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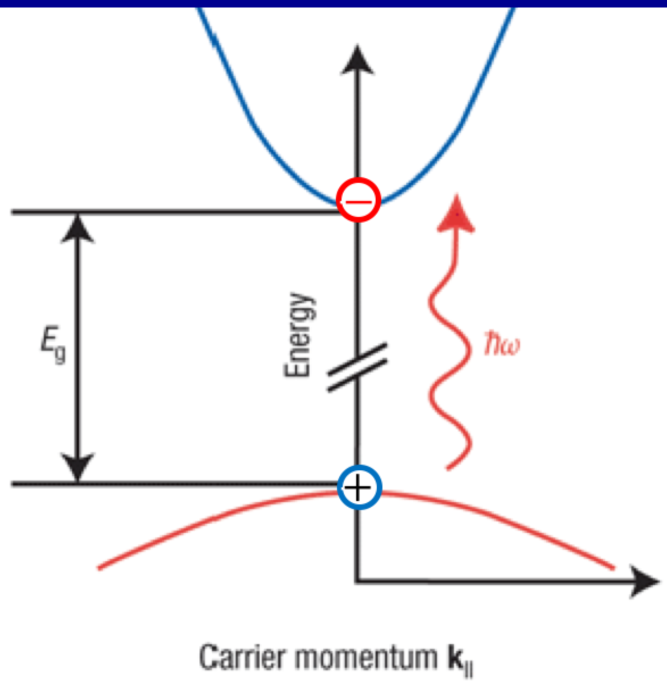
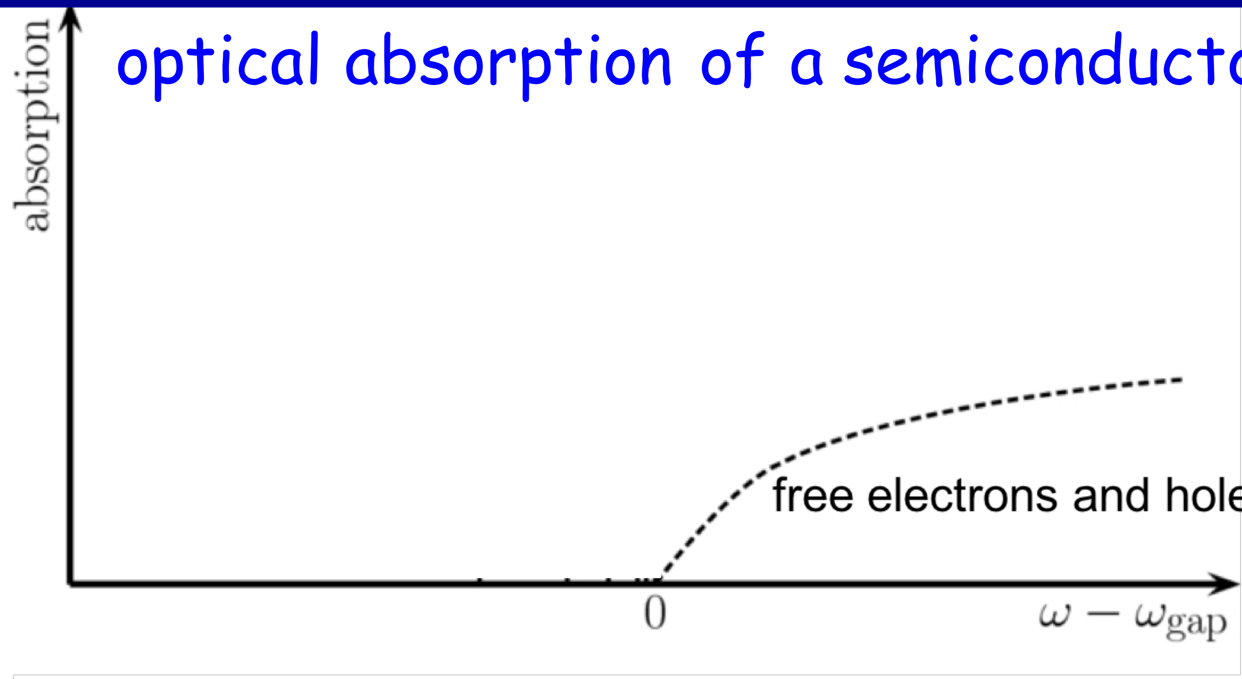
MESA+ INSTITUTE FOR NANOTECHNOLOGY

