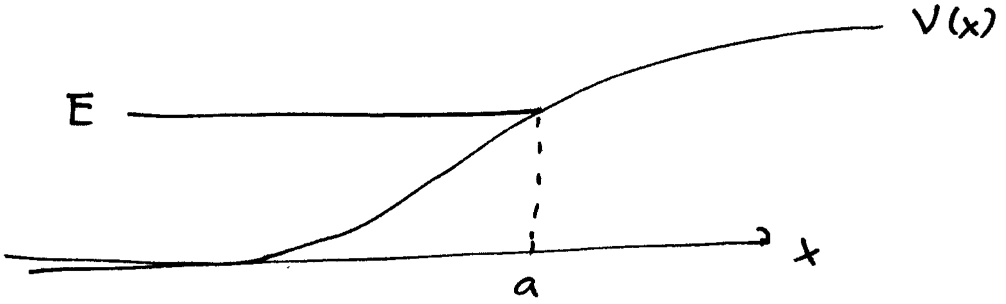
The connection formulas at a classical turning point

The Classical Turning Point:



Change dependent and independent variables

$$v(x) = \sqrt{k(x)}\ \psi(x) \quad \text{and} \quad y = \int^{x} k(x)\,dx$$

$$\frac{d}{dx} = \frac{dy}{dx}\frac{d}{dy} = k(x)\frac{d}{dy}$$

$$\frac{d^2}{dx^2} = \frac{d^2y}{dx^2}\frac{d}{dy} + \left(\frac{dy}{dx}\right)^2\frac{d^2}{dy^2} = k'(x)\frac{d}{dy} + k^2(x)\frac{d^2}{dy^2} = k^2\frac{d^2}{dy^2} + k\frac{dk}{dy}\frac{d}{dy}$$

So the time-independent Schrödinger Eq. becomes

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

$$\frac{d^2\psi}{dx^2} + k^2(x)\,\psi(x) = 0 \Rightarrow \cancel{\frac{d^2\psi}{dy^2}}$$

$$\frac{d^2}{dx^2}\left[k^{-1/2}(x)\,v(x)\right] + k^{3/2}v(x) = 0$$

$$\left(k^2(y)\frac{d^2}{dy^2} + k\frac{dk}{dy}\frac{d}{dy}\right)\left(\frac{1}{k^{1/2}(y)}v(y)\right) + k^{3/2}(y)v(y) = 0 \qquad k^{-3/2}\frac{d^2v}{dy^2}$$

$$\cancel{k^2\left\{v(y)\frac{-1/2(-3/2)}{k^{5/2}} + 2\frac{dv}{dy}k^{-3/2}(-1/2)\frac{dk}{dy} + k\frac{dk}{dy}(-1/2)k^{-3/2}v(y) + k\frac{dk}{dy}\frac{1}{k^{1/2}}\frac{dv}{dy}\right\} + k^{3/2}(y)\,v(y) = 0}$$

$$\left(k^2\frac{d^2}{dy^2} + k\frac{dk}{dy}\frac{d}{dy}\right)\left(\frac{1}{k^{1/2}}v(y)\right) + k^{3/2}v(y) = 0$$

$$\frac{d^2}{dy^2}\frac{1}{k^{1/2}}v(y) = \frac{d}{dy}\left(-\frac{1}{2k^{3/2}}k'v + \frac{1}{k^{1/2}}v'\right) = +\frac{3}{4k^{5/2}}k'^2v + -\frac{1}{2k^{3/2}}k''v +$$

$$-\frac{1}{2k^{3/2}}k'v' - \frac{1}{2k^{3/2}}k'v' + \frac{1}{k^{1/2}}v'' = -\frac{3}{4k^{5/2}}k'^2v - \frac{1}{2k^{3/2}}k''v - \frac{k'}{k^{3/2}}v' + \frac{v''}{k^{1/2}}$$

$$kk'\frac{d}{dy}\left(k^{-1/2}v\right) = kk'^2\left(-\frac{1}{2}\right)k^{-3/2}v + k^{1/2}k'v'$$

$\Longrightarrow$

$$k^2\left(\frac{v''}{k^{1/2}} - \frac{k'}{k^{3/2}}v' - \frac{1}{2k^{3/2}}k''v + \frac{3}{4k^{5/2}}k'^2v\right) + k^{1/2}k'v' - \frac{k'^2}{2k^{1/2}}v + k^{3/2}v = 0$$

$$k^{3/2}v'' + k^{3/2}v \underbrace{- k'k^{1/2}v' + k^{1/2}k'v'}_{\text{cancel}} + \left(\frac{3}{4\cancel{k}} - \frac{1}{2}\right)\frac{k'^2}{k^{1/2}}v = 0$$

$$-\frac{k^{1/2}}{2}vk''$$

$$v'' + v\left[1 - \frac{1}{2k}k'' + \frac{1}{4k^2}k'^2\right] = 0$$

$$\Longrightarrow \boxed{\frac{d^2v}{dy^2} + v(y)\left[1 - \frac{1}{2k(y)}\frac{d^2k}{dy^2} + \frac{1}{4k^2(y)}\left(\frac{dk}{dy}\right)^2\right] = 0}$$

The WKB approximation means dropping the two terms that are proportional to k'^2 and k'' in favor of 1.

