Advanced Quantum Mechanics

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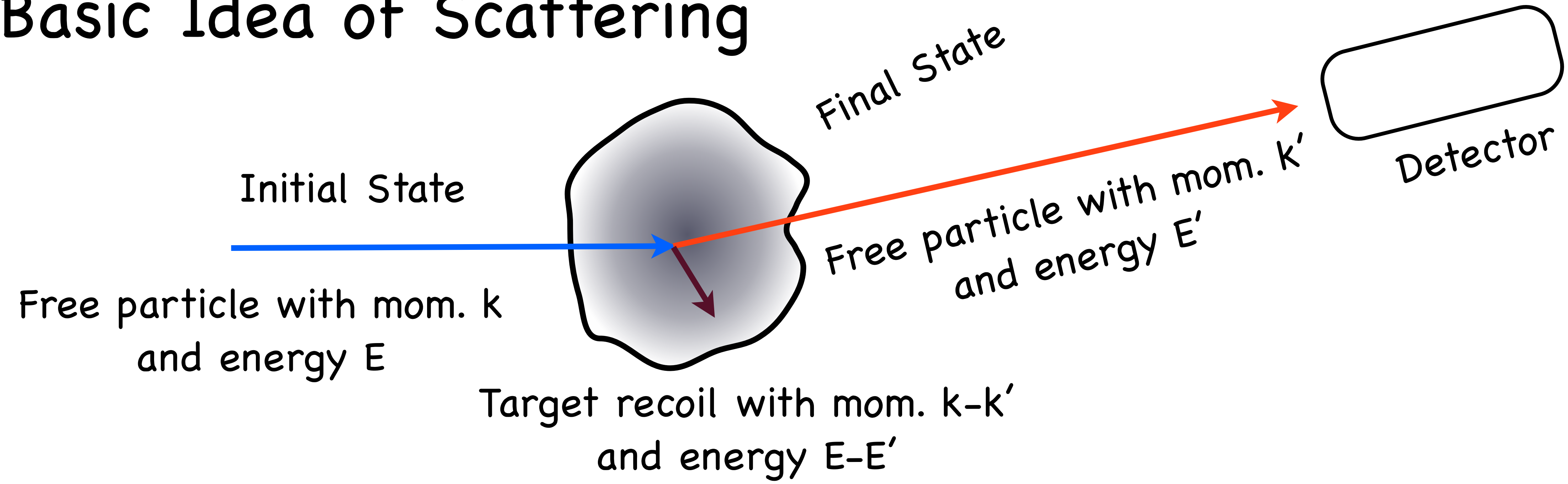
Scattering Theory

Ref : Sakurai, Modern Quantum Mechanics
Taylor, Quantum Theory of Non-Relativistic Collisions
Landau and Lifshitz, Quantum Mechanics

The Basic Idea of Scattering



Examples:

- Almost all of high energy experiments ...
- Neutron Scattering for materials, light scattering
- Rutherford's original experiment of scattering of α particles by gold foil
- Scattering of electrons by impurities

Info obtained from scattering:

- Interaction potential between the target and the incident particles

  Nuclear potentials, atomic potentials, beyond SM terms?

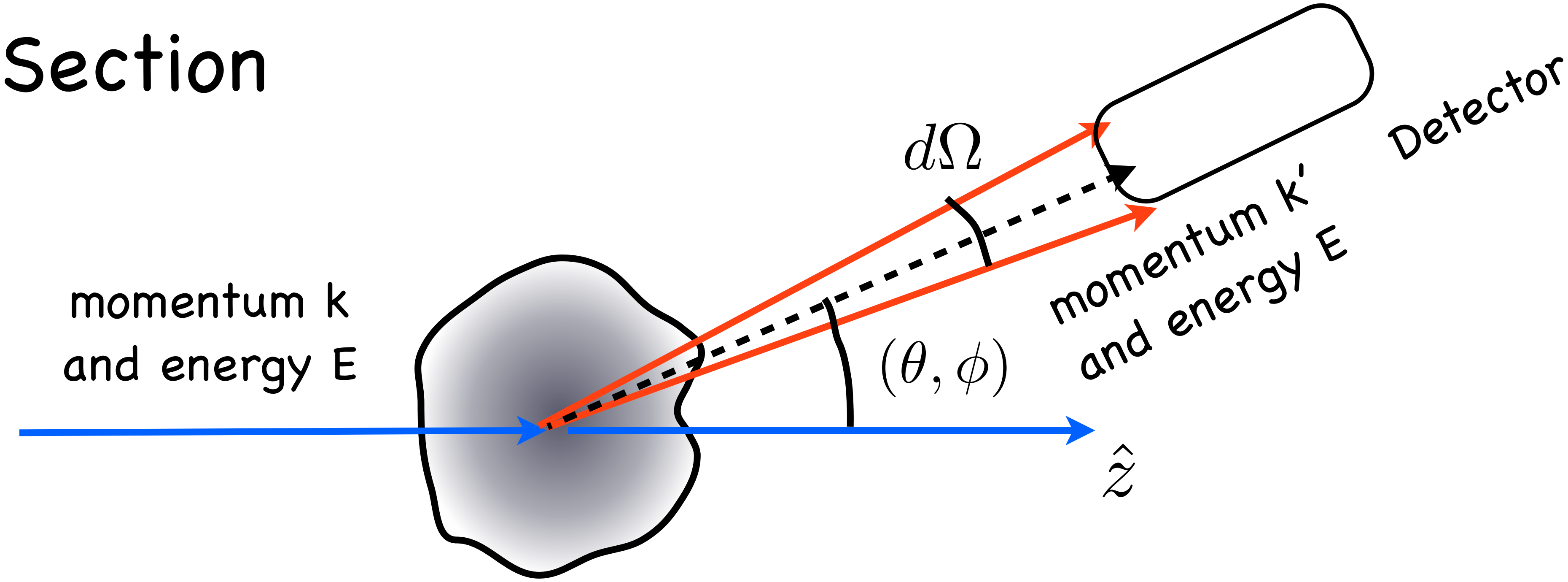
- Spatial structure of target matter distribution

  Rutherford and nucleus, neutrons and spin patterns, form and structure factors

- Excitation Spectrum of the target

  Inelastic Scattering -- energy dumped into target

Scattering Cross Section



Measureable Quantities:

Differential Cross Section:

$$\frac{d\sigma}{d\Omega} d\Omega = \frac{\text{No. of particles scattered into the solid angle } d\Omega \text{ around } \hat{k}' = (\theta, \phi) \text{ per unit time}}{\text{Number of incident particles crossing unit area normal to z dirn. per unit time}}$$

Total Cross Section: Obtained by integrating the differential cross section over all solid angles

Assumptions:

- The particle interacts with the target through a finite range potential, so that far away from the target (both for incident and scattered beams) a free particle state is obtained.

