fredag 23. september 2016 08.42

Repulsion between two electrons:

$$V(\vec{r}_1, \vec{r}_2) = \frac{\beta}{|\vec{r}_1 - \vec{r}_2|} \qquad \beta = 1.44 \text{ eV nm}$$

$$= \frac{\beta}{r}$$

$$\Rightarrow \text{Our eq.: } \left(-\frac{\hbar^2}{m}\frac{d^2}{dr^2} + \frac{kr^2}{4} + \frac{\beta}{r}\right) u(r) = E_r\, u(r)$$

The general form:

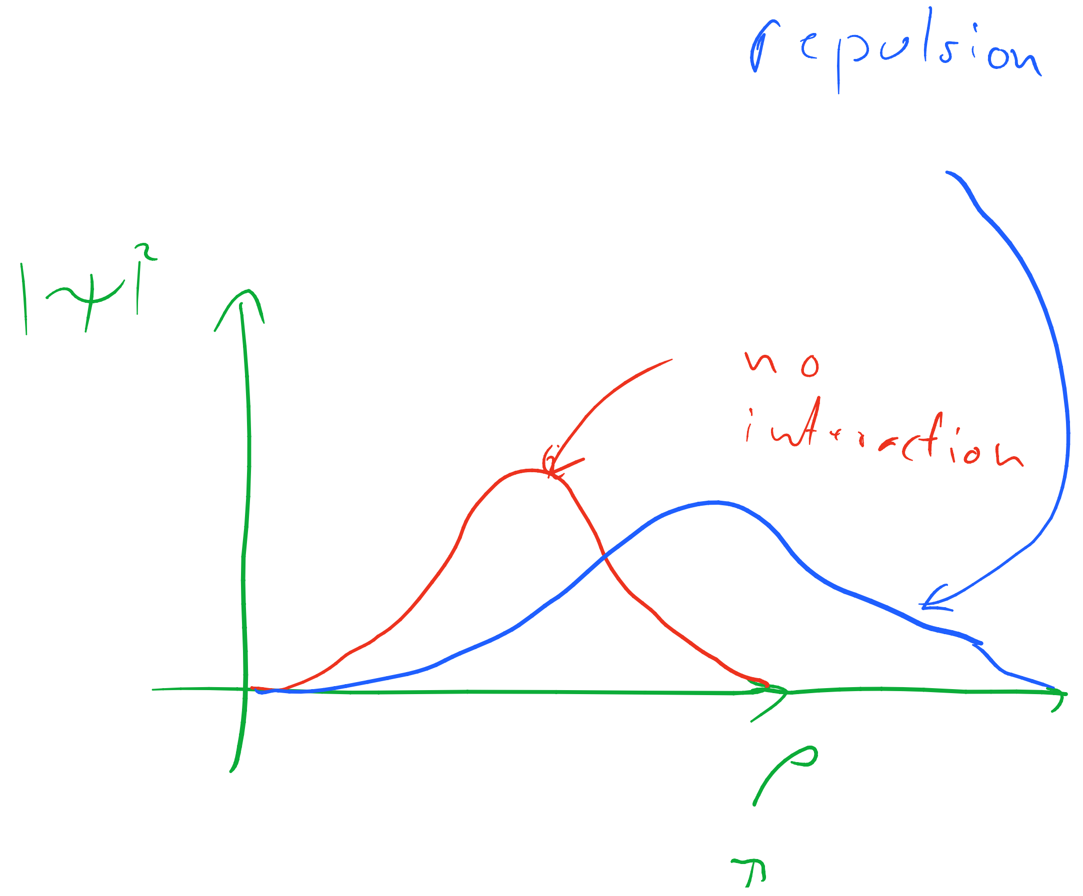
$$-\frac{d^2}{d\rho^2}\psi(\rho) + V(\rho)\psi(\rho) = \lambda\psi(\rho)$$