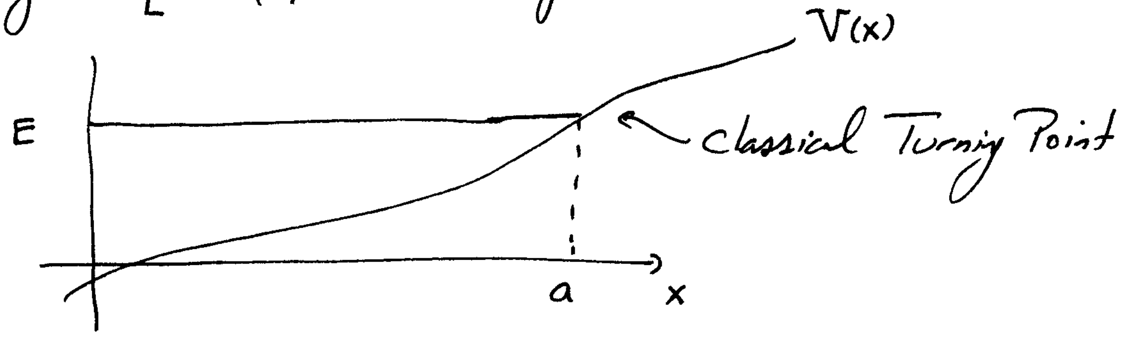
$\Longrightarrow$ $v \cong Ae^{iy} + Be^{-iy}$ for the classically allowed region

$v \cong Ce^{|y|} + De^{-|y|}$ in the classically forbidden region.

How do we link these solutions?

WKB Continued:

$$\frac{d^2 v}{dy^2} + \left[\frac{1}{4k^2}\left(\frac{dk}{dy}\right)^2 - \frac{1}{2k}\frac{d^2 k}{dy^2} + 1\right] v = 0$$



Far from the classical turning point $x < a$ we have

$$\frac{d^2 v}{dy^2} + v \cong 0 \Rightarrow v \cong e^{iy}A + Be^{-iy}$$

Far from the classical turning point: $x > a$ we have.

$$v \cong Ce^{|y|} + De^{-|y|}$$

How can we relate the coefficients $\begin{pmatrix} A \\ B \end{pmatrix}$ to $\begin{pmatrix} C \\ D \end{pmatrix}$?

Now we need to integrate the full S-equation!

Assumption: $V(x) \rightarrow E$ linearly: $V(x) - E = \alpha(x-a)$ near $x = a$. ($\alpha > 0$)

Then $k(x) = \sqrt{\frac{2m\alpha(a-x)}{\hbar^2}}$, $x < a$

$K(x) = i\sqrt{\frac{2m\alpha(x-a)}{\hbar^2}}$, $x > a$

Now put these into $y = \int_a^x k(x)dx$

↖ set lower limit to a. $y(a) = 0$

Y is a measure of the distance to the classical turning point.

$$\int \sqrt{a-x}\, dx \doteq \frac{2}{3}(a-x)^{3/2}(-1)$$

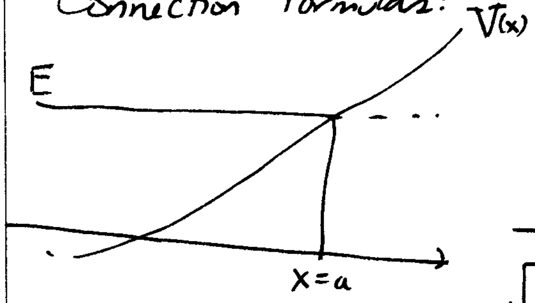
$$\int \sqrt{x-a}\, dx = \frac{2}{3}(x-a)^{3/2}(+1)$$

$$\Longrightarrow \quad y = \begin{cases} \frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(a-x)^{3/2} e^{i\pi}, & x < a \\ \frac{2}{3}\left(\frac{2m\alpha}{\hbar^2}\right)^{1/2}(x-a)^{3/2} e^{-i\pi/2}, & x > a \end{cases}$$

Write in terms of k and take the derivatives.

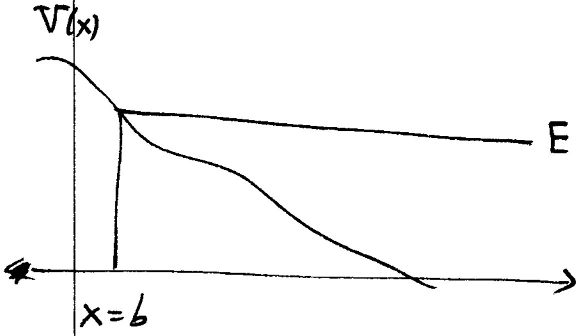
$$\Longrightarrow \quad \frac{d^2v}{dy^2} + \left(1 + \frac{5}{36y^2}\right)v = 0$$

Connection Formulas:



$$\frac{2}{\sqrt{k}}\cos\left(\int_x^a k\,dx - \frac{1}{4}\pi\right) \longleftrightarrow \frac{1}{\sqrt{K}} e^{-\int_a^x K\,dx}$$

$$\frac{1}{\sqrt{k}}\sin\left(\int_x^a k\,dx - \frac{1}{4}\pi\right) \longleftrightarrow -\frac{1}{\sqrt{K}} e^{\int_a^x K\,dx}$$



$$\frac{1}{\sqrt{K}} e^{-\int_x^b K\,dx} \longleftrightarrow \frac{2}{\sqrt{k}}\cos\left(\int_b^x k\,dx - \pi/4\right)$$

$$-\frac{1}{\sqrt{K}} e^{\int_x^b K\,dx} \longleftrightarrow \frac{1}{\sqrt{k}}\sin\left(\int_b^x k\,dx - \pi/4\right)$$

Best Explanation I think:

Quantum Mechanics 2nd Ed.
E. Merzbacher
Wiley + Sons (1970)

Application of WKB to Bound States.