Project 1: Excitons

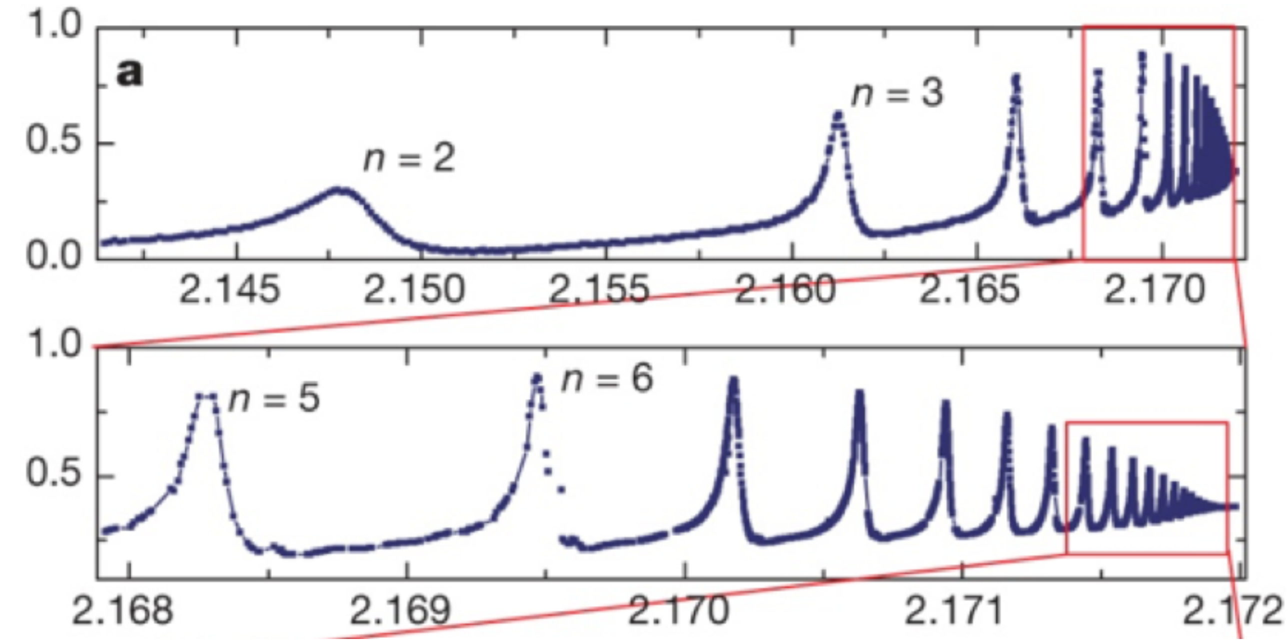
Project 1: Excitons $\hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$





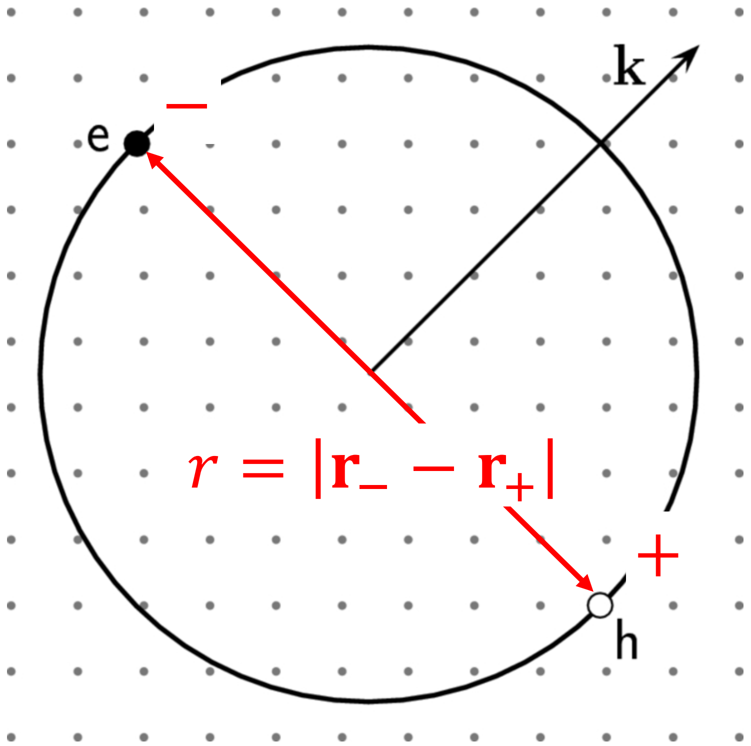
Excitons in Cu_2O

Kazimierczuk et al,
Nature 514, 343 (2014)



