

Title: Scientific Computation (PHYS 608) - Lecture 8

Date: Nov 04, 2009 10:30 AM

URL: <http://pirsa.org/09110083>

Abstract:

Differential Equations

Differential Equations

Initial Value Problems

IVP

$$x' = f(t, x)$$

$$x(a) = S$$

Differential Equations

Initial Value Problems

IVP

$$\left. \begin{array}{l} x' = f(t, x) \\ x(a) = S \end{array} \right\}$$

\Rightarrow Solve for $x(t)$

Differential Equations

Initial Value Problems

I V P

$$\left. \begin{array}{l} x' = f(t, x) \\ x(a) = S \end{array} \right\}$$

\Rightarrow Solve for $x(t)$

Later

Boundary Value Problems

Differential Equations

Initial Value Problems

I V P

$$\left. \begin{array}{l} x' = f(t, x) \\ x(a) = S \end{array} \right\}$$

\Rightarrow Solve for $x(t)$

Later

Boundary Value Problem

$$a_2(x) \frac{d^2 y}{dx^2} + a_1(x) \frac{dy}{dx} + a_0(x) y =$$

Differential Equations

Initial Value Problems

IVP

$$\left. \begin{array}{l} x' = f(t, x) \\ x(a) = S \end{array} \right\}$$

\Rightarrow Solve

Later

Boundary Value Problem

$$a_2(x) \frac{d^2 y}{dx^2} + a_1(x) \frac{dy}{dx} + a_0(x) y = f(x)$$

$$y(a) = y_0$$

$$y(b) = y_1$$

Differential Equations

Initial Value Problems

IVP

$$\left. \begin{aligned} x' &= f(t, x) \\ x(a) &= S \end{aligned} \right\}$$

\Rightarrow Solve for $x(t)$

Later

Boundary Value Problem

$$a_2(x) \frac{d^2 y}{dx^2} + a_1(x) \frac{dy}{dx} + a_0(x) y =$$

$$b(x) = y_0$$

$$y(t) = y_1$$

Differential Equations

Initial Value Problems

IVP

$$\left. \begin{aligned} x' &= f(t, x) \\ x(a) &= S \end{aligned} \right\}$$

\Rightarrow Solve for $x(t)$

Later

Boundary Value Problem

$$a_2(x) \frac{d^2 y}{dx^2} + a_1(x) \frac{dy}{dx} + a_0(x) y = 0$$

$$y(a) = y_0$$

$$y(b) = y_1$$

Take



B

same Problem

$$+ a_1(x) \frac{dy}{dx} + a_0(x)y = 0$$
$$y_0 \quad y(t) = y_1$$

Today

Schrodinger's Equation in any potential Well

Schrodinger's Equation in ^{any} potential Well 1D

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi(r)}{dr^2} + V(r) \psi(r) = E \psi(r)$$

Bound-States

Schrödinger's Equation in ^{any} potential Well - 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r) \quad \text{Bound-States}$$

↳ Eigenvalue

Schrodinger's Equation in ^{any} potential well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bowling

↳ Eigenvalue

Schrodinger's Equation in ^{any} potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r) \quad \text{Bound-States}$$

↳ Eigenvalue



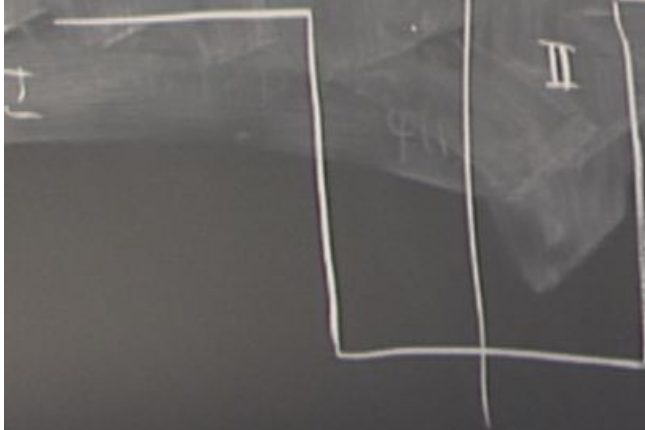
Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue

Region I, III



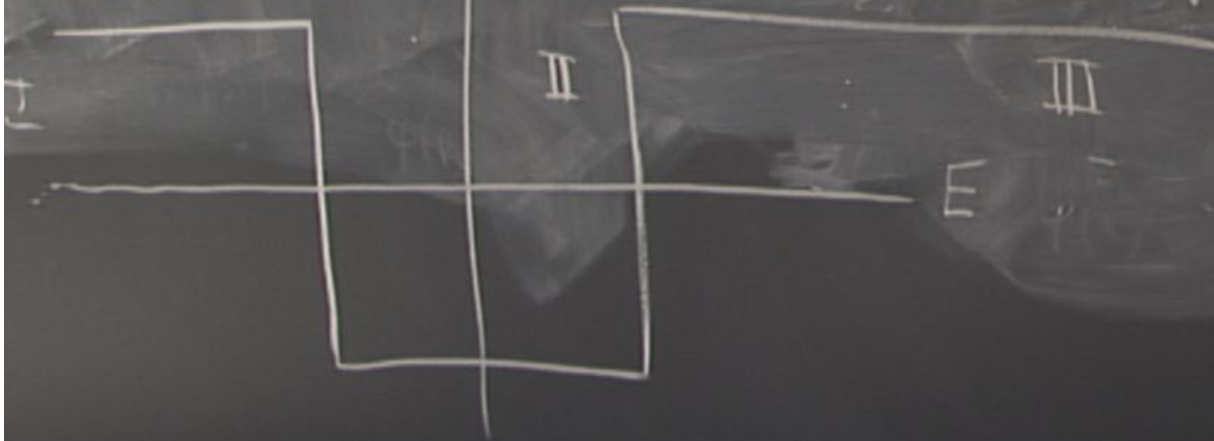
Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue

Region I, III

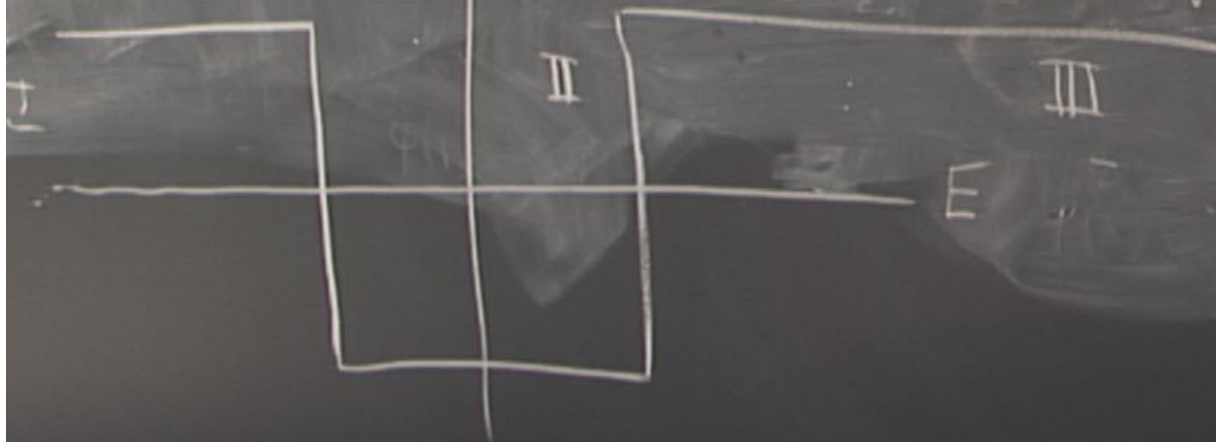


Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V-E) \psi(x)$$

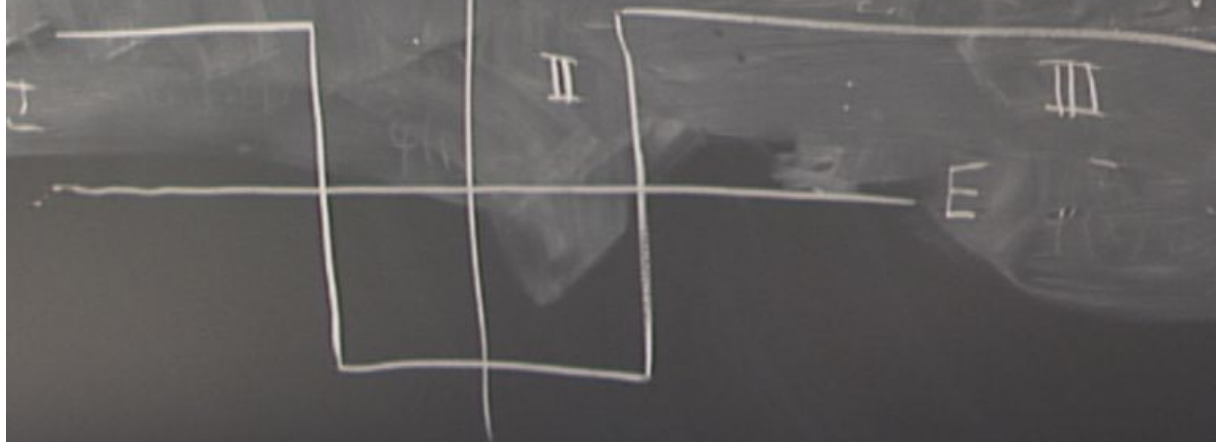
$$= \lambda^2 \psi(x)$$

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V-E) \psi(x)$$

$$= \lambda^2 \psi(x)$$

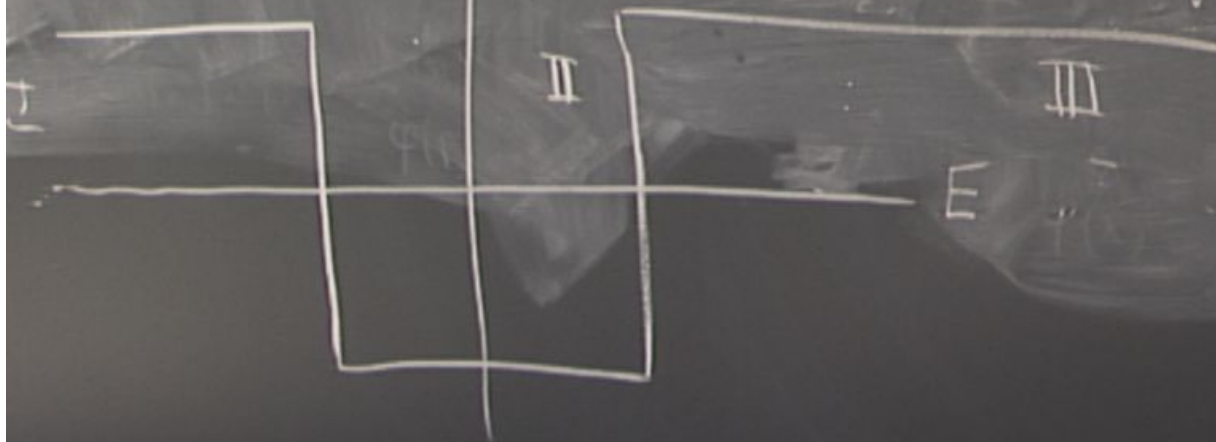
$\lambda > 0$

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\begin{aligned} \frac{d^2 \psi}{dx^2} &= \frac{2m}{\hbar^2} (V-E) \psi(x) \\ &= \lambda^2 \psi(x) \end{aligned}$$

$\lambda > 0$

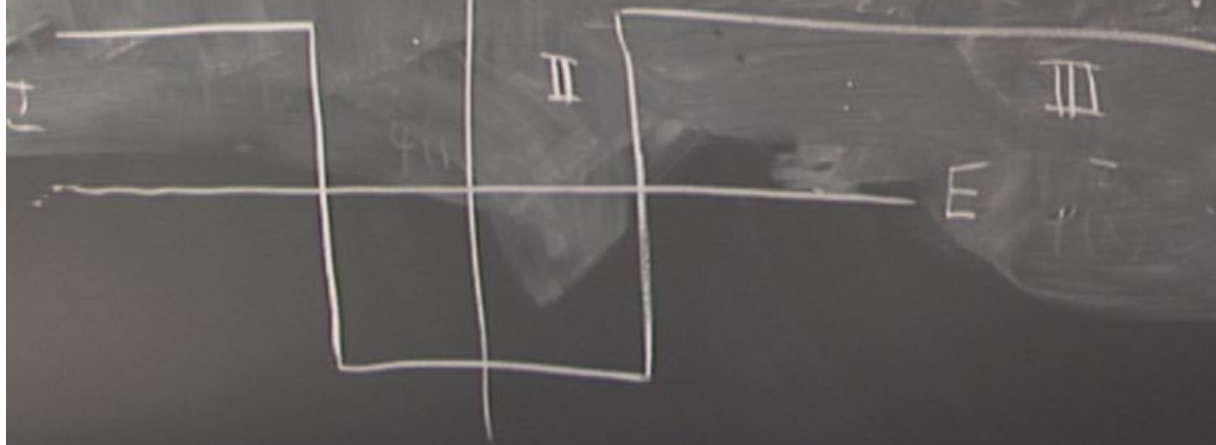
$$e^{-\lambda x}$$

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V-E) \psi(x)$$

$$= \lambda^2 \psi(x) \quad \lambda > 0$$

$$e^{\pm \lambda x}$$

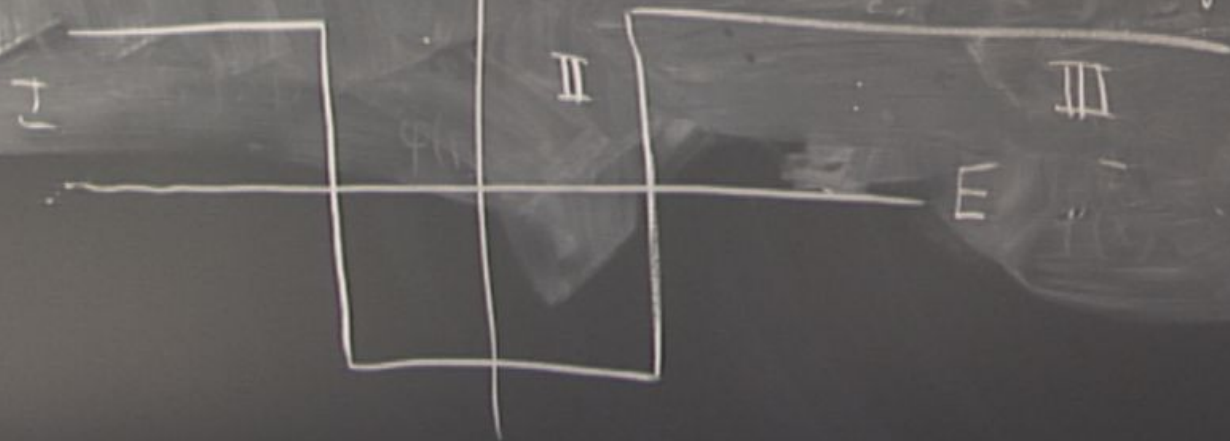
We need to tell the computer that
we don't want $e^{+\lambda x}$ as a solution
in region III

