Quantum Mechanics II

WKB

Derivation; Properties & Connection Formulae; Application

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WKB

Derivation

Extra!

- 1926: Gregor **W**entzel, Hans **K**ramers & Léon **B**rillouin
- also: Francesco Carlini (1817), Joseph **Liouville** (1837), George **Green** (1837), Lord Rayleigh (John Strutt, 1912), Richard Gans (1915), Harold **J**effreys (1923)
- Focus on 1-dimensional physics:

$$\widehat{H}\psi = E\psi \qquad \widehat{H} = -\frac{\hbar^2}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W(x) \qquad \psi(x) = e^{iu(x)}$$

- Substituting yields:

$$(u'(x))^2 = k^2(x) + iu''(x) \qquad k(x) := \sqrt{\tfrac{2M}{\hbar^2}\left[E - W(x)\right]}$$

- …which is a non-linear, inhomogeneous 2nd order differential equation—*vs*. the linear, homogeneous Schrödinger equation.
- But, it admits an iterative (“fixed point”) method of solving.

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WKB

Derivation

$$(u'(x))^2 = k^2(x) + i u''(x)$$

$$k(x) := \sqrt{\tfrac{2M}{\hbar^2}\,[E - W(x)]}$$

Extra!

- Too hard to solve exactly. However, if $k(x) = k$ were constant,
  - $u(x) = \pm k{\cdot}x + C$, so $u'(x) = \pm k$ and $u''(x) = 0$,
  - and $\psi(x) = \mathrm{A}\, e^{ik\cdot x} + \mathrm{B}\, e^{-ik\cdot x}$ would be the exact solution.

"piece-wise constant" potentials

- For "sufficiently slowly-varying potentials," start with

$$u_0'(x) = \pm k(x) \qquad u_0(x) = \pm \int \mathrm{d}x\, k(x) + C \qquad u_0''(x) \mapsto 0$$

ignored!

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WKB

Derivation

$$(u'(x))^2 = k^2(x) + iu''(x)$$

$$k(x) := \sqrt{\tfrac{2M}{\hbar^2}\left[E - W(x)\right]}$$

Extra!

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"piece-wise constant" potentials

- For "sufficiently slowly-varying potentials," start with

$$u_0'(x) = \pm k(x) \qquad u_0(x) = \pm \int dx\, k(x) + C \qquad u_0''(x) \mapsto 0$$

ignored!

- …and iterate

$$u_0''(x) = \pm k'(x) \qquad u_1(x) = \pm \int dx\, \sqrt{k^2(x) + iu_0''(x)} + C$$

$$u_2(x) = \pm \int dx\, \sqrt{k^2(x) + iu_1''(x)} + C$$

- …so the n^{th} iteration is

$$u_n(x) = \pm \int dx\, \sqrt{k^2(x) + iu_{n-1}''(x)} + C$$

- If $u_0(x)$ was a good start, $u_\infty(x)$ is exact.

WKB

$$u_1(x) = \pm \int dx\, \sqrt{k^2(x) + i u_0''(x)} + C$$

Derivation

Extra!

- Still not soluble exactly, in general.
- Approximate:

$$\sqrt{k^2 + ik'} = k\sqrt{1 + \frac{ik'}{k^2}} \approx k\left[1 + \frac{ik'}{2k^2} + \ldots\right] = k + \frac{i}{2}\frac{k'}{k} + \ldots$$

$$\begin{aligned} u_1(x) &= \pm \int dx\, \sqrt{k^2 \pm ik'} \\ &\approx \pm \int dx\, k\left[1 \pm \frac{ik'}{2k^2} + \ldots\right] \\ &= \pm \int dx\, k + \frac{i}{2}\int dx \frac{k'}{k} + \ldots \\ &= \pm \int dx\, k + \frac{i}{2}\int \frac{dk}{k} + \cdots \\ &= \pm \int dx\, k + \frac{i}{2}\ln\left[k(x)\right] + \ldots \end{aligned}$$

$$\begin{aligned} \psi(x) &= e^{iu(x)} \\ &= e^{\pm i \int dx\, k - \frac{1}{2}\ln[k(x)] + C} \\ &= e^{C} e^{\pm i \int dx\, k} e^{-\frac{1}{2}\ln[k(x)]} \end{aligned}$$

$$\rightarrow \frac{A}{\sqrt{k(x)}} e^{+i\int dx\, k} + \frac{B}{\sqrt{k(x)}} e^{-i\int dx\, k}$$

WKB

$$k(x) := \sqrt{\tfrac{2M}{\hbar^2}[E - W(x)]}$$

$$\psi_{\text{WKB}}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int \mathrm{d}x\; k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int \mathrm{d}x\; k(x)}$$

Properties & Connection Formulae

Extra!

