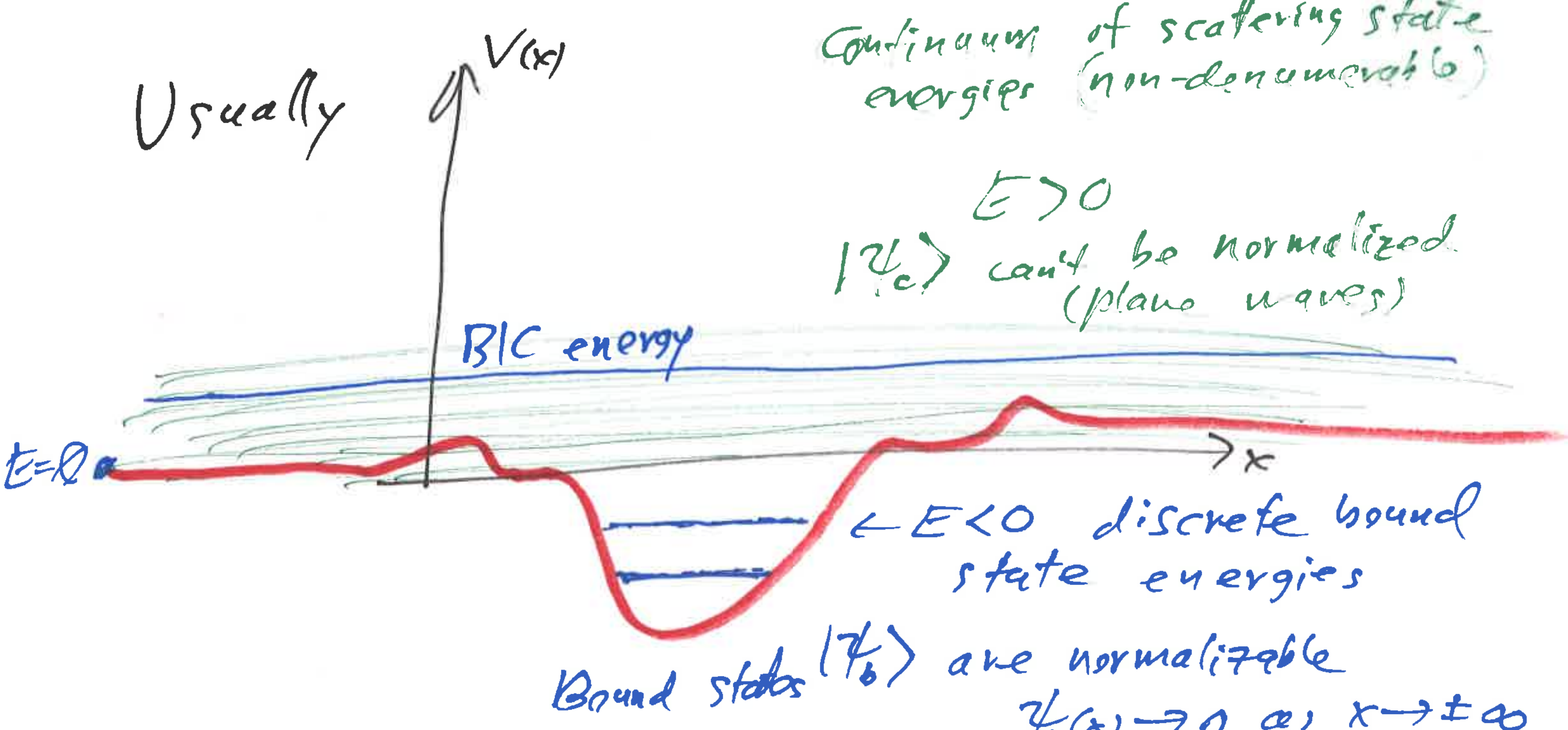
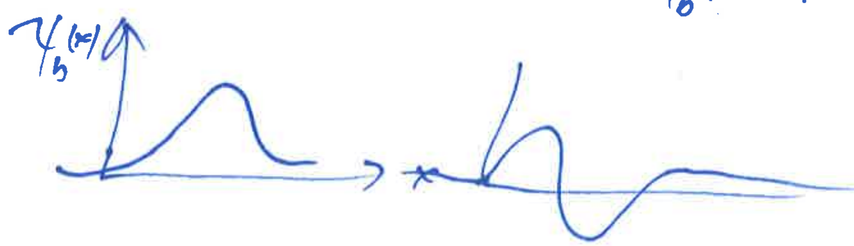
Bound State in the Continuum (BIC)

1929 John von Neumann + Eugene Wigner

Phys. Z 30, p 465–467

Usually





BIC has energy $E>0$ in the continuum but has the $\psi(r)$ of a bound state, spatially localized,

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"On Positive Eigenvalues of One-Body Schrödinger Operators" Barry Simon

DEFINE $g(r) \equiv 2r - \sin 2r$

$$V(r) = \frac{-32\sin(r)}{\left[1+g(r)^2\right]^2}\left[g(r)^3\cos(r) - 3g(r)^2\sin^3(r) + g(r)\cos(r) + \sin^3(r)\right]$$

$E = +1 > 0$ $\qquad\qquad \psi(r) = \dfrac{\sin(r)}{r\left[1+g(r)^2\right]}$

Expect only scattering states for $E>0$.