Wannier excitons $\hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$

simple model: electron + hole, Coulomb interaction



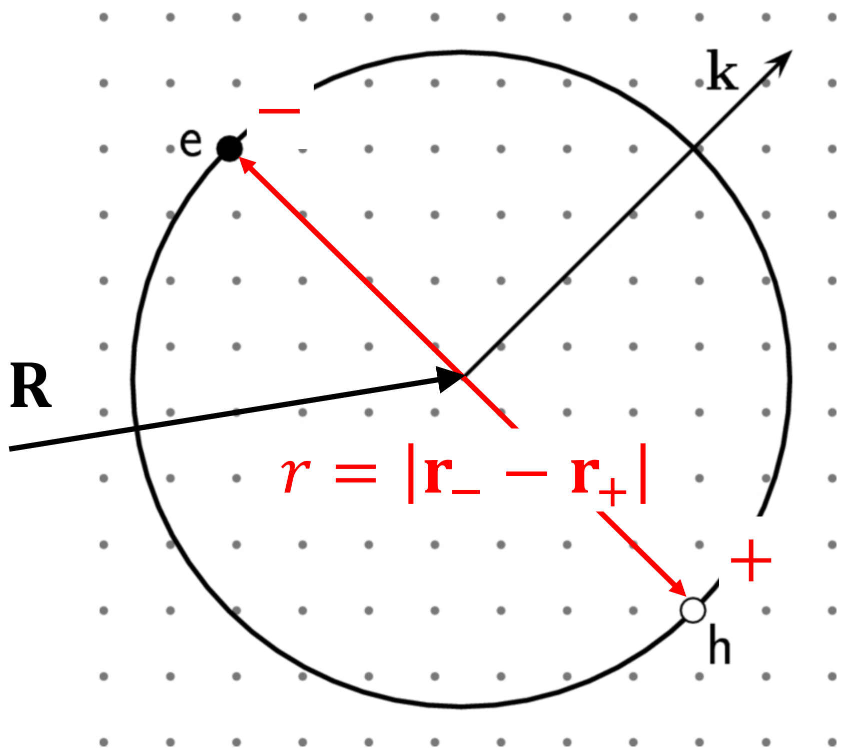
$$V(\mathbf{r}_-, \mathbf{r}_+) = -\frac{e^2}{4\pi\epsilon}\frac{1}{|\mathbf{r}_- - \mathbf{r}_+|}$$

Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2m_-}\nabla_-^2 - \frac{\hbar^2}{2m_+}\nabla_+^2 + V(\mathbf{r}_-, \mathbf{r}_+)\right\}\Psi(\mathbf{r}_-, \mathbf{r}_+) = E\Psi(\mathbf{r}_-, \mathbf{r}_+)$$

Wannier excitons $\hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$

simple model: electron + hole, Coulomb interaction



$$V(\mathbf{r}_-, \mathbf{r}_+) = -\frac{e^2}{4\pi\epsilon}\frac{1}{|\mathbf{r}_- - \mathbf{r}_+|}$$

$$\mathbf{r} = \mathbf{r}_- - \mathbf{r}_+ = (r, \theta, \phi)$$

solution:

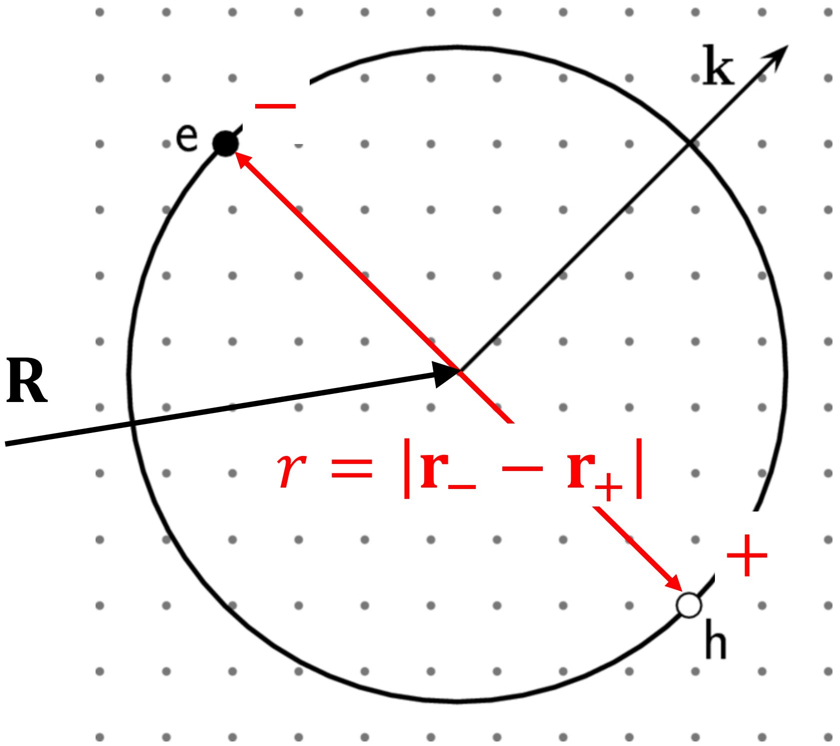
$$\Psi = \exp[i\mathbf{k}\cdot\mathbf{R}]Y_l^m(\theta,\phi)\zeta_{nl}(r)/r$$

Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2m_-}\nabla_-^2 - \frac{\hbar^2}{2m_+}\nabla_+^2 + V(\mathbf{r}_-, \mathbf{r}_+)\right\}\Psi(\mathbf{r}_-, \mathbf{r}_+) = E\Psi(\mathbf{r}_-, \mathbf{r}_+)$$

Wannier excitons $\hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$

simple model: electron + hole, Coulomb interaction



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solution:

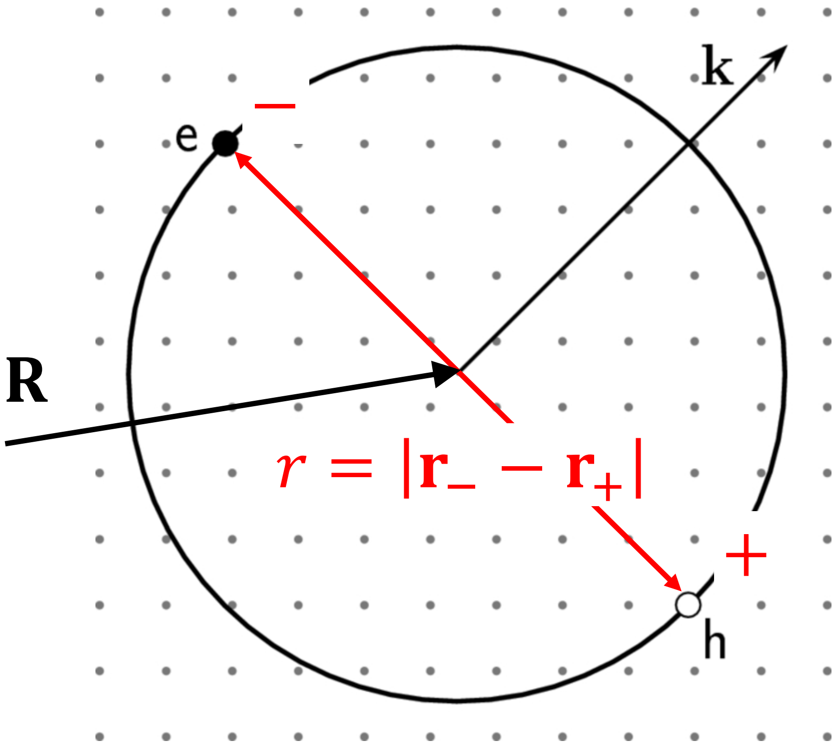
$$\Psi = \exp[i\mathbf{k}\cdot\mathbf{R}]Y_l^m(\theta,\phi)\zeta_{nl}(r)/r$$

radial Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right\}\zeta_{nl}(r) = E_{nl}\zeta_{nl}(r)$$