Schrodinger's Equation in any potential Well - 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V-E) \psi(x)$$

$$= -\lambda^2 \psi(x) \quad \lambda > 0$$

$$e^{\pm \lambda x}$$

We need to tell the computer that
we don't want $e^{+\lambda x}$ as a solution
in region III

Strategy

$$\psi(x = -c)$$

We need to tell the computer that
we don't want $e^{+\lambda x}$ as a solution
in region III

Strategy

$$\psi(x=-c) = 0$$

We need to tell the computer that we don't want $e^{+\lambda x}$ as a solution in region III

Strategy

$$\psi(x=-c) = 0$$

then integrate towards the right

We need to tell the computer that
we don't want $e^{+\lambda x}$ as a solution
in region III

Strategy

$$\psi(x=-c) = 0$$

then integrate towards the right

Try to get $\psi(x=-c+h)$

← step

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V-E) \psi(x)$$

$$= \lambda^2 \psi(x) \quad \lambda > 0$$

$$e^{\pm \lambda x}$$

We need to tell the computer that
we don't want $e^{+\lambda x}$ as a solution
in region III

Strategy

$$\psi(x=-c) = 0$$

then integrate towards the right

Try to get $\psi(x=-c+h)$

← step

Numerov's Method

Numerov's Method

Valid for 2nd equation
with no 1st
derivative

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ap

Numerov's Method

Valid for 2nd equation
with no 1st
derivative

Numerov's Method

Valid for 2nd equation
with no 1st
derivative

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

Numerov's Method

Valid for 2nd equation
with no 1st
derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

Numerov's Method

Valid for 2nd equation
with no 1st
derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

Numerov's Method

Valid for 2nd equation
with no 1st
derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x)\psi(x) = 0$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x)\psi(x) = 0$$

If we look

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x)\psi(x) = 0$$

If we look

$$\psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)}$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remin te

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x) = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2}$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remin te

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

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Numerov's Method

Valid for 2nd equation with no 1st derivative

Page 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x)\psi(x) = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)}$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Page 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x) = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + \mathcal{O}(h^4)$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remin te

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x) = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + O(h^4)$$

Trick Apply $1 + \frac{1}{12} \frac{d^2}{dx^2}$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x)\psi(x) = 0$$

If we look

$$\psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)}$$

$$\psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} = \frac{h^2}{12}\psi^{(4)}$$

$$\frac{h^4}{4!}\psi^{(4)}$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remin te

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x))\psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} k^2(x) = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + \mathcal{O}(h^4)$$

Trick Apply $1 + \frac{1}{12} \frac{d^2}{dx^2}$ to (1)

$\psi^{(2)}$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)}$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2\psi}{dx^2} + k^2(x) \psi = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} + \dots \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} - \dots \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + \mathcal{O}(h^4)$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Page 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2\psi}{dx^2} + k^2(x) \psi = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + O(h^4)$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remin te

$$\frac{d^2 \psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2 \psi}{dx^2} + k^2(x) \psi = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h \psi^{(1)} + \frac{h^2}{2!} \psi^{(2)} + \frac{h^3}{3!} \psi^{(3)} + \frac{h^4}{4!} \psi^{(4)} \\ \psi(x-h) = \psi(x) - h \psi^{(1)} + \frac{h^2}{2!} \psi^{(2)} - \frac{h^3}{3!} \psi^{(3)} + \frac{h^4}{4!} \psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12} \psi^{(4)} + \mathcal{O}(h^4)$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x) \psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi]$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] =$$

Substitute in (2)

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] =$$

Substitute in (2)

Numerov's Method

Valid for 2nd equation with no 1st derivative

Pang 104

Remin te

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2\psi}{dx^2} + k^2(x) \psi = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} + \dots \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} - \dots \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + \mathcal{O}(h^4)$$

Numerov's Method

Valid for 2nd equation with no 1st derivative

Page 104

Remember

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V(x)) \psi(x) = 0$$

$$\rightarrow \textcircled{1} \quad \frac{d^2\psi}{dx^2} + k^2(x) \psi = 0$$

If we look

$$\begin{cases} \psi(x+h) = \psi(x) + h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} + \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \\ \psi(x-h) = \psi(x) - h\psi^{(1)} + \frac{h^2}{2!}\psi^{(2)} - \frac{h^3}{3!}\psi^{(3)} + \frac{h^4}{4!}\psi^{(4)} \end{cases}$$

$$\psi^{(2)} \approx \frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} - \frac{h^2}{12}\psi^{(4)} + O(h^4) \quad \textcircled{2}$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x) \psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] =$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2}$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x) \psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] =$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2}$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x) \psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] =$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2} + \mathcal{O}\left(\frac{1}{\hbar^4}\right)$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] =$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2} + \mathcal{O}\left(\frac{1}{\hbar^4}\right) + k^2(x)\psi$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} + \mathcal{O}\left(\frac{1}{h^4}\right) + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

Trick Apply $1 + \frac{\hbar^2}{12} \frac{d^2}{dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2}{12} \frac{d^2}{dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2} + \mathcal{O}\left(\frac{\hbar^4}{12}\right) + k^2(x)\psi + \frac{\hbar^2}{12} \frac{d^2}{dx^2} [k^2 \psi] = 0$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} + \textcircled{1} \left(\frac{\hbar^4}{12} \right) + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

→ Remonte

$$\psi(x+h) = \dots \psi(x)$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} + \textcircled{1} \left(\frac{\hbar^4}{12} \right) + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

→ Remonte

$$\psi(x+h) = \dots \psi(x) \dots \psi(x-h)$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2} + \mathcal{O}\left(\frac{\hbar^4}{\hbar^2}\right) + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

→ Remonte

$$\psi(x+h) = \dots \psi(x) \dots \psi(x-h)$$

Trick Apply $1 + \frac{\hbar^2 d^2}{12 dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2} + \mathcal{O}\left(\frac{1}{h^4}\right) + k^2(x)\psi + \frac{\hbar^2 d^2}{12 dx^2} [k^2 \psi] = 0$$

→ Remonte

$$\psi(x+h) = \dots \psi(x) \dots \psi(x-h)$$

Trick Apply $1 + \frac{\hbar^2}{12} \frac{d^2}{dx^2}$ to (1)

$$\psi^{(2)} + \frac{\hbar^2}{12} \psi^{(4)} + k^2(x) \psi + \frac{\hbar^2}{12} \frac{d^2}{dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{\hbar^2} + \textcircled{1} \left(\frac{\hbar^4}{12} \right) + k^2(x) \psi + \frac{\hbar^2}{12} \frac{d^2}{dx^2} [k^2 \psi] = 0$$

→ Remonte

$$\psi(x+h) = \dots \psi(x) \dots \psi(x-h)$$

Trick Apply $1 + \frac{h^2}{12} \frac{d^2}{dx^2}$ to (1)

$$\psi^{(2)} + \frac{h^2}{12} \psi^{(4)} + k^2(x)\psi + \frac{h^2}{12} \frac{d^2}{dx^2} [k^2 \psi] = 0$$

Substitute in (2)

$$\frac{\psi(x+h) + \psi(x-h) - 2\psi(x)}{h^2}$$

$$+ (1) \left(\frac{h^4}{12} \right) + k^2(x)\psi + \frac{h^2}{12} \frac{d^2}{dx^2} [k^2 \psi] = 0$$

Works because
no 1st derivative

→ Rewrite

$$\psi(x+h) = \dots \psi(x) \dots \psi(x-h)$$

Approximate

$$\frac{d^2[\psi^2]}{dx^2} =$$

$$k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - \psi''(x)$$

①

= 0

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} =$$

$$\frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2}$$

→ ①

= 0

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} =$$

$$\frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

①

= 0

Approximate

$$\frac{d^2[\psi]}{dx^2}$$

=

$$\frac{h^2(x+h)\psi(x+h) + h^2(x-h)\psi(x-h) - 2h^2(x)\psi(x)}{h^2}$$

+ $\mathcal{O}(h^2)$

→ ①

= 0

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3)

→ (1)

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

→ (1)

= 0

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x)$$

= 0

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x) + h^2 k^2(x)\psi +$$

$$\frac{h^2}{12} [k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)]$$

= 0

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x) + h^2 k^2(x)\psi + \frac{h^2}{12} [k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)] = 0$$

Isolate

$$\psi(x+h) = \frac{1}{1 + \frac{h^2}{12} k^2(x+h)} \left[\dots \right]$$

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x) + h^2 k^2(x)\psi +$$

$$\frac{h^2}{12} [k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)]$$

= 0

Isolate

$$\psi(x+h) = \frac{1}{1 + \frac{h^2}{12} k^2(x+h)} \left[\dots \right]$$

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x) + h^2 k^2(x)\psi +$$

$$\frac{h^2}{12} [k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)]$$

= 0

Isolate

$$\psi(x+h) = \frac{1}{1 + \frac{h^2}{12} k^2(x+h)} [2\psi(x) + \frac{h^2}{12} k^2(x+h)\psi(x+h) + \frac{h^2}{12} k^2(x-h)\psi(x-h) - 2\psi(x) - \frac{h^2}{12} k^2(x)\psi(x)]$$

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x) + h^2 k^2(x)\psi +$$

$$\frac{h^2}{12} [k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)] = 0$$

Isolate

$$\psi(x+h) = \frac{1}{1 + \frac{h^2}{12} k^2(x+h)} \left[2\psi(x) - \psi(x-h) - \frac{h^2}{12} k^2(x)\psi(x) + \frac{h^2}{12} k^2(x-h)\psi(x-h) \right]$$

$$\psi(x+h) = \frac{1 + \frac{h^2}{12} k^2 (x+h)}{1 + \frac{h^2}{12} k^2 (x+h)}$$

Approximate

$$\frac{d^2 [k^2 \psi]}{dx^2} = \frac{k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)}{h^2} + \mathcal{O}(h^2)$$

Substitute into (3) after mult. by h^2

$$\psi(x+h) + \psi(x-h) - 2\psi(x) + h^2 k^2(x)\psi +$$

$$= 0 \quad \frac{h^2}{12} [k^2(x+h)\psi(x+h) + k^2(x-h)\psi(x-h) - 2k^2(x)\psi(x)]$$

Isolate

$$\psi(x+h) = \frac{1}{1 + \frac{h^2}{12} k^2(x+h)} \left[2\psi(x) - \psi(x-h) - h^2 k^2(x)\psi(x) - \frac{h^2}{12} k^2(x-h)\psi(x-h) + \frac{2h^2}{12} k^2(x)\psi(x) \right]$$

$$\psi(x+h) = \frac{2\left(1 - \frac{5}{12}k^2(x)\right)\psi(x) -}{1 + \frac{h^2}{12}k^2(x+h)}$$

$$\psi(x+h) = \frac{2\left(1 - \frac{5}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

$$\psi(x+h) = \frac{2\left(1 - \frac{5}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

$$\psi(x=c) = 0$$

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

$$\psi(x=c) = 0$$

Should c depend
on E

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

$$\psi(x=c) = 0$$

$$\psi(x=-c+h) = \epsilon$$

Should c depend
on E

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

$$\psi(x=c) = 0$$

$$\psi(x=-c+h) = \epsilon$$

Should c depend
on E

(Fix by norm)

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

$$\psi(x=c) = 0$$

$$\psi(x=-c) = 0$$

c depend
on E

by normalizing

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

$$\psi(x=c) = 0$$

$$\psi(x=-c+h) = \epsilon$$

Should c depend on E

(Fix by normalizing)

$$\psi(x+h) = \frac{2\left(1 - \frac{5h^2}{12}k^2(x)\right)\psi(x) - \left(1 + \frac{h^2}{12}k^2(x-h)\right)\psi(x-h)}{1 + \frac{h^2}{12}k^2(x+h)}$$

Strategy II

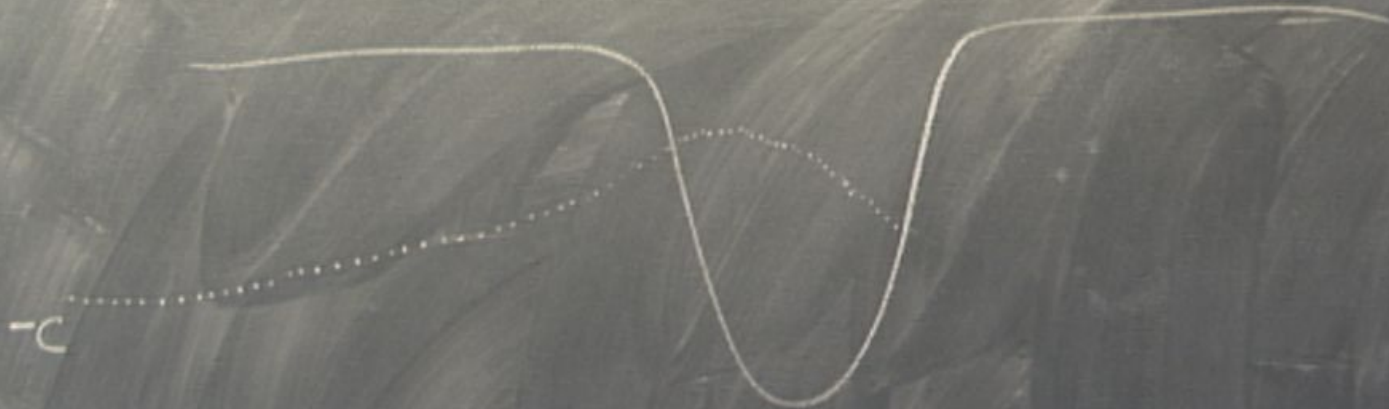
$$\psi(x=c) = 0$$

$$\psi(x=-c+h) = +\epsilon$$

Should c depend on E

(Fix by normalizing)
Fixed throughout all

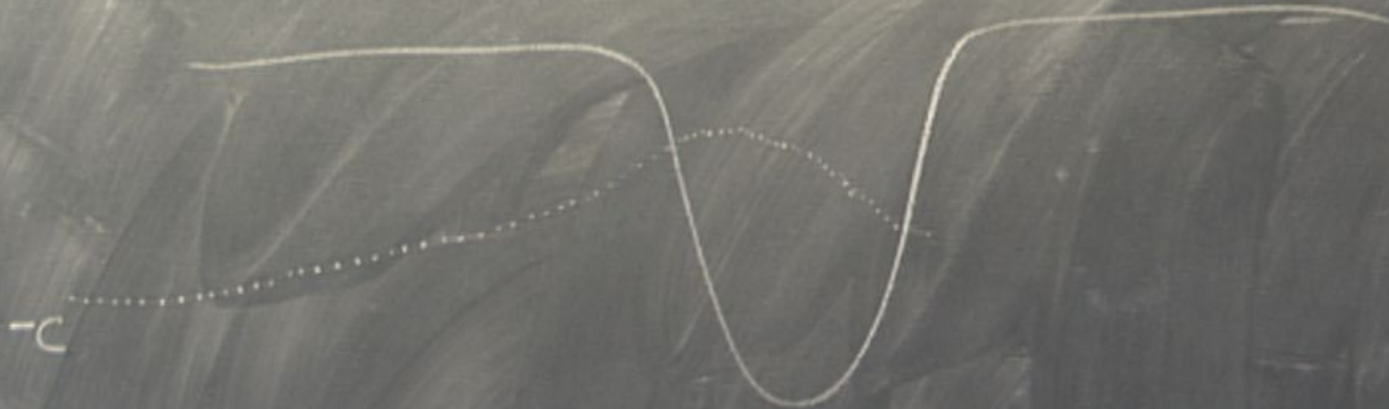
Problems



$=0$

Why?