Exception: Coulomb Scattering — long range potential .... will not treat in this course

Collision of Particles

Two body problem: $$\left[-\frac{\nabla_1^2}{2m_1} - \frac{\nabla_2^2}{2m_2} + V(r_1 - r_2) - E\right]\psi(r_1, r_2) = 0$$

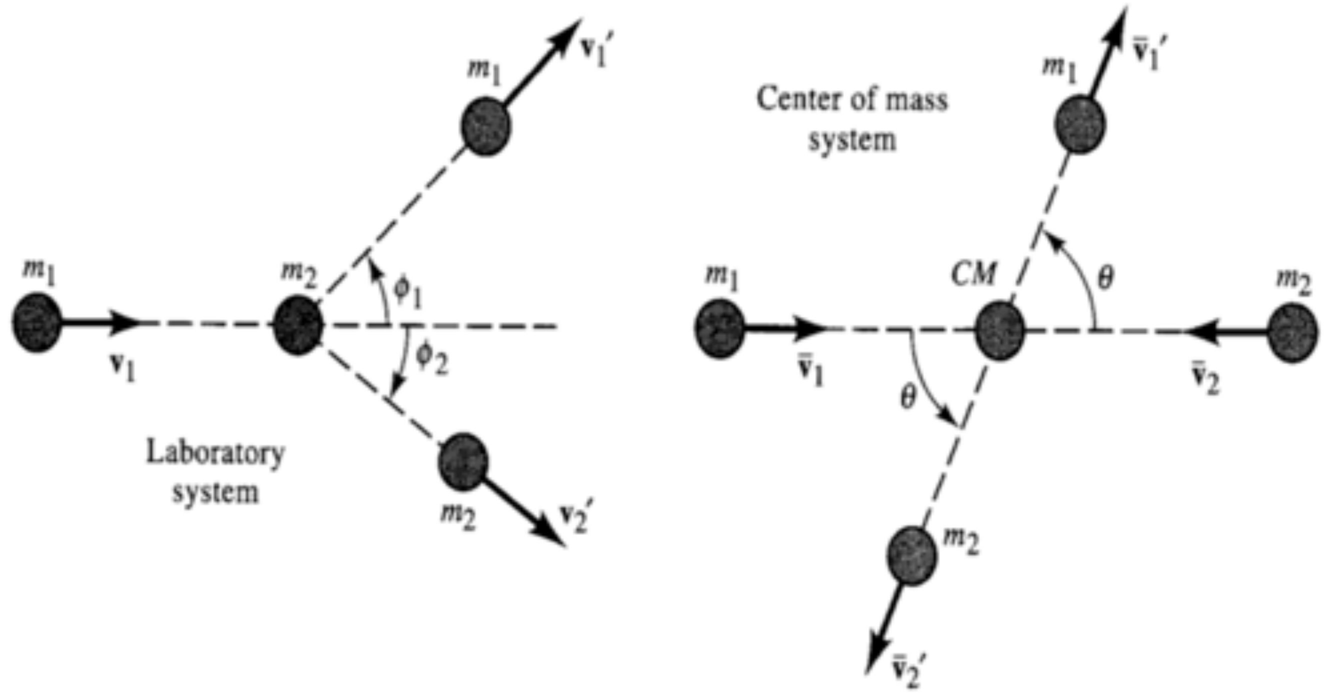
Center of mass and relative co-ordinates $$\vec{R} = \frac{m_1\vec{r_1} + m_2\vec{r_2}}{m_1 + m_2} \qquad \vec{r} = \vec{r_1} - \vec{r_2}$$

Reduced Mass: $$\frac{1}{m^*} = \frac{1}{m_1} + \frac{1}{m_2}$$

Now $$\frac{\nabla_1^2}{2m_1} + \frac{\nabla_2^2}{2m_2} = \frac{\nabla_R^2}{2(m_1 + m_2)} + \frac{\nabla_r^2}{2m^*}$$

$$\psi(r_1, r_2) \to \psi(r)\phi(R)$$

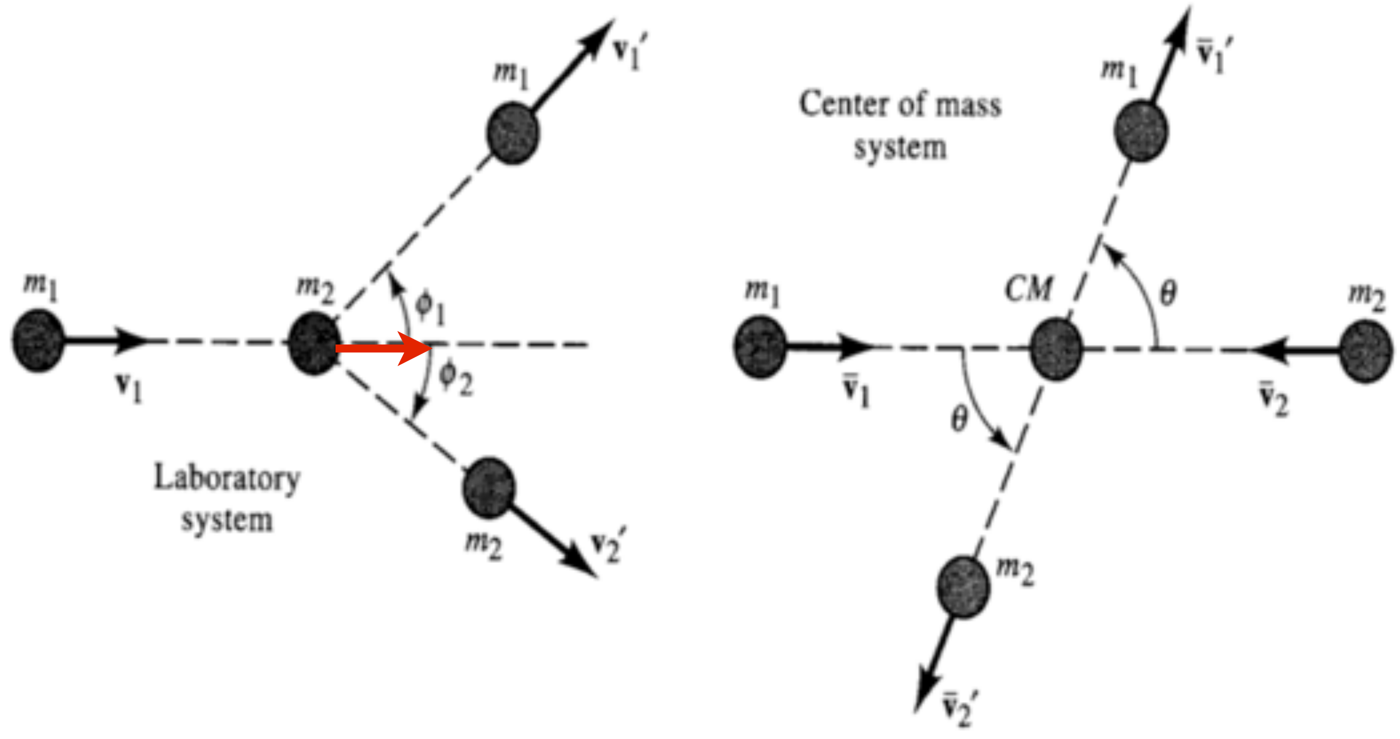
$$\left[-\frac{\nabla_r^2}{2m^*} + V(r) - (E - E_{com})\right]\psi(r) = 0$$