Asymptotic Values of $V(r) \to -\dfrac{8\sin(2r)}{r} \to 0$ for large r

Numerical Approximations to Solutions of the TISE

e.g. 1-dim Quantum Harmonic Oscillator

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

Problem: $[V(x)] = [E] = \frac{L^2 M}{T^2}$, $[x] = L$, $[m] = M$

$[\hbar] = \frac{L^2 M}{T}$, etc.

Computers deal with dimensionless quantities

$\Rightarrow$ non-dimensionalize

Define $u \equiv \frac{x}{l_0}$ where l_0 is a constant length

$[u] = 1$

$x = u l_0$, $dx = du\, l_0$, $\psi(u l_0) \equiv f(u) \neq \psi(u)$

TISE: $$-\frac{\hbar^2}{2m}\frac{1}{l_0^2}\frac{d^2 f(u)}{du^2} + \frac{m}{2}\omega^2 l_0^2 u^2 f(u) = E\, f(u)$$

$$f''(u) - \frac{m^2\omega^2 l_0^4}{\hbar^2} u^2 f(u) = -\frac{2m l_0^2 E}{\hbar^2} f(u)$$

Choose $l_0 = \left(\frac{\hbar}{m\omega}\right)^{1/2}$ or ($2x$ or $17x$ or $\sqrt{\pi}\,x$)

$$f''(u) - u^2 f(u) = -\frac{E}{\left(\frac{1}{2}\hbar\omega\right)} f(u)$$

Define $\epsilon = \frac{E}{\frac{1}{2}\hbar\omega}$

$E = \epsilon\left(\frac{1}{2}\hbar\omega\right)$

$$f''(u) - (u^2 - \epsilon) f(u) = 0 \qquad \text{everything dimensionless}$$

Now we need a numerical integration method.

For pedagogy: (Forward) Euler method, aka 1st order Runge-Kutta RK1

error $\propto h^2$ ← h is stepsize (not Planck constant)

Second-order Runge-Kutta (RK2): error $\propto h^3$

Fourth-order Runge-Kutta (RK4): error $\propto h^5$

Why not continue? RK8, RK16?

Diminishing returns: more operations per step.

Forward Euler is unstable. ⇒ Backward Euler

(use right side of the interval instead of left)

Express of 2nd-order D.E. as a pair of coupled 1st-order equations

$$y_1(u) \equiv f(u)$$

$$y_1'(u) = f'(u) \equiv y_2(u)$$

$$y_2(u) = y_1'(u)$$

$$y_2(u) = f'(u)$$

$$y_2'(u) = f''(u) = (u^2 - \epsilon) f(u)$$

$$= (u^2 - \epsilon) y_1(u)$$

Taylor Expansion: Expand $g(x)$ around $x=k$

x dependence

$$g(x) = \frac{1}{0!} g(x)\Big|_{x=k} + \frac{1}{1!}\frac{dg}{dx}\Big|_{x=k}(x-k) + \frac{1}{2!}\frac{d^2g}{dx^2}\Big|_{x=k}(x-k)^2 + \cdots$$

Incremental form

x-dependence

$$g(x+h) = \frac{1}{0!}g(x) + \frac{1}{1!}h\frac{dg(x)}{dx} + \frac{1}{2!}h^2\frac{d^2g(x)}{dx^2}$$

$$f(u+h) = f(u) + h\frac{df}{du} + \cdots$$

$$f'(u+h) = f'(u) + h\frac{d^2f}{du^2} + \cdots$$

$$y_1(u+h) = y_1(u) + h\,y_2(u)$$

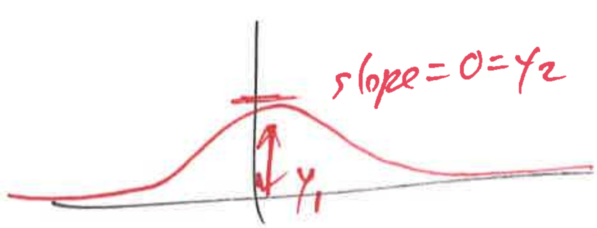
$$y_2(u+h) = y_2(u) + h(u^2-\epsilon)\,y_1(u)$$