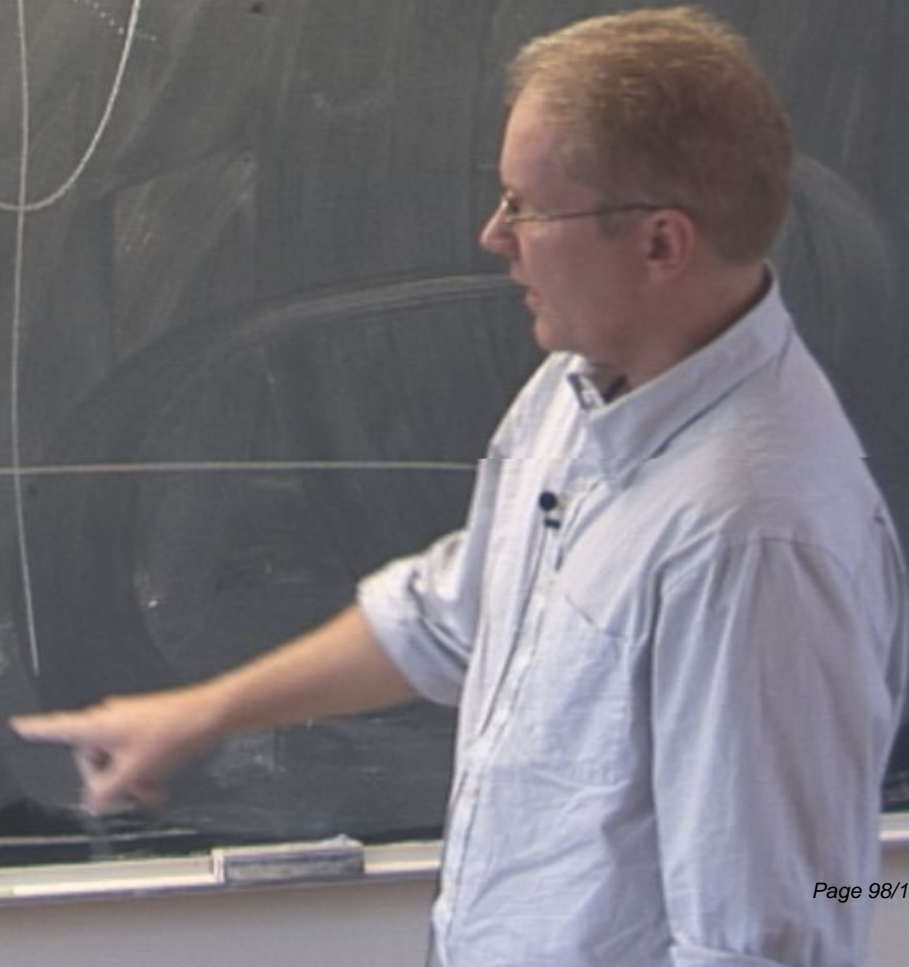
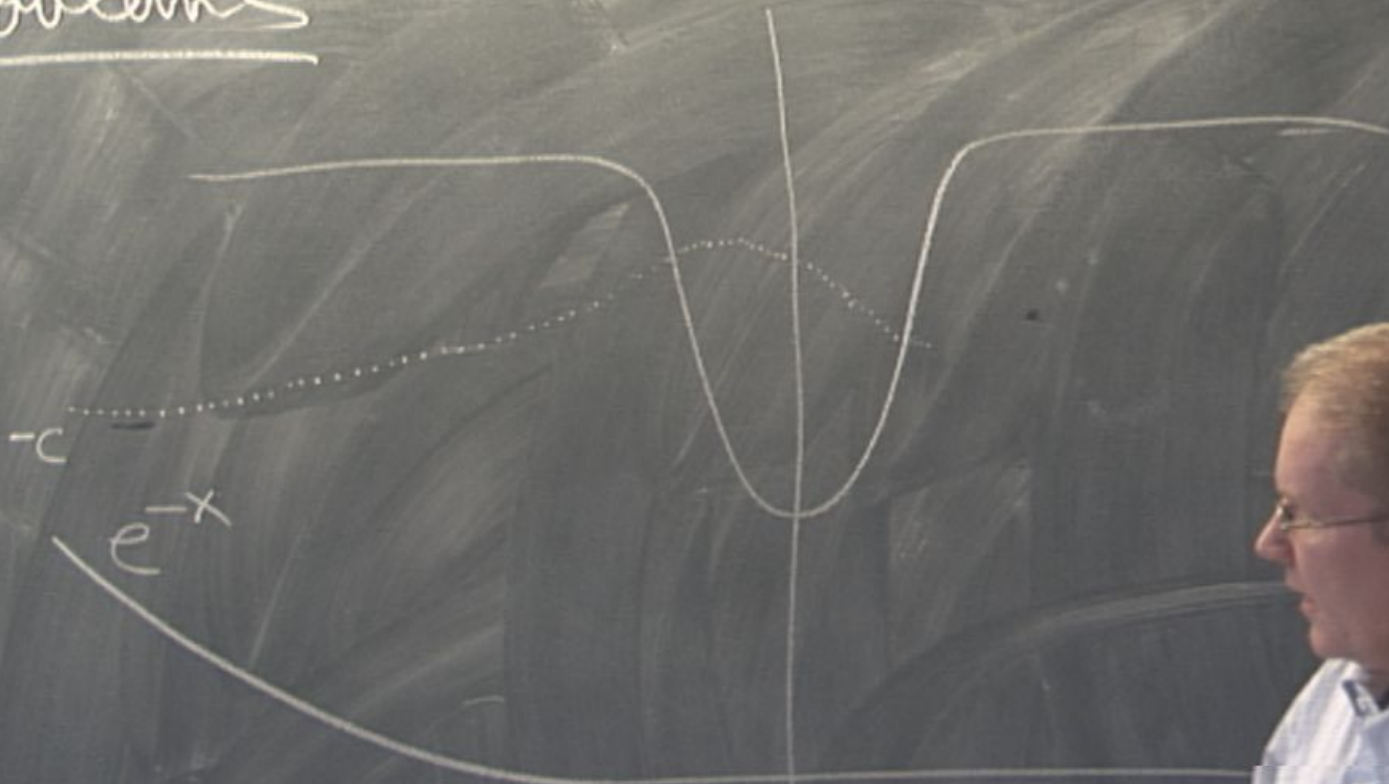
Probleme



=0

Why?