Wannier excitons $\qquad \hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$

simple model: electron + hole, Coulomb interaction

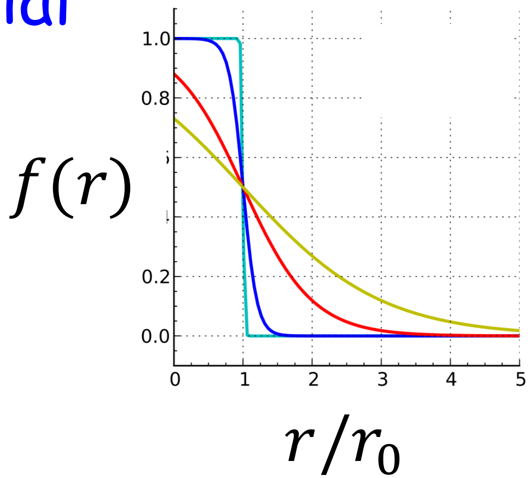


$$V(r) = -\frac{e^2}{4\pi\epsilon}\frac{1}{r}$$

which ϵ ?

$$V(r) = -\frac{e^2}{4\pi}\frac{1}{r}\left[\frac{f(r)}{\epsilon_e} + \frac{1-f(r)}{\epsilon_v}\right]$$

Haken potential



$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right\}\zeta_{nl}(r) = E_{nl}\zeta_{nl}(r)$$

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Project 1: Excitons numerical approach

Numerical approach $\hat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$

radial Schrödinger equation:

$$\left\{-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r)\right\}\zeta(r) = E\zeta(r)$$

define natural units
of energy and distance V_0 $\quad r_0 = \dfrac{\hbar}{\sqrt{2\mu V_0}}$

step 0: dimensionless Schrödinger equation:

$$\frac{d^2\zeta(\rho)}{d\rho^2} = \{W(\rho) - \lambda\}\zeta(\rho)$$

with $\lambda = \dfrac{E}{V_0}$ $\quad \rho = \dfrac{r}{r_0}$

and $W(\rho) = \dfrac{V(\rho)}{V_0} + \dfrac{l(l+1)}{\rho^2}$

Solving $\widehat{H}\,\psi(\mathbf{r}) = E\,\psi(\mathbf{r})$ by shooting

dimensionless Schrödinger equation:

$$\frac{d^2\zeta(\rho)}{d\rho^2} = \{W(\rho) - \lambda\}\zeta(\rho)$$

unknowns: eigenvalue λ , eigenfunction $\zeta(\rho)$

iterative technique: "shooting"

start with guess $\lambda^{(0)}$

iterate $\lambda^{(0)} \to \zeta^{(0)}(\rho) \to \lambda^{(1)} \to \zeta^{(1)}(\rho) \to \lambda^{(2)} \to \cdots$

until converged

Finite differencing

step $\lambda \rightarrow \zeta\,(\rho)$

$$\frac{d^2\zeta\,(\rho)}{d\rho^2} = \{W(\rho) - \lambda\,\}\zeta\,(\rho)$$

finite difference

$$\frac{d^2\zeta\,(\rho)}{d\rho^2} = \frac{1}{h^2}\{\zeta\,(\rho + h) - 2\zeta\,(\rho) + \zeta\,(\rho - h)\}$$