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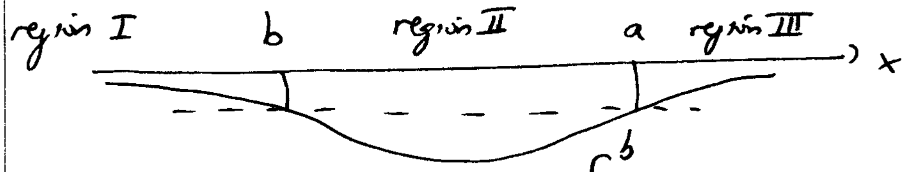


Region I: $\psi_1 \cong \frac{1}{\sqrt{K}} e^{-\int_x^b K\,dx}$ $\quad x < b$

Region II: $\psi_2 \cong \frac{2}{\sqrt{k}} \cos\left(\int_b^x k\,dx - \pi/4 \right)$ $\quad b < x < a$

Region III: $\psi_3 \cong \frac{1}{\sqrt{K}} e^{-\int_a^x K\,dx}$

Rewrite the wavefunction in region II:

$$\psi_2 \cong \frac{2}{\sqrt{k}} \cos\left(\int_b^a dx\,k - \int_x^a k\,dx - \pi/4 \right)$$

$$= \frac{2}{\sqrt{k}} \left\{ \cos\left(\int_b^a k\,dx\right) \cos\left(\int_x^a k\,dx + \pi/4\right) + \sin\left(\int_b^a k\,dx\right) \sin\left(\int_x^a k\,dx + \pi/4\right) \right\}$$

$$= \frac{2}{\sqrt{k}} \left\{ -\cos\left(\int_b^a k\,dx\right) \sin\left(\int_x^a k\,dx - \pi/4\right) + \sin\left(\int_b^a k\,dx\right) \cos\left(\int_x^a k\,dx - \pi/4\right) \right\}$$

Using $\cos(\alpha + \pi/4) =$
$\cos(\alpha - \pi/4 + \pi/2) =$
$= -\sin(\alpha - \pi/4)$

Using $\sin(\alpha + \pi/4)$
$= \sin(\alpha - \frac{\pi}{4} + \pi/2)$
$= \cos(\alpha - \pi/4)$

ⓓ

Looking at the connection formulas the first term connects to a growing exponential! We need that coefficient to be zero!

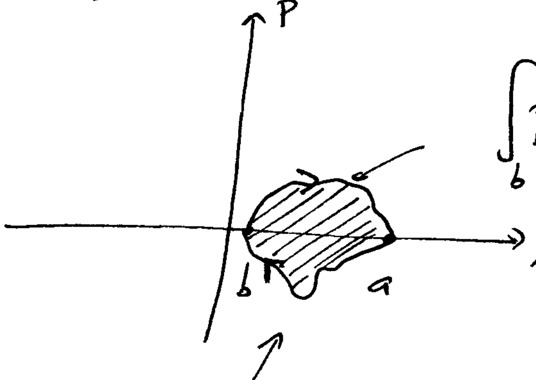
$$\Longrightarrow \cos\left(\int_a^b k(x)\,dx\right) = 0 \Longrightarrow$$

$$\int_a^b k(x)\,dx = n\pi + \pi/2 \;;\quad n \in \mathbb{Z}.$$

This equation determines the discrete values of E.

$$\int_a^b \sqrt{\frac{2m}{\hbar^2}(E - V(x))}\,dx = (n + 1/2)\,\pi$$

What does this mean? Consider the classical phase space portrait of the motion. $p = \hbar k(x) = \sqrt{2m(E - V(x))}$



$$\int_b^a p\,dx = (n + 1/2)\,\pi\,\hbar = \frac{(n+1/2)\,h}{2}$$

or

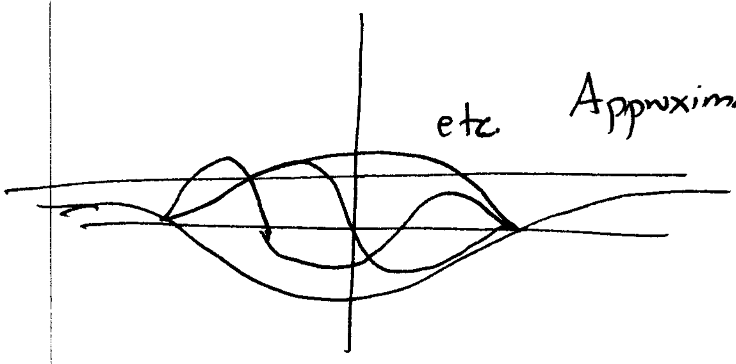
$$2\int_b^a p\,dx = (n + 1/2)\,h \longleftarrow$$

area enclosed by the classical path.

bounded motion of the classical particle

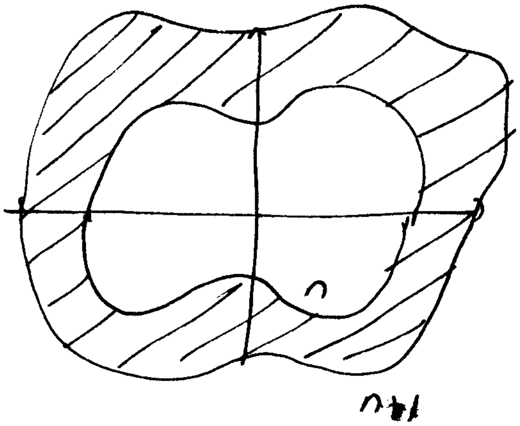
Old QM: Phase Integral $J = \oint p(x)\,dx = (n + 1/2)\,h \leftarrow$ is quantized in units of h.

$\Longrightarrow \frac{1}{2}n + \frac{1}{4}$ "wavelengths" have to fit between $\underline{\underline{b}}$ and $\underline{\underline{a}}$. n = # nodes of the wavefunction



Approximate bound state wavefunctions.

Note also that the area of phase space per state is h.



extra area $= (n+1+1/_2)h - (n+1/_2)h$

$= h$ ← reasonable to take h as the fundamental unit of the volume of phase space. See the usual treatment in statistical physics.