Probleme

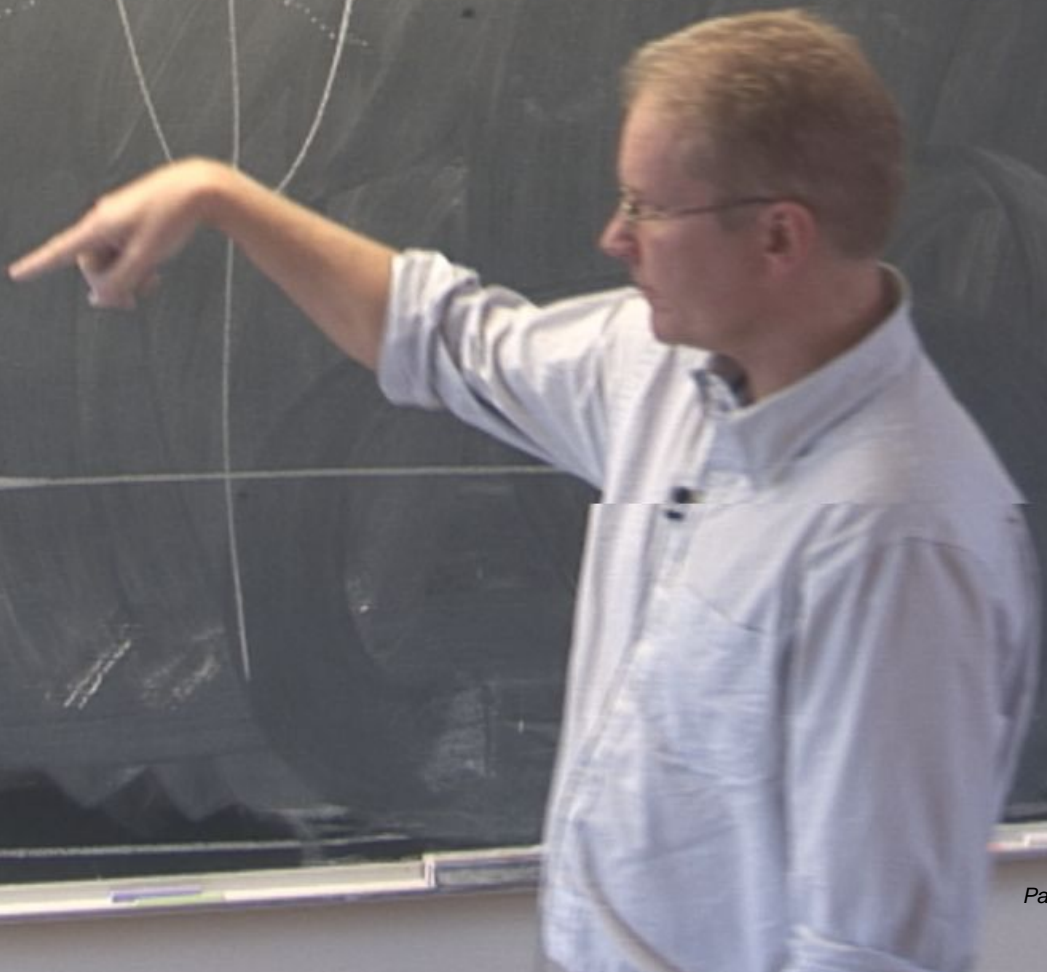


Probleme

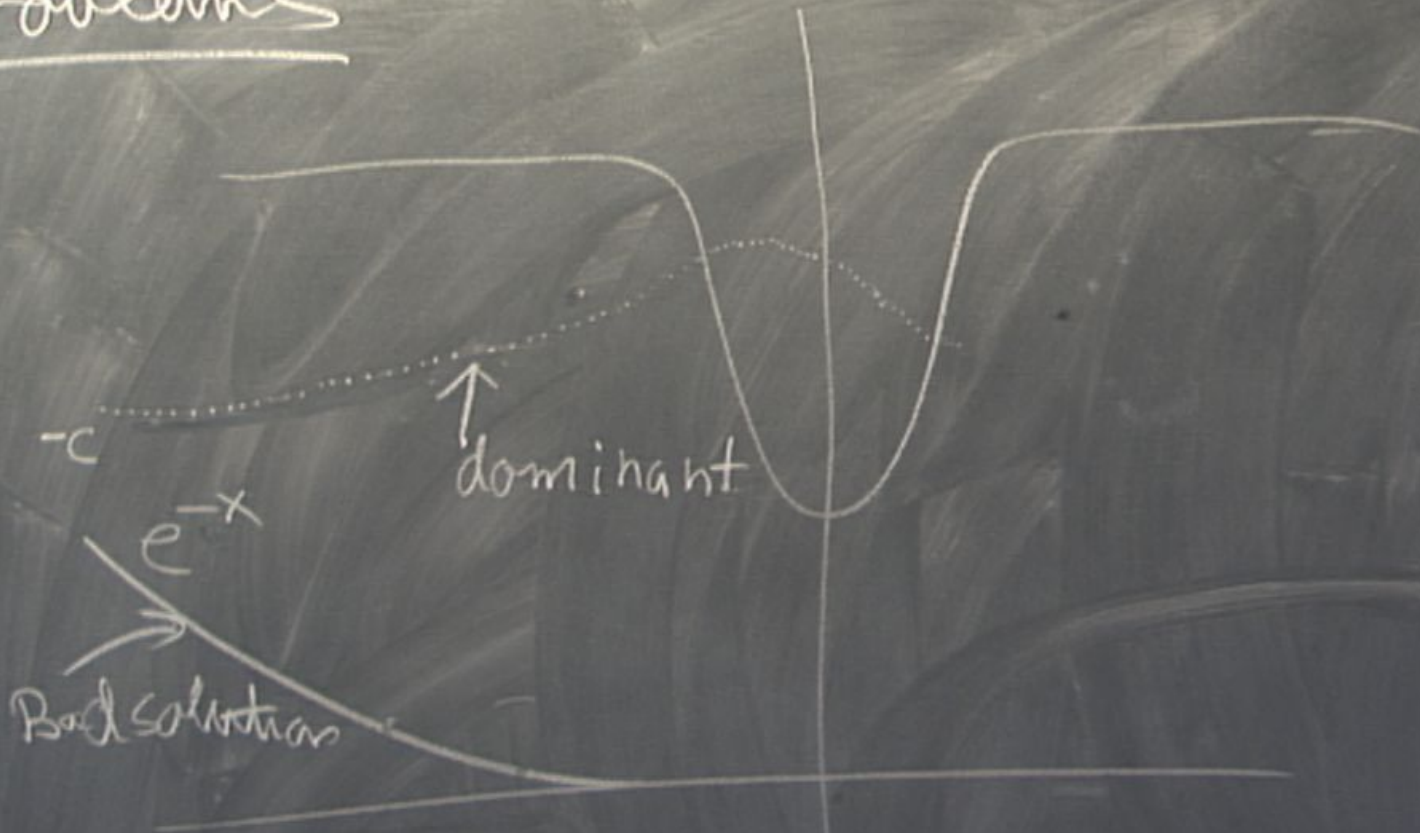
$-c$

e^{-x}

Bad solution



Probleme



e^{-x}
Bad solution

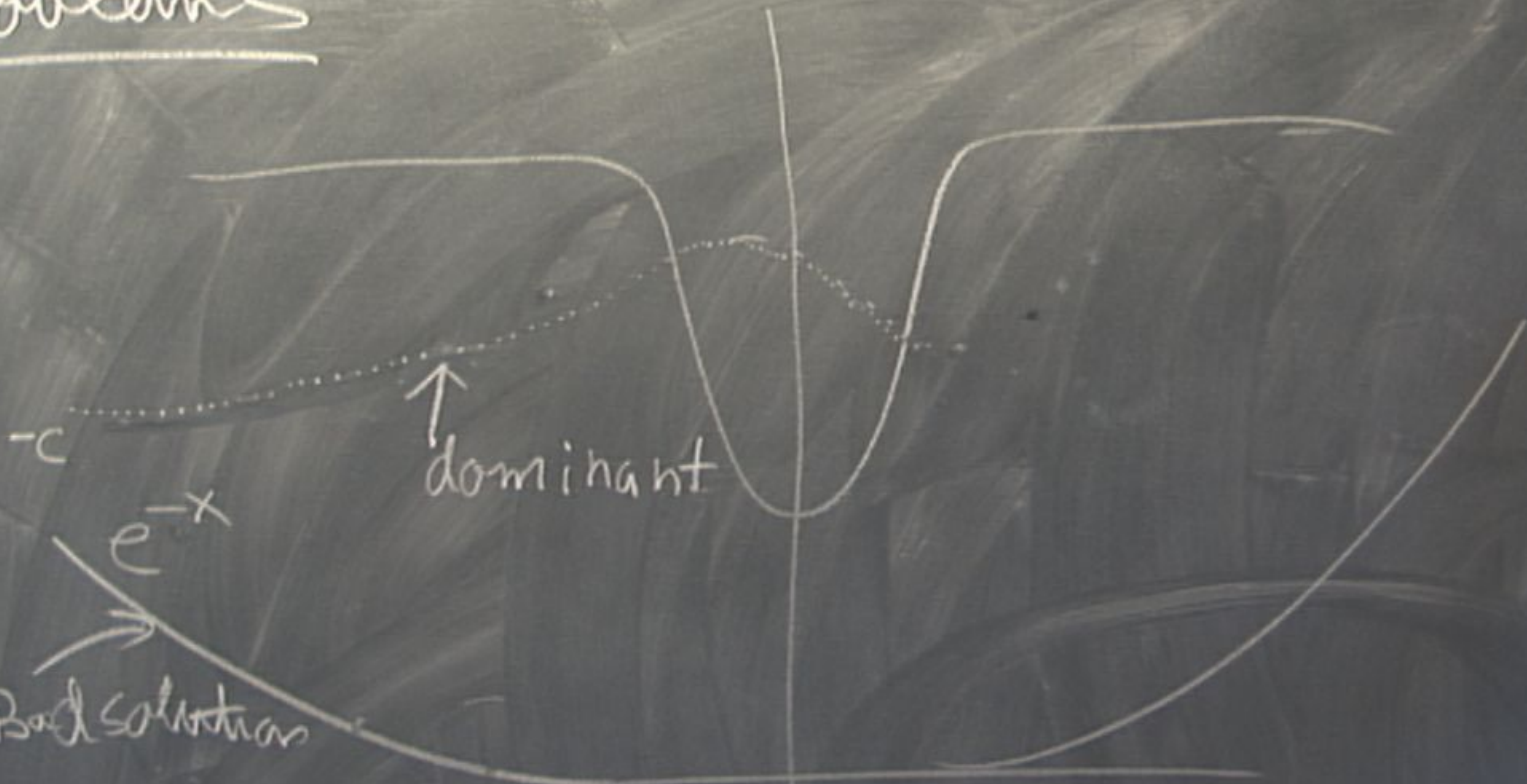
dominant

$-c$

$= 0$

Wahy

Probleme



Bad solution

dominant

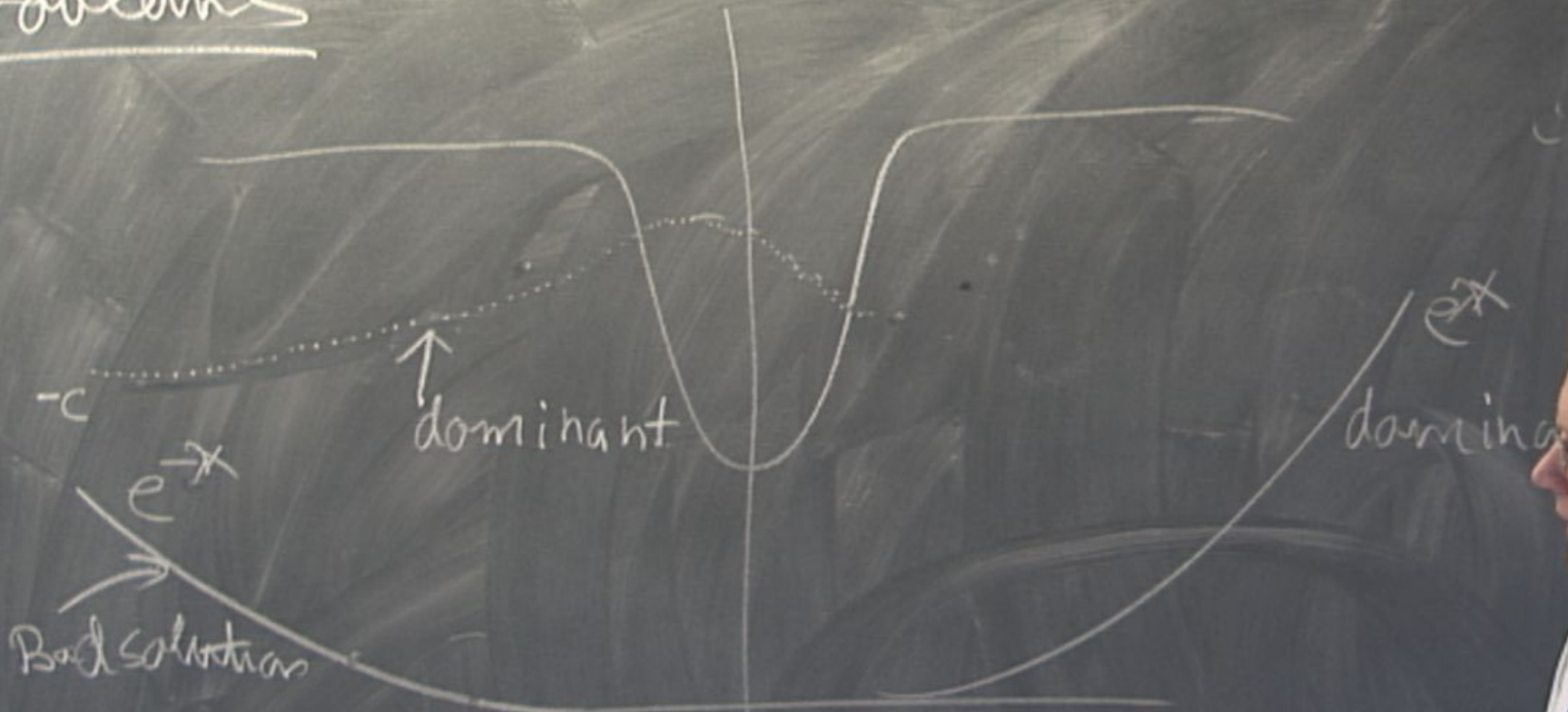
e^{-x}

$-c$

$= 0$

Why?

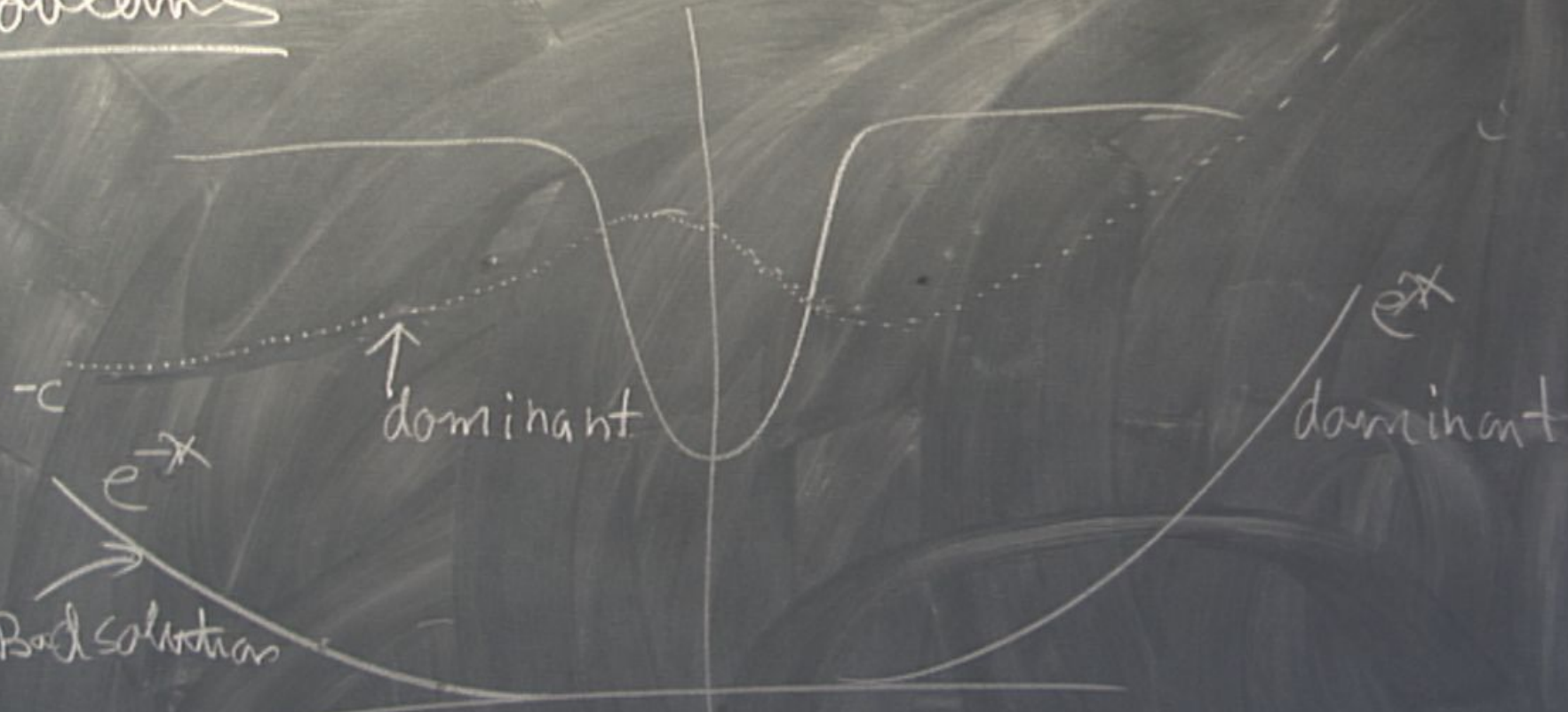
Probleme



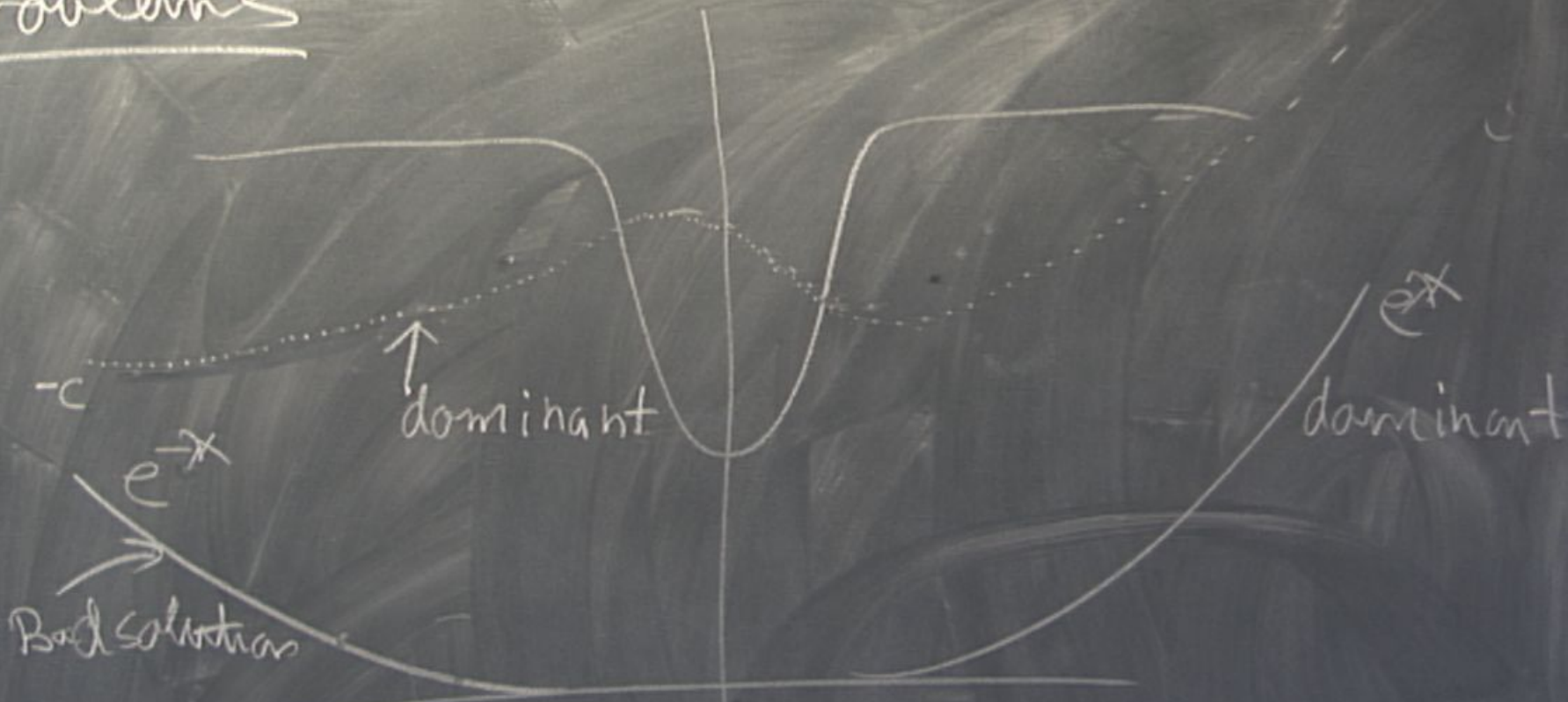
= 0

Why?