Effective 1-body problem in relative co-ordinates with reduced mass and energy

Shooting particles at targets look like 2 moving particles colliding with each other in COM frame. Thus scattering problem also tells us about say interaction between atoms in a gas, where there is no fixed target to shoot at.

Lab vs. C.O.M. Frame



C.O.M. velocity: $v' = \frac{m_1}{m_1 + m_2} v_1$

C.O.M. Frame:

$$\bar{v}_2 = v' \qquad \bar{v}_1 = \frac{m_2 v}{m_1 + m_2}$$

Conservation of momentum and energy:

$$\bar{v'}_2 = \bar{v}_2 \quad \bar{v'}_1 = \bar{v}_1$$

$$\tan(\phi_1) = \frac{\sin\theta}{\gamma + \cos\theta} \qquad \gamma = \frac{m_1}{m_2}$$

Relation between differential scattering cross sections in lab vs C.O.M. frame

Physically, the same number of particles are scattered towards the same solid angle, irrespective of which frame we choose to measure it.

$$\sigma_L(\phi_1, \chi) \sin\phi_1 d\phi_1 d\chi = \sigma_C(\theta, \phi) \sin\theta d\phi d\theta \qquad \sigma_L(\phi_1, \chi) = \frac{(1 + \gamma^2 + 2\gamma\cos\theta)^{1/2}}{|1 + \gamma\cos\theta|} \sigma_C(\theta, \phi)$$

Setting up the Problem: Free Particles

A free particle with a given momentum will remain in that momentum state forever.

Time Evolution Operator:

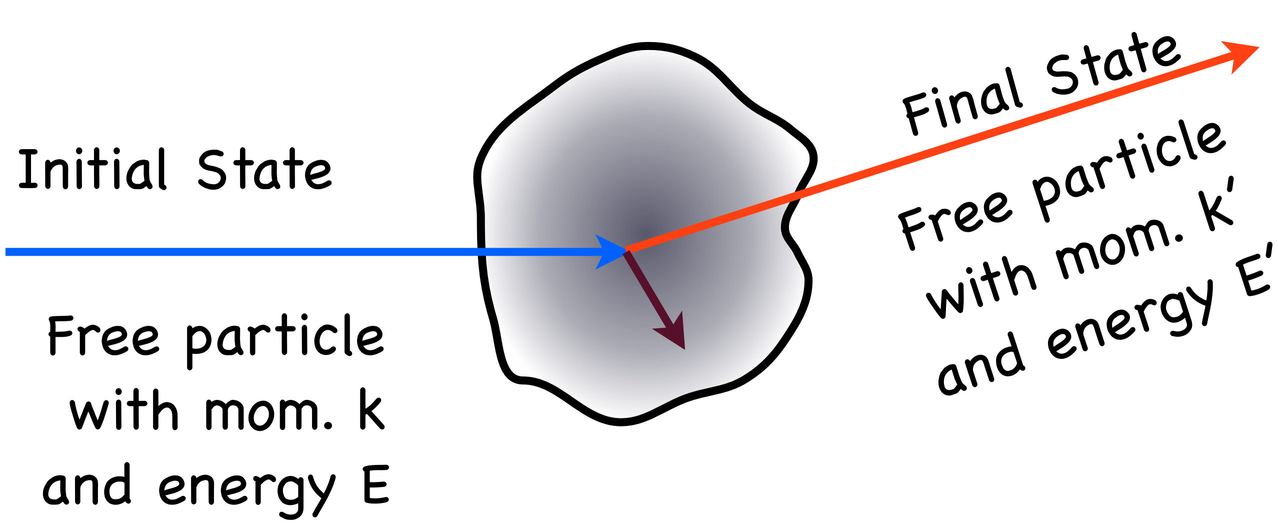
$$U(\vec{k},t;\vec{k'},t') = \delta(\vec{k}-\vec{k'})e^{-i\frac{k^2}{2m}(t-t')} \qquad \psi_k(t) = \int d^dk' U(\vec{k},t;\vec{k'},t')\psi(\vec{k'},t')$$

Retarded Propagator

$$G_0^R(\vec{k},t;\vec{k'},t') = -i\Theta(t-t')\delta(\vec{k}-\vec{k'})e^{-i\frac{k^2}{2m}(t-t')} \qquad G_0^R(\vec{k},\omega) = \frac{1}{(\omega + i0^+ - \frac{k^2}{2m})}$$