So, what is $i G^+(k_2, k_1; t_2-t_1)$ for our free particle?

$$\psi(x,t_1) = \varphi_{k_1}(x) \qquad \psi(x,t_2) = \varphi_{k_1}(x)\, e^{-i\varepsilon_{k_1}(t_2-t_1)}$$

Prob amplitude to find the particle in state k_2 at time t_2:

$$\int dx\, \psi(x,t_2)\,\varphi^*_{k_2}(x) = e^{-i\varepsilon_{k_1}(t_2-t_1)} \underbrace{\int dx\, \varphi_{k_1}(x)\,\varphi^*_{k_2}(x)}_{\delta_{k_1 k_2}}$$

$\Longrightarrow$

$$\underset{\uparrow}{G_0^+}(k_2,k_1,t_2-t_1) = -i\,\theta(t_2-t_1)\,e^{-i\varepsilon_{k_1}(t_2-t_1)}\,\delta_{k_1,k_2}$$

To remind us that this is for free particles

Or: $G_0^+(k_2, k_1, t_2-t_1) = \delta_{k_1 k_2}\, G_0^+(k_1, t_2-t_1)$ where

$$G_0^+(k_2, t_2-t_1) = \begin{cases} -i\,\theta(t_2-t_1)\,e^{-i\varepsilon_k(t_2-t_1)}, & t_2 \neq t_1 \\ 0 & t_2 = t_1 \end{cases}$$

This function is considerably simpler in the frequency domain:

$$G_0^+(k,\omega) = -i\int_{-\infty}^{\infty} dt\ \theta(t)\, e^{i\omega t}\, e^{-i\varepsilon_k t}$$

$$= -1\,\frac{1}{\omega-\varepsilon_k}\, e^{i(\omega-\varepsilon_k)t}\Big|_0^\infty = \frac{1}{\omega-\varepsilon_k} - \underset{\substack{\uparrow\\ \text{Whoops!}}}{\frac{e^{i(\omega-\varepsilon_k)\infty}}{\omega-\varepsilon_k}}$$

To fix this we multiply in $e^{-\delta t}$ where δ is infinitesimal such that $\delta \times \infty = \infty$:

Then $G_0^+(k, t_2-t_1) = -i\,\theta(t_2-t_1)\, e^{-i(\varepsilon_k - i\delta)(t_2-t_1)}$

and $\boxed{G_0^+(k,\omega) = \frac{1}{\omega - \varepsilon_k + i\delta}}$ ← "modified" free propagator in the ω-domain

Note: The usual way to get this is to note that

$$\theta(t) = -\lim_{\delta\to 0}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi i}\,\frac{e^{-i\omega t}}{\omega+i\delta}$$ and do the integral by poles.

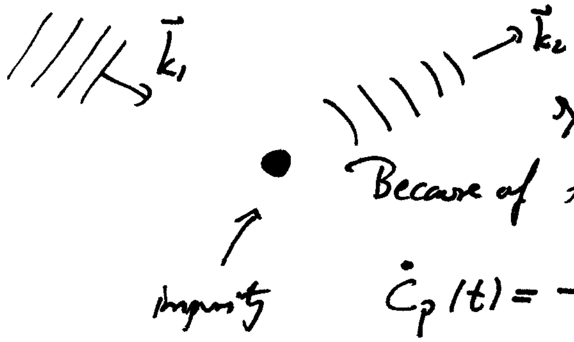
How to use the propagator: A game of quantum pin-ball!

[For more detail see: Richard D. Mattuck "A Guide to Feynman diagrams in the many body problem Dover, New York.]

We will take a result from perturbation theory (Chapter 5) and, at this point, take it to be physically explained, but not proved. We will revisit this point later, but for now let's see what we can do!

Consider there to be a po localized "impurity" potential $V(\vec r - \vec R)$ centered at $\vec R$ in the system:

Plane waves will scatter off of this potential



$C_\ell(t)$ = prob amplitude that the system is in state ℓ at time t.

Because of the perturbation

$$\dot C_p(t) = -i\sum_\ell V_{p\ell}\, C_\ell(t)\, e^{-i(\varepsilon_p-\varepsilon_\ell)(t-t_0)}$$

at $t_0 = t_M$, we are in state $\vec k_1$ i.e. $C_\ell = \delta_{\ell k_1}$

and $V_{p\ell} = +\int d^3\vec{r}\; \varphi_p^*(\vec{r})\, V(\vec{r}-\vec{R})\, \varphi_\ell(\vec{r})$

At time t_m ← Time when the scattering event occurs!

$$\dot{C}_{k_2}(t_m) = -i \int d^2\vec{r}\, \varphi_p^*(\vec{r})\, V(\vec{r}-\vec{R})\, \varphi_\ell(\vec{r}) = -i\, V_{p\ell}$$

What is the probability amplitude to go from $\vec{k}_1$ at t_1 to k_2 at t_2?

$$i\, G_1^+(\vec{k}_2, t_2, \vec{k}_1, t_1) = i\, G_0^+(k_2, t_2-t_m)\left(-i\, V_{k_2k_1}\right) i G_0^+(k_1, t_m-t_1)$$

But the interaction could have happened at any time $t_1 < t_m < t_2$

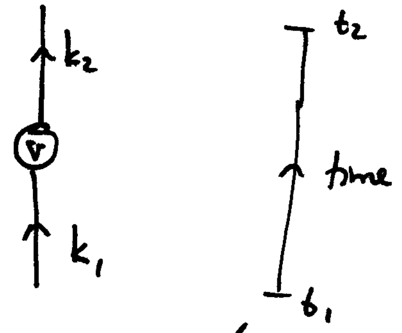
$\Longrightarrow$

$$i\, G_1^+(k_2, t_2, k_1, t_1) = i\int_{-\infty}^{\infty} dt_m\; G_0^+(k_2, t_2-t_m)\, V_{k_2k_1}\, G_0^+(k_1, t_m-t_1)$$

↑ one interaction w/ the potential

← θ-functions keep the times in order...

A picture:



Why can't you interact w/ the potential multiple times?

