



# Bounding the Bogoliubov coefficients.

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## Abstract:

We have all seen the WKB estimate for barrier penetration probability.

Unfortunately, the WKB estimate is an example of an uncontrolled approximation, and you do not know if it is high or low.

In this talk I will explain some rigorous bounds that you can place on barrier penetration probabilities, or equivalently on the Bogoliubov coefficients associated with a time-dependent potential.

This is an example of finding new physics in an old and apparently well-understood area.



## Background:

Bounding the Bogoliubov coefficients.  
(with Petarpa Boonserm)

e-Print: [arXiv:0801.0610 \[quant-ph\]](https://arxiv.org/abs/0801.0610)

Annals of Physics (2008) in press.

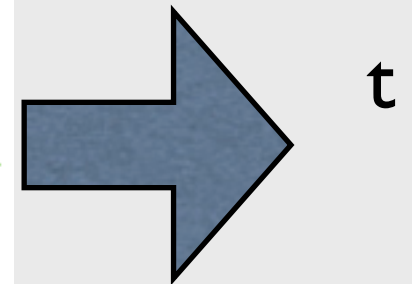
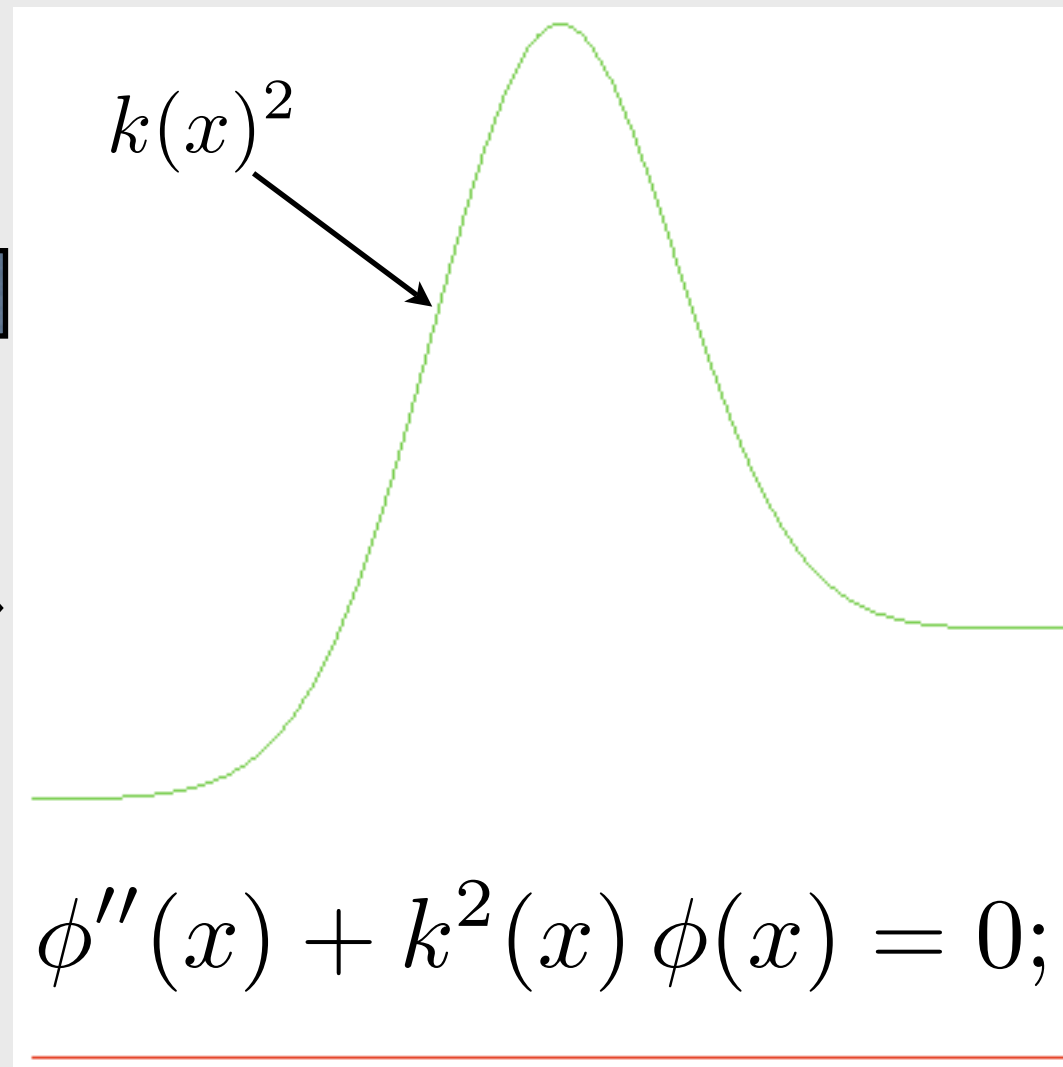
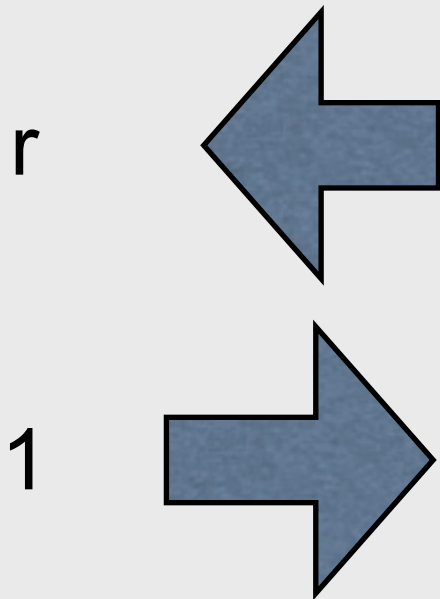
Some general bounds for 1-D scattering.

e-Print arXiv: [quant-ph/9901030](https://arxiv.org/abs/quant-ph/9901030)

[Physical Review A59 \(1999\) 427--438](#)



## Scattering:



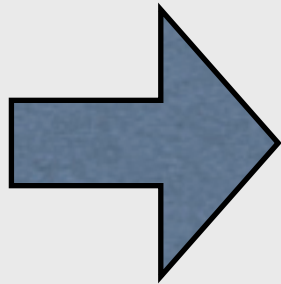
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$$1 = |t|^2 + |r|^2$$

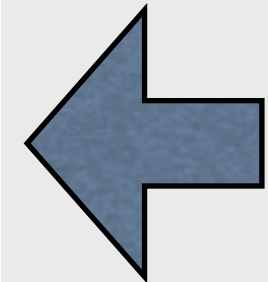
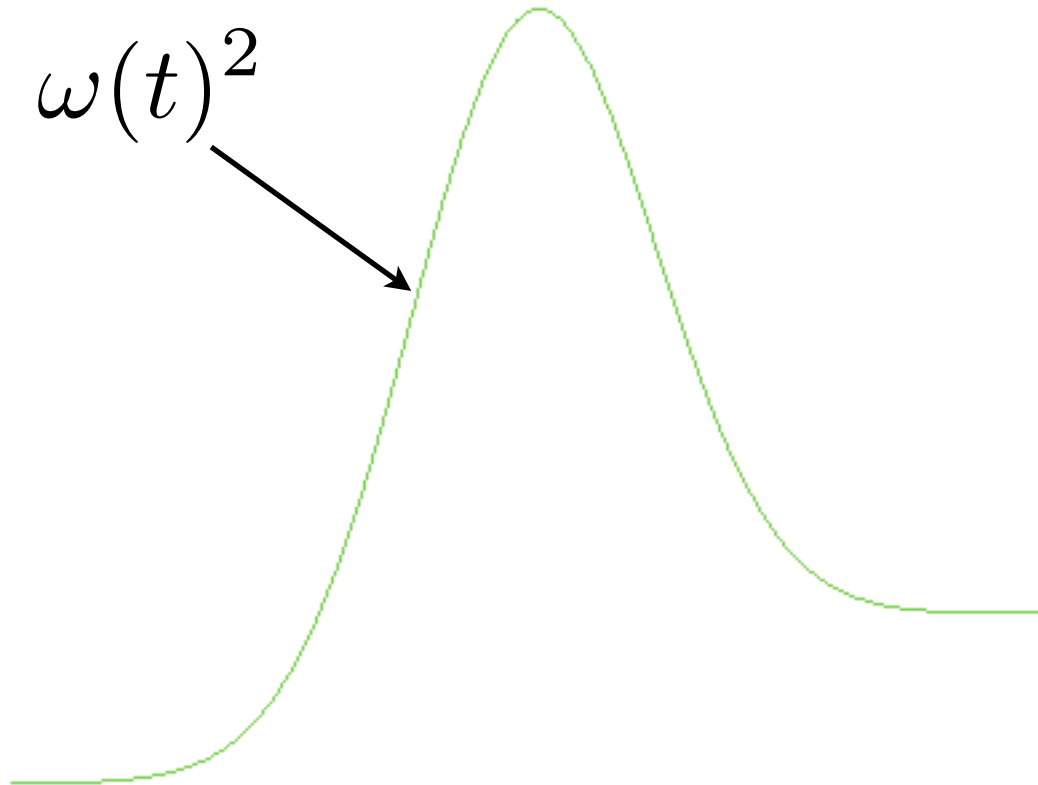
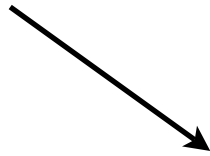


# Parametric oscillator:

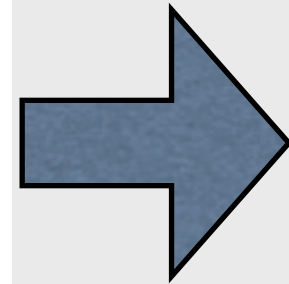
1



$\omega(t)^2$



$\beta$



$\alpha$

$$\ddot{\phi}(t) + \omega^2(t) \phi(t) = 0.$$

---

$$|\alpha|^2 - |\beta|^2 = 1$$



## Equivalences:

$$|\alpha| \leftrightarrow \frac{1}{|t|} \qquad |\beta| \leftrightarrow \frac{|r|}{|t|}$$