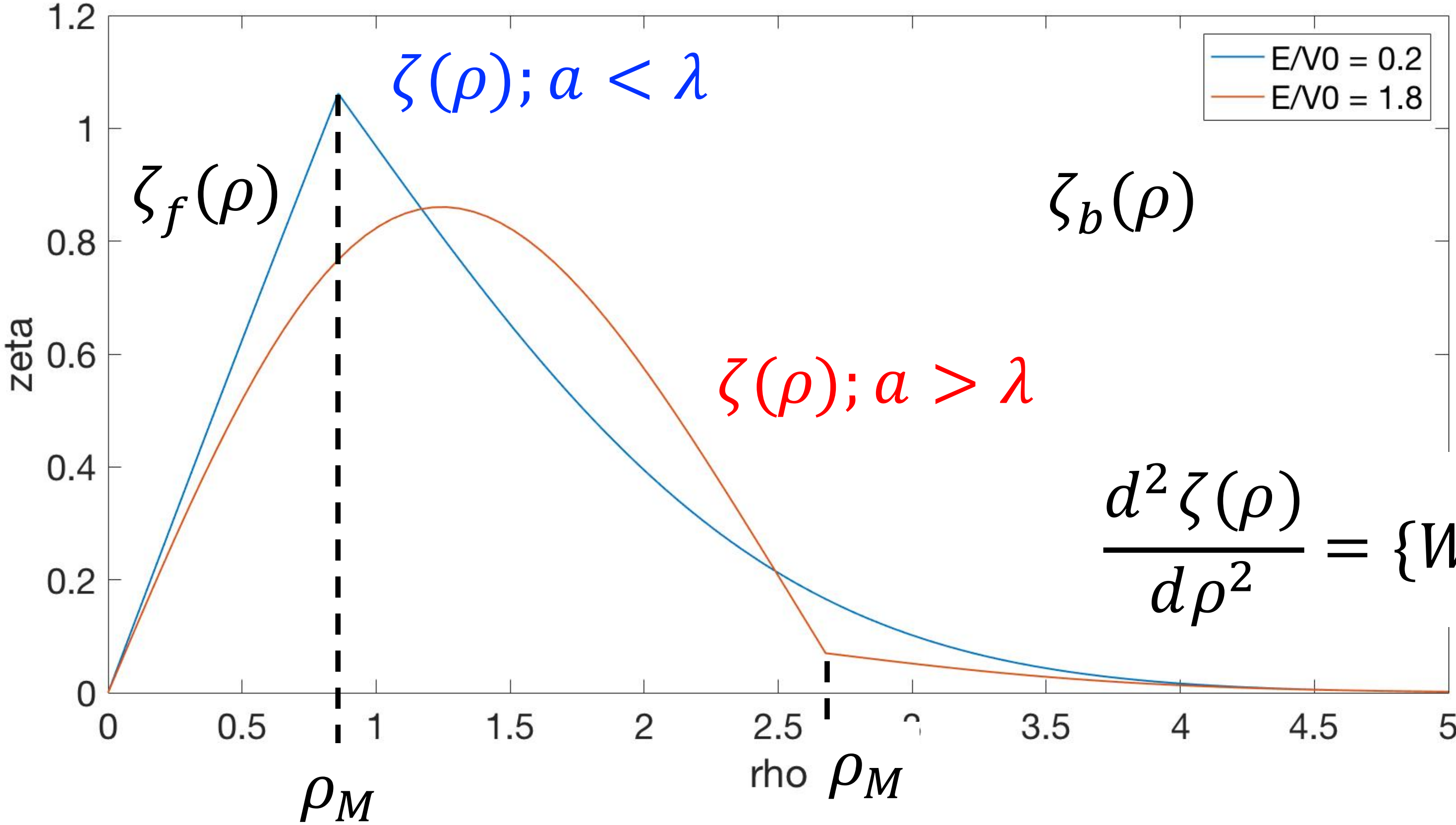
forward propagation

$$\zeta_f(\rho + h) = 2\zeta_f(\rho) - \zeta_f(\rho - h) + h^2\{W(\rho) - \lambda\,\}\zeta_f(\rho)$$

and backward propagation

$$\zeta_b(\rho - h) = 2\zeta_b(\rho) - \zeta_b(\rho + h) + h^2\{W(\rho) - \lambda\,\}\zeta_b(\rho)$$