Probleme

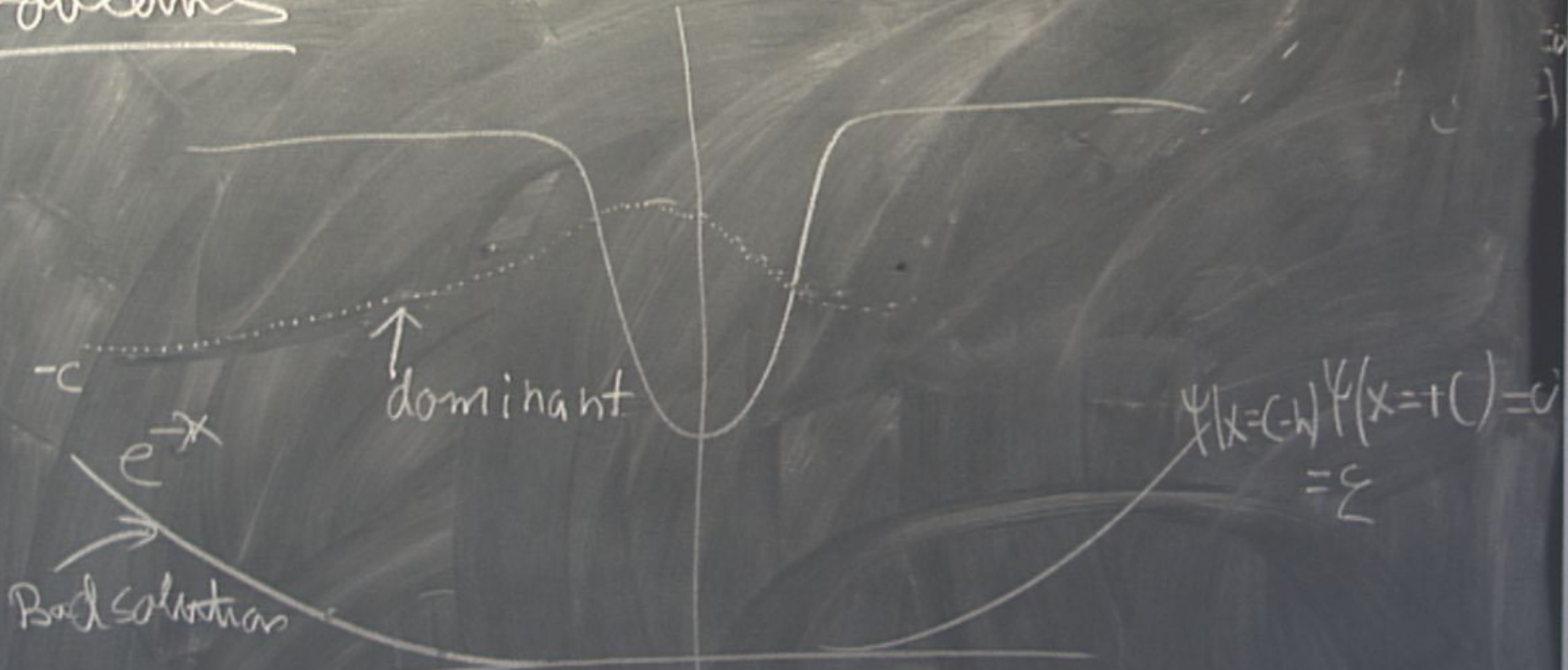


Problems



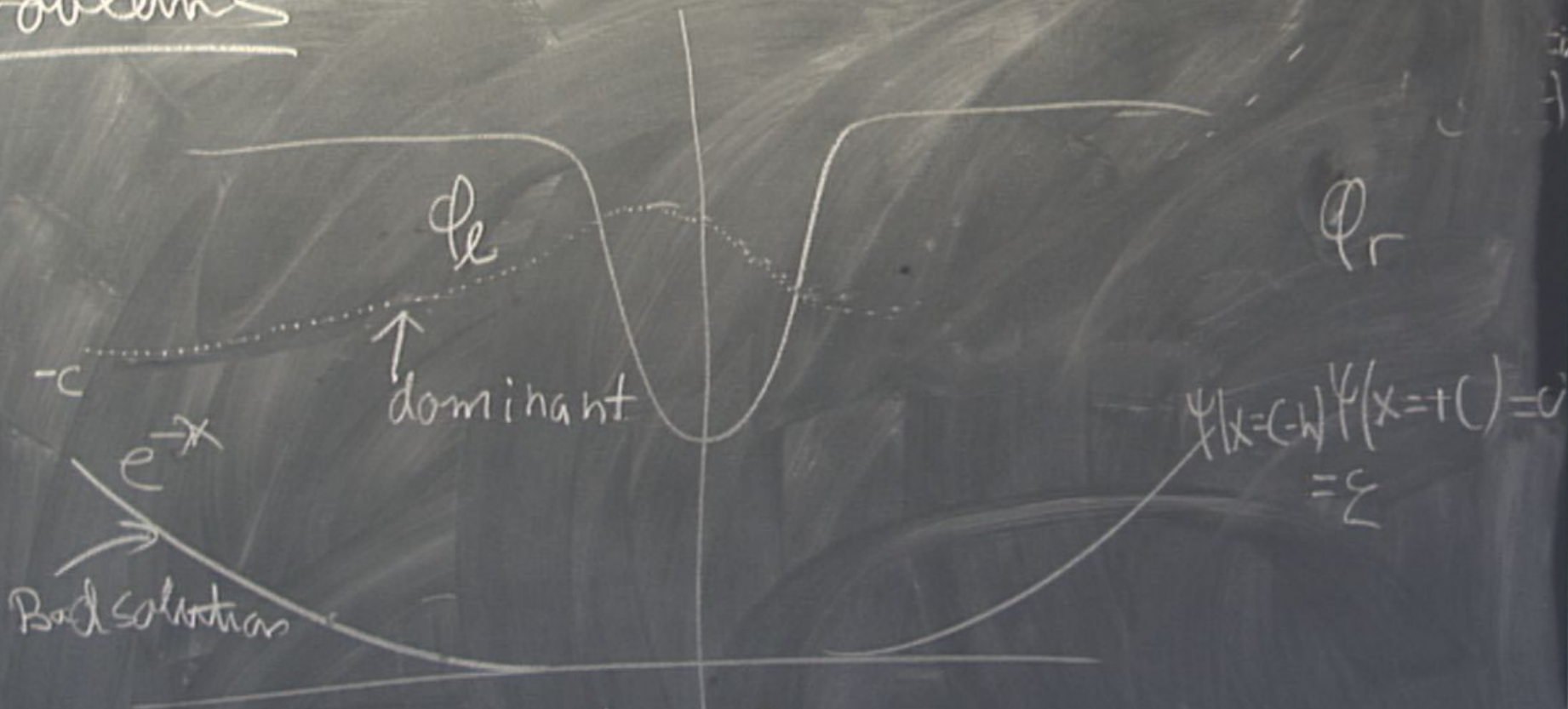
Have to integrate also from right to left.

Problems



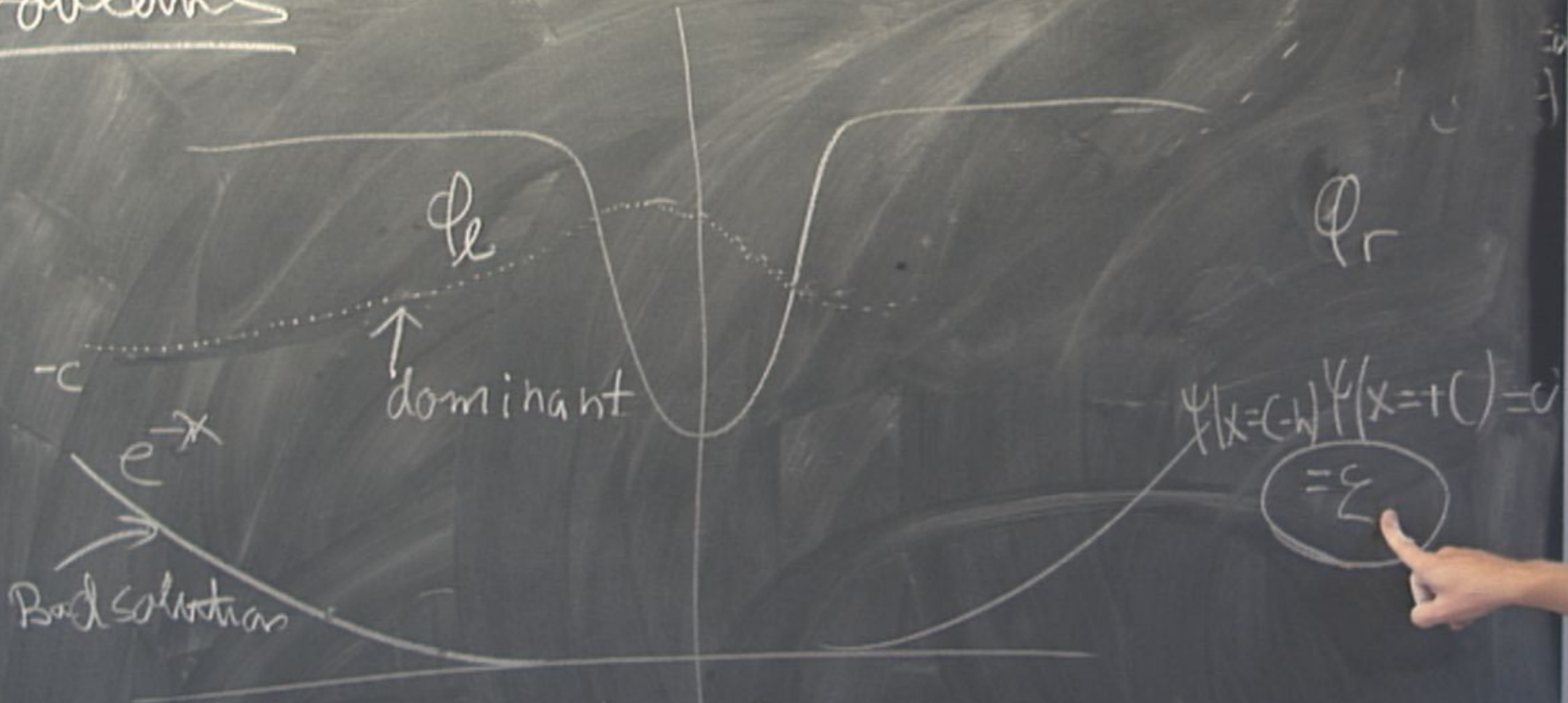
Have to integrate also from right to left.

Problems



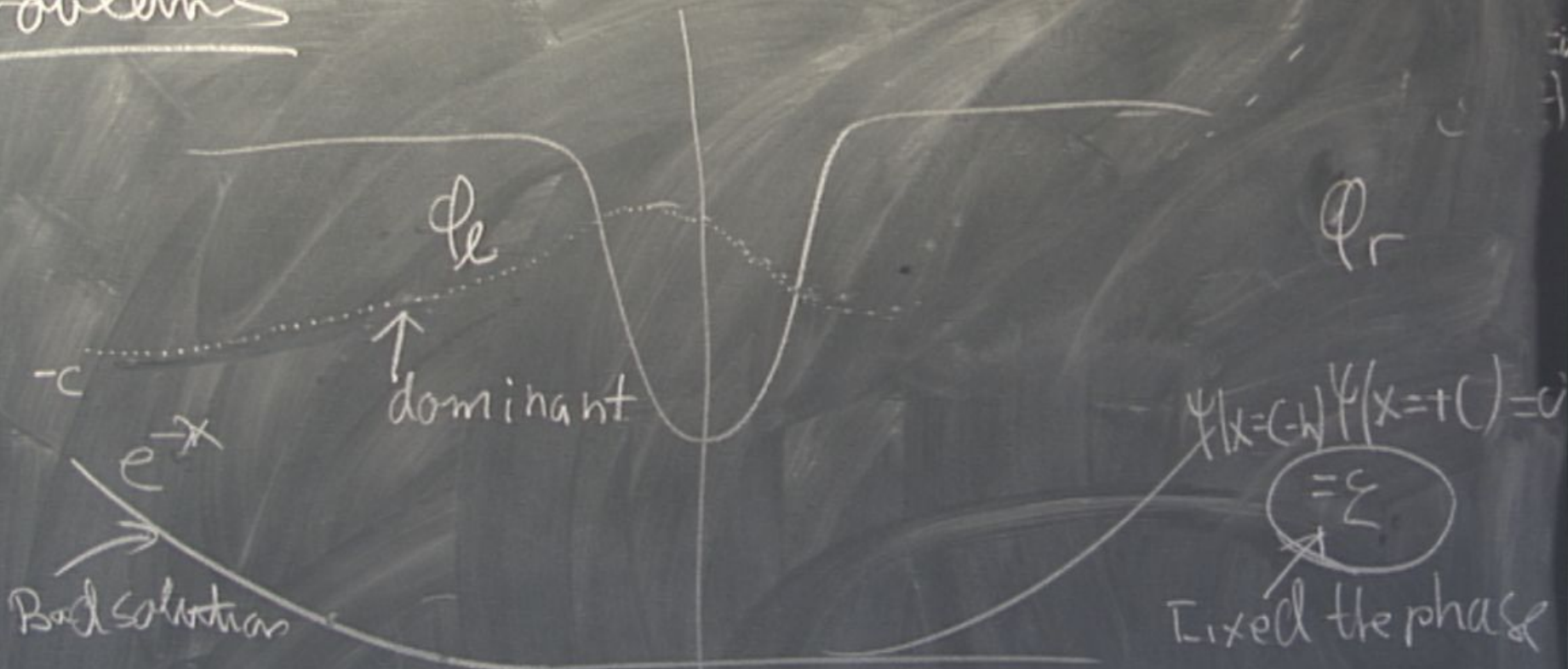
Have to integrate also from right to left.

Problems



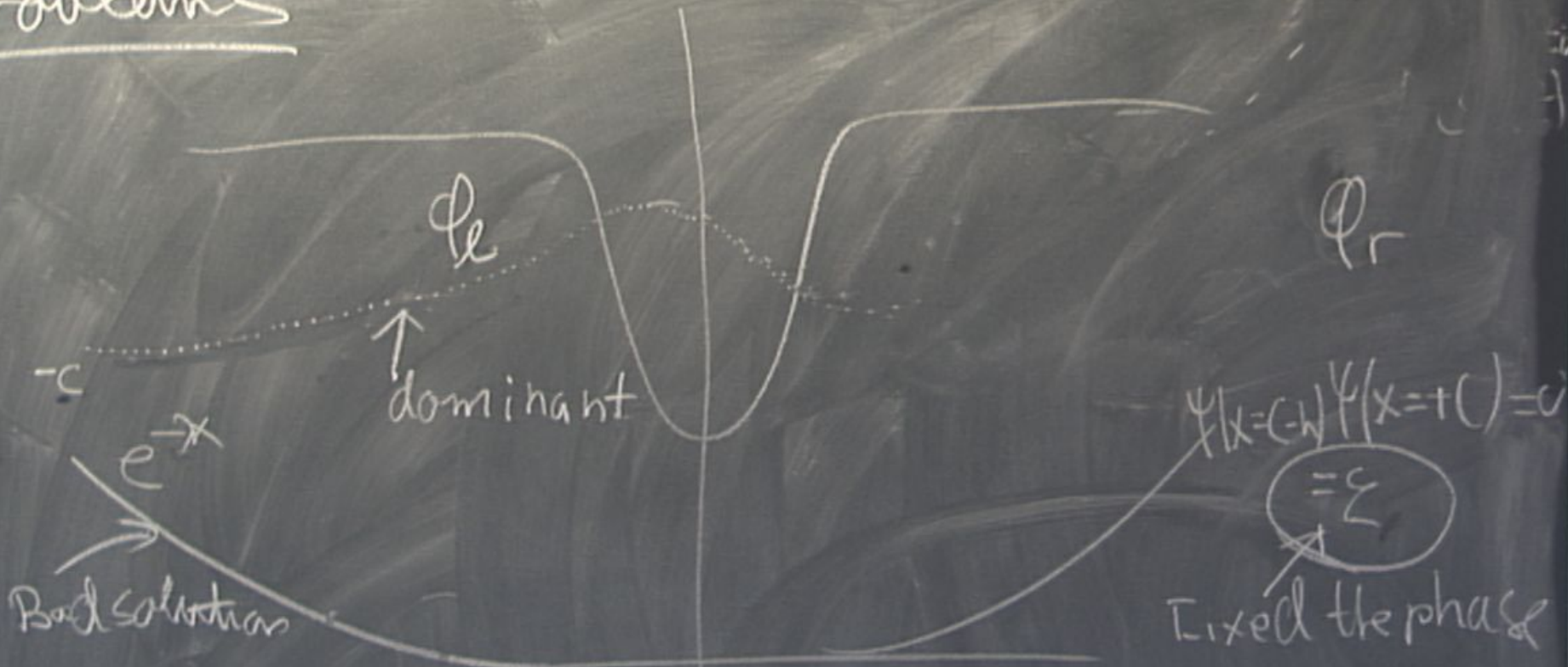
Have to integrate also from right to left

