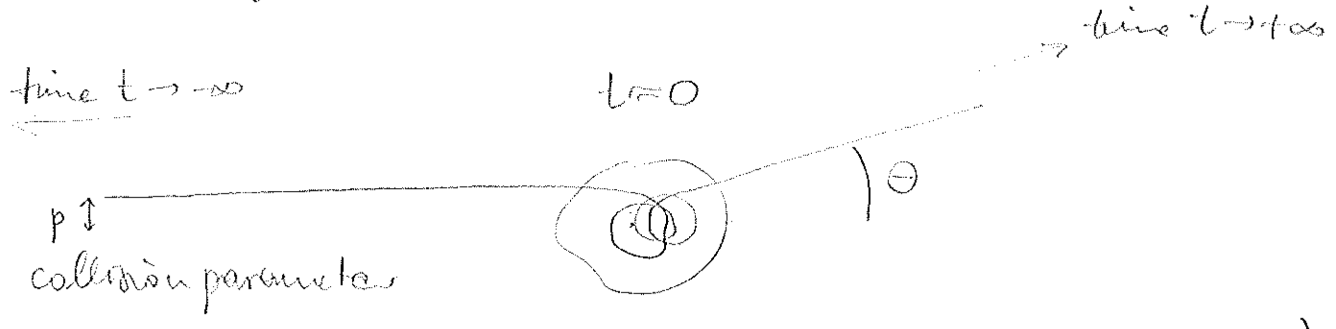
Time-dependent scattering theory.

We now consider scattering in its natural conceptual setting, namely as a time-dependent phenomenon. When a wave packet scatters off some obstacle, the long-time behaviour is not described by a simple limit as time gets long, since the scattered packet will move out of any bounded region in most cases. What one needs to construct limits is a dynamics one can compare to.

In classical mechanics, scattering at a short-range potential is schematically described



asymptotically (or, for finite-range potentials, exactly)

$$\vec{x}(t) \sim \vec{a}_- + \vec{v}_- t \quad \text{as } t \to -\infty$$

$$\vec{x}(t) \sim \vec{a}_+ + \vec{v}_+ t \quad \text{as } t \to +\infty.$$

The scattering operator is defined as the map

$$S: (\vec{a}_-, \vec{v}_-) \longrightarrow (\vec{a}_+, \vec{v}_+)$$

(which is nonlinear)

(2)

If we define $\Omega_\pm$ by

$$\Omega_+(\vec{a}_-, \vec{v}_-) = (\vec{x}(0), \dot{\vec{x}}(0))$$
$$\Omega_-(\vec{a}_+, \vec{v}_+) = (\vec{x}(0), \dot{\vec{x}}(0))$$

then

$$S : (\vec{a}_-, \vec{v}_-) \xrightarrow[\Omega_+]{} (\vec{x}(0), \dot{\vec{x}}(0)) \xrightarrow[\Omega_-^{-1}]{} (\vec{a}_+, \vec{v}_+)$$

becomes

$$S = \Omega_-^{-1} \circ \Omega_+$$

It is, of course, a physically and mathematically interesting question whether $\Omega_\pm$, Ω_-^{-1}, and S exist, whether they are everywhere defined, etc. They can in fact not be everywhere def'd if the effective radial potential $V_{eff}(r) = V(r) + \frac{L^2}{2mr^2}$ has a maximum, because then particles can get captured at certain energies ...

