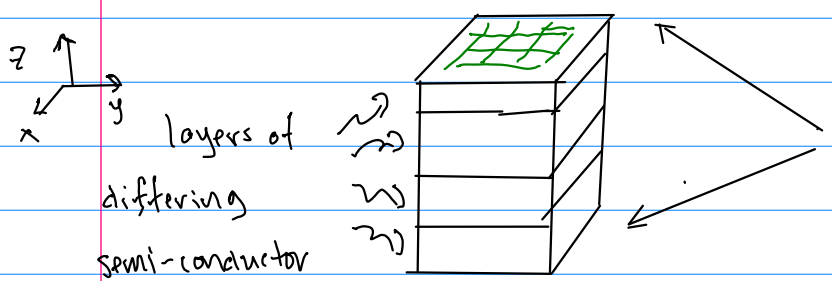
Also, fortunately, numerical methods for many of the common computational tasks have been well studied. However, there are many methods to choose from and good choices depend on an awareness of some of the specific features of the computational tasks that arise when constructing simulations involving quantum mechanical behavior.

In addition, many simulations are based on coupled systems, and while each sub-system itself may be composed of equations whose solutions can be obtained using "conventional" methods, the methods for combining subsystem solutions can be tricky.

So, there are aspects of numerical methods for many common problems that are useful to know about, and, knowing them will increase the likelihood that you will be able to develop/explore/use simulations of systems involving quantum mechanical behavior.

Exposition plan: Present and discuss the techniques and details in the context of creating a simulation based on a Schroedinger-Poisson model for determining electron density in a layered semi-conductor. The perspective I'm going to take is "here is a coupled system of PDE's - let's create a simulation based on this system of PDE's". I'm generally not going to get into a discussion of the physics involved - e.g., it's being picked for expository reasons.

Device: A layed semi-conductor periodic or infinite in transverse directions.



low temperature ⇒ electrons associated with atoms in the material are 'frozen' in.

Equations / mathematical model.

* The electrostatic potential is the sum of

ϕ_D : (1) The potential induced by gate bias and any 'static' charge

$\tilde{\phi}$: (2) The potential induced by the density of "mobile" electrons

ϕ_B : (3). A bandshift potential

Associated with each material is a band shift - a fixed potential offset from the ambient potential

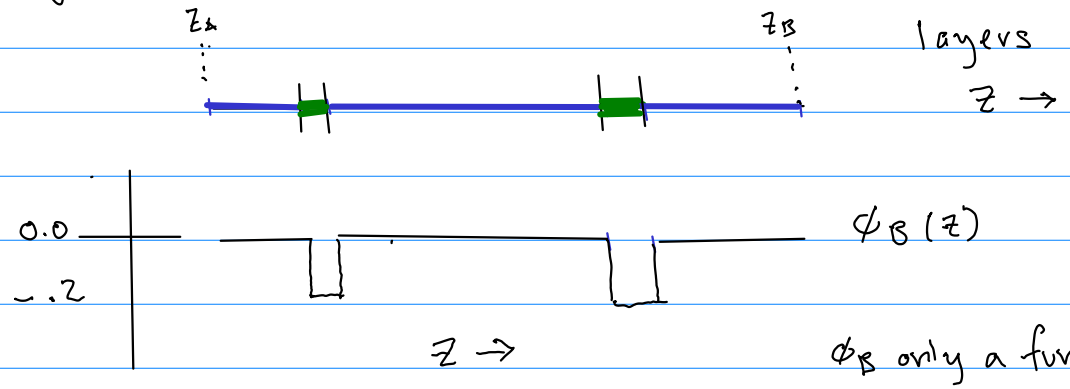
$\phi = \tilde{\phi} + \phi_D + \phi_B$

mat-1 : band shift −.2

mat-2 : band shift 0

Bandshift potential ϕ_B ?

ϕ_B is "given"



ϕ_B only a function of z.

ϕ_D: "Doping" potential

Assume dielectric factor is uniform in each layer - but different layers may have different dielectric factors.