The two problems are formally completely equivalent,  
and one can treat them completely interchangeably:

$$|\alpha| = \cosh Q \qquad |\beta| = \sinh Q \qquad |t| = \operatorname{sech} Q \qquad |r| = \tanh Q$$

Put a bound on the functional “Q”...

$$Q = Q[k(x)] = Q[\omega(t)]$$



Equivalences:

$$T = |t|^2 = \operatorname{sech}^2 Q$$

$$N = |\beta|^2 = \sinh^2 Q$$

$$R = |r|^2 = \tanh^2 Q$$

$$T \leftrightarrow \frac{1}{1 + N}$$



Simple case:  
(spatial)

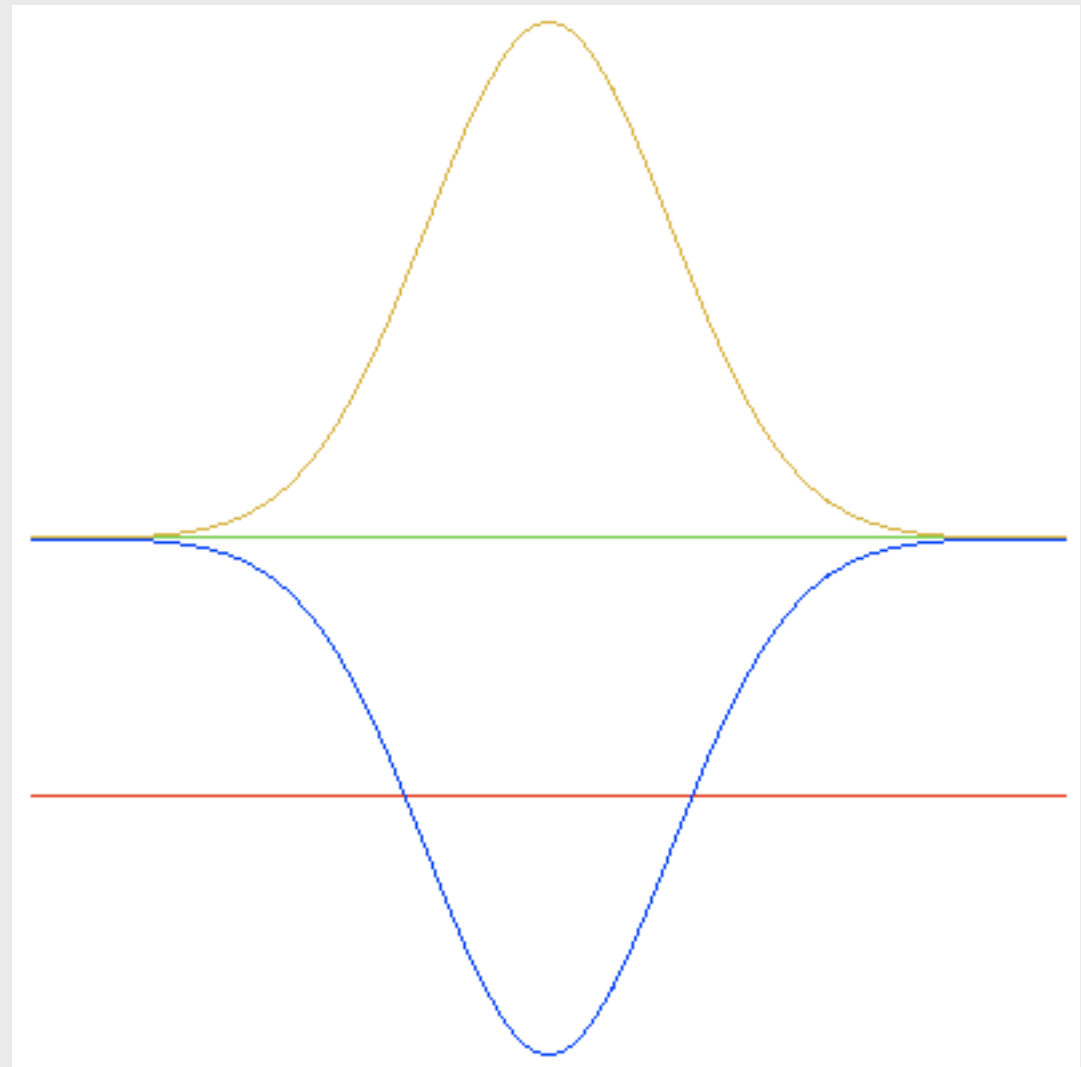
$$k_{\infty} = k(+\infty) = k(-\infty)$$

$$T = |t|^2 = \operatorname{sech}^2 Q$$

$$R = |r|^2 = \tanh^2 Q$$

**Theorem:**

$$Q \leq \oint \left| \frac{k_{\infty}^2 - k(x)^2}{2k_{\infty}} \right| dx$$



**Proof:** Let's delay that for now....



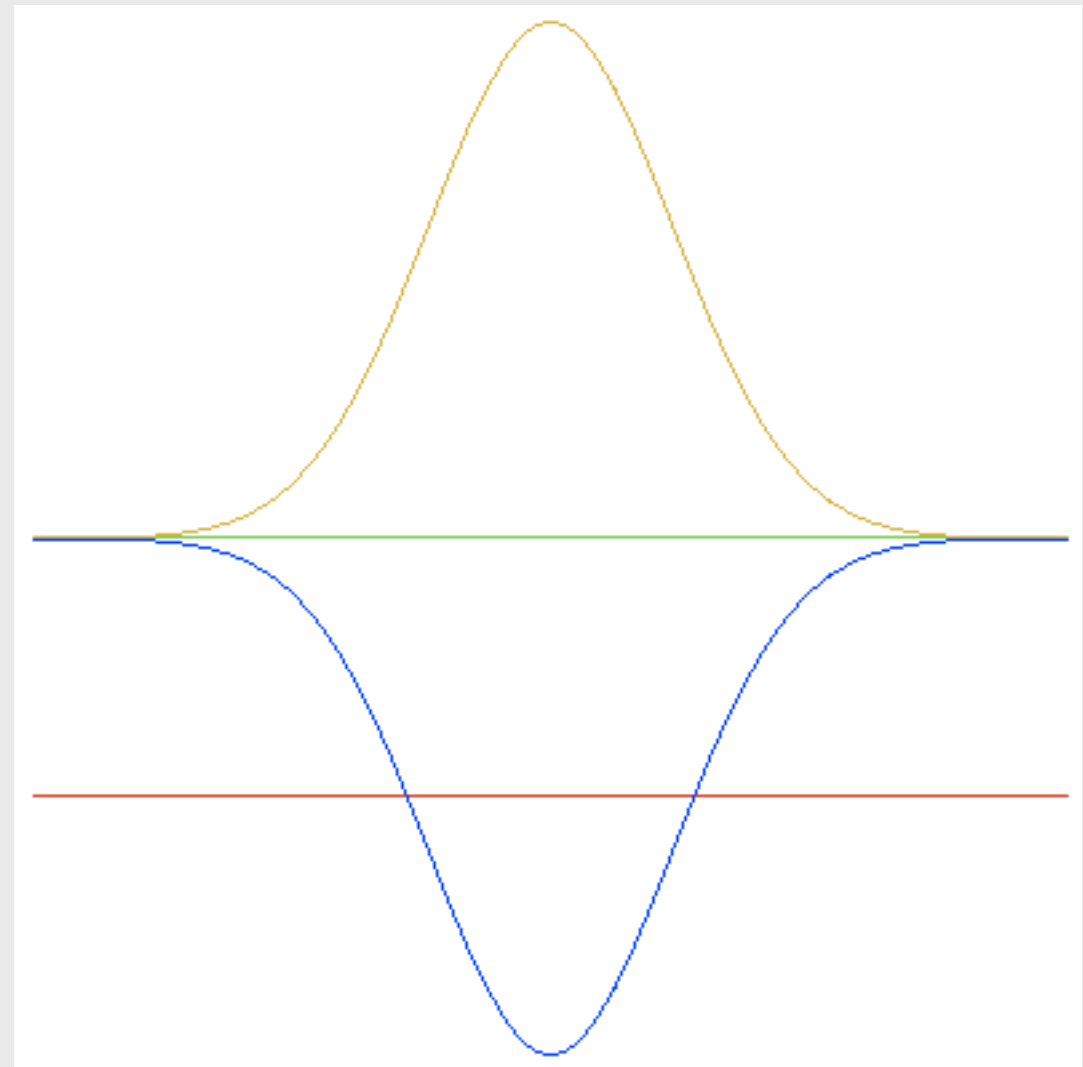
Simple case:  
(temporal)

$$\omega_{\infty} = \omega(+\infty) = \omega(-\infty)$$

$$N = |\beta|^2 = \sinh^2 Q$$

**Theorem:**

$$Q \leq \oint \left| \frac{\omega_{\infty}^2 - \omega(t)^2}{2\omega_{\infty}} \right| dt$$



**Proof:** Let's delay that for now....



These bounds

$$Q \leq \oint \left| \frac{k_{\infty}^2 - k(x)^2}{2k_{\infty}} \right| dx$$

$$Q \leq \oint \left| \frac{\omega_{\infty}^2 - \omega(t)^2}{2\omega_{\infty}} \right| dt$$

are limited to situations where the asymptotic limits of the potential are equal, but are otherwise very general...

They work perfectly well in the “classically forbidden” region:

$$k(x)^2 < 0$$

$$\omega(t)^2 < 0$$



## Comments:

Two significantly different proofs have been developed (arXiv: 0810.0610 [quant-ph], and quant-ph/9901030).

Many consistency checks against known exact solutions are presented in quant-ph/9901030.

I have not seen anything like these bounds anywhere else.