$\dot{r}^2 = 2m(E - V_{eff}(r))$

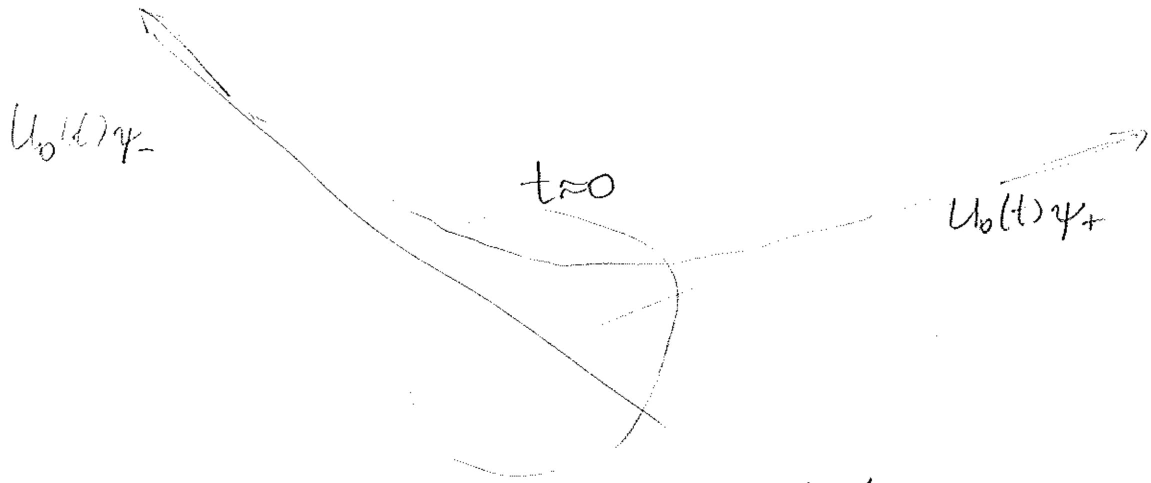
$1/r$

For Coulomb, $\Omega_\pm$ don't exist; comparison dynamics does not have straight lines.

asymptotic completeness?

The wave operators (alias Møller operators)

In QM, we proceed similarly, and compare to free motion. Schematically



The true time evolution is $\psi(t) = U(t)\psi_0$ with $U(t) = e^{-itH}$ ("$\hbar = 1$"),

where the wave packet is assumed to come in at very early times, $t \to -\infty$, and leave at late times $t \to \infty$, i.e. with

$$H_0 = \frac{p^2}{2m},$$

we expect

$$\psi(t) \approx U_0(t)\psi_\pm \quad \text{as } t \to \pm\infty.$$

More precisely, we ask if

$$\| \psi(t) - U_0(t)\psi_\pm \| \xrightarrow[t \to \pm\infty]{} 0$$

[where $\|\psi\| = \sqrt{\langle \psi | \psi \rangle}$ is the standard Hilbert space norm]

$$\psi(t) - U_0(t)\psi_\pm = U(t)\psi_0 - U_0(t)\psi_\pm$$

$$= U(t)\left(\psi_0 - U(t)^{-1}U_0(t)\psi_\pm\right)$$

Because $U(t)$ is unitary,

$$\|\psi(t) - U_0(t)\psi_\pm\| = \|\psi_0 - U(t)^{-1}U_0(t)\psi_\pm\|$$

This suggests the definition

$$\Omega_\pm = \lim_{t\to\mp\infty}\left(U(t)^{-1}U_0(t)\right)$$

Again, an obvious question is if this limit exists, and in what sense.
(this question can be asked, and the $\Omega_\pm$ are useful, for general H and H_0)

The limit does not exist in operator norm, unless $H = H_0$, in which case $\Omega_\pm = 1$,

If ϕ is an eigenvector of H_0, $H_0\phi = \epsilon\phi$, then $U(t)^{-1}U_0(t)$ does not converge as $t\to\infty$, unless $H = H_0$.

In general, therefore, the def. of $\Omega_\pm$ involves a projection: $\Omega_\pm = \lim U(t)^{-1} U_0(t) P_{ac}(H_0)$

Since H_0 has only a.c. spectrum in our case, we can omit it.

The limit is a strong limit, i.e. holds when applied to ψ: $\Omega_\pm = s\text{-}\lim_{t \to \mp\infty} U(t)^{-1} U_0(t)$.

Then $\psi_0 = \Omega_\pm \psi_\mp$.

Because $U(t)$ and $U_0(t)$ are unitary, $\Omega_\pm$ are isometries:

$$\| \Omega_\pm \psi \| = \|\psi\|.$$

However, because of the limit taken,

$$R_\pm = \mathrm{Ran}\, \Omega_\pm = \{ \Omega_\pm \phi : \phi \in \mathcal{H} \}$$

are not equal to $\mathcal{H}$.

For an arbitrary isometry Ω (with $R = \mathrm{ran}\, \Omega$)

$$\Omega^* = \begin{cases} \Omega^{-1} & \text{on } R \\ 0 & \text{on } R^\perp. \end{cases}$$

Thus $\Omega^* \Omega = \mathbb{1}$, $\Omega \Omega^* = P_R$

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Because of

$$e^{-itH}\, e^{isH}\, e^{-isH_0}\, \psi$$

$$= e^{i(s-t)H}\, e^{-i(s-t)H_0}\, e^{-itH_0}\, \psi$$

we get for $s \to \pm\infty$

$$e^{-itH}\, \Omega_\pm = \Omega_\pm\, e^{-itH_0} \qquad \text{for all } t$$

(intertwining relation; for this reason, the $\Omega_\pm$ are also called intertwiners) (1)

This implies that $R_\pm$ is invariant under e^{-itH} and that $H\restriction_{R_\pm}$ is unitarily equivalent to $H_0\restriction