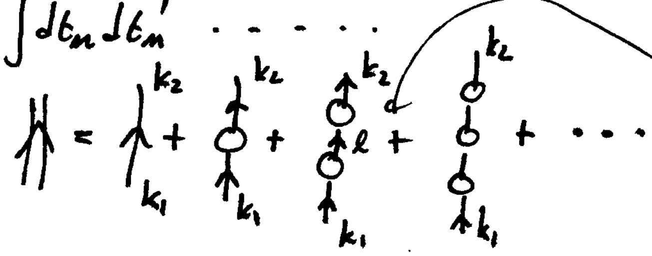
Ans: Of course you can!

$\Longrightarrow$

$$G^+(k_2, t_2, k_1, t_1) = G_0^+(k_1, t_2-t_1)\,\delta_{k_1k_2} + \int_{-\infty}^{\infty} dt_m\, G_0^+(k_2, t_2-t_m)\, V_{k_2k_1} \cdot$$

$$\cdot\, G_0^+(k_1, t_m-t_1) + \int dt_m\, dt_m' \;\ldots\ldots$$

or in pictures



need a sum over intermediate states.

Observe that the integrals over time are simple in the frequency domain: $I(t_2-t_1) = \int_{-\infty}^{\infty} f(t_2-t')\, g(t'-t_1)\, dt' = \int_{-\infty}^{\infty} dt' \int \frac{d\omega}{2\pi}\frac{d\nu}{2\pi} \times$

$$\times\ e^{-i\omega(t_2-t') - i\nu(t'-t_1)}\, \tilde{f}(\omega)\, \tilde{g}(\nu)$$

$$\Rightarrow I(t_2-t_1) = \int \frac{d\omega d\nu}{(2\pi)^2} \tilde{f}(\omega)\tilde{g}(\nu)\, e^{-i\omega t_2} e^{+i\nu t_1} \underbrace{\int_{-\infty}^{\infty} dt'\, e^{-it'(\nu-\omega)}}_{2\pi\,\delta(\nu-\omega)}$$

$$I(t_2-t_1) = \int \frac{d\omega}{(2\pi)} e^{-i(t_2-t_1)\omega} \tilde{f}(\omega)\tilde{g}(\omega) \quad \text{or}$$

$$\tilde{I}(\omega) = \tilde{f}(\omega)\, \tilde{g}(\omega).$$

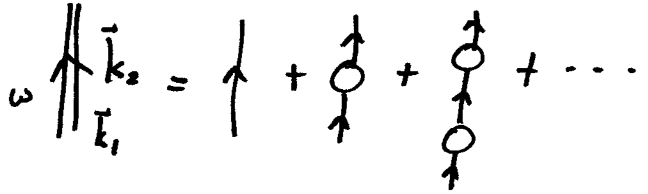
so in $\vec{k},\omega$ space

$i\, G^{+}(k_2,k_1,\omega) = \omega$  Full propagator

$i\, G_0^{+}(k,\omega) =$  $\vec{k},\omega$ Free propagator $= \dfrac{i}{\omega - \varepsilon_k + i\delta}$

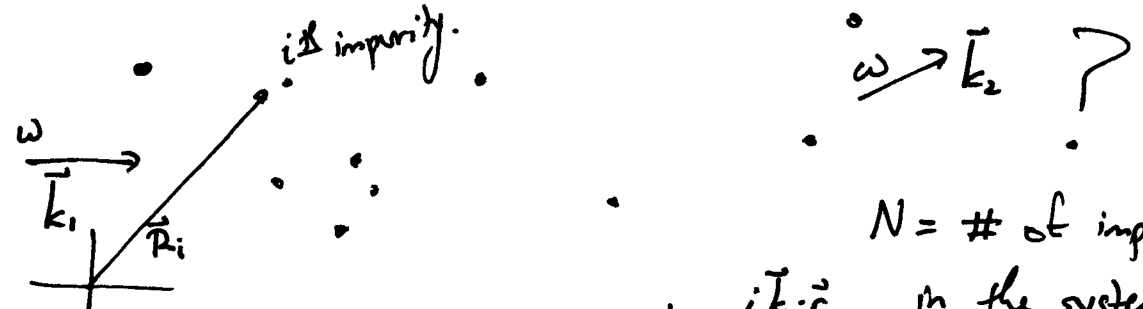
$-i\, V_{k\ell} =$  Interaction w/ the impurity potential.

and

 or

$$G^{+}(\vec{k}_{2,1},\omega) = G_0(k,\omega)\, \delta_{\vec{k}_1\vec{k}_2} + G_0^{+}(k_2,\omega)\, V_{k_2k_1}\, G_0^{+}(k_1,\omega) + \cdots$$

Now, to our problem with random impurities



N = # of impurity sites in the system.

Taking our plane waves $\varphi_{\vec{k}} = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{r}}$

↑ volume of the system.

so $\langle \varphi_k | \varphi_{\vec{k}'} \rangle = 1 \qquad \delta_{k,k'}$ ← Note: Different normalization than in Chapter One.