- Wherever $E > W(x)$, kinetic energy is positive ☺
  - $k(x)$ is real and $\psi_{\text{WKB}}(x)$ is oscillatory.
- Wherever $E < W(x)$, kinetic energy is negative ☹
  - $k(x)$ is imaginary and $\psi_{\text{WKB}}(x)$ is non-oscillatory.
  - Write

$$\kappa(x) := -ik(x) = \sqrt{\tfrac{2M}{\hbar^2}[W(x) - E]} \qquad k(x) = i\kappa(x)$$

$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int \mathrm{d}x\; \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int \mathrm{d}x\; \kappa(x)}$$

- Transition from one to another:
  - If $W(x)$ goes across E discontinuously, $W(x) \neq E$, $\psi_{\text{WKB}}(x)$ is well-defined.
  - If $W(x)$ goes across E continuously, $W(x_*) = E$, $\psi_{\text{WKB}}(x_*) \to \infty$

$$[W(x) - E] = F_1(x - x_*) + \ldots \qquad \frac{1}{\sqrt{\sqrt{x - x_*}}}\, e^{\int \mathrm{d}x\, \sqrt{x - x_*}} \xrightarrow{x \to x_*} \frac{1}{\sqrt[4]{0}}\, e^{0^{3/2}}$$

not a pole; branch-cut

WKB

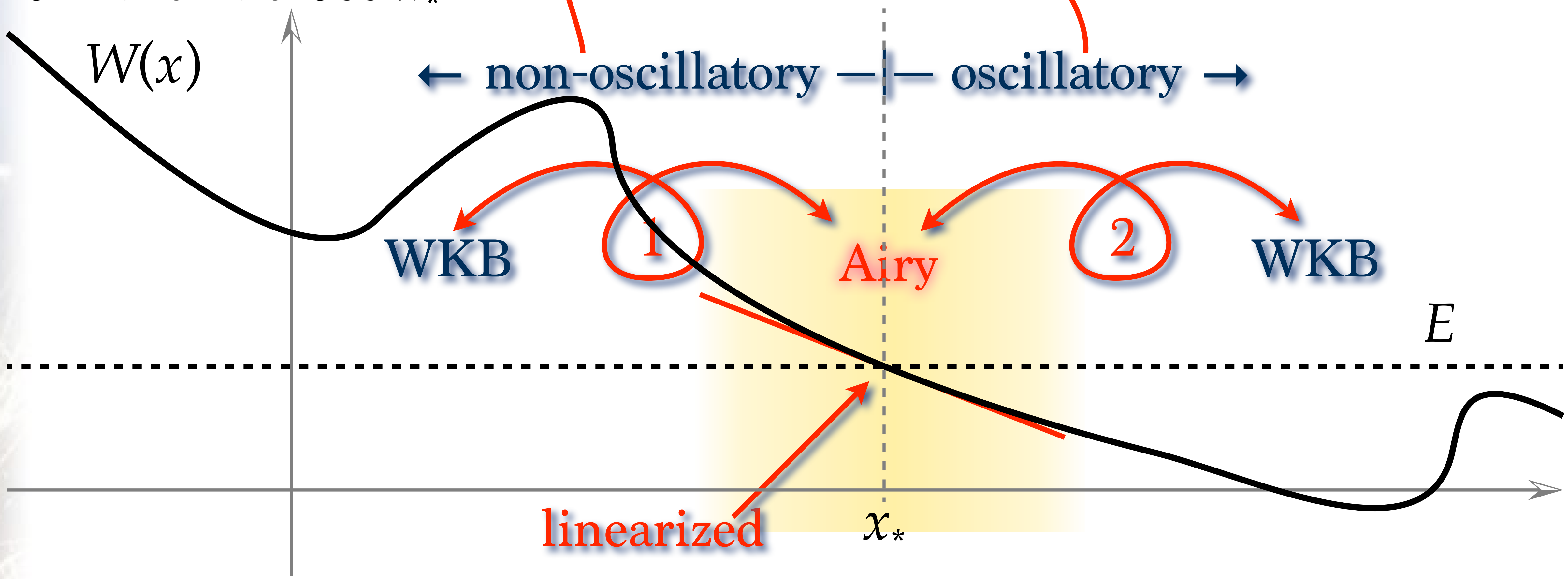
$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int \mathrm{d}x\ \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int \mathrm{d}x\ \kappa(x)}$$

$$\psi_{\text{WKB}}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int \mathrm{d}x\ k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int \mathrm{d}x\ k(x)}$$