This is the causal propagator, which propagates forward in time

$$\psi_k(t) = i\int d^dk' G_0^R(\vec{k},t;\vec{k'},t')\psi(\vec{k'},t')$$



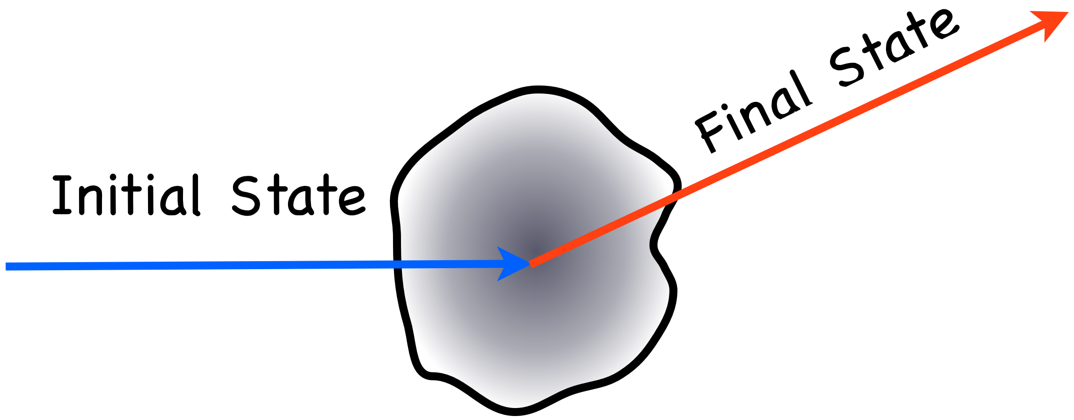
The Scattering Amplitude is related to the

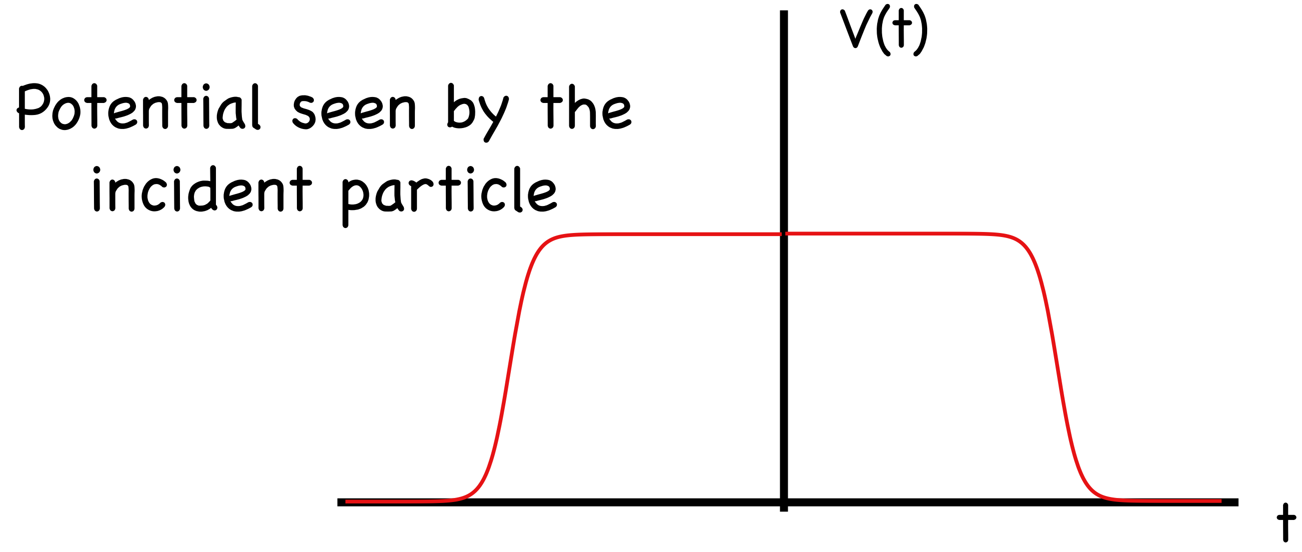
matrix element of the

Time Evolution Operator in presence of Interaction

between different momentum states

Interactions and Propagator





- We assume that the potential is turned on from 0 at t= -∞.
- It is also switched off as t --> ∞.
- The exact manner of turning on/ switching off does not matter as long as it is done far in past/future.
- This mimics the fact that at large negative and positive times, the particle is out of the interaction region

Formal Solution:

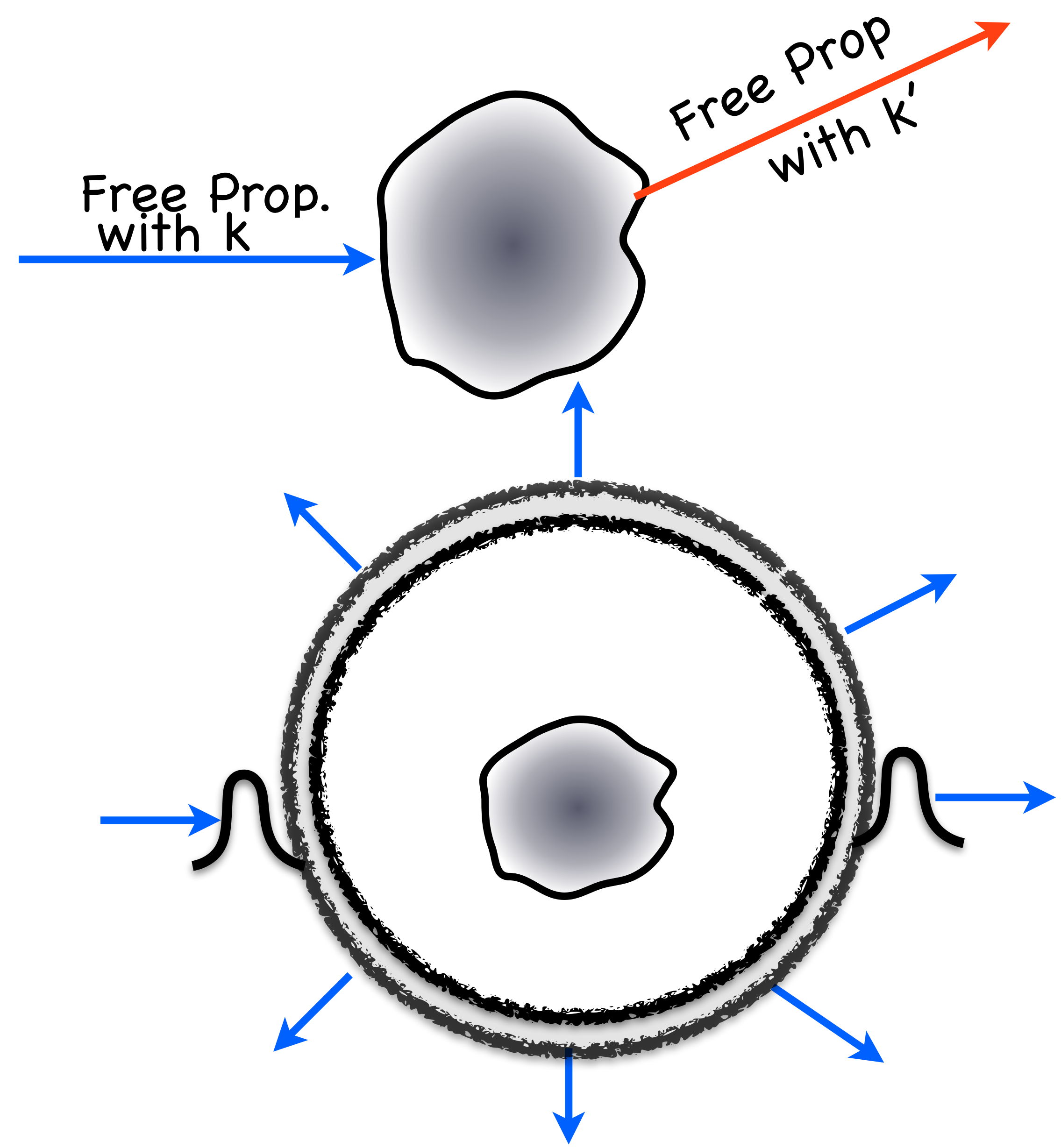
$$|\psi^{(+)}(r,t)\rangle = i\int dr' G^R(r,t;r't')|\phi(r',t')\rangle$$

