LAPW Notes

Radial Schroedinger equation:

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \frac{l(l+1)}{2r^2} + V_{\mathrm{KS}}(r) - \epsilon_{nl}\right] u_{nl}(r) = 0 \tag{1}$$

Numerov integration

$$x''(t) = f(t)x(t) + u(t) \tag{2}$$

$$x(h) + x(-h) = 2x(0) + h^2\left[f(0)x(0) + u(0)\right] + \frac{2}{4!}h^4 x^{(4)}(0) + O(h^6) \tag{3}$$

For $O(h^4)$ algorithm, we can neglect $x^{(4)}$ term and get the following:

$$x_{i+1} - 2x_i + x_{i+1} = h^2(f_i x_i + u_i) \tag{4}$$

From the differential equation we can get:

$$x^{(4)} = \frac{\mathrm{d}^2 x''(t)}{\mathrm{d}t^2} = \frac{\mathrm{d}^2}{\mathrm{d}t^2}(f(t)x(t) + u(t)) \tag{5}$$

which can be approximated by:

$$x^{(4)} \approx \frac{f_{i+1}x_{i+1} + u_{i+1} - 2f_i x_i - 2u_i + f_{i-1}x_{i-1} + u_{i-1}}{h^2} \tag{6}$$

Using this we can write:

$$x_{i+1} - 2x_i + x_{i-1} = h^2\left(f_i x_i + u_i\right) + \tag{7}$$

$$\frac{h^2}{12}\left(f_{i+1}x_{i+1} + u_{i+1} - 2f_i x_i - 2u_i + f_{i-1}x_{i-1} + u_{i-1}\right) \tag{8}$$

Using $w_i = x_i\left(1 - \frac{h^2}{12}f_i\right) - \frac{h^2}{12}u_i$ we have the following scheme:

$$w_{i+1} - 2w_i + w_{i-1} = h^2\left(f_i x_i + u_i\right) + O(h^6) \tag{9}$$