"Intial" Conditions = Boundary Conditions

even states

$y_1(0) = 1$ (say)

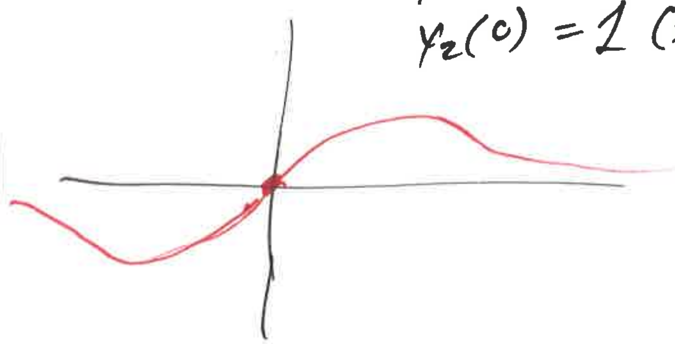
$y_2(0) = 0$



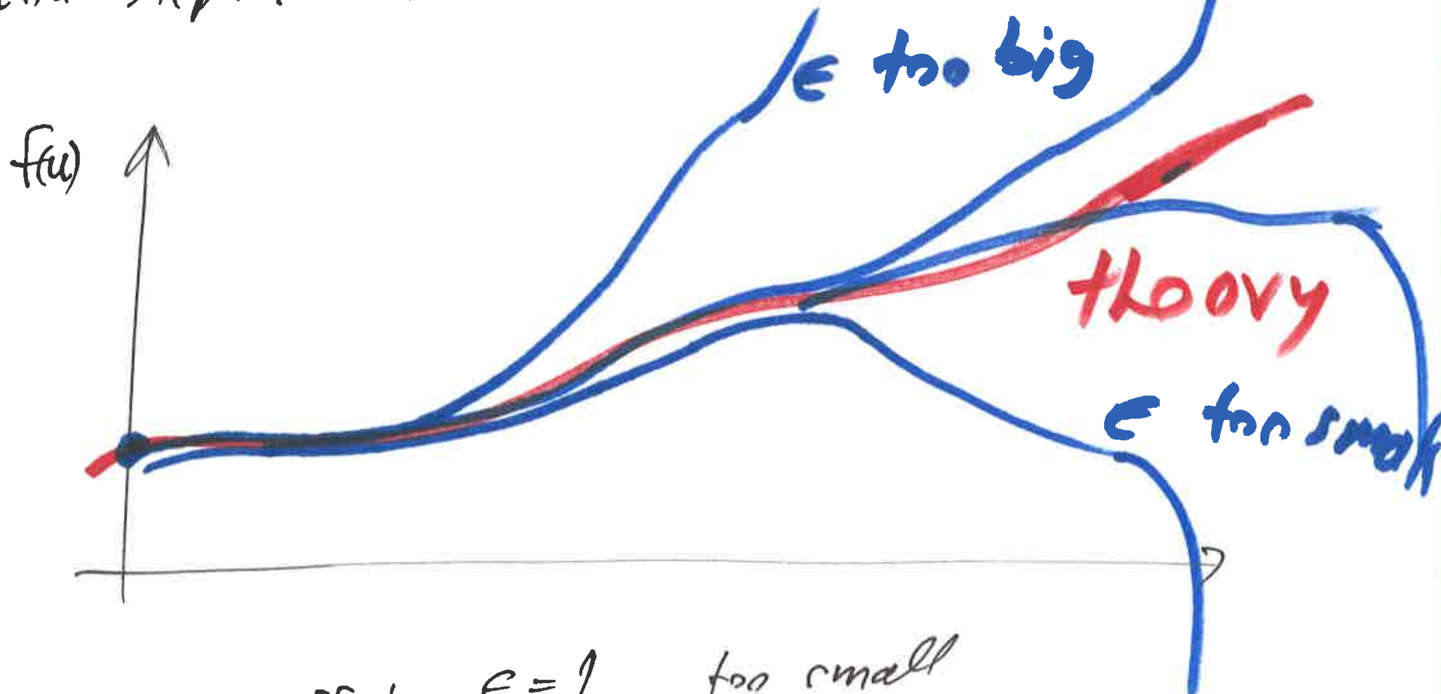
odd states

$y_1(0) = 0$

$y_2(0) = 1$ (say)



If we want f(u) between $u=0$ and $u=10$ with step size $h=0.01$, then need 1,000 steps



guess: $\epsilon = 1$ too small
$\epsilon = 2$ too big
$\epsilon = 1.005$ too big
$\epsilon = 1.004$ too small
$\epsilon = 1.0045$ too small
$\epsilon = 1.0046$ too big

can program the computer to do this.