$|\phi(r',t')\rangle$ → Free initial state

G^R → (as yet unknown) propagator in presence of interaction

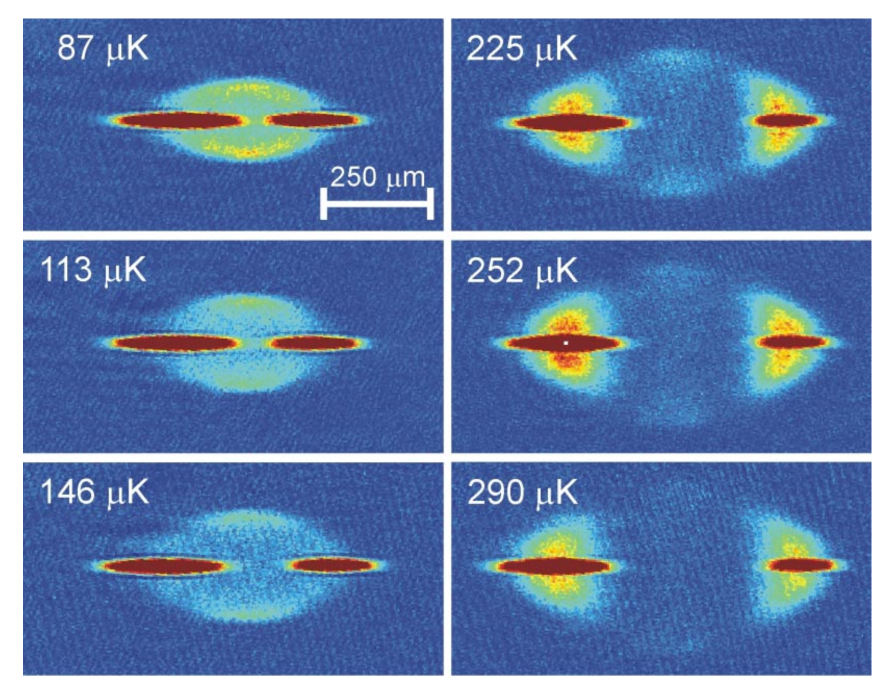
The Wave Packet Picture

We are talking about initial and final states with fixed momenta. This sets the boundary cond. for the scattering problem



We are also talking about a particle localized in real space, which “feels” the potential as it moves in time

Need to think about scattering of wave-packets. E.g. time spent in interaction region only has meaning for wave-packets, not for k eigenstates



Will continue to talk about what happens to an initial k state. Can reconstruct what happens to wave-packet by linear superposition.

Interactions and Propagator

$$V_I(t) = e^{iH_0t}V(t)e^{-iH_0t}$$

$$G^R(r,t;r',t') = -i\Theta(t-t')U(r,t;r',t') = -i\Theta(t-t')e^{-iH_0t}T[e^{-i\int_{t'}^{t}dt_1V_I(t_1)}]e^{iH_0t'}$$

Back to Schrodinger picture

Time Evolution Operator in Interaction Representation

Back to Schrodinger picture

$$G^R(r,t;r',t') = -i\Theta(t-t')e^{-iH_0t}T[e^{-i\int_{t'}^{t}dt_1V_I(t_1)}]e^{iH_0t'}$$

$$= -i\Theta(t-t')e^{-iH_0t}\left[1 - i\int_{t'}^{t}dt_1V_I(t_1) - \int_{t'}^{t}dt_1V_I(t_1)\int_{t'}^{t_1}dt_2V_I(t_2) + \ldots\right]e^{iH_0t'}$$

Note Time Ordering

$$= -i\Theta(t-t')e^{-iH_0t}\left[1 + \sum_n(-i)^n\int_{t'}^{t}dt_1e^{iH_0t_1}V(t_1)e^{-iH_0t_1}\int_{t'}^{t_1}dt_2e^{iH_0t_2}V(t_2)e^{-iH_0t_2}\ldots\right.$$
$$\left.\int_{t'}^{t_{n-1}}dt_ne^{iH_0t_n}V(t_n)e^{-iH_0t_n}\right]e^{iH_0t'}$$

Interactions and Propagator

$$= -i\Theta(t-t')e^{-iH_0 t}\left[1+\sum_n (-i)^n \int_{t'}^{t} dt_1 e^{iH_0 t_1} V(t_1) e^{-iH_0 t_1} \int_{t'}^{t_1} dt_2 e^{iH_0 t_2} V(t_2) e^{-iH_0 t_2} \ldots \int_{t'}^{t_{n-1}} dt_n e^{iH_0 t_n} V(t_n) e^{-iH_0 t_n}\right] e^{iH_0 t'}$$

Now $G_0^R(r,t;r',t') = -i\Theta(t-t')e^{-iH_0(t-t')}$

n^{th} order term: combine the $\exp(-iH_0\, t_i)$ and $\exp(iH_0 t_{i+1})$ Insert $\int dr_i\, |r_i\rangle\langle r_i| = 1$ in between

(n+1) propagators : (n+1) factors of i, and time ordering takes care of theta fn.

$$\int dr_1 \int dt_1 \ldots \int dr_n \int dt_n G_0^R(r,t;r_1,t_1)V(t_1)G_0^R(r_1,t_1;r_2,t_2)V(t_2)\ldots G_0^R(r_{n-1},t_{n-1};r_n,t_n) V(t_n)G_0^R(r_n,t_n;r',t')$$