These are **not** JWKB-like bounds.  
JWKB theory would lead to integrals such as:

$$\int_{\text{forbidden}} |k(x)| dx$$

$$\int_{\text{forbidden}} |\omega(t)| dt$$



## Reprise:

$$T = |t|^2 = \operatorname{sech}^2 Q \geq \operatorname{sech}^2 \oint \left| \frac{k_\infty^2 - k(x)^2}{2k_\infty} \right| dx$$

$$R = |r|^2 = \tanh^2 Q \leq \tanh^2 \oint \left| \frac{k_\infty^2 - k(x)^2}{2k_\infty} \right| dx$$

$$N = |\beta|^2 = \sinh^2 Q \leq \sinh^2 \oint \left| \frac{\omega_\infty^2 - \omega(t)^2}{2\omega_\infty} \right| dt$$

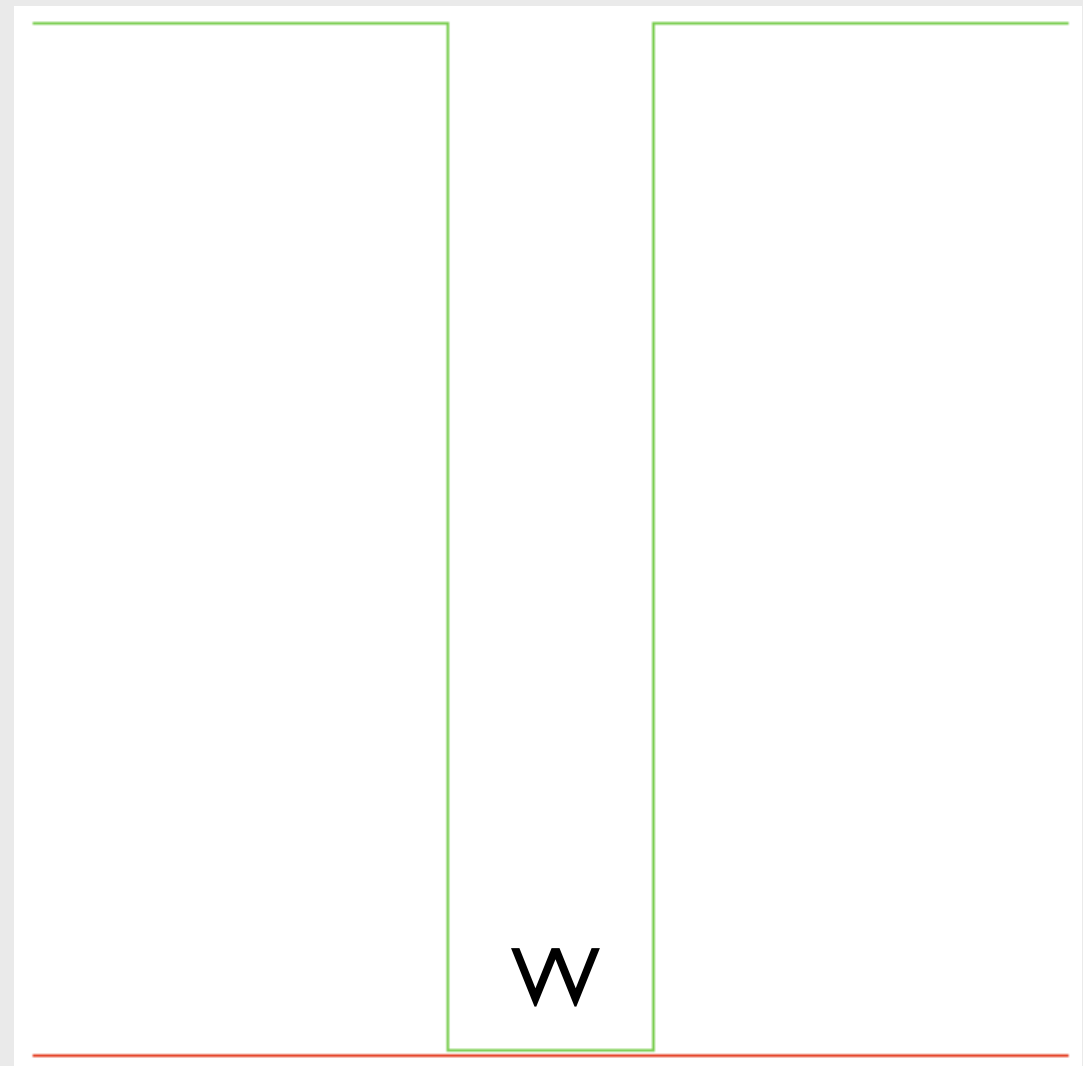
There are situations where these bounds are  
arbitrarily close to saturation...



$$T_{\text{exact}} = \frac{1}{1 + k_{\infty}^2 W^2/4}$$

$$T_{\text{bound}} = \text{sech}^2(k_{\infty} W/2)$$

Arbitrarily close for  
narrow wells  
( $W \Rightarrow 0$ ).

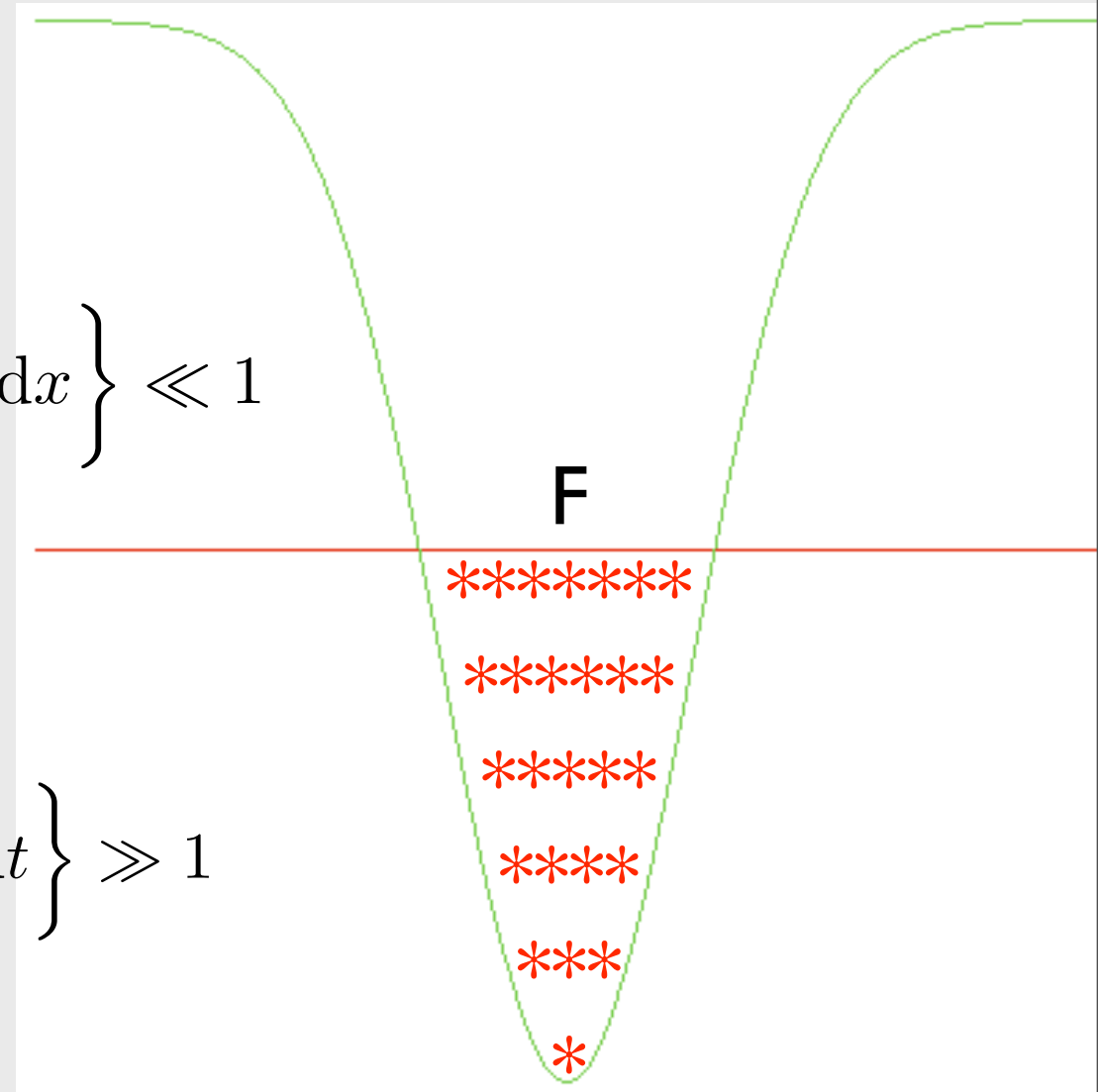




# Compare JWKB:

$$T \approx \exp \left\{ -2 \int_{\text{forbidden}} |k(x)| dx \right\} \ll 1$$

$$N \approx \exp \left\{ +2 \int_{\text{forbidden}} |\omega(t)| dt \right\} \gg 1$$





More general  
bound:  
(spatial)

Need  $\varphi'(x)^2 > 0$ .