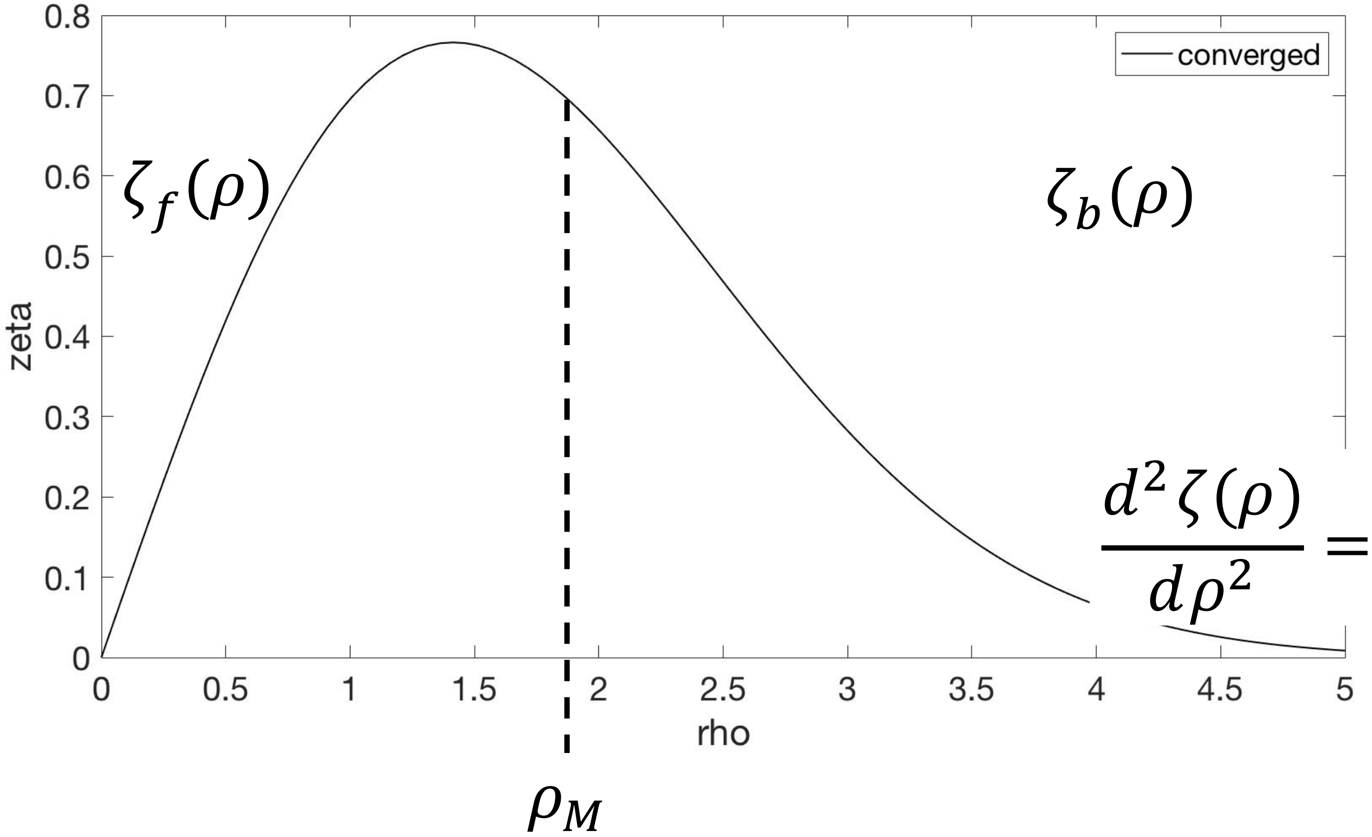
Solution for $a \neq \lambda$



$$\frac{d^2\zeta(\rho)}{d\rho^2} = \{W(\rho) - a\}\zeta(\rho)$$

$$f(a) = \frac{d\,\zeta_b(\rho_M)}{d\rho} - \frac{d\,\zeta_f(\rho_M)}{d\rho}$$ changes sign at $a = \lambda$

Solution for $a = \lambda$



$$\frac{d^2\zeta(\rho)}{d\rho^2} = \{W(\rho) - a\}\zeta(\rho)$$

$$f(a) = \frac{d\,\zeta_b(\rho_M)}{d\rho} - \frac{d\,\zeta_f(\rho_M)}{d\rho} = 0 \quad \text{at } a = \lambda$$

gives the solution to the eigenvalue problem !!

Numerical approach: tricks of the trade (1)

Numerov's method: use higher order expansion improves accuracy

$$\frac{d^2\zeta(\rho)}{d\rho^2} = \frac{1}{h^2}\{\zeta(\rho+h) - 2\zeta(\rho) + \zeta(\rho-h)\} + \frac{h^2}{12}\frac{d^4\zeta(\rho)}{d\rho^4}$$

trick: write 4th derivative as a 2nd derivative

$$\frac{d^4\zeta(\rho)}{d\rho^4} = \frac{d^2}{d\rho^2}\left\{\frac{d^2\zeta(\rho)}{d\rho^2}\right\} = \frac{d^2}{d\rho^2}\{W(\rho)-\lambda\}\zeta(\rho) \equiv \frac{d^2 g(\rho)}{d\rho^2}$$
$$= \frac{1}{h^2}\{g(\rho+h) - 2g(\rho) + g(\rho-h)\}$$

4th order accuracy at 2nd order costs !!