Impurity potential $W(\vec{r}-\vec{R}_i)$

$$\Rightarrow \quad -iV_{\ell k}(\vec{R}_i) = \frac{-i}{(\sqrt{\Omega})^2}\int d^3\vec{r}\; e^{-i\vec{\ell}\cdot\vec{r}}\, e^{+i\vec{k}\cdot\vec{r}}\, W(\vec{r}-\vec{R}_i)$$

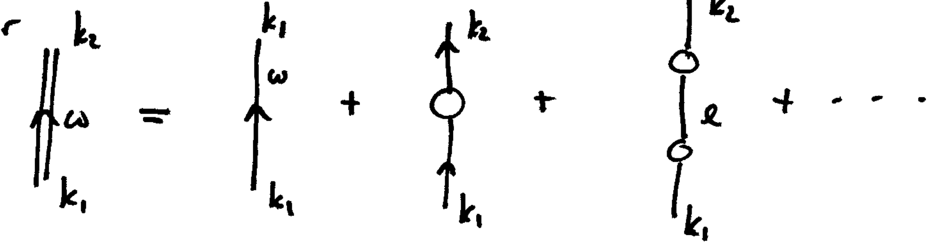
$$= \frac{-i}{\Omega}\, e^{-i(\vec{\ell}-\vec{k})\cdot\vec{R}_i} \underbrace{\int d^3r'\, e^{-i(\vec{\ell}-\vec{k})\cdot\vec{r}'}\, W(\vec{r}')}_{W_{\ell k}}$$

So

$$G^+(\vec{k}_2,\vec{k}_1,\omega) = G_0^+(\vec{k}_1,\omega)\,\delta_{k_1k_2} + G_0^+(\vec{k}_2,\omega)\sum_i^N V_{k_2k_1}(\vec{R}_i)\, G_0^+(\vec{k}_1,\omega)$$

$$+ \; G_0^+(\vec{k}_2,\omega)\sum_{\ell}\sum_{\substack{i=1\\ j=1}}^{N} V_{k_2\ell}(\vec{R}_i)\, G_0^+(\vec{\ell},\omega)\, V_{\ell k_1}(\vec{R}_j)\; G_0^+(\vec{k}_1,\omega) + \cdots$$

or



no interaction one interaction two interactions at the same or different sites i,j

Can we average or exalt over the random placement of scattering sites?

Ans: Yes and we will get a meaningful average applicable to large systems: — "self-averaging" see Kohn and Luttinger (1957).

Average $\langle G^+ \rangle$:

A. Note $$\left\langle G_0^+(\vec{k}_2)\, G_0^+(\vec{k}_1) \sum_{i=1}^{N} V(\vec{R}_i)_{k_2 k_1} \right\rangle = G_0^+(\vec{k}_2) G_0^+(\vec{k}_1) \frac{W_{k_1 k_2}}{\Omega} \cdot$$

$$\cdot \left\langle \underset{\underset{N\left\langle e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{R}_i}\right\rangle}{\uparrow}}{\sum_{i=1}^{N}} e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{R}_i} \right\rangle$$

Prob of finding any specific impurity in a volume $d^3\vec{R}_i$ at point $\vec{R}_i = \frac{1}{\Omega}$

$$\Rightarrow N\left\langle e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{R}_i}\right\rangle = N\frac{1}{\Omega}\underset{\uparrow}{\int} d^3\vec{R}_i\, e^{-i(\vec{k}_1-\vec{k}_2)\cdot\vec{R}_i} = \frac{\Omega N}{\Omega}\,\delta_{k_1,k_2} \leftarrow$$

Contributes to forward scattering!

Sidebar on Integrals:

Periodic b.c. $e^{ik(x+L)} = e^{ikx} \Rightarrow e^{ikL} = 1 \quad k = \frac{2\pi n}{L} \quad n \in \mathbb{Z}$. so

$$\int_{-L/2}^{L/2} dx\, e^{-ikx} = \frac{2}{\cancel{2}k}\sin(kL/2) = 0 \text{ unless } k = 0.$$

B. What about two scattering events?

We need to distinguish between types of double scattering:

Scattering from two different defects

Scattering from the same defect <u>twice</u>.

Consider the appropriate terms in the perturbation series:

2. $$\sum_{\vec{l}} G_0^+(\vec{l}) \left\langle \sum_i V_{k_2 l}(\vec{R}_i)\, V_{l k_1}(\vec{R}_i) \right\rangle$$ ← Scattering from the same defect twice.

$$= \sum_{\vec{l}} G_0^+(\vec{l})\, \frac{W_{k_2 l}\, W_{l k_1}}{\Omega^2} \left\langle \sum_i e^{-i(\vec{k}_2 - \vec{l} + \vec{l} - \vec{k}_1)\cdot \vec{R}_i} \right\rangle$$

Average over the position of the impurities

We've done this before!

$$\Downarrow$$

$$\underline{N}\ \delta_{k_1 k_2}$$

$$= \frac{N}{\Omega^2} \sum_{\vec{l}} G_0^+(\vec{l})\, W_{k_2 l}\, W_{l k_1}\, \delta_{k_1 k_2}$$

Change the sum into an integral: $\sum_{\vec{l}} \to \int dl$ or $\sum_{l} = \frac{1}{\Delta l}\int dl$

And : $|\vec{l}| = \frac{2\pi n}{L}$ $n = 0, 1, 2, \ldots$

$$\Delta l = \frac{2\pi}{L}\Delta n = \frac{2\pi}{L}$$

So $\sum_{l} = \frac{L}{2\pi}\int dl$ – or in 3D $\sum_{\vec{l}} = \frac{L^3}{(2\pi)^3}\int d^3\vec{l}$

↖ $\frac{\Omega}{(2\pi)^3}$

$$= \delta_{k_1 k_2}\left(\frac{N}{\Omega}\right)\int \frac{d^3\vec{l}}{(2\pi)^3}\, G_0^+(\vec{l})\, W_{k_2 l}\, W_{l k_1}$$

↖ Proportional to the density of impurities/scattering sites.

1. Scattering from two different impurities

$$\sum_{\vec{l}} G_0^+(\vec{l}) \left\langle \sum_{i \neq j}^{N} V_{k_2 l}(\vec{R}_i)\, V_{l k_1}(\vec{R}_j) \right\rangle$$

Two different impurities.

$$= \sum_{\vec{l}} G_0^+(\vec{l}) \frac{W_{k_2 l} W_{l k_1}}{\Omega^2} \left\langle \sum_{i \neq j}^{N} e^{-i(\vec{k}_2-\vec{l})\cdot\vec{R}_i}\, e^{-i(\vec{k}_1-\vec{l})\cdot\vec{R}_j} \right\rangle$$

How do we do the averaging?