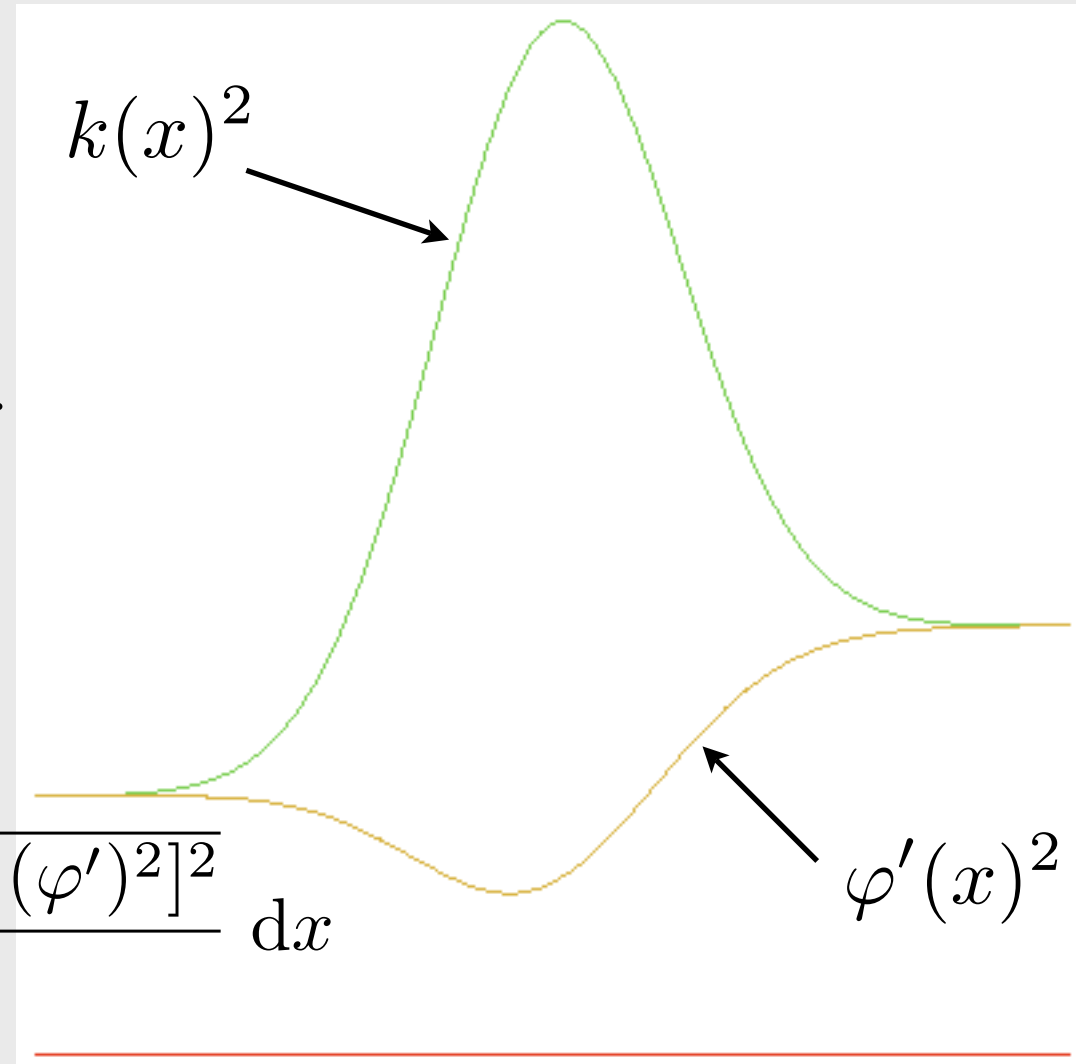
Permit  $k_{-\infty} \neq k_{+\infty}$ .

$\varphi'(x)$  essentially arbitrary.

$$T = |t|^2 = \text{sech}^2 Q$$

**Theorem:**

$$Q \leq \oint \frac{\sqrt{(\varphi'')^2 + [k^2 - (\varphi')^2]^2}}{2|\varphi'|} dx$$



Generalizes previous bound.



More general  
bound:  
(temporal)

Need  $\dot{\varphi}(t)^2 > 0$ .

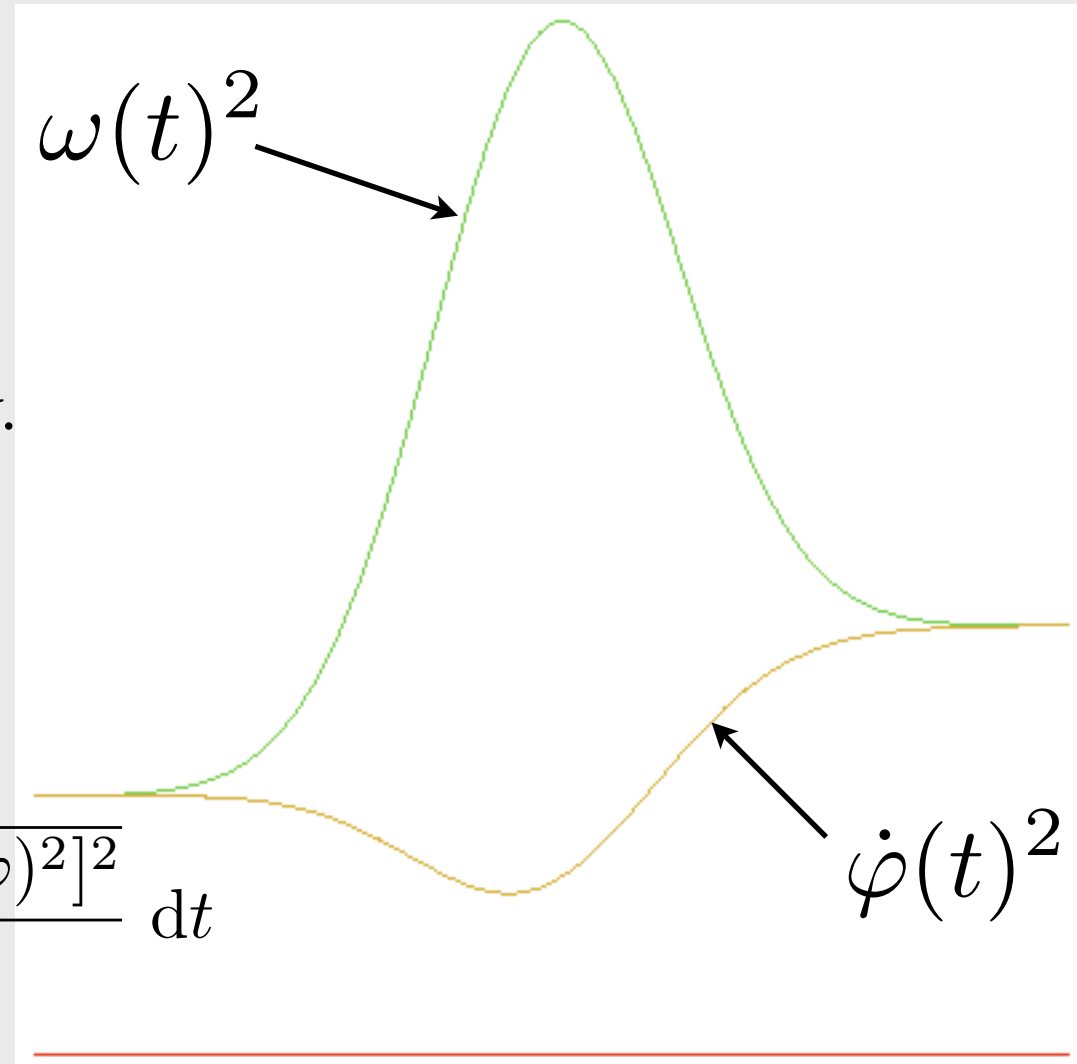
Permit  $\omega_{-\infty} \neq \omega_{+\infty}$ .

$\dot{\varphi}(t)$  essentially arbitrary.

$$N = |\beta|^2 = \sinh^2 Q$$

**Theorem:**

$$Q \leq \oint \frac{\sqrt{(\ddot{\varphi})^2 + [\omega^2 - (\dot{\varphi})^2]^2}}{2|\dot{\varphi}|} dt$$



Generalizes previous bound.



Reprise:

$$T \geq \operatorname{sech}^2 \left\{ \oint \frac{\sqrt{(\varphi'')^2 + [k^2 - (\varphi')^2]^2}}{2|\varphi'|} dx \right\}$$

$$R \leq \tanh^2 \left\{ \oint \frac{\sqrt{(\varphi'')^2 + [k^2 - (\varphi')^2]^2}}{2|\varphi'|} dx \right\}$$

$$N \leq \sinh^2 \left\{ \oint \frac{\sqrt{(\ddot{\varphi})^2 + [\omega^2 - (\dot{\varphi})^2]^2}}{2|\dot{\varphi}|} dt \right\}$$



Special case of  
this more  
general bound:



$$\varphi'(x) = k(x) \quad \dot{\varphi}(t) = \omega(t)$$

(Thus no “classically forbidden” region allowed.)

$$Q \leq \frac{1}{2} \oint \frac{|k'|}{|k|} dx \quad Q \leq \frac{1}{2} \oint \frac{|\dot{\omega}|}{|\omega|} dt$$

$$T \geq \text{sech}^2 \left\{ \frac{1}{2} \oint \frac{|k'|}{|k|} dx \right\} \quad N \leq \sinh^2 \left\{ \frac{1}{2} \oint \frac{|\dot{\omega}|}{|\omega|} dt \right\}$$



## Application:

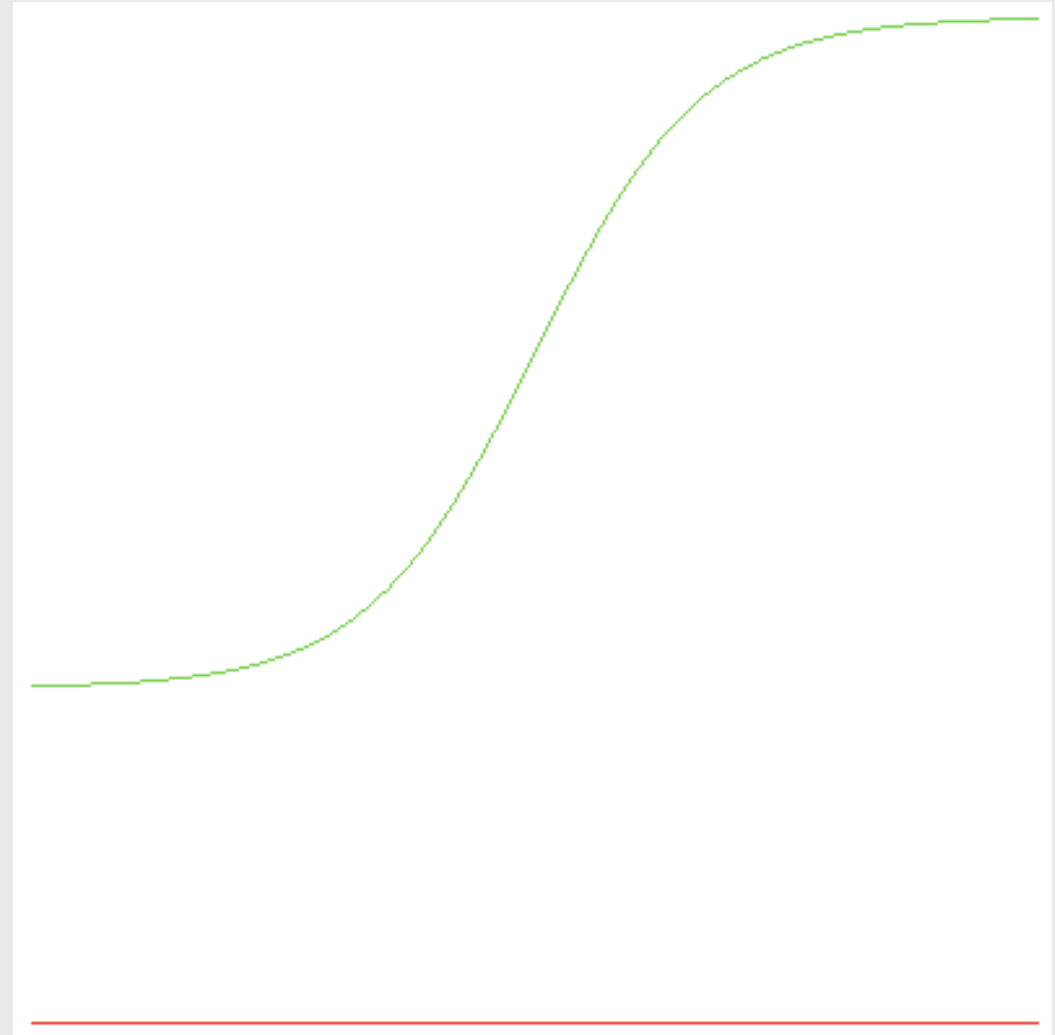
$$T \geq \operatorname{sech}^2 \left\{ \frac{1}{2} \ln \left[ \frac{k_{+\infty}}{k_{-\infty}} \right] \right\}$$