When discretized

$$-\frac{(\psi_{i+1} + \psi_{i-1} - 2\psi_i)}{h^2} + V_i\psi_i = \lambda\psi_i$$

Two types of potential

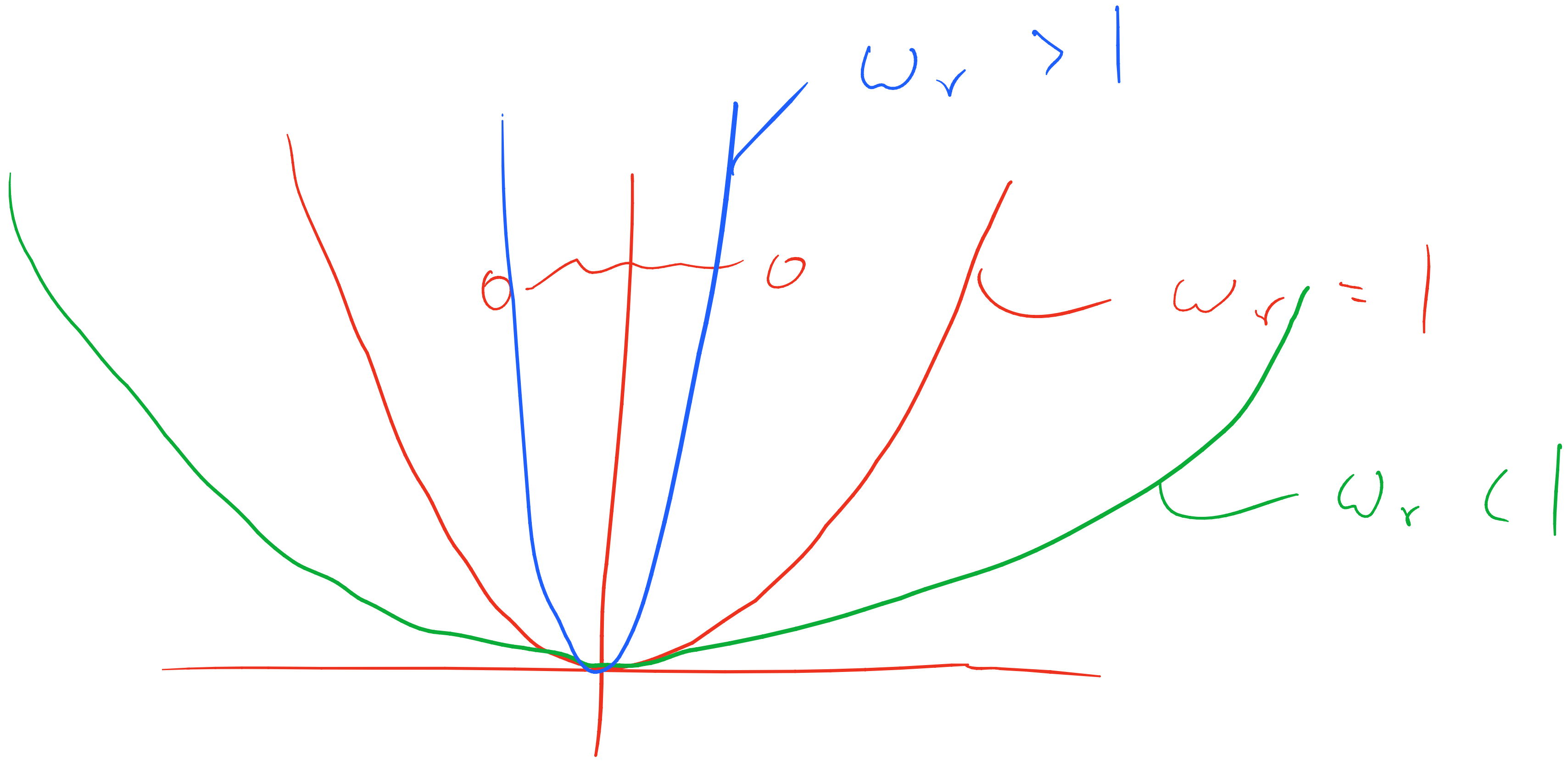
(i) $V_i = \rho_i^2$



(i) $V_i = \rho_i$

(ii) $V_i = \omega_r^2 \rho_i + \frac{1}{\rho_i}$

relative distance



General symmetric/hermitian square matrix A

Schur decomposition:

$$T = S^T A S \qquad S^T = S^{-1} \qquad S^T S = \mathbb{1}$$

tridiagonal

Eigenvalue and eigenvector algo:

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$$\overset{A}{\begin{bmatrix} \times & \times & \cdots & \times \\ \times & \times & & \vdots \\ \vdots & & \ddots & \vdots \\ \times & \cdots & \cdots & \times \end{bmatrix}} \xrightarrow[1]{\text{Phase}} \overset{T}{\begin{bmatrix} \times & \times & & & 0 \\ \times & \times & \times & & \\ & \times & \times & \ddots & \\ & & \ddots & \ddots & \times \\ 0 & & & \times & \times \end{bmatrix}} \xrightarrow[2]{\text{Phase}} \overset{D}{\begin{bmatrix} \times & & & 0 \\ & \times & & \\ & & \ddots & \\ 0 & & & \times \end{bmatrix}}$$