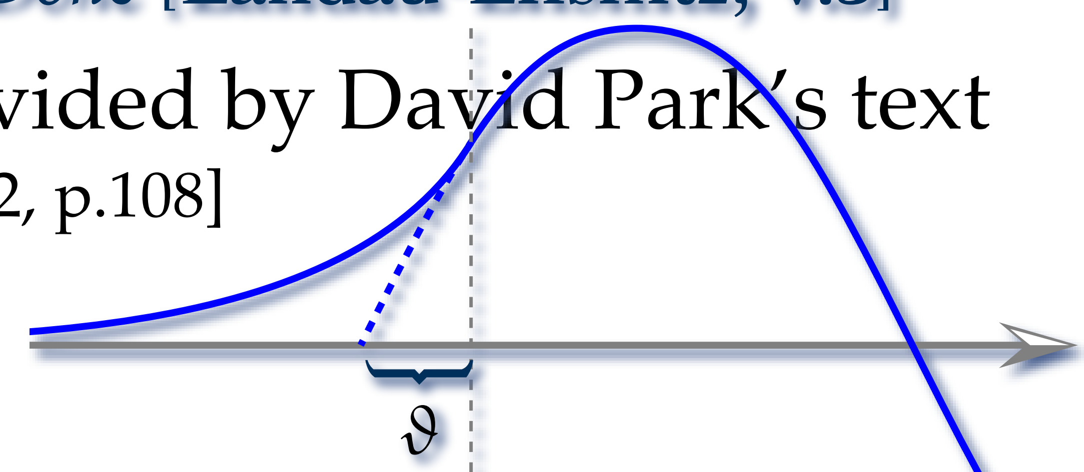
Properties & Connection Formulae

Extra!

- To match across x_*



- So, match: WKB_L—Airy—WKB_R ***Done*** **[Landau-Lifshitz, v.3]**
- Use the “connection formulae” provided by David Park’s text [Introduction to Quantum Physics, 3rd ed., 1992, p.108]
- Phase-shift: $\vartheta = e^{i\pi/4}$



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$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int \mathrm{d}x\ \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int \mathrm{d}x\ \kappa(x)}$$

$$\psi_{\text{WKB}}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int \mathrm{d}x\ k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int \mathrm{d}x\ k(x)}$$

Properties & Connection Formulae

Extra!

- For the non-oscillatory form:
  - The C-term diverges for $x \to -\infty$; the D-term diverges for $x \to +\infty$
- All integrals are computed with x_* as the lower limit
- Then:

Barrier to Left	**Barrier to Right**
$C = (\vartheta^* A + \vartheta B)$	$C = \tfrac{1}{2}(\vartheta^* A + \vartheta B)$
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- The lower limit x^* in all integrals must refer to the transition point, *i.e.*, the classical turning point of the conn. formulae.
- In general: discontinuous $W(x)/E$ crossing = no phase-shift
- …continuous $W(x)/E$ crossing = $\pi/4$ phase-shift

QM II

WKB

Applications

$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int \mathrm{d}x\ \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int \mathrm{d}x\ \kappa(x)}$$

$$\psi_{\text{WKB}}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int \mathrm{d}x\ k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int \mathrm{d}x\ k(x)}$$

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$$\phi := \int_a^b \mathrm{d}\xi\ k(\xi) = \int_a^b \mathrm{d}\xi\ \sqrt{\tfrac{2M}{\hbar^2}[E - W(x)]}$$