$$N \leq \sinh^2 \left\{ \frac{1}{2} \ln \left[ \frac{\omega_{+\infty}}{\omega_{-\infty}} \right] \right\}$$

Rewrite as:

$$T \geq \left( \frac{2}{\sqrt{k_{+\infty}/k_{-\infty}} + \sqrt{k_{-\infty}/k_{+\infty}}} \right)^2$$

$$N \leq \left( \frac{\sqrt{\omega_{+\infty}/\omega_{-\infty}} - \sqrt{\omega_{-\infty}/\omega_{+\infty}}}{2} \right)^2$$





## Application:

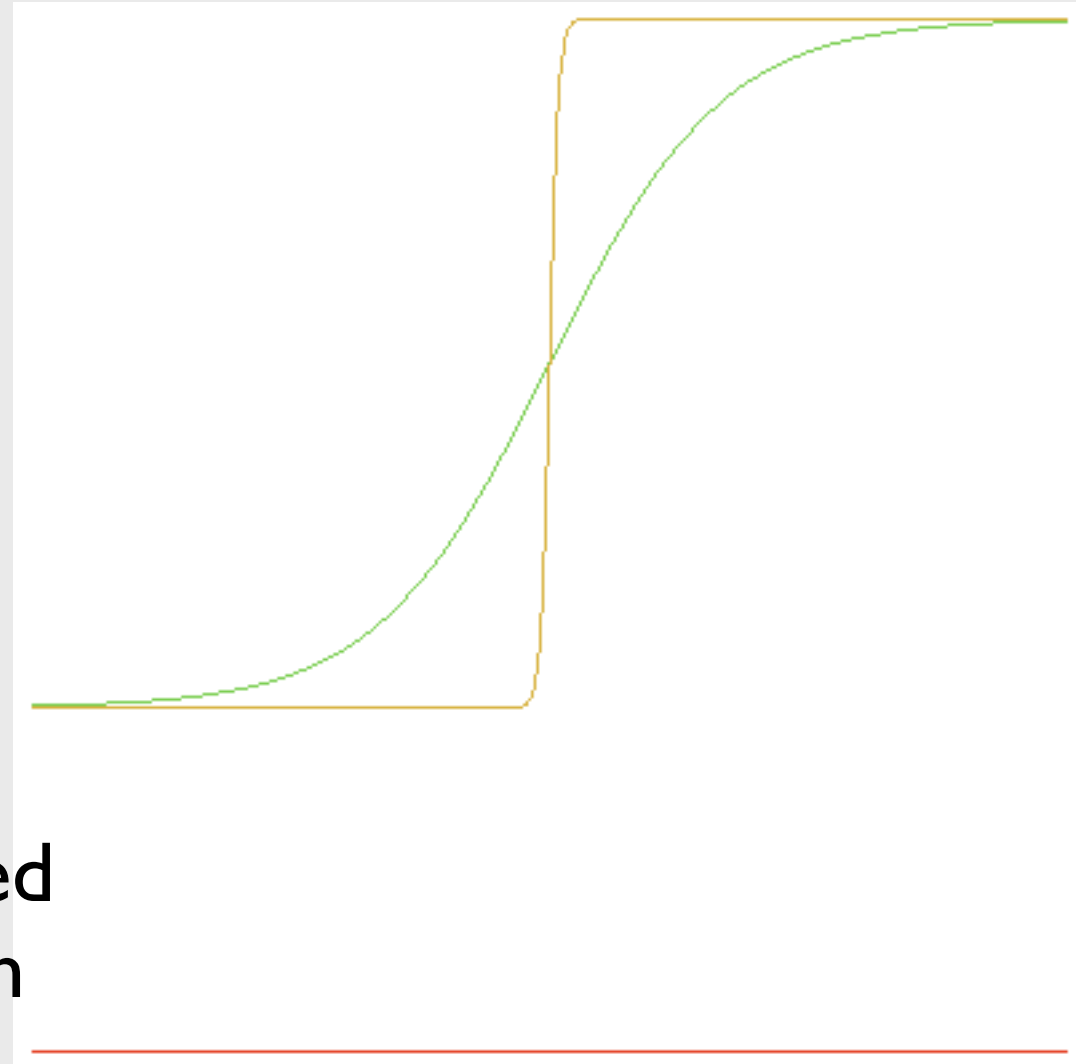
Rewrite as:

$$T \geq \frac{4k_{+\infty}k_{-\infty}}{(k_{+\infty} + k_{-\infty})^2}$$

$$N \leq \frac{(\omega_{+\infty} - \omega_{-\infty})^2}{4\omega_{+\infty}\omega_{-\infty}}$$

These bounds are saturated  
by a “sudden” step...

Sharp corners are guaranteed  
to be the best for reflection  
and particle production...





## Discussion:

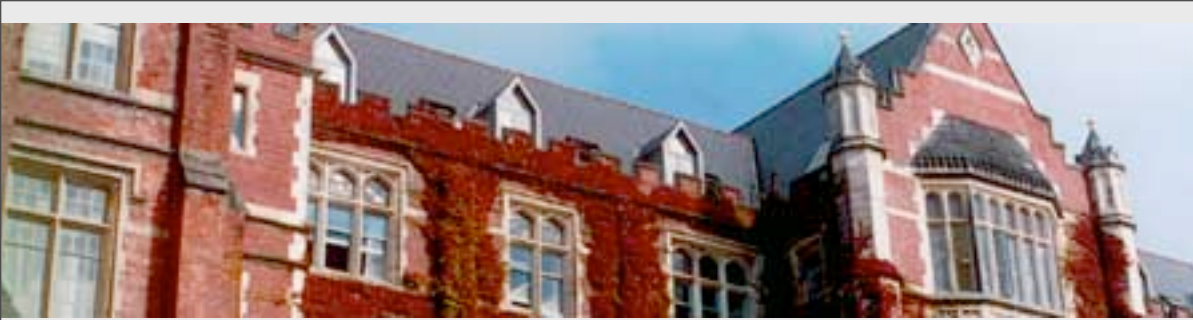
These are some very unexpected results...

How on earth did I (discover/ derive/ prove) these bounds?

Ultimately it was a side-effect of trying to understand  
the Birrell and Davies discussion of the  
adiabatic vacuum and  
cosmological particle production...

(Though the connection is somewhat tenuous.)

(And I'm still not sure I fully understand Birrell and Davies;  
there's got to be more you can say...)



## Strategy:

Pick a convenient basis:

$$\frac{\exp(+i\varphi)}{\sqrt{\varphi'}} \quad \frac{\exp(-i\varphi)}{\sqrt{\varphi'}}.$$

Define position-dependent Bogoliubov coefficients:

$$\psi(x) = a(x) \frac{\exp(+i\varphi)}{\sqrt{\varphi'}} + b(x) \frac{\exp(-i\varphi)}{\sqrt{\varphi'}}.$$

Restrict with an “auxiliary condition”:

$$\frac{d}{dx} \left( \frac{a}{\sqrt{\varphi'}} \right) e^{+i\varphi} + \frac{d}{dx} \left( \frac{b}{\sqrt{\varphi'}} \right) e^{-i\varphi} = 0.$$



The first derivative is simple...

$$\frac{d\psi}{dx} = i\sqrt{\varphi'} \{a(x) \exp(+i\varphi) - b(x) \exp(-i\varphi)\}.$$

As long as  $\varphi(x)$  is real (some generalizations possible):

$$\mathcal{J} = \text{Im} \left\{ \psi^* \frac{d\psi}{dx} \right\} = \{|a|^2 - |b|^2\}.$$

So then:

$$|a|^2 - |b|^2 = 1.$$



## Strategy:

Rewrite the  
Schrodinger  
equation  
in terms of  
 $a(x)$  and  $b(x)$ ...

$$\begin{aligned}\frac{d^2\psi}{dx^2} &= \frac{d}{dx} \left( i \frac{\varphi'}{\sqrt{\varphi'}} \{ae^{+i\varphi} - be^{-i\varphi}\} \right) \\ &= \frac{(i\varphi')^2}{\sqrt{\varphi'}} \{ae^{+i\varphi} + be^{-i\varphi}\} \\ &\quad + i\varphi' \left\{ \frac{d}{dx} \left( \frac{a}{\sqrt{\varphi'}} \right) e^{+i\varphi} - \frac{d}{dx} \left( \frac{b}{\sqrt{\varphi'}} \right) e^{-i\varphi} \right\} \\ &\quad + i \frac{\varphi''}{\sqrt{\varphi'}} \{ae^{+i\varphi} - be^{-i\varphi}\}\end{aligned}$$

Two distinct  
forms...