Problems



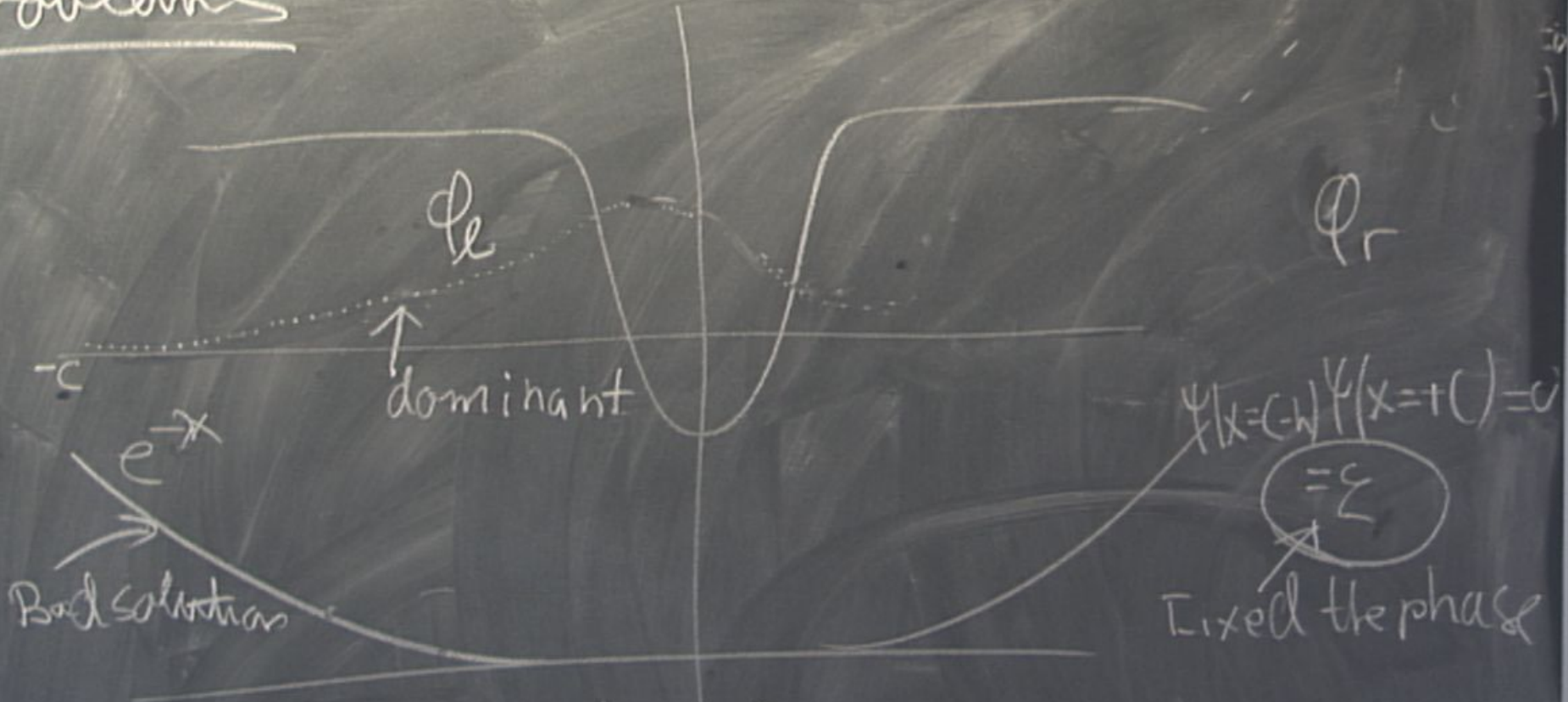
Have to integrate also from right to left

Problems



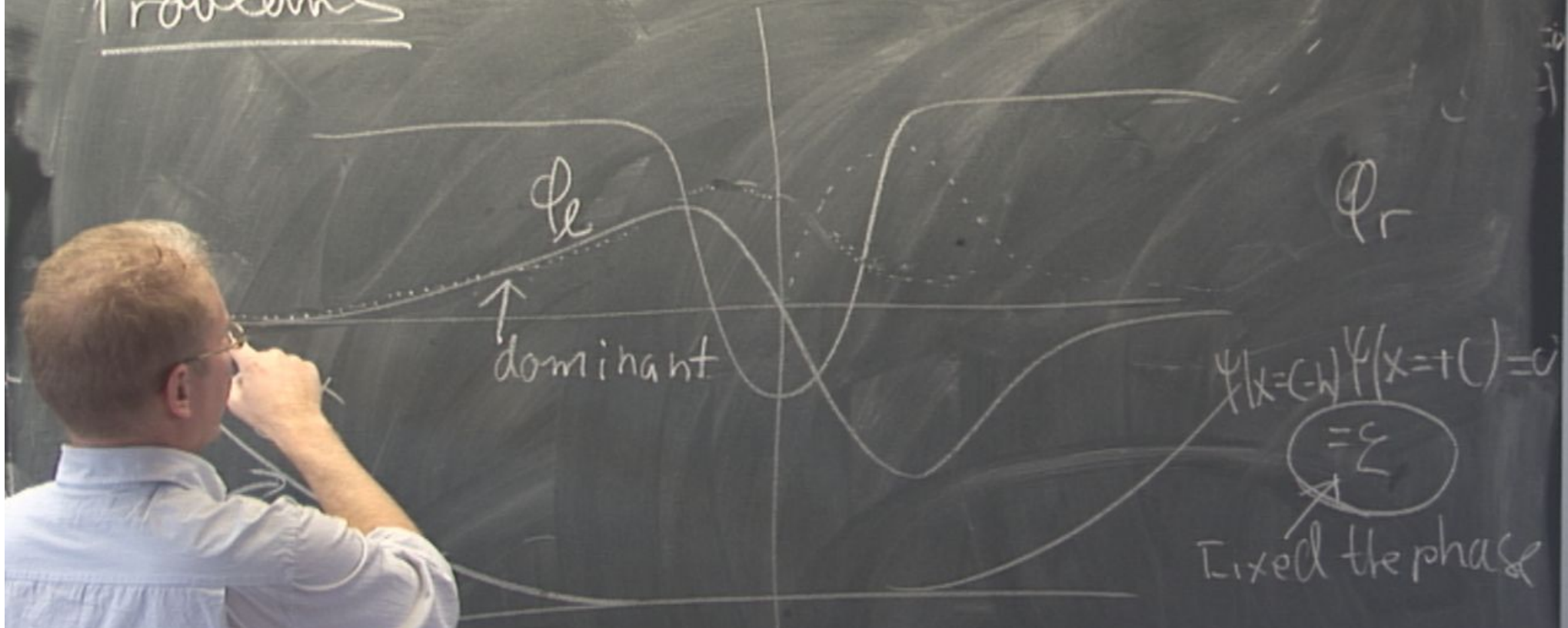
Have to integrate also from right to left

Problems



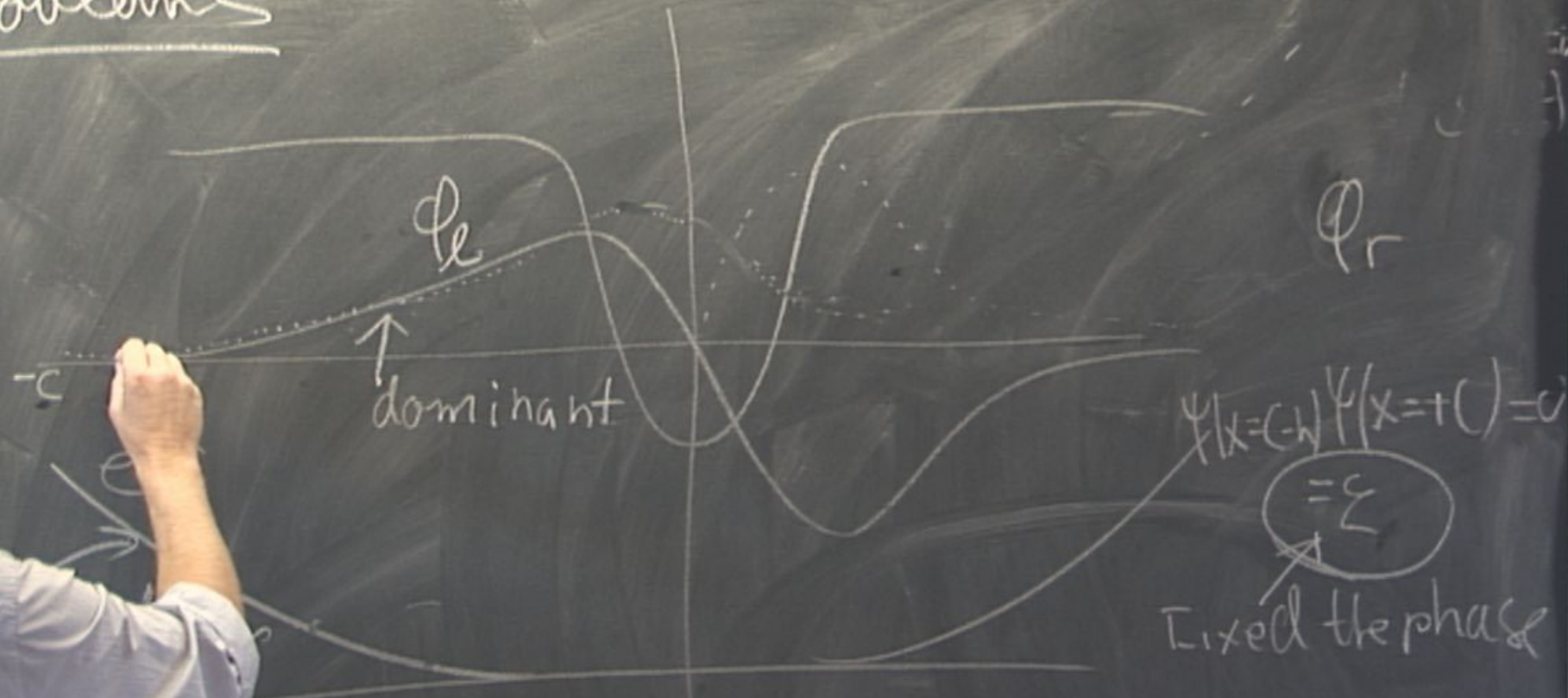
Have to integrate also from right to left

Problems



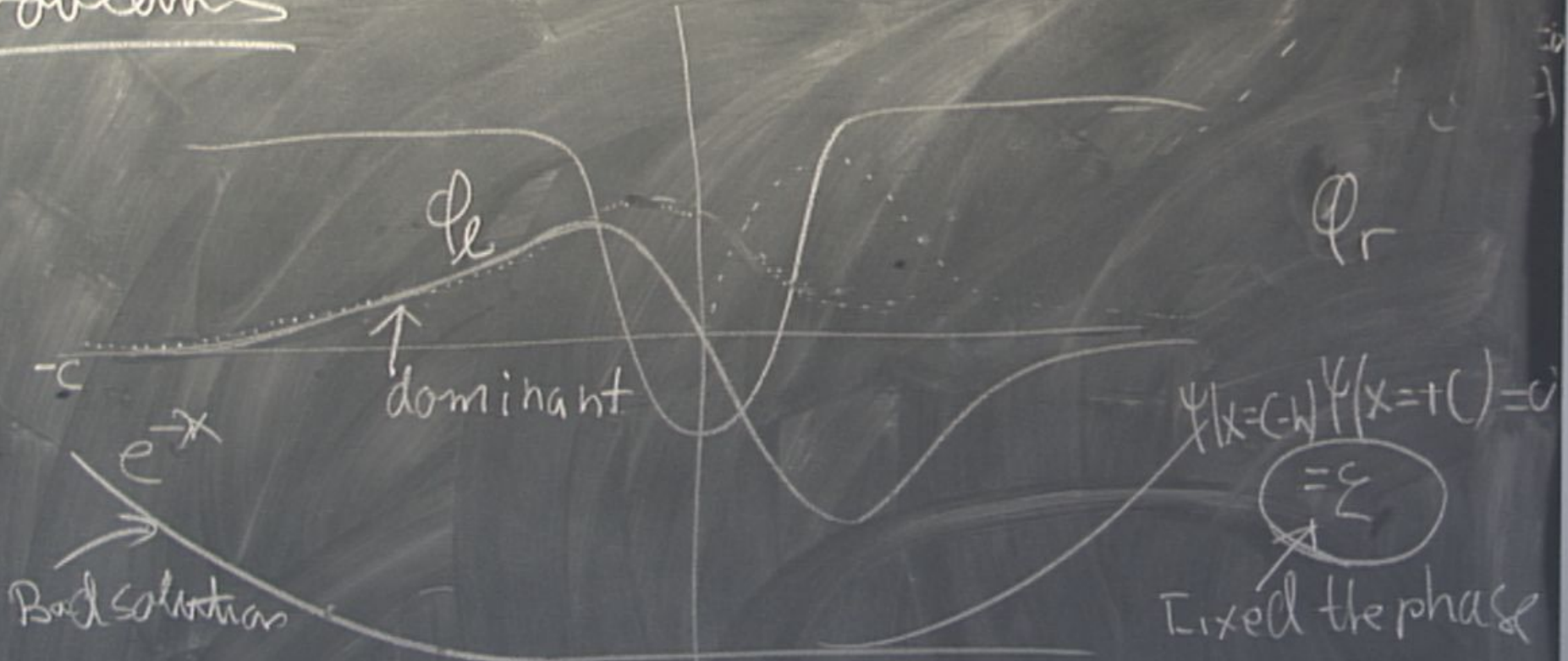
integrate also from right to left

Problems



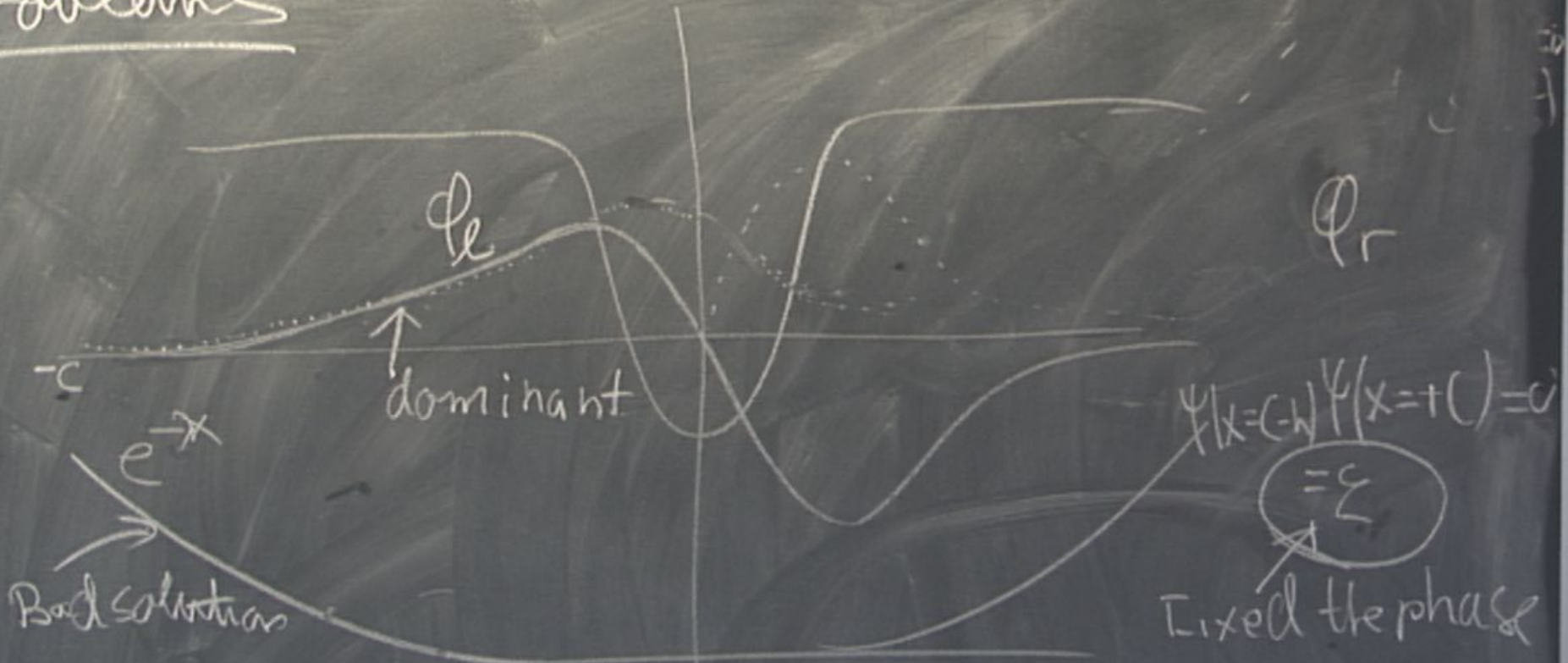
are to interpret also from right to left

Problems



Have to integrate also from right to left.

