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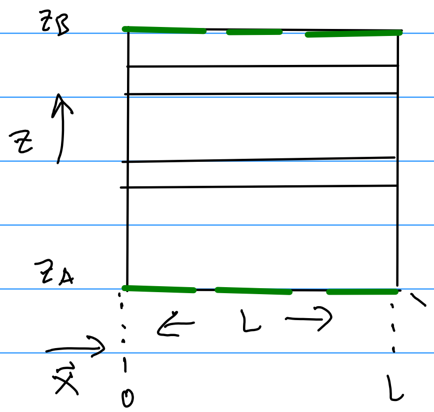
The electrostatic problem in a 2D layered semi-conductor.



$$\frac{d}{dz}\left(\kappa(z)\frac{d\phi}{dz}\right) + \kappa(z)\frac{d^2\phi}{dx^2} = -\rho(x,z)$$

$$\phi(x, z_A) = g_A(x) \qquad \phi(x, z_B) = g_B(x)$$

Assume periodic in x.

Solution? How might we do it analytically? Ansatz.

$$\phi(x,z) = \sum_{k=-\infty}^{\infty} a_k(z)\, e^{\frac{2\pi i k x}{L}}$$

Fourier modes in the transverse direction whose coefficients depend on z.

Equations for the $a_k(z)$?

For each k, insert into the equation and equate coefficients of Fourier modes.

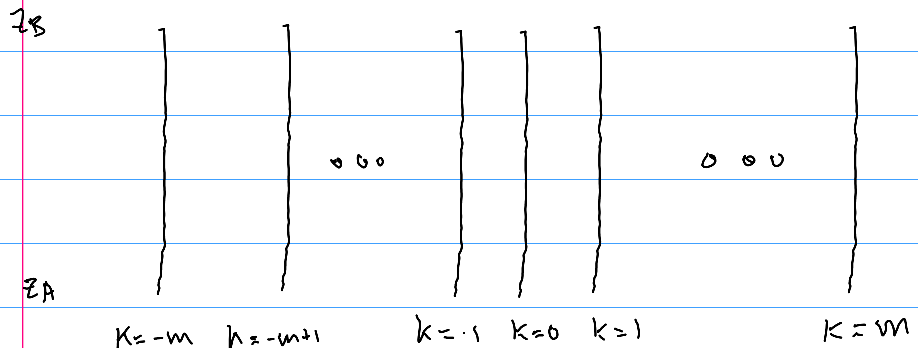
(*) $$\frac{d}{dz}\kappa(z)\frac{d}{dz}a_k(z) - \frac{4\pi^2 k^2}{L^2}a_k(z) = -b_k(z) \qquad a_k(z_A) = c_A^k \quad a_k(z_B) = c_B^k$$

where $b_k(z)$, c_A^k, c_B^k are the coefficients of the Fourier expansion of $\rho(x,z)$, $g_A(x)$ and $g_B(x)$ respectively.

$$\rho(x,z) = \sum_{k=-\infty}^{\infty} \underline{b_k(z)}\, e^{\frac{2\pi i k}{L}x} \qquad g_A(x) = \sum_{k=-\infty}^{\infty} \underline{c_A^k}\, e^{\frac{2\pi i k x}{L}} \qquad g_B(z) = \sum_{k=-\infty}^{\infty} \underline{c_B^k}\, e^{\frac{2\pi i k x}{L}}$$

For each Fourier mode, k, we have an ODE in z whose solution determines the Fourier coefficients of ϕ. The solution to this ODE can be solved numerically using essentially the same techniques as used for the Poisson equation in the 1D Schroedinger-Poisson equations.

So, pick some # of modes, say all $k \in [-m\ m]$



(I) For each z determine $b_k(z)$ so $\rho(x,z) = \sum_{k=-m}^{m}{}' \, b_k(z)\, e^{2\pi i \frac{k}{L} x}$

and c_A^k so $g_A(x) = \sum_{k=-m}^{m}{}' \, c_A^k \, e^{\frac{2\pi i k x}{L}}$

c_B^k so $g_B(z) = \sum_{k=-m}^{m}{}' \, c_B^k \, e^{\frac{2\pi i k x}{L}}$

(II) Solve for each $k \in [-m, m]$ the $2m+1$ ODE's

$$\frac{d}{dz} \kappa(z) \frac{d}{dz} a_k(z) - \frac{4\pi^2 k^2}{L^2} a_k(z) = -b_k(z) \qquad a_k(z_A) = c_A^k \quad a_k(z_B) = c_B^k$$

(III) $$\phi(x,z) \overset{\sim}{=} \sum_{k=-m}^{m}{}' \, a_k(z)\, e^{\frac{2\pi i k x}{L}}$$

A numerical procedure results when numerical methods are use to carry out (I), (II), and (III).

For (I), if one is doing the calculations analytically, then the coefficients are determined using the standard formulas:

$$b_k(z) = \int_0^L \frac{1}{\sqrt{L}} e^{\frac{-2\pi i k x}{L}} \rho(x,z)\, dx \qquad c_k^A = \int_0^L \frac{1}{\sqrt{L}} e^{\frac{-2\pi i k x}{L}} g_A(x)\, dx$$

$$c_k^B = \int_0^L \frac{1}{\sqrt{L}} e^{\frac{-2\pi i k x}{L}} g_B(x)\, dx$$

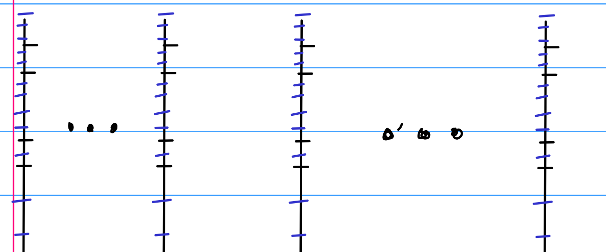
If one uses a uniform grid in the x-direction, and the Trapezoidal method of approximating the integrals so

$$b_k(z) \doteq \sum_{j=0}^{N_x-1} \rho(x_j, z) \frac{e^{\frac{-2\pi i k x_j}{L}}}{\sqrt{L}}$$

Then the work to evaluate all necessary sums for a specified value of z can be accomplished with one call to a Fast Fourier Transform (FFT) routine.

For (III), again using a uniform grid in the x-direction, all values of $\phi(x_j, z) = \sum_{k=-m}^{m} a_k(z) e^{\frac{-2\pi i k x_j}{L}}$ at x_j for a fixed z can be carried out using one call to an FFT routine.

What about (II)? Use the same procedure as was used to solve Poisson's equation in the 1D Schroedinger-Poisson.
The mesh in the z-direction can be semi-uniform - there is no requirement that the mesh in the z-direction be uniform.



$k=-m$ $\quad k=-1$ $\quad k=0$ $\quad k=m$

For each k solve an ODE for $a_k(z)$ in the z direction.

Computational work?

number of z grid points

number of transverse Fourier modes = number of x grid points, N_x $\Rightarrow O\left(N_x \cdot \log_2(N_x) \cdot N_z\right)$

$\therefore$ $O(N_x \log_2(N_x) \cdot N_z) \approx O(N_x N_z) = O($total number of grid points$)$
$(O(N))$

$\Rightarrow$ A "fast direct method".

What's interesting about the resulting numerical method is that it isn't derived by first discretizing and the solving the resulting linear system.

More details about this solution procedure can be found in.

C. R. Anderson, T. C. Cecil, “A Fourier–Wachspress method for solving
Helmholtz’s equation in three-dimensional layered domains”,
J. of Comput. Phys., 205, 706-71, (2005)