Prob of getting an impurity at $\vec{R}_i$ and $\vec{R}_j$:

$$N(N-1)\, \frac{d^3\vec{R}_i}{\Omega}\, \frac{d^3\vec{R}_j}{\Omega}.$$

$$\Rightarrow$$

$$= \sum_{\vec{l}} G_0^+(\vec{l}) \frac{W_{k_2 l} W_{l k_1}}{\Omega^2} \frac{N(N-1)}{\Omega^2} \int d^3R_i\, d^3R_j\, e^{-i(\vec{k}_2-\vec{l})\cdot\vec{R}_i}\, e^{-i(\vec{k}_1-\vec{l})\cdot\vec{R}_j}$$

$$= \sum_{\vec{l}} G_0^+(\vec{l}) \frac{W_{k_2 l} W_{l k_1}}{\Omega^2} \frac{N(N-1)}{\Omega^2} \Omega^2 \underline{\delta_{k_2 l}\, \delta_{k_1 l}}$$

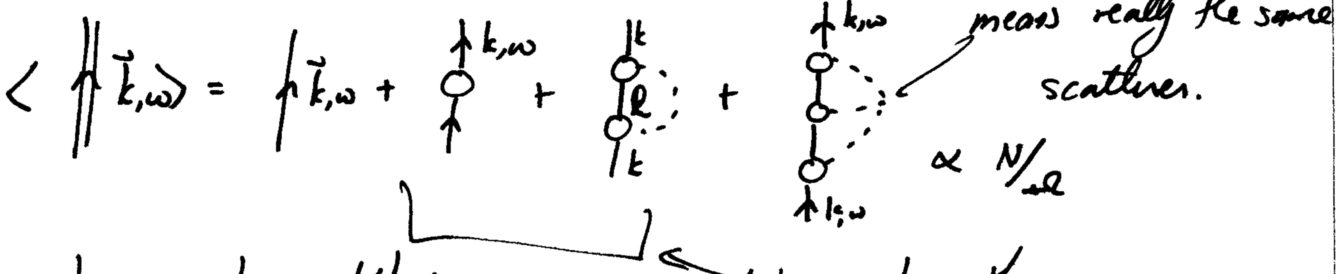
Use this to do the sum!

$$\cong \left(\frac{N}{\Omega}\right)^2 \cancel{\sum_{\vec{l}}} G_0^+(\vec{k}_1)\, W_{k_1 k_2} W_{k_2 k_1} \delta_{k_1 k_2}$$

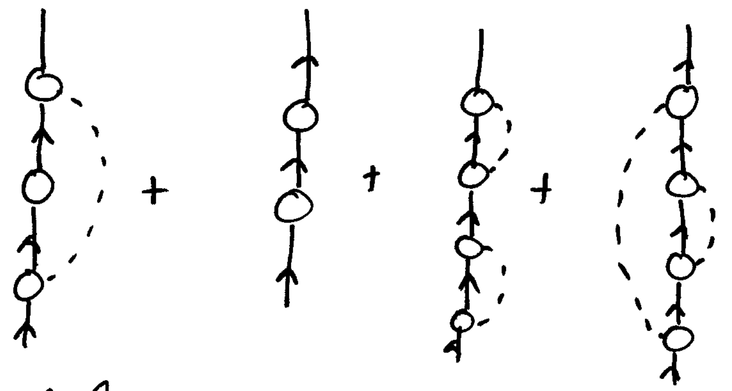
Proportional to the square of the density.

Thus in the low density limit two interactions w/ the same defect matter more than interactions w/ different scatterers.

Let's focus on the single impurity case!



whereas terms like:



$\propto (N/\Omega)^2$

Doing the final sum:

$$1 + x + x^2 + \cdots = \frac{1}{1-x} \quad \text{and}$$

$$G\left[1 + x + x^2 + \cdots\right] = G\,\frac{1}{1-x}$$

what is x? x = { $= -iW_{lk}$ combined w/ $\uparrow k = iG_0^+(k) = \frac{i}{\omega - \varepsilon_k + i\delta}$

$$\Rightarrow G_0^+(k_1)\,x = \frac{N}{\Omega} W_{k_1k_1}\, G_0^+(k_1) + \frac{N}{\Omega}\int G_0^+(k_1)\, W_{k_1 l}\, W_{l k_1}\, G_0^+(\vec l)\,\frac{d^3\vec l}{(2\pi)^3}$$

$$\Rightarrow \langle G(\vec k,\omega)\rangle = \frac{1}{G_0^{+\,-1}(k,\omega) \cancel{+} - \left(W_{kk}\frac{N}{\Omega} + \frac{N}{\Omega}\int\frac{d^3\vec l}{(2\pi)^3}\,\frac{|W_{k,l}|^2}{\omega - \varepsilon_l + i\delta}\right)}$$

or

$$\langle G(\vec k,\omega)\rangle = \frac{1}{\omega - \varepsilon_k + i\delta - \Sigma(\vec k,\omega)}$$

Where

$$\underset{\underset{\text{"Self-energy"}}{\uparrow}}{\Sigma(\vec{k},\omega)} = \frac{N}{\Omega}\left\{ W_{kk} + \int\frac{d^3\vec{l}}{(2\pi)^3}\,\frac{|W_{kl}|^2}{\omega-\varepsilon_l+i\delta}\right\}$$

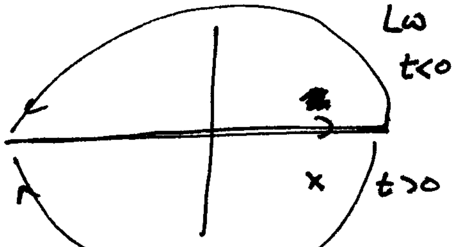
How do we interpret this result?

Break Σ into real and imaginary parts.

$$\frac{1}{\omega-\varepsilon_k-\Sigma} = \frac{1}{\omega-\varepsilon_k-\underset{\underset{\delta\varepsilon_k}{\nearrow}}{\mathrm{Re}\,\Sigma}-i\,\underset{\underset{1/\tau_k}{\nwarrow}}{\mathrm{Im}\,\Sigma}}$$

Let's go back to the time domain:

$\overset{+}{G}$on $$\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-i\omega t}\,\frac{d\omega}{\omega-(\varepsilon_k+\delta\varepsilon_k)+i/\tau_k} = \underset{\underset{\text{usual bit}}{\nearrow}}{\theta(t)}\, \underset{\underset{\text{quasi-particle energy}}{\uparrow}}{e^{-i(\varepsilon_k+\delta\varepsilon_k)t}}\; \underset{\text{lifetime of the state.}}{e^{-t/\tau_k}}$$



pole: $\omega = \varepsilon_k+\delta\varepsilon_k \mp i/\tau_k$

So, how do we get the real and imaginary parts?

$$\mathrm{Re}\,\Sigma(k)\Big|_{\omega=\varepsilon_k} = \frac{N}{\Omega}W_{kk} + \lim_{\delta\to 0}\frac{N}{\Omega}\int\frac{d^3\vec{l}}{(2\pi)^3}\,\frac{|W_{kl}|^2(\varepsilon_k-\varepsilon_l)}{(\varepsilon_k-\varepsilon_l)^2+\delta^2} \leftarrow \text{using } \omega=\varepsilon_k$$

$$= \frac{N}{\Omega}W_{kk} + \frac{N}{\Omega}\,\mathcal{P}\int\frac{d^3\vec{l}}{(2\pi)^3}\,\frac{|W_{kl}|^2}{(\varepsilon_k-\varepsilon_l)}$$

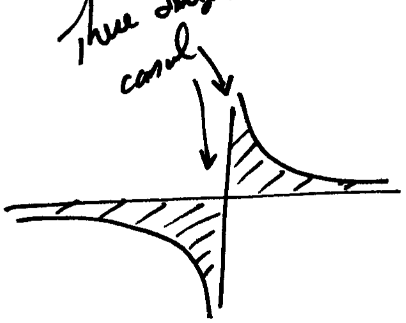
$$\mathrm{Im}\,\Sigma(k)\Big|_{\omega=\varepsilon_k} = -\lim_{\delta\to 0}\frac{N}{\Omega}\int\frac{d^3\vec{l}}{(2\pi)^3}\,|W_{kl}|^2\,\frac{\delta}{(\varepsilon_k-\varepsilon_l)^2+\delta^2} = -\pi\frac{N}{\Omega}\int\frac{d^3\vec{l}}{(2\pi)^3}\,|W_{kl}|^2\,\delta(\varepsilon_k-\varepsilon_l)$$

What is the $\mathcal{P}$? and how to get the limits $\delta \to 0$.

Consider: $$\frac{1}{\omega-\varepsilon_\ell+i\delta} = \frac{1}{(\omega-\varepsilon_\ell)^2+\delta^2}(\omega-\varepsilon_\ell-i\delta)\Bigg|_{\omega=\varepsilon_k}$$

$$= \frac{\varepsilon_k-\varepsilon_\ell}{(\varepsilon_k-\varepsilon_\ell)^2+\delta^2}$$ ← This is a function of $|\vec{\ell}|$

in the limit that $\delta \to 0$ is this finite?



An example: $$\mathrm{Re}\int_{-a}^{b}\frac{dx}{x+i\delta}$$

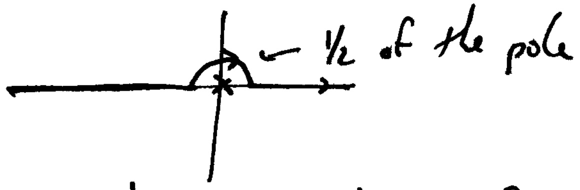
$$= \mathrm{Re}\int_{-a}^{b}\frac{dx\,(x-i\delta)}{x^2+\delta^2} = \int_{-a}^{b}\frac{dx}{x} = \lim_{\delta\to 0}\left\{\log(b)-\log(\delta)+\log(-\delta)-\log(-a)\right\}$$

$$= \lim_{\delta\to 0}\left\{\log\left(\frac{b}{\delta}\right)\cdot\log\left(\frac{-\delta}{-a}\right)\right\} = \lim_{\delta\to 0}\log(b/a) = \log(b/a)$$

Or, just do the integral $\int_{-a}^{b} dx\,\frac{x}{x^2+\delta^2} = \log(b/a)$

What about the imaginary part?

$$\mathrm{Im}\int_{-\infty}^{\infty} dx\,\frac{f(x)}{x+i\delta} = -\lim_{\delta\to 0}\int dx\,\frac{f(x)\,\delta}{x^2+\delta^2} = -i\pi f(0)$$



or $$\frac{1}{x+i\delta} = \mathcal{P}\frac{1}{x} - i\pi\delta(x)$$ ← A short-hand to remember this result.

So: We have an interesting result

$$\varepsilon_k+\delta\varepsilon_k = \varepsilon_k + \frac{N}{\Omega}W_{kk} + \frac{N}{\Omega}\mathcal{P}\int\frac{d^3\vec{\ell}}{(2\pi)^3}\frac{|W_{\ell k}|^2}{\varepsilon_k-\varepsilon_\ell}$$ ← 2nd order Perturbation Theory

$$\tau_k^{-1} = \pi\frac{N}{\Omega}\int\frac{d^3\vec{\ell}}{(2\pi)^3}|W_{\ell k}|^2\,\delta(\varepsilon_k-\varepsilon_\ell)$$ ← Fermi's Golden Rule

Transition rate out of the k-state.