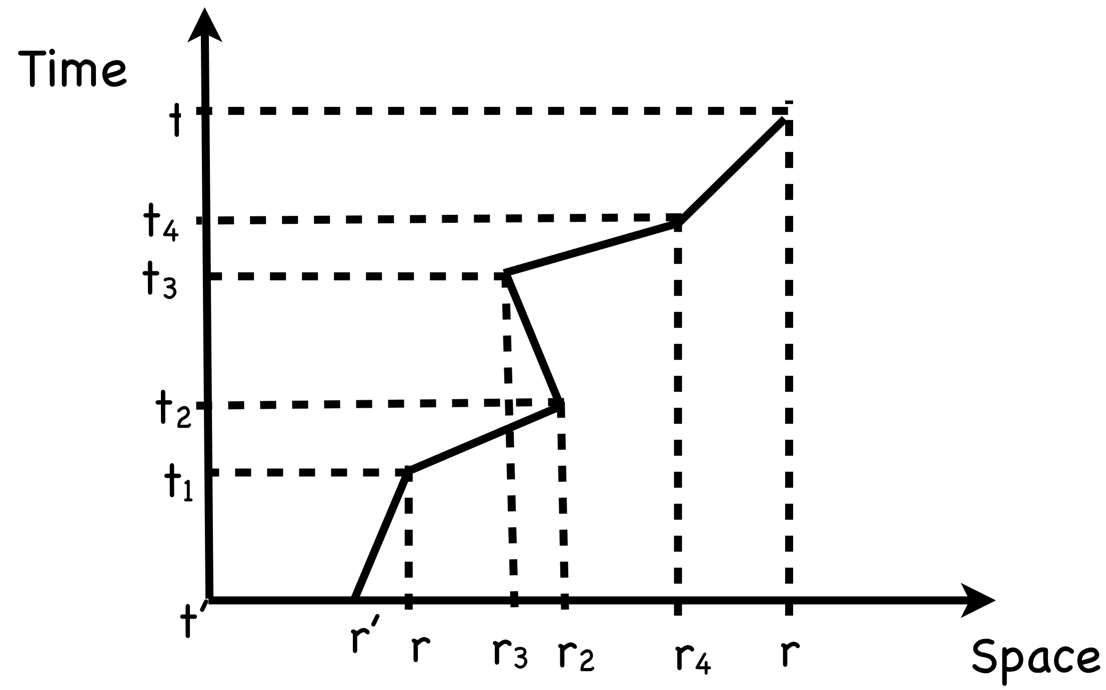
$$G^R = G_0^R + G_0^R V G_0^R + G_0^R V G_0^R V G_0^R + \ldots = G_0^R + G_0^R V G^R$$

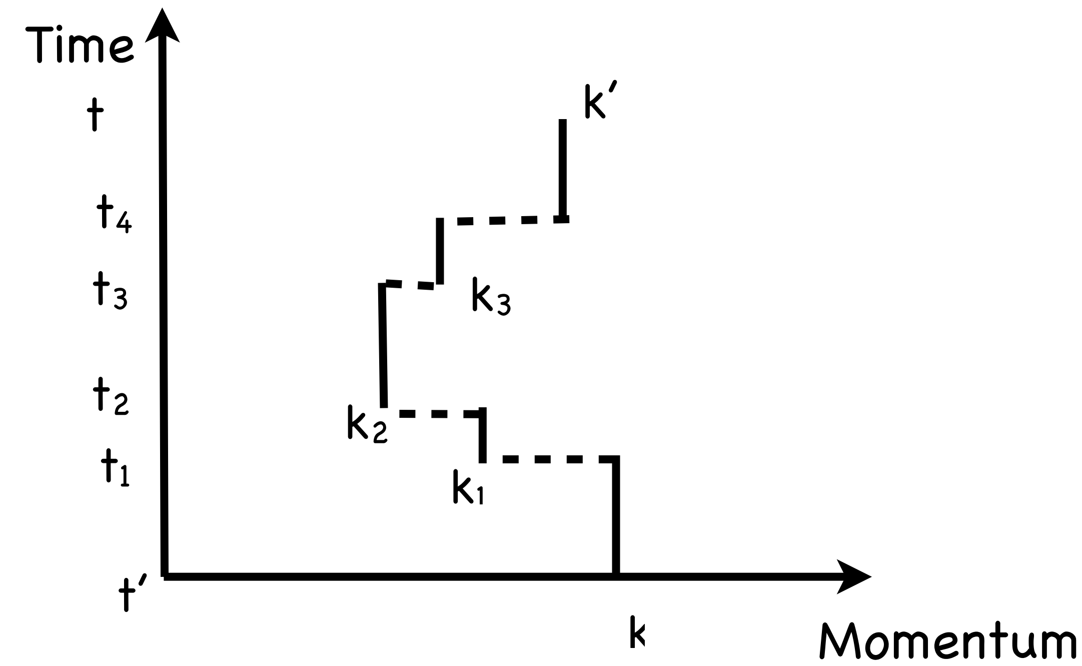
where

$$G_0^R V G_0^R = \int dr_1 \int dt_1 G_0^R(r,t;r_1,t_1)V(t_1)G_0^R(r_1,t_1;r',t')$$

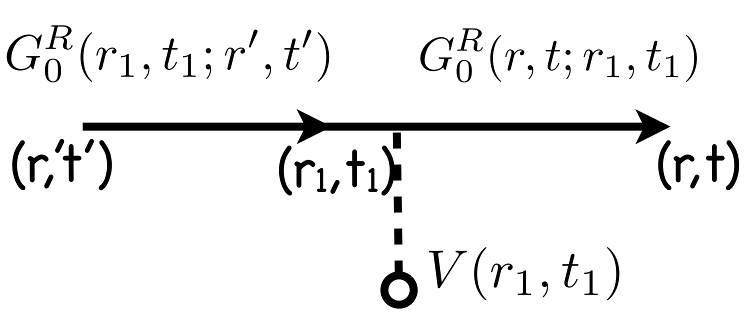
is to be thought of in Matrix Multiplication sense [matrix in (r,t) co-ord]