- Smooth potential well
  - Two transition points, a & b
  - Left transition, "Barrier to Left," $x_* = a$
  - Right transition, "Barrier to Right," $x_* = b$
- So,

$$\psi_L(x) = \frac{\cancel{C}}{\sqrt{\kappa(x)}}\, e^{-\int_a^x \mathrm{d}\xi\ \kappa(\xi)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int_a^x \mathrm{d}\xi\ \kappa(\xi)}$$

diverges $x < a$

$$\psi_M(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int_a^x \mathrm{d}\xi\ k(\xi)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int_a^x \mathrm{d}\xi\ k(\xi)}$$

$$= \frac{Ae^{+i\phi}}{\sqrt{k(x)}}\, e^{+i\int_b^x \mathrm{d}\xi\ k(\xi)} + \frac{Be^{-i\phi}}{\sqrt{k(x)}}\, e^{-i\int_b^x \mathrm{d}\xi\ k(\xi)}$$

$$\psi_R(x) = \frac{C'}{\sqrt{\kappa(x)}}\, e^{-\int_b^x \mathrm{d}\xi\ \kappa(\xi)} + \frac{\cancel{D'}}{\sqrt{\kappa(x)}}\, e^{+\int_b^x \mathrm{d}\xi\ \kappa(\xi)}$$

diverges $x > b$

- $A = A(D)$ & $B = B(D)$, $C' = C'(Ae^{+i\phi}, Be^{-i\phi})$ and $D'(Ae^{+i\phi}, Be^{-i\phi}) = 0$!

QM II

WKB

$$\psi_{WKB}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int dx\ \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int dx\ \kappa(x)}$$

$$\psi_{WKB}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int dx\ k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int dx\ k(x)}$$

Applications

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- Left→Middle: $A = \vartheta^* D$ & $B = \vartheta D$
- M→R:

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WKB

Applications

$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int \mathrm{d}x\ \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int \mathrm{d}x\ \kappa(x)}$$

$$\psi_{\text{WKB}}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int \mathrm{d}x\ k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int \mathrm{d}x\ k(x)}$$

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$$= \frac{1}{2}\left(\vartheta^*(\vartheta^* D\, e^{i\phi}) + \vartheta(\vartheta D\, e^{-i\phi})\right)$$

$$= \frac{1}{2}\left(e^{-i\pi/2} D\, e^{i\phi} + e^{i\pi/2} D\, e^{-i\phi}\right)$$

$$= D\frac{-ie^{i\phi} + ie^{-i\phi}}{2} = D\frac{e^{i\phi} - e^{-i\phi}}{2i} = D\sin(\phi)$$

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Barrier to Right

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WKB

$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int \mathrm{d}x\ \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int \mathrm{d}x\ \kappa(x)}$$

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$$\begin{aligned} C' &= \tfrac{1}{2}\big(\vartheta^*(A\,e^{i\phi}) + \vartheta(B\,e^{-i\phi})\big) \\ &= \tfrac{1}{2}\big(\vartheta^*(\vartheta^* D\,e^{i\phi}) + \vartheta(\vartheta D\,e^{-i\phi})\big) \\ &= \tfrac{1}{2}\big(e^{-i\pi/2} D\,e^{i\phi} + e^{i\pi/2} D\,e^{-i\phi}\big) \\ &= D\frac{-ie^{i\phi}+ie^{-i\phi}}{2} = D\frac{e^{i\phi}-e^{-i\phi}}{2i} = D\sin(\phi) \end{aligned}$$

- …and:

$$\begin{aligned} D' &= \big(\vartheta(A\,e^{i\phi}) + \vartheta^*(B\,e^{-i\phi})\big) \\ &= \big(\vartheta(\vartheta^* D\,e^{i\phi}) + \vartheta^*(\vartheta D\,e^{-i\phi})\big) \\ &= \big(D\,e^{i\phi} + D\,e^{-i\phi}\big) \\ &= 2D\frac{e^{i\phi}+e^{-i\phi}}{2} = 2D\cos(\phi) \stackrel{!}{=} 0 \end{aligned}$$

QM II

WKB

Applications

$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int dx\, \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int dx\, \kappa(x)}$$

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$$= 2D\frac{e^{i\phi}+e^{-i\phi}}{2} = 2D\cos(\phi) \overset{!}{=} 0$$

$$\phi = \begin{cases}(2n+\frac{1}{2})\pi\\(2n+\frac{3}{2})\pi\end{cases}$$

$$\phi = \int_a^b dx\sqrt{\tfrac{2M}{\hbar^2}[E-W(x)]}$$

WKB

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$$\psi_{\text{WKB}}(x) = \frac{C}{\sqrt{\kappa(x)}}\, e^{-\int dx\, \kappa(x)} + \frac{D}{\sqrt{\kappa(x)}}\, e^{+\int dx\, \kappa(x)}$$