Problems



Have to integrate also from right to left

Consistent Phase Choice

Integrate P_e from $-C$ up to $X_m + h^h$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $X_m + h$

Integrate Q_r from $+C$ down to $X_m - h$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $X_m + h$

Integrate Q_r from $+C$ down to $X_m - h$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r / Q_e(x_m)$$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r / Q_e(x_m)$$

Consistent Phase Choice

Integrate \mathcal{P}_e from $-C$ up to $x_m + h$

Integrate \mathcal{P}_r from $+C$ down to $x_m - h$

$$\mathcal{P}_r \rightarrow \mathcal{P}_r / \mathcal{P}_e(x_m)$$

Automatically $\mathcal{P}_r(x_m) = \mathcal{P}_e(x_m)$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r / Q_e(x_m)$$

Automatically $Q_r(x_m) = Q_e(x_m)$

$$Q_r(\cdot) = Q_r(\cdot) / Q_e(x_m)$$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from C down to $x_m - h$

$$Q_r \rightarrow \frac{Q_e(x_m)}{Q_r(x_m)}$$

Automatically

$$Q_r(x_m)$$

$$Q_e(x_m)$$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r \frac{Q_e(x_m)}{Q_r(x_m)}$$

Automatically $Q_r(x_m) = Q_e(x_m)$

$$Q_r(\cdot) = Q_r(\cdot) \frac{Q_e(x_m)}{Q_r(x_m)}$$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r \frac{Q_e(x_m)}{Q_r(x_m)}$$

Automatically $Q_r(x_m) = Q_e(x_m)$

$$Q_r(\cdot) = Q_r(\cdot) \frac{Q_e(x_m)}{Q_r(x_m)}$$

Match the slopes

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h^h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r \frac{Q_e(x_m)}{Q_r(x_m)}$$

Automatically $Q_r(x_m) = Q_e(x_m)$

$$Q_r(\cdot) = Q_r(\cdot) \frac{Q_e(x_m)}{Q_r(x_m)}$$

Consistent Phase Choice

Integrate Q_e from $-C$ up to $x_m + h$

Integrate Q_r from $+C$ down to $x_m - h$

$$Q_r \rightarrow Q_r \frac{Q_e(x_m)}{Q_r(x_m)}$$

Automatically $Q_r(x_m) = Q_e(x_m)$

$$Q_r(\cdot) = Q_r(\cdot) \frac{Q_e(x_m)}{Q_r(x_m)}$$

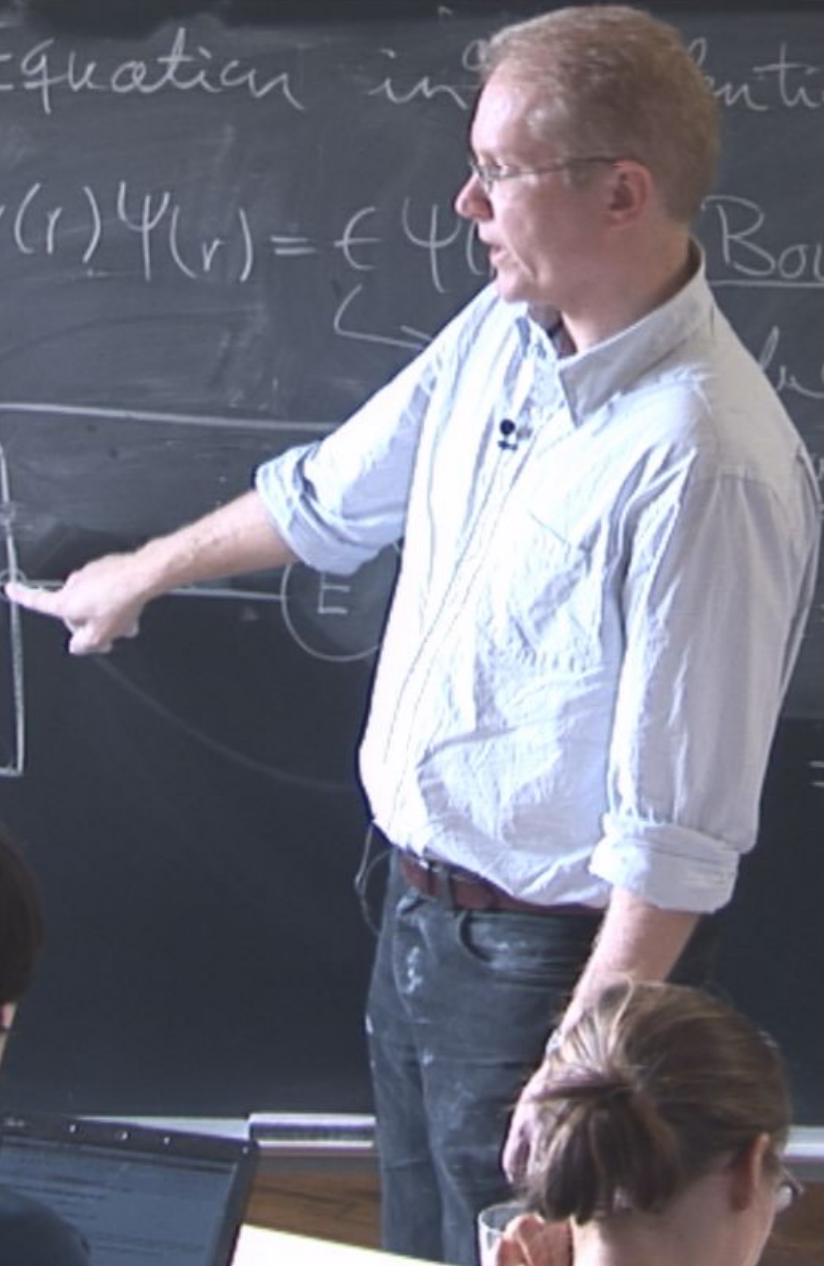
x_m cannot be a node of the eigenfunction

— x_m cannot be a node of the eigenfunction

Schrödinger's Equation in 1D Potential Well

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States



Region I, III

$$= \frac{2m}{\hbar^2} (V-E) \psi(x)$$
$$= \lambda^2 \psi(x)$$

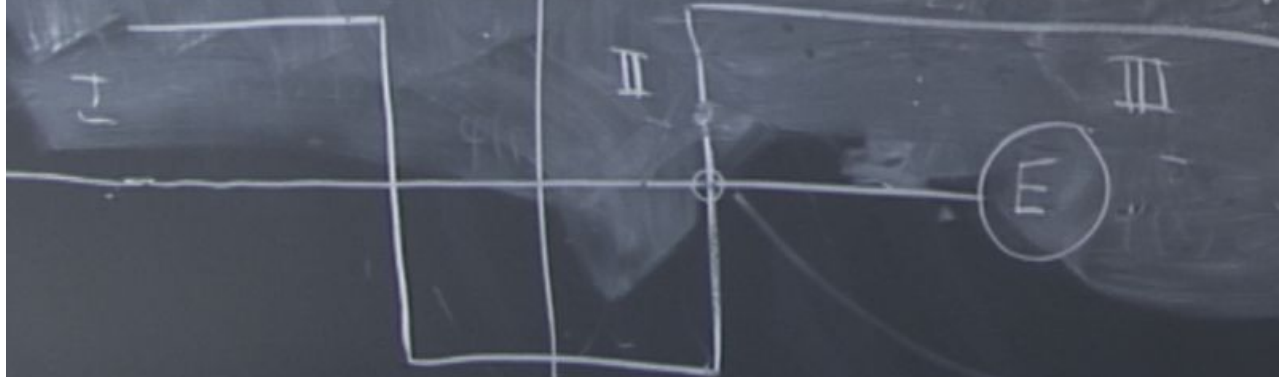
$\lambda > 0$

$$e^{\pm \lambda x}$$

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r) \quad \text{Bound-States}$$

↳ Eigenvalue



Region I, III

$$\frac{d^2 \psi}{dx^2} = \frac{2m}{\hbar^2} (V-E) \psi(x)$$

$$= \lambda^2 \psi(x) \quad \lambda > 0$$

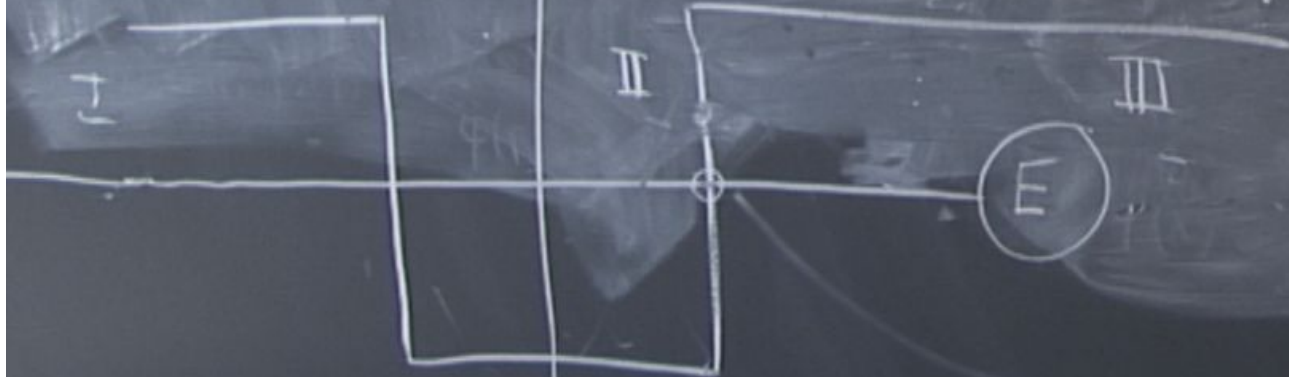
$$e^{\pm \lambda x}$$

Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

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Region I, III

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$$= -\lambda^2 \psi(x) \quad \lambda > 0$$

$$e^{\pm \lambda x}$$

— x_m cannot be a node of the eigenfunction

Match the Slopes

— x_m cannot be a node of the eigenfunction

Match the Slopes

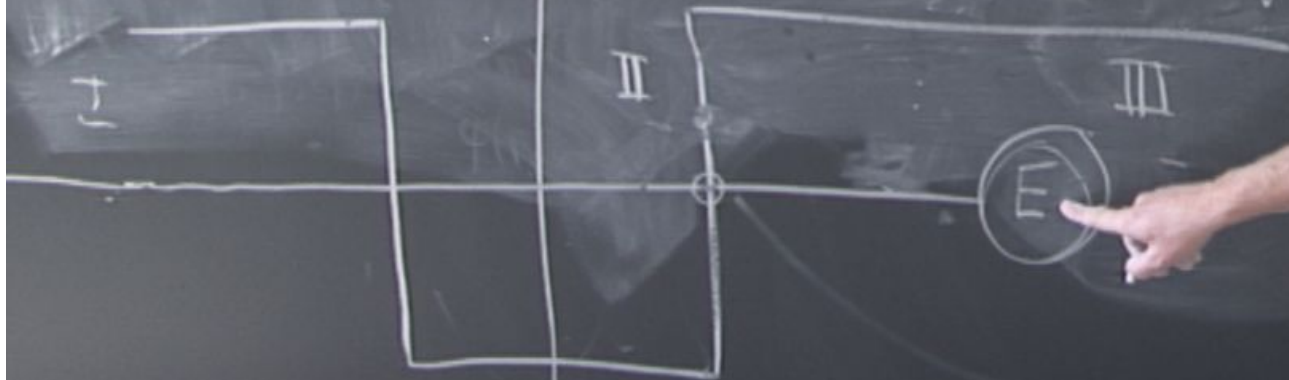
$F(E)$

Schrodinger's Equation in any potential well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound States

↳ Eigenvalue

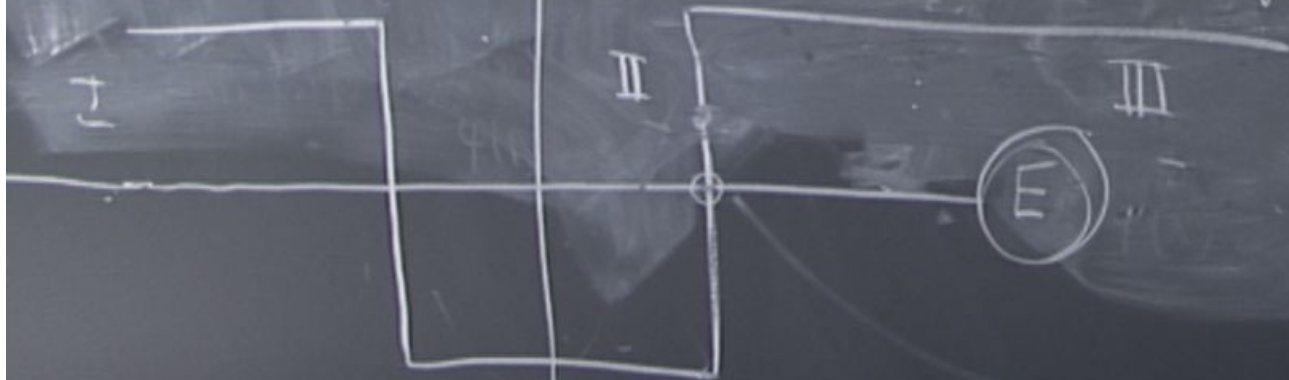


Schrodinger's Equation in any potential Well 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

Bound-States

↳ Eigenvalue



Region I, III

$$\begin{aligned} \frac{d^2\psi}{dx^2} &= \frac{2m}{\hbar^2} (V-E) \psi(x) \\ &= \lambda^2 \psi(x) \end{aligned}$$