Pictorial Representations and Feynman Diagrams

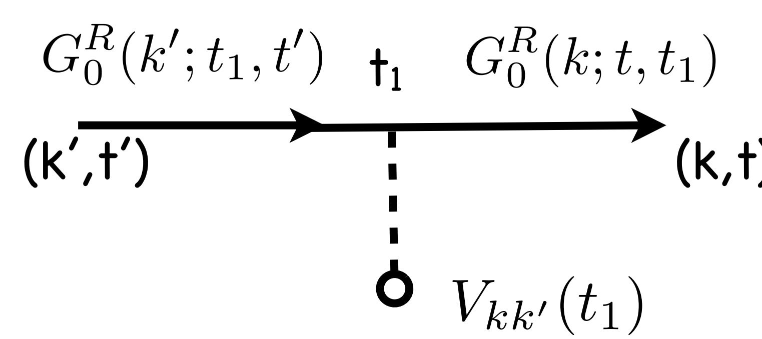


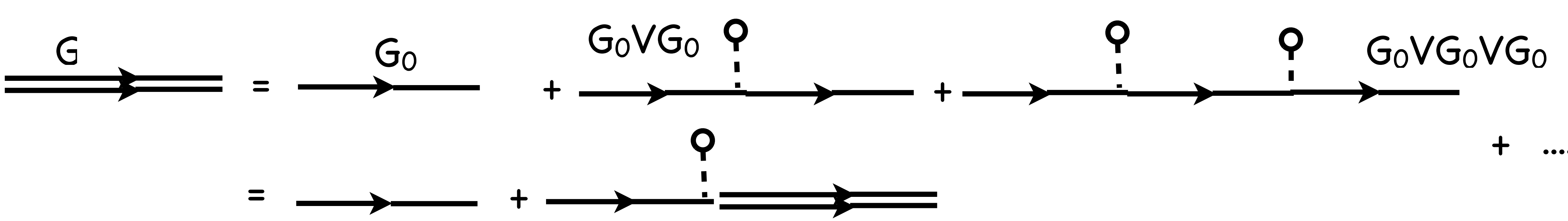


- Should not be literally interpreted as trajectories of particles
- OK as long as you read it as "free propagation followed by scattering event followed by ...."
- Remember to integrate over all co-ordinates (space+time or momentum+time) in between

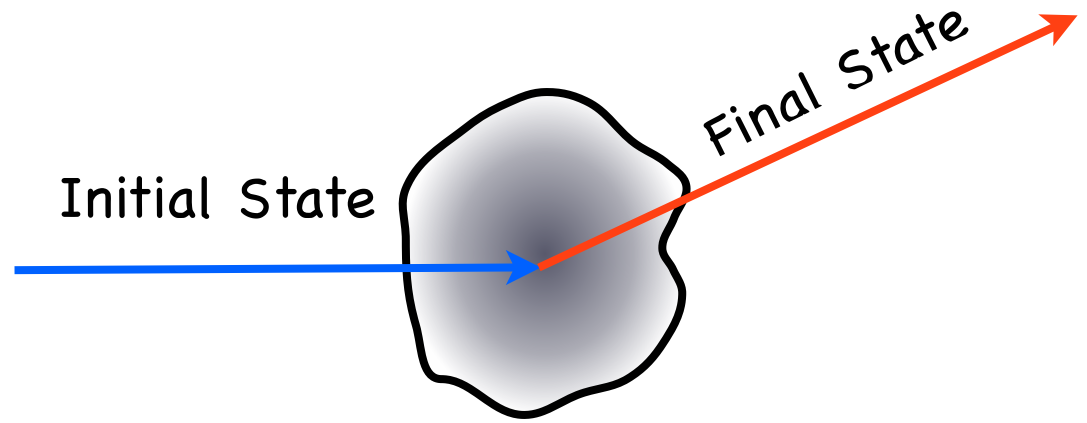


Feynman Diagrams





Scattering Matrix (S-Matrix)



Back to the scattering problem.

Incident particle in a free particle (momentum)state (in-state), which will be scattered by the potential into different free-particle (momentum)states (out states) far from the interaction region.

S-matrix is the matrix, with indices corresponding to a free-particle (say momentum) basis, whose matrix element (say $\alpha\beta$), gives the probability amplitude of obtaining the state $|\varphi_\alpha\rangle$ after scattering, if we started with $|\varphi_\beta\rangle$ as the incident state.

$$S_{\alpha\beta} = \langle \phi_\alpha | \psi_\beta^{(+)}(t \to \infty) \rangle = Lt_{t\to\infty, t'\to-\infty} iG^R(\alpha, t; \beta, t')$$

- S Matrix is unitary (Probability Conservation)
- S Matrix commutes with generators of symmetries of the full Hamiltonian (incl. potential), which are represented by unitary operators (rotation, translation etc).
- For time reversal invariant Hamiltonians, $\langle -\alpha | S | -\beta \rangle = \langle \beta | S | \alpha \rangle$

Reciprocity Property

S-Matrix and T (Transition) Matrix

$$S_{\alpha\beta} = \langle \phi_\alpha | \psi_\beta^{(+)}(t \to \infty) \rangle = Lt_{t\to\infty, t'\to-\infty} iG^R(\alpha, t; \beta, t')$$

Remember

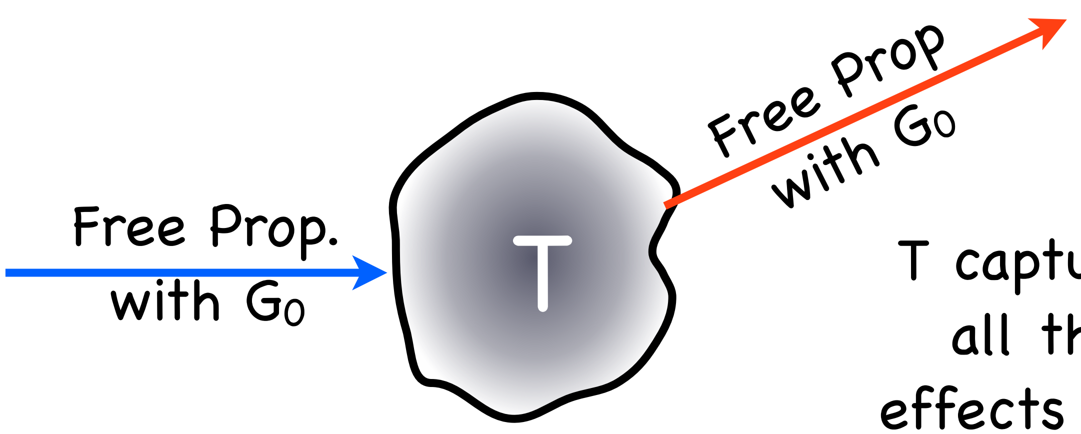
$$G^R = G_0^R + G_0^R V G_0^R + G_0^R V G_0^R V G_0^R + \ldots = G_0^R + G_0^R V G^R$$