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- …and: $$\begin{aligned} D' &= \big(\vartheta(A\, e^{i\phi}) + \vartheta^*(B\, e^{-i\phi})\big) \\ &= \big(\vartheta(\vartheta^* D\, e^{i\phi}) + \vartheta^*(\vartheta D\, e^{-i\phi})\big) \\ &= \big(D\, e^{i\phi} + D\, e^{-i\phi}\big) \\ &= 2D\frac{e^{i\phi}+e^{-i\phi}}{2} = 2D\cos(\phi) \stackrel{!}{=} 0 \end{aligned}$$

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$$\phi = \int_a^b dx \sqrt{\frac{2M}{\hbar^2}[E - W(x)]}$$

Energy quantization

WKB

Applications

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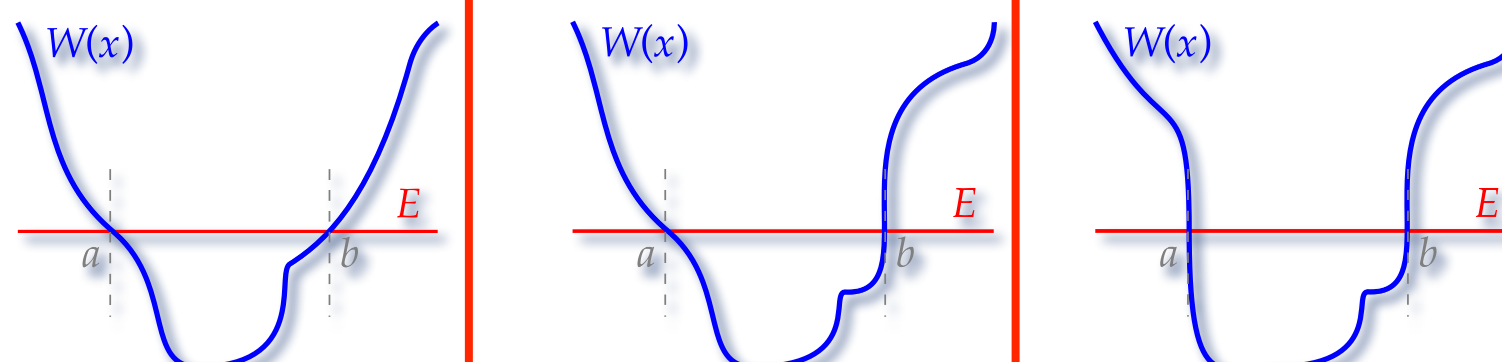
$$\psi_{\rm WKB}(x) = \frac{A}{\sqrt{k(x)}}\, e^{+i\int {\rm d}x\ k(x)} + \frac{B}{\sqrt{k(x)}}\, e^{-i\int {\rm d}x\ k(x)}$$

- Potential well w/ transition points $x_* = a$ and $x_* = b$
- The energy-quantization relation is:

$$\int_a^b {\rm d}x \sqrt{\frac{2M}{\hbar^2}[E - W(x)]} = \begin{cases}(2n+\frac{1}{2})\pi \\ (2n+\frac{3}{2})\pi\end{cases} = \begin{cases}(2n+\frac{3}{4})\pi \\ (2n+\frac{7}{4})\pi\end{cases} = \begin{cases}(2n+1)\pi \\ (2n+2)\pi\end{cases}$$

symmetric

antisymmetric



- Whenever $W(x)$ crosses E discontinuously

$$\triangle\psi(x) = 0 = \triangle\psi'(x)$$

- Whenever $W(x)$ crosses E continuously

WKB connection formulae

Barrier to Left

$$\begin{aligned} C &= (\vartheta^* A + \vartheta B) \\ D &= \tfrac{1}{2}(\vartheta A + \vartheta^* B) \\ A &= \tfrac{1}{2}\vartheta C + \vartheta^* D \\ B &= \tfrac{1}{2}\vartheta^* C + \vartheta D \end{aligned}$$

Barrier to Right

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Quantum Mechanics II

Now, go forth and calculate!!

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