$$= -\frac{\varphi'^2}{\sqrt{\varphi'}} \{ae^{+i\varphi} + be^{-i\varphi}\} \quad ***$$

$$+ \frac{2i\varphi'}{\sqrt{\varphi'}} \frac{da}{dx} e^{+i\varphi} - i \frac{\varphi''}{\sqrt{\varphi'}} be^{-i\varphi}$$

$$= -\frac{\varphi'^2}{\sqrt{\varphi'}} \{ae^{+i\varphi} + be^{-i\varphi}\} \quad ***$$

$$- \frac{2i\varphi'}{\sqrt{\varphi'}} \frac{db}{dx} e^{-i\varphi} + i \frac{\varphi''}{\sqrt{\varphi'}} ae^{+i\varphi}.$$

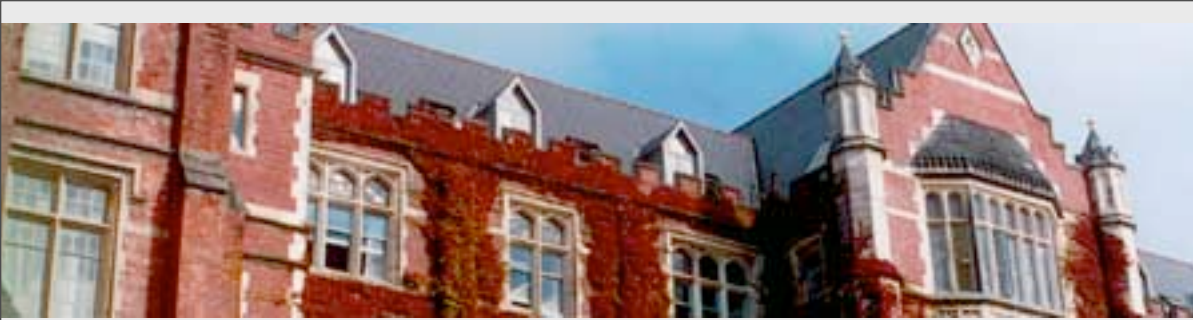


Strategy:

The Schrodinger equation is equivalent to:

$$\frac{da}{dx} = +\frac{1}{2\varphi'} \left\{ \varphi'' b \exp(-2i\varphi) + i [k^2(x) - (\varphi')^2] (a + b \exp(-2i\varphi)) \right\},$$

$$\frac{db}{dx} = +\frac{1}{2\varphi'} \left\{ \varphi'' a \exp(+2i\varphi) - i [k^2(x) - (\varphi')^2] (b + a \exp(+2i\varphi)) \right\}.$$



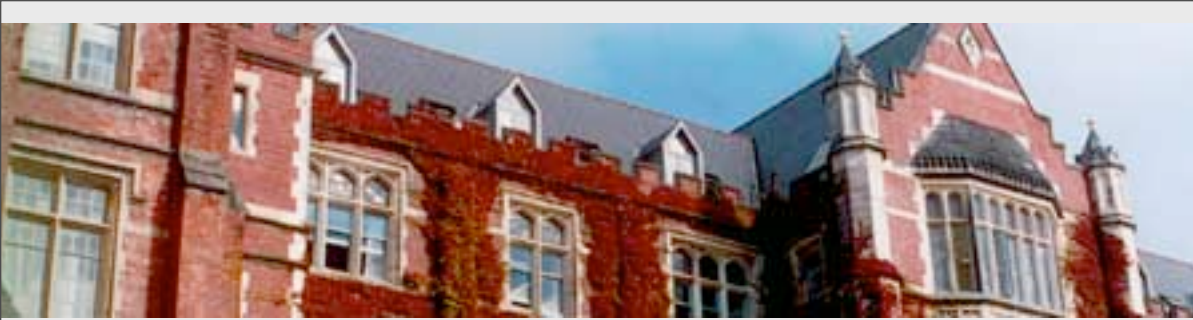
Strategy:

Calculate:

$$\frac{d|a|}{dx} = \frac{1}{2|a|} \left( a^* \frac{da}{dx} + a \frac{da^*}{dx} \right)$$

Obtain:

$$\begin{aligned} \frac{d|a|}{dx} = & \frac{1}{2|a|} \frac{1}{2\varphi'} \left( \varphi'' [a^* b \exp(-2i\varphi) + ab^* \exp(+2i\varphi)] \right. \\ & \left. + i[k^2 - (\varphi')^2] [a^* b \exp(-2i\varphi) - ab^* \exp(+2i\varphi)] \right) \end{aligned}$$



**Strategy:**

**Implying:**

$$\frac{d|a|}{dx} = \frac{1}{|a|} \frac{1}{2\varphi'} \operatorname{Re} \left( \begin{bmatrix} \varphi'' + i[k^2 - (\varphi')^2] & [a^* b \exp(-2i\varphi)] \end{bmatrix} \right).$$

**Use:**  $\operatorname{Re}(X) \leq |X|$

**Then:** 
$$\frac{d|a|}{dx} \leq \frac{|\varphi'' + i[k^2 - (\varphi')^2]|}{2|\varphi'|} |b|$$

$$\frac{d|a|}{dx} \leq \frac{\sqrt{(\varphi'')^2 + [k^2 - (\varphi')^2]^2}}{2|\varphi'|} |b|.$$



**Integrate:**

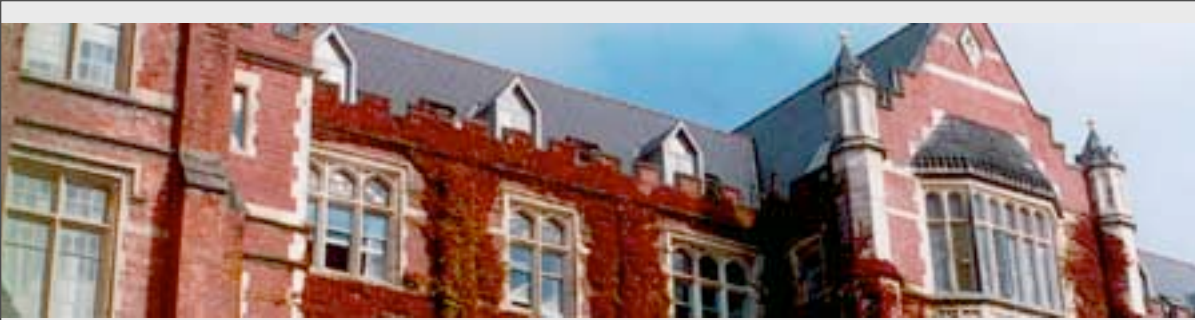
$$\vartheta[\varphi(x), k(x)] \equiv \frac{\sqrt{(\varphi'')^2 + [k^2(x) - (\varphi')^2]^2}}{2|\varphi'|},$$

**(definition)**

$$\frac{d|a|}{dx} \leq \vartheta \sqrt{|a|^2 - 1}.$$

$$\left\{ \cosh^{-1} |a| \right\} \Big|_{x_i}^{x_f} \leq \int_{x_i}^{x_f} \vartheta \, dx.$$

$$\cosh^{-1} |\alpha| \leq \int_{-\infty}^{+\infty} \vartheta \, dx.$$



Conclude:

$$|\alpha| \leq \cosh \left( \int_{-\infty}^{+\infty} \vartheta \, dx \right) .$$

$$|\beta| \leq \sinh \left( \int_{-\infty}^{+\infty} \vartheta \, dx \right) .$$

$$T \geq \operatorname{sech}^2 \left( \int_{-\infty}^{+\infty} \vartheta \, dx \right) ,$$

$$R \leq \tanh^2 \left( \int_{-\infty}^{+\infty} \vartheta \, dx \right) .$$

This is **one** proof,  
(quant-ph/9901030).

Distinct proof in  
arXiv:0801.0610  
[quant-ph]

I am certain that  
significant  
generalizations  
are still possible...