A fixed charge (+ or −), typically due to doping

$$\frac{\partial}{\partial z}\left(\chi(z)\frac{\partial}{\partial z}\right)\phi_D + \chi(z)\frac{\partial^2\phi_D}{\partial y^2} + \chi(z)\frac{\partial^2\phi_D}{\partial x^2} = -\rho_D$$

$\phi_D(x,y,z_A) = g_A(x,y)$ $\quad$ $\phi_D(x,y,z_B) = g_B(x,y)$

$\chi(z)$ = dielectric factor

$\chi(z)$ will often be a <u>discontinuous</u> function of z.

$\tilde{\phi}$: Potential due to mobile electron charge density.

$$\frac{\partial}{\partial z}\left(\chi(z)\frac{\partial}{\partial z}\right)\tilde{\phi} + \chi(z)\frac{\partial^2\tilde{\phi}}{\partial y^2} + \chi(z)\frac{\partial^2\tilde{\phi}}{\partial x^2} = -\rho_e$$

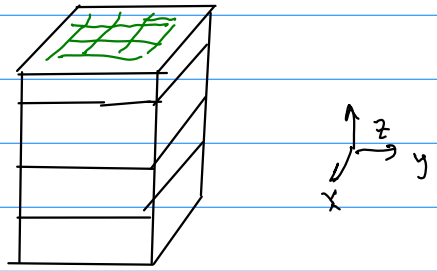
$\tilde{\phi}(x,y,z_A) = 0 \quad \tilde{\phi}(x,y,z_B) = 0$

$\chi(z)$ = dielectric factor

Notation for convenience $\Delta_x \phi = \frac{\partial}{\partial z}\left(\chi(z)\frac{\partial}{\partial z}\right)\phi + \chi(z)\frac{\partial^2\phi}{\partial y^2} + \chi(z)\frac{\partial^2\phi}{\partial x^2}$

Electrostatic potential.

$$\phi(\vec{x}) = \tilde{\phi}(\vec{x}) + \phi_D(\vec{x}) + \phi_B(\vec{x}) \qquad \vec{x} \in \mathbb{R}^3$$



ϕ_B : given

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

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

mmm

What are the equations for ρ_e - the electron density?

If $\psi_j(\vec{x})$ is the single particle wave function with energy E_j then

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

E_f = Fermi energy. (2 for double occupancy)

So: determine single particle states, add up densities associated with each state, if the state has a sufficiently low energy level.

Equations?

Single particle Schroedinger equation

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

$m_r(z)$ = effective mass - constant in each layer, but may be discontinuous across layers.

$$V(\vec{x})=\tilde{\phi}(\vec{x})+\phi_D(\vec{x})+\phi_B(\vec{x})$$

Notational convenience $\Delta_m=-\frac{\hbar^2}{2}\left[\frac{\partial}{\partial z}\frac{1}{m_r(z)}\frac{\partial}{\partial z}+\frac{1}{m_r(z)}\frac{\partial^2}{\partial y^2}+\frac{1}{m(z)}\frac{\partial^2}{\partial x^2}\right]$

So, the equations for the density become

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

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

Since $\tilde{\phi}(\vec{x})$ is determined by $\rho_e(\vec{x})$, and $\rho_e(\vec{x})$ is determined by $\tilde{\phi}(\vec{x})$, there is a coupling between the potential and the states of the system. A non-linear coupling.

Equations / tasks required to obtain a solution of the Schroedinger - Poisson.

(0) Determine ϕ_D such that

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

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

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

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

$$\rho_{e,i} = 2 \sum_{j < E_f} \psi_j^*(\vec{x}) \psi_j(x)$$

what's being presented in these following lectures is a 1D version of many of the ideas in.

C. R. Anderson. "Efficient solution of the Schroedinger–Poisson equations in layered semiconductor devices", J. of Comp. Phys., 228, 4745-4756, (2009)

However, the discretization of the electrostatics problem will be done using finite volume discretizations instead of the procedure based upon Wachspress' method.