$\lambda > 0$
 $e^{\pm \lambda x}$

x_m cannot be a node of the eigenfunction

Match the Slopes

$F(E)$

x_m cannot be a node of the eigenfunction

Match the Slopes

$$F(E) = \phi_e'$$

x_m cannot be a node of the eigenfunction

Match the Slopes

$$F(E) = \frac{\varphi_l'(x_m) - \varphi_r'(x_m)}{2h \varphi_r(x_m)}$$

— x_m cannot be a node of the eigenfunction

Match the Slopes

$$F(E) = \frac{\psi'_e(x_m) - \psi'_r(x_m)}{2h \psi_r(x_m)}$$
$$= \frac{\psi_e(x_{m+h}) - \psi_e(x_{m-h}) - (\psi_r(x_{m+h}) - \psi_r(x_{m-h}))}{2h \psi_r(x_m)}$$

— x_m cannot be a node of the eigenfunction

Match the Slopes

$$\begin{aligned} F(E) &= \frac{\psi'_e(x_m) - \psi'_r(x_m)}{2h \psi_r(x_m)} \\ &= \frac{\psi_e(x_{m+h}) - \psi_e(x_{m-h}) - (\psi_r(x_{m+h}) - \psi_r(x_{m-h}))}{2h \psi_r(x_m)} \end{aligned}$$

ℓ

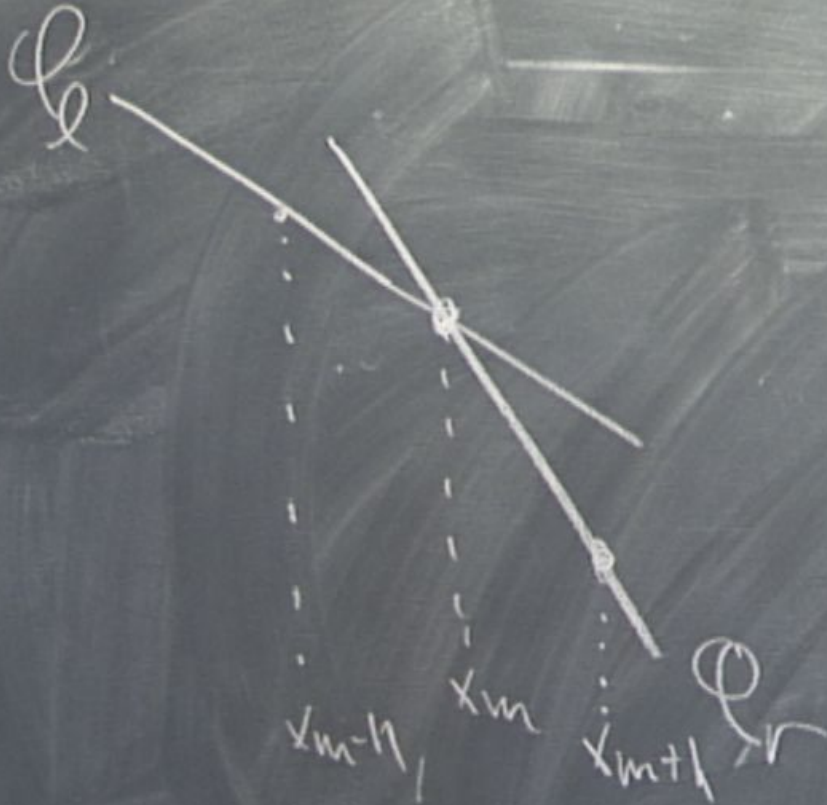


ℓ

\mathcal{L}

x_{m-1} , x_m , x_{m+1}

\mathcal{Q}



\mathcal{E}



x_{m-1} , x_m , x_{m+h}

$$F(E) > C$$

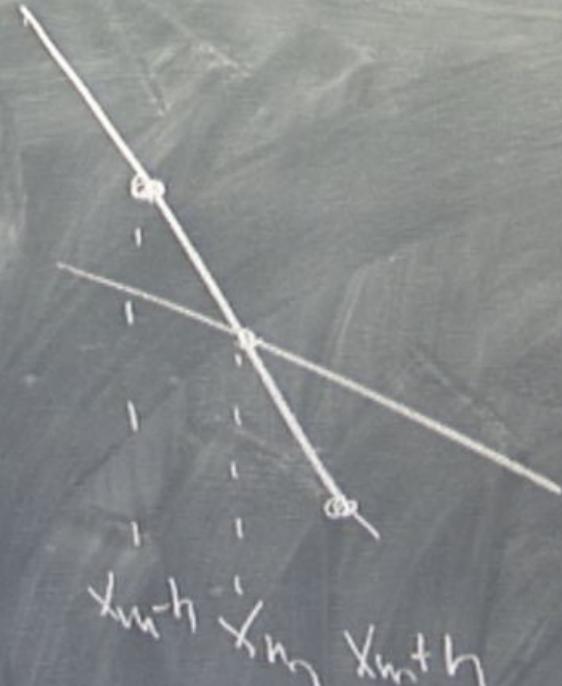


x_{m-1} , x_m , x_{m+h}

\mathcal{E}



$$F(E) > 0$$



$$F(E) < 0$$

- ① Plot $F(E)$ Start E below the bottom of well
- ② increase E

- ① Plot $F(E)$ Start E below the bottom of well
- ② $F(E)$ increase E



- ① Plot $F(E)$ Start E below the bottom of well
② $F(E)$ increase E



- ① Plot $F(E)$ Start E below the bottom of well increase E



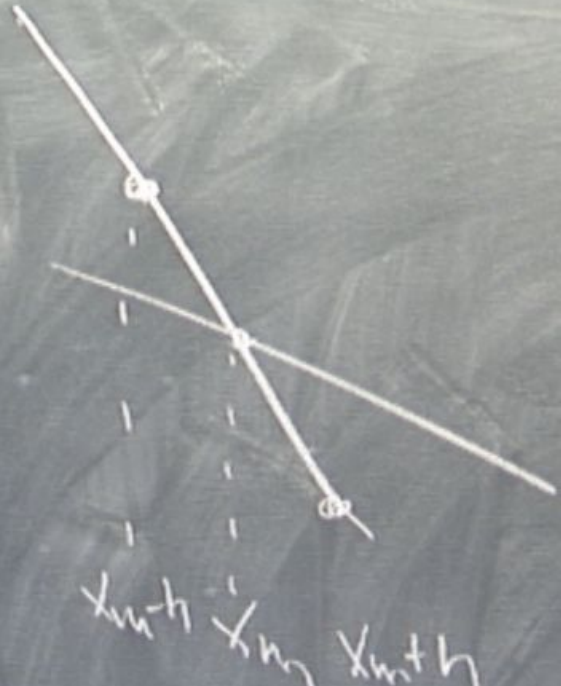
determine $[a, b]$

- ③ Run bisection on $f(E)$ on the $[a, b]$

\mathcal{L}

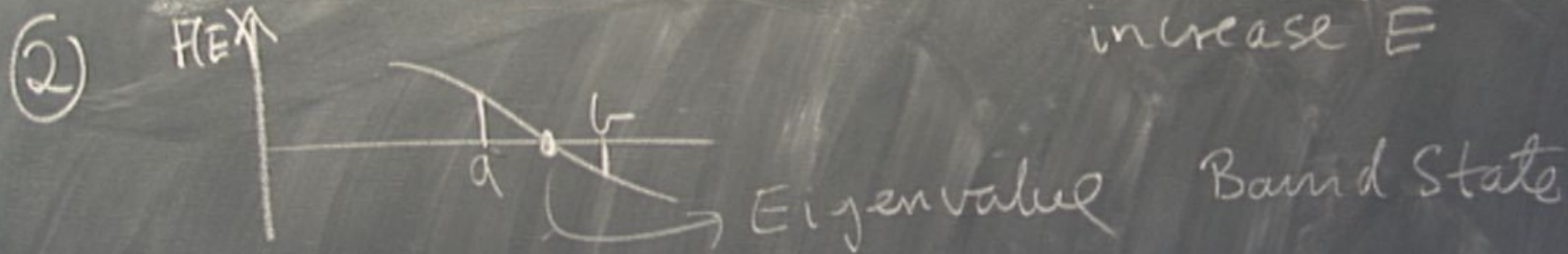


$$F(s) > 0$$



$$F(s) < 0$$

- ① Plot $F(E)$ Start E below the bottom of well
increase E



determine $[a, b]$

- ③ Run bisection on $f(E)$ on the $[a, b]$

- ① Plot $F(E)$ Start E below the bottom of well increase E

② $F(E)$



Eigenvalue

Band

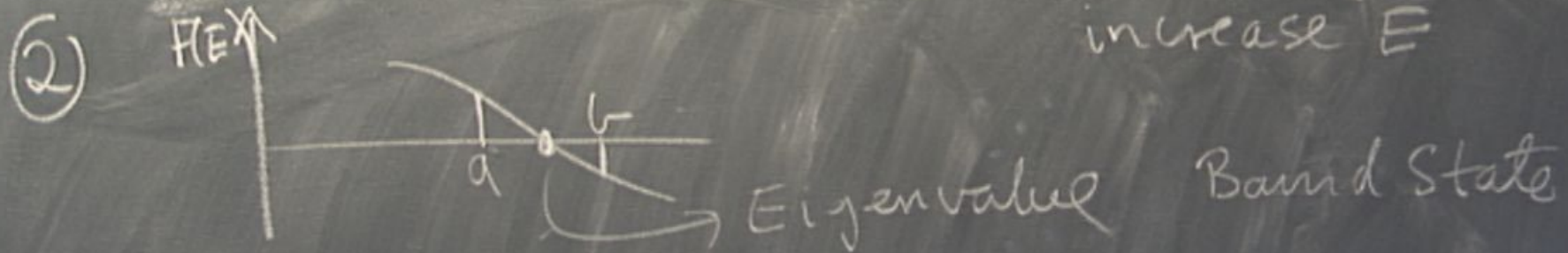
determine $[a, b]$

- ③ Run bisection on $f(E)$ on the

$f(E)$

$\phi_r(x_m)$

- ① Plot $F(E)$ Start E below the bottom of well
 increase E



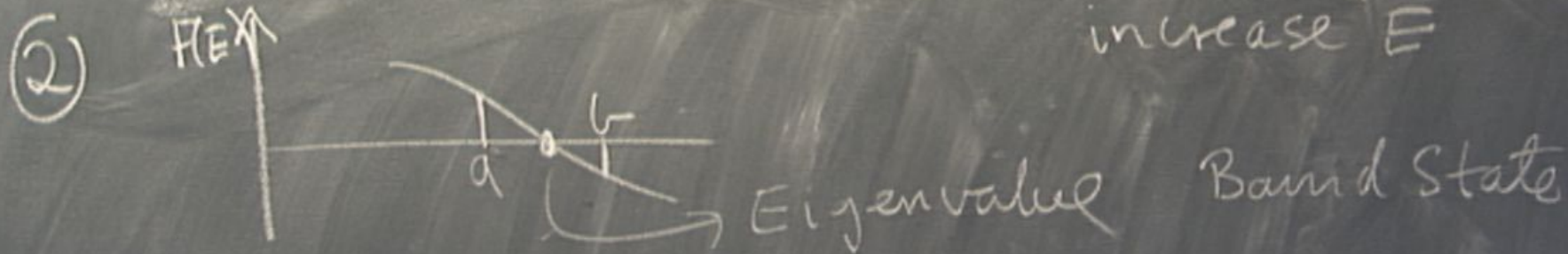
determine $[a, b]$

- ③ Run bisection on $f(E)$ on the $[a, b]$

$f(E)$

$\varphi_r(x_m)$

- ① Plot $F(E)$ Start E below the bottom of well increase E



determine $[a, b]$

- ③ Run bisection on $f(E)$ on the $[a, b]$

$f(E)$

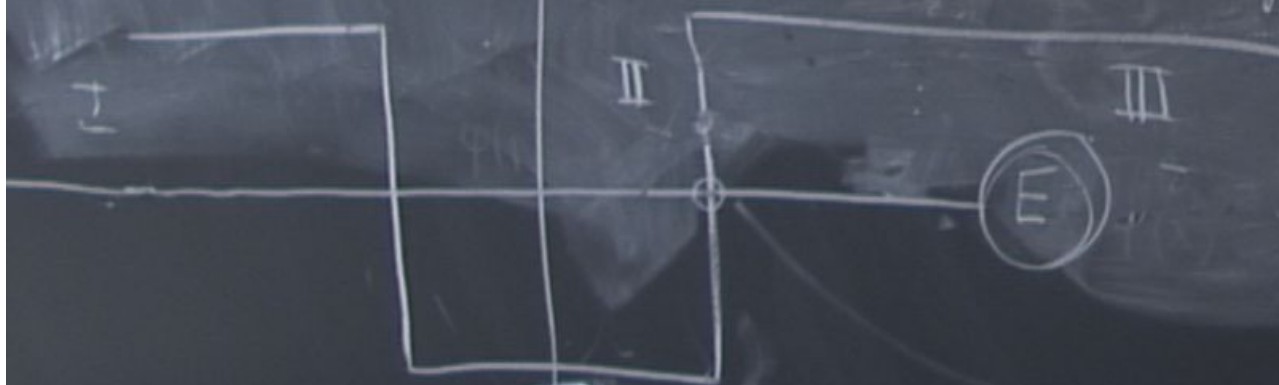
$\psi_r(x_m)$

Schrodinger's Equation in any potential $V(r)$ 1D

$$-\frac{\hbar^2}{2m} \nabla^2 \psi + V(r) \psi(r) = E \psi(r)$$

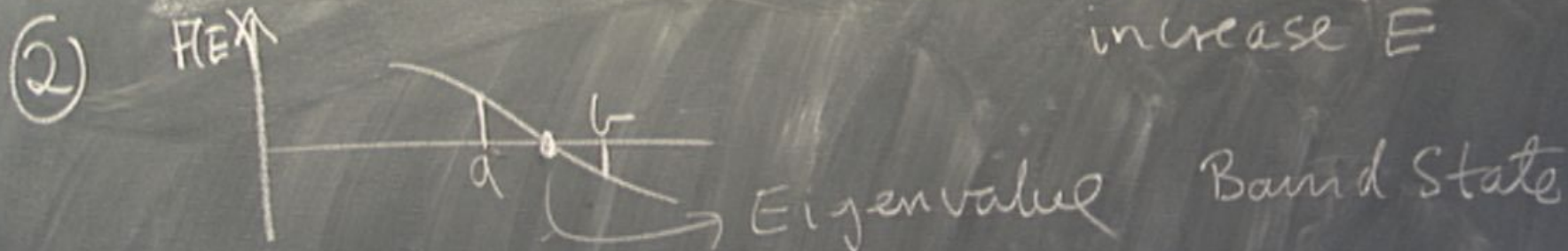
Bound-States

\hookrightarrow Eigenvalue



$$\frac{d^2 \psi}{dx^2} =$$

- ① Plot $F(E)$ Start E below the bottom of well increase E



determine $[a, b]$

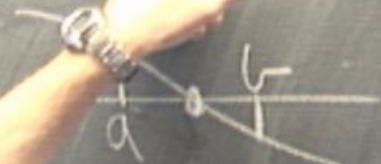
- ③ Run bisection on $f(E)$ on the $[a, b]$

$f(E)$

$\varphi_r(x_m)$

- ① Plot $F(E)$ Start E below the bottom of well increase E
- ②

$F(E)$



Eigenvalue Band State

etermine $[a, b]$

Run bisection on $f(E)$ on the $[a, b]$

$f(E)$

$\psi_r(x_m)$