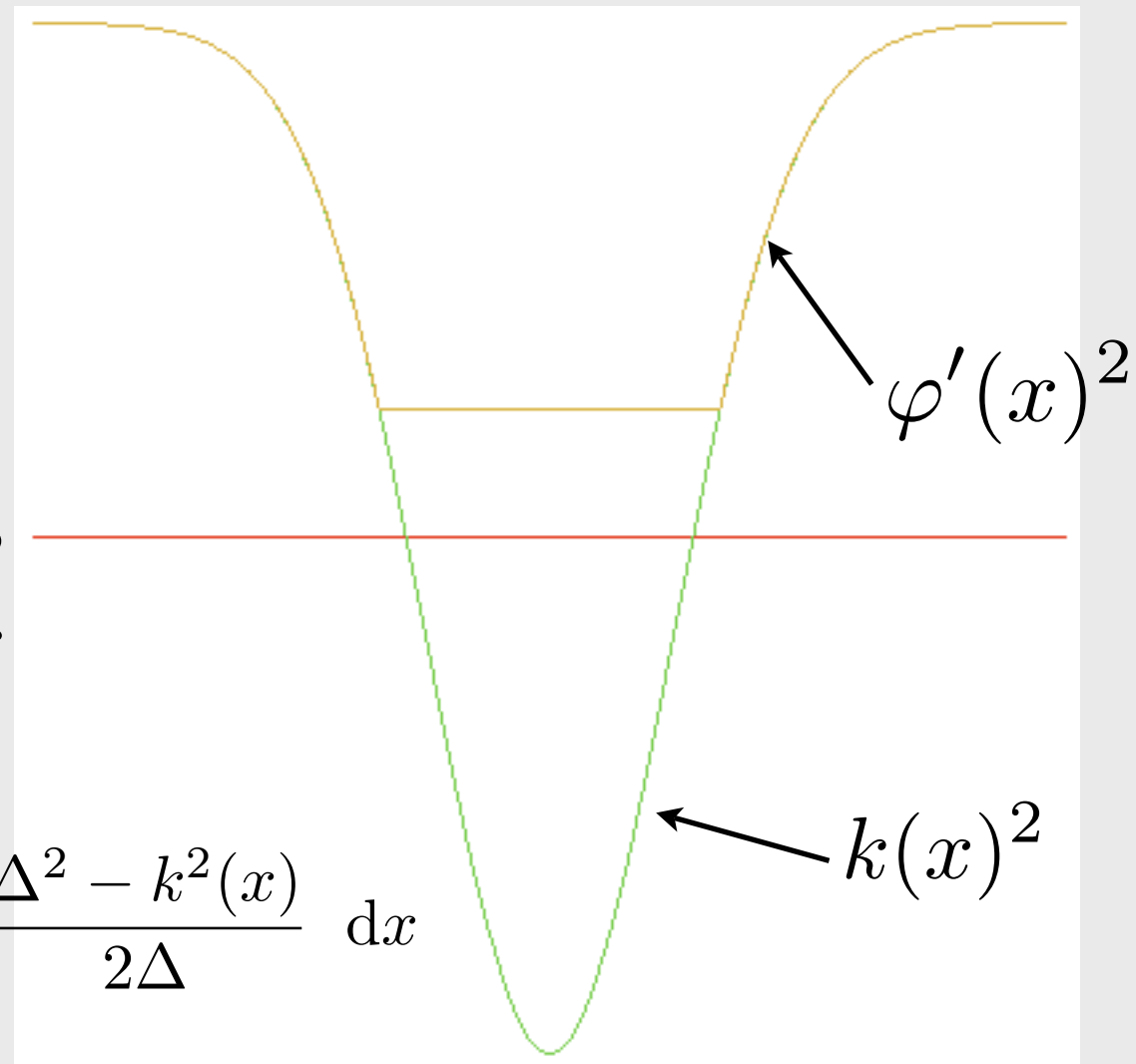


Another  
application:

$$\forall \Delta > 0$$

Let  $\phi'(x)$  track  $k(x)$  until  
one gets close to the  
classically forbidden region,  
then hold  $\phi'(x)$  constant...

$$Q \leq \frac{1}{2} \ln \left[ \frac{k_{+\infty} k_{-\infty}}{\Delta^2} \right] + \int_{\Delta^2 - k^2 > 0} \frac{\Delta^2 - k^2(x)}{2\Delta} dx$$



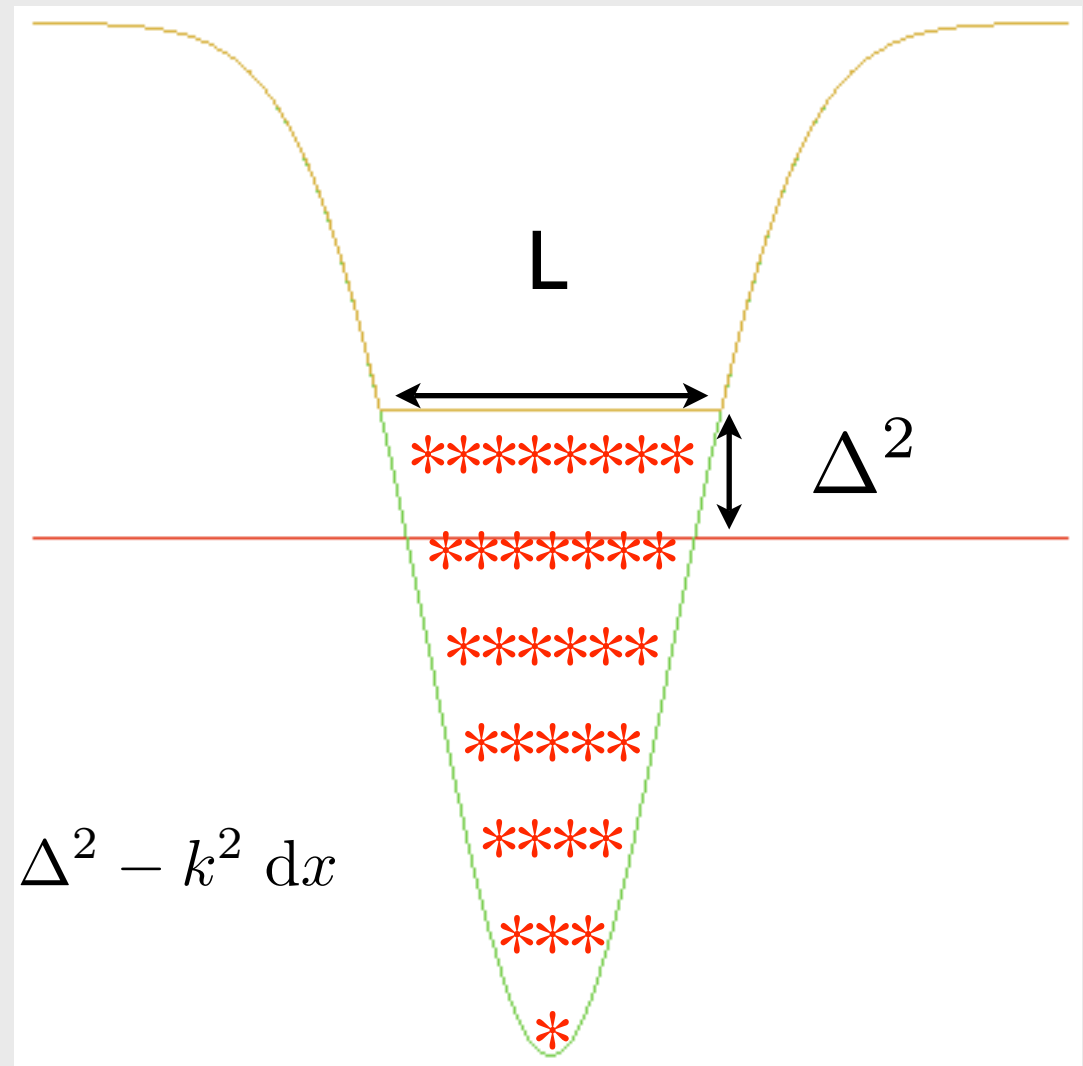


Extremize to find the “best” value for Delta...

$$L_{\Delta} = \int_{\Delta^2 - k^2 > 0} 1 \, dx$$

Horrible nonlinear  
equation for Delta...

$$\Delta L_{\Delta} + (\Delta L_{\Delta})^2 = L_{\Delta} \int_{\Delta^2 - k^2 > 0} \Delta^2 - k^2 \, dx$$





Another  
application:

$$\Delta = \frac{\int_{\Delta^2 - k^2 > 0} \Delta^2 - k^2 \, dx}{1 + \Delta L_\Delta}$$

$$\Delta \leq \int_{k^2 < 0} |k^2(x)| \, dx$$

$$\Delta \geq \int_{k^2 < 0} |k^2(x)| \, dx - \Delta^2(L_\Delta - L_0)$$



Another  
application:

For shallow wells:

$$L_{\Delta} \int_{\Delta^2 - k^2 > 0} \Delta^2 - k^2 \, dx \ll 1$$

We can then approximate:

$$\Delta \lesssim \int_{k^2 < 0} |k^2(x)| \, dx$$

[Remember: bound holds for *\*all\** Delta.]



Another  
application:

So we certainly can certainly assert:

Choose: 
$$\Delta = \int_{k^2 < 0} |k^2(x)| \, dx$$

Deduce:

$$Q \leq \frac{1}{2} \ln \left[ \frac{k_{+\infty} k_{-\infty}}{\Delta^2} \right] + \int_{\Delta^2 - k^2 > 0} \frac{\Delta^2 - k^2(x)}{2\Delta} \, dx$$

But this bound might not be “optimal”.  
(And finding a general “optimal” bound is  
exceedingly difficult.)



## Comparison with JWKB:

If there is no forbidden region then:

$$T_{\text{JWKB}} = 1$$

But for (almost all) potentials without a forbidden region there will still be *\*some\** scattering, so:

$$T_{\text{exact}} < 1$$

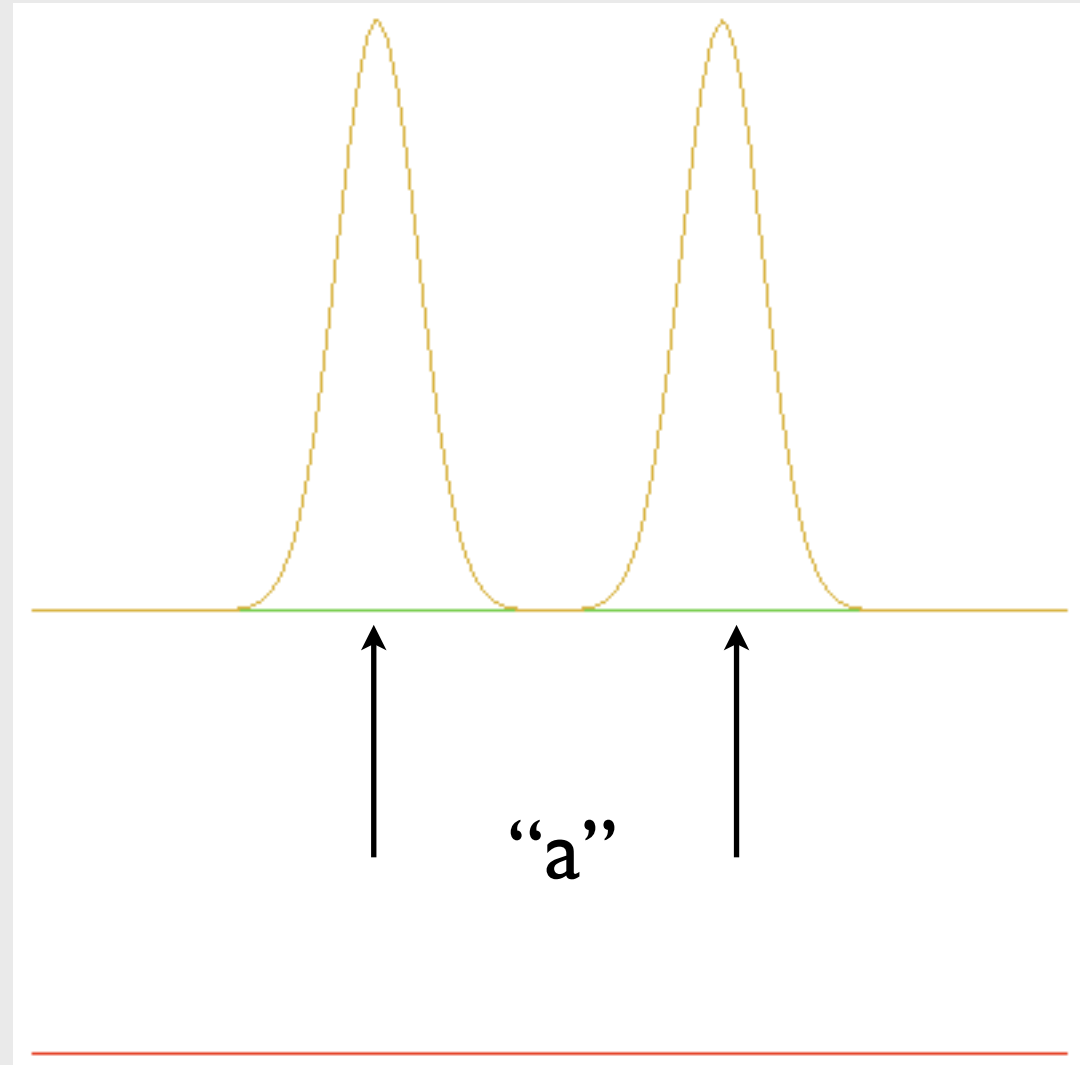
So there definitely are situations where JWKB *\*over-estimates\** the transmission probability.