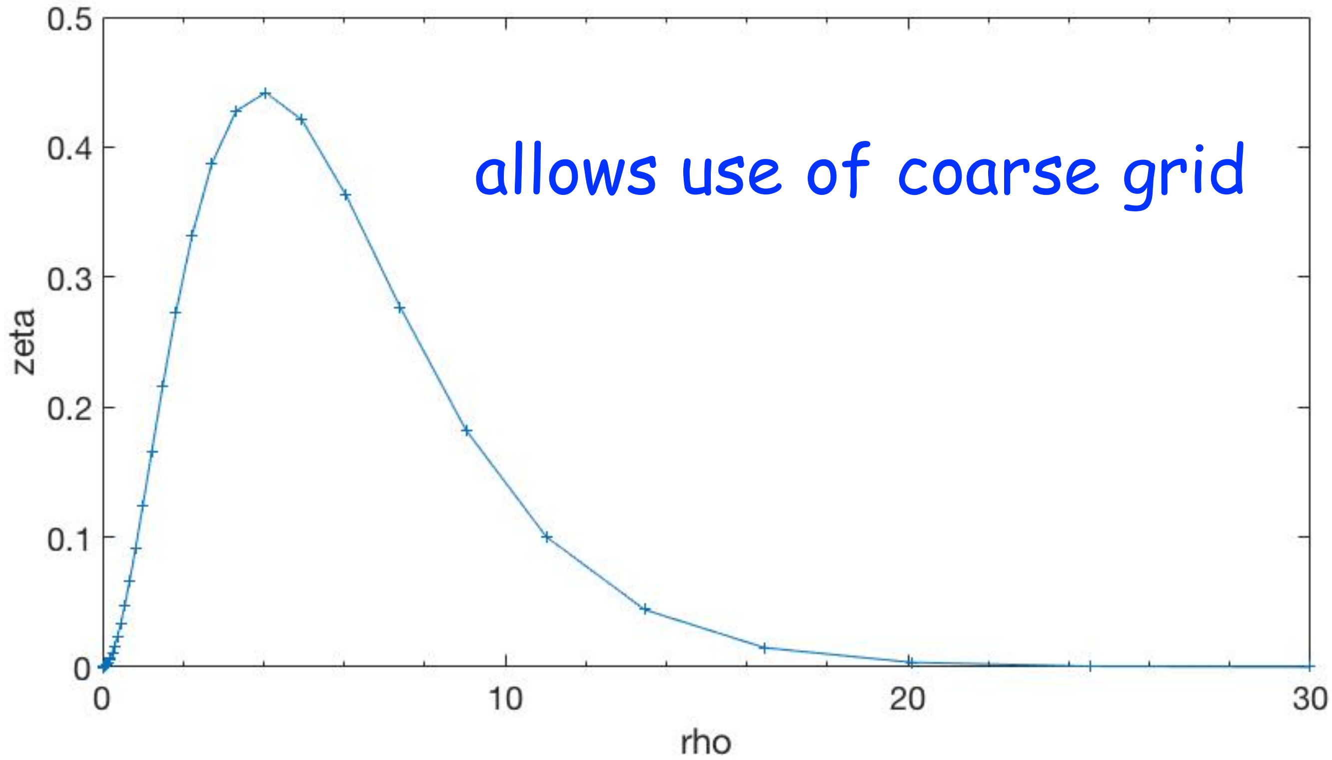
Numerical approach: tricks of the trade (2)

logarithmic grid: non-equidistant grid makes calculation more efficient

$$u(\rho) = \ln(\rho + \tau) = jh;\ j = 1, \dots, N \qquad \zeta(\rho) \to \rho(u)^{\frac{1}{2}}\eta(u)$$

modified eigenvalue equation

$$\frac{d^2\eta\,(u)}{du^2} = \left[\{W(u) - \lambda\}\{\rho(u) + \tau\}^2 + \tfrac{1}{4}\right]\eta\,(u)$$



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Too fast for you?

use the lecture notes:

they are brilliant !!