Ankara University

Numerical Solution of Particle in 1D Potential

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1 Numerical Solution of Particle in 1D Potential

First lets assume the problem with particle in 1D potential with nonuniform shape.

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{x}) \tag{1}$$

$$\hat{H}\Psi^{(0)}(x) = E^0\Psi^{(0)}(x) \tag{2}$$

Wavefucntion of this corresponded second order differential equation is summation of primitive wavefunctions with different k points and related factors.

$$\Psi^{(0)}(x) = \int_{-\infty}^{\infty} a_k e^{ikx} dk \tag{3}$$

$$\Psi^{(0)}(x) = \sum_i^N a_i e^{ik_i x} \tag{4}$$

Wave functions is nothing but just functional of $\{a_i\}_N$ and $\{k_i\}_N$ set.

$$\Psi^{(0)}[\{a_i\},\{k_i\}](x) = \sum_i^N a_i e^{ik_i x} \tag{5}$$

Which means that by changing the paramteres of $\{a_i\}_N$ and $\{k_i\}_N$ we can construct any wavefunction which is solution of given Hamiltonian.

Lets assume we have energy E_{system} of given system corresponded potental $V(r)$. If wavefunctions $\Psi_{system}(x)$ is the solution of given system then that statement is always true.

$$\int_{-\infty}^{\infty}\left[\frac{\Big(-\frac{\hbar^2}{2m}\nabla^2\Psi^{(0)}[\{a_i\},\{k_i\}](x) + V(x)\Psi^{(0)}[\{a_i\},\{k_i\}(x)\Big)}{\Psi^{(0)}[\{a_i\},\{k_i\}](x)} - E_{system}\right]dx = 0 \tag{6}$$

This is cost function in discrete form and in true k and a values this statement is true:

$$C = \sum_j\left[\frac{\Big(-\frac{\hbar^2}{2m}\nabla^2\Psi^{(0)}[\{a_i\},\{k_i\}](x_j) + V(x)\Psi^{(0)}[\{a_i\},\{k_i\}(x_j)\Big)}{\Psi^{(0)}[\{a_i\},\{k_i\}](x_j)} - E_{system}\right] \approx 0 \tag{7}$$

Also cost function is the functional of a and k.

$$C[\{a_i\},\{k_i\}] \approx 0 \tag{8}$$