## Comparison with JWKB:

There are also situations  
where JWKB definitely  
**\*under-estimates\*** the  
transmission probability.

Consider a “repeated”  
potential, with the two  
repeats separated by  
distance “a”.





## Resonant tunnelling:

For such a “repeated” potential, one can encounter “resonant tunnelling”.

It is an “easy” exercise to see that:

$$T_2(a) = \frac{T_1^2}{1 + 2R_1 \cos[2k_\infty a - \phi(t)] + R_1^2}$$

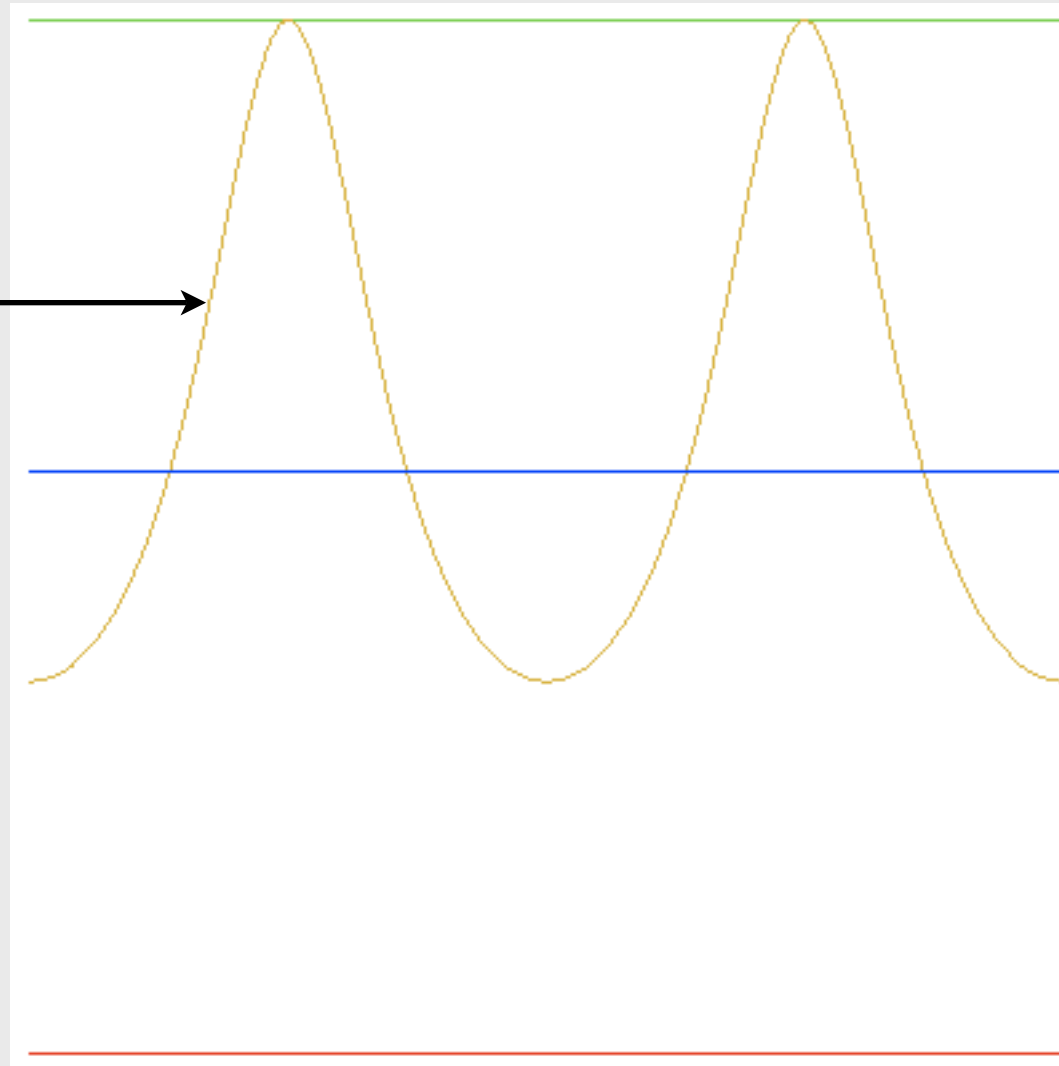
Thus, as the separation “a” is adjusted the exact transmission probability oscillates between:

$$T_2(a) \in \left[ \frac{T_1^2}{(1 + R_1)^2}, 1 \right]$$



# Resonant tunnelling:

$T_2(a)$



1

$T_1^2$

0



## Resonant tunnelling:

Proof: Describe the effect of each individual potential by a “transfer matrix” [ Jones matrix ]:

$$\begin{bmatrix} \alpha_1 & \beta_1 \\ \beta_1^* & \alpha_1^* \end{bmatrix} \quad \begin{bmatrix} \alpha_1 & \beta_1 e^{2ika} \\ \beta_1^* e^{-2ika} & \alpha_1^* \end{bmatrix}$$

As long as the 2 potentials do not overlap:

$$\begin{bmatrix} \alpha_2(a) & \beta_2(a) \\ \beta_2^*(a) & \alpha_2^*(a) \end{bmatrix} = \begin{bmatrix} \alpha_1 & \beta_1 \\ \beta_1^* & \alpha_1^* \end{bmatrix} \begin{bmatrix} \alpha_1 & \beta_1 e^{2ika} \\ \beta_1^* e^{-2ika} & \alpha_1^* \end{bmatrix}$$



## Resonant tunnelling:

Matrix multiply:

$$\alpha_2(a) = \alpha_1^2 + |\beta_1|^2 e^{2ika}$$

Evaluate:

$$T_2(a) = \frac{1}{|\alpha_2(a)|^2} = \frac{1}{\left| |\alpha_1^2| e^{2i\phi_\alpha} + |\beta_1|^2 e^{2ika} \right|^2}$$

$$T_2(a) = \frac{T_1^2}{1 + 2R_1 \cos[2k_\infty a - \phi(t)] + R_1^2}$$



## Comparison with JWKB:



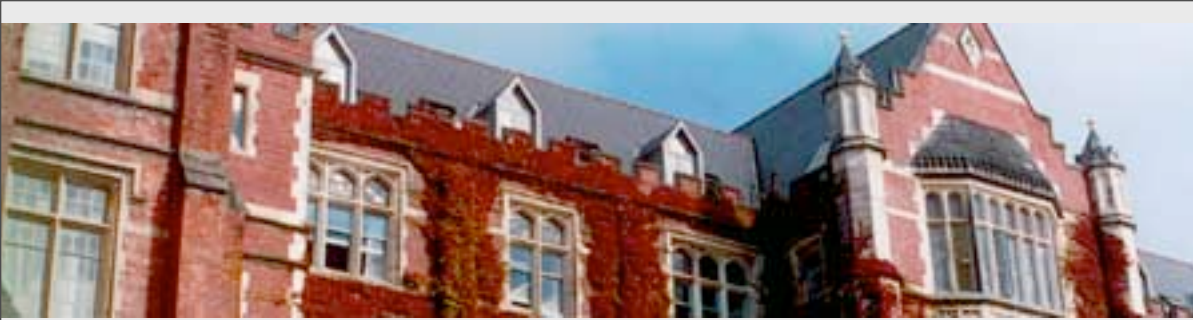
But for all potentials with a forbidden region:

$$T_{1,\text{JWKB}} < 1 \quad T_{2,\text{JWKB}} = T_{1,\text{JWKB}}^2 < 1$$

But we have just seen that there are some choices  
of the separation “a” for which

$$T_{2,\text{exact}} = 1$$

That is, there are some potentials for which the  
JWKB estimate is an **\*under-estimate\*** of the  
true transmission probability.



This is what I mean by an “uncontrolled approximation”.

JWKB is sometimes high, sometimes low, and there is no (known) a-priori estimate of just how good/ bad JWKB might be in a specific situation.

Given this, the “a priori” bounds I discussed earlier seem (at present) to be the best one can do.

Is there room for improvement?



Reprise:

$$T \geq \operatorname{sech}^2 \left\{ \oint \frac{\sqrt{(\varphi'')^2 + [k^2 - (\varphi')^2]^2}}{2|\varphi'|} dx \right\}$$

$$R \leq \tanh^2 \left\{ \oint \frac{\sqrt{(\varphi'')^2 + [k^2 - (\varphi')^2]^2}}{2|\varphi'|} dx \right\}$$

$$N \leq \sinh^2 \left\{ \oint \frac{\sqrt{(\ddot{\varphi})^2 + [\omega^2 - (\dot{\varphi})^2]^2}}{2|\dot{\varphi}|} dt \right\}$$



- Probably there are “optimal” bounds still waiting to be discovered...
- Definitely there are “more general” bounds in the process of being discovered...
- Just because it’s quantum mechanics, it does not mean that everything has already been done...
- Watch this space....