There is a part in G^R which is just free propagation. Makes sense to isolate this from parts which depend on the potential

The part involving V has the unknown interacting propagator G^R sitting in it. We would like to write this in terms of G_0^R and push the effects of multiple scattering into a new object T.

$$G^R = G_0^R + G_0^R V G^R = G_0^R + G_0^R T G_0^R$$

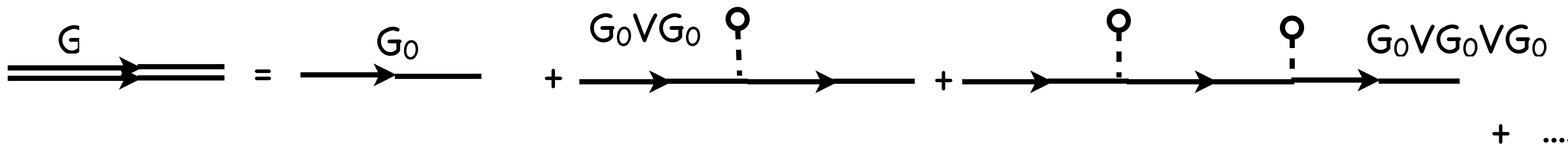
Will later relate T to measureables



T captures all the effects of V incl. multiple scatterings

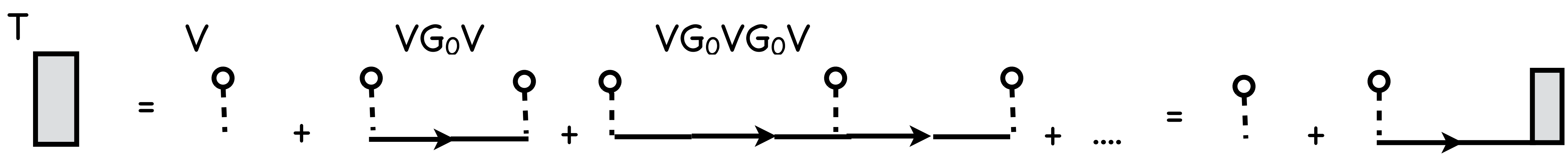
The T Matrix

The defining Equation: $VG = TG_0$ $\qquad$ $T = VGG_0^{-1}$



Now $$G = G_0 + G_0 V G_0 + .. = [1 - G_0 V]^{-1} G_0$$

So $$T = V[1 - G_0 V]^{-1} = V + V G_0 V + V G_0 V G_0 V + \ldots = V + V G_0 T$$



$$T^{-1} = V^{-1} - G_0$$

Integral Equation Form:

$$T(r,t;r',t') = \delta(r-r')\delta(t-t')V(r,t) + V(r,t)G_0^R(r,t;r',t')V(r',t')$$

$$+ \int d^d r_1 dt_1 V(r,t) G_0^R(r,t;r_1,t_1) V(r_1,t_1) G_0^R(r_1,t_1;r',t') V(r',t') + \ldots$$

Elastic Scattering and S(E)

Elastic scattering: energy of the particle is conserved, i.e. E'=E, |k'|=|k|.

V is essentially const. in time, other than being turned off at large +(-) T_0. $V(r,t) = V(r)$

In this case

$$G^R(r,t;r',t') = G^R(r,r',t-t')$$

Fourier Transform:

$$G^R(\alpha,\beta,\omega) = G_0^R(\alpha,\beta,\omega) + \sum_{\gamma\delta} G_0^R(\alpha,\gamma,\omega)V_{\gamma\delta}G^R(\delta,\beta,\omega)$$

$$S_{\alpha\beta} = iLt_{t\to\infty,t'\to-\infty} e^{iE(t-t')}G^R(\alpha,t;\beta,t') = iLt_{t\to\infty,t'\to-\infty}\int d\omega G^R(\alpha,\beta,\omega)e^{i(E-\omega)(t-t')}$$

Now $\displaystyle\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}G_0^R(\vec{k'},\vec{k},\omega)e^{i(E-\omega)(t-t')} = -i\delta_{\vec{k'},\vec{k}}e^{i(E-k^2/2m)(t-t')}$

As t-t' becomes large, the fn oscillates rapidly unless $E=k^2/2m$

$$S_{\vec{k},\vec{k'}}(E) = \delta_{\vec{k'},\vec{k}}\delta(E-k^2/2m) + iLt_{t\to\infty,t'\to-\infty}\sum_{k_1}\int\frac{d\omega}{2\pi}G_0^R(k,\omega)V_{kk1}G^R(k_1,k',\omega)e^{i(E-\omega)(t-t')}$$

Incident wave

Involves G rather than G_0

Scattered to different out states

Scattering (S) and Transition (T) Matrices

$$S_{\vec{k},\vec{k'}}(E) = \delta_{\vec{k'},\vec{k}}\delta(E-k^2/2m) + iLt_{t\to\infty,t'\to-\infty}\sum_{k_1}\int\frac{d\omega}{2\pi}G_0^R(k,\omega)V_{kk1}G^R(k_1,k',\omega)e^{i(E-\omega)(t-t')}$$

Incident wave

Involves G rather than G_0

Scattered to different out states

Let us define the Transition (T) matrix such that : $(VG^R)_{\alpha\beta}=(TG_0{}^R)_{\alpha\beta}$

$$iLt_{t\to\infty,t'\to-\infty}e^{iE(t-t')}\int dt_1\int dt_2 G_0^R(k',t,t_1)T_{k'k}(t_1,t_2)G_0^R(k,t_2,t')$$

$$= -iLt_{t\to\infty,t'\to-\infty}e^{i(E-(k')^2/2m)t}e^{-i(E-k^2/2m)t'}\int\frac{d\omega}{2\pi}\int dt_1\int dt_2 T_{k'k}(\omega)e^{-i(\omega-(k')^2/2m)t_1}e^{i(\omega-k^2/2m)t_2}$$

$$= -2\pi i\delta(E-(k')^2/2m)\delta(E-k^2/2m)T_{k'k}(E)$$

$T_{kk'}(E)$ incorporates all the effects of scattering in the interction region

$$S_{\vec{k}\vec{k'}}(E) = \delta(E-(k')^2/2m)\delta(E-k^2/2m)[\delta_{\vec{k}\vec{k'}} - 2\pi i T_{k'k}(E)]$$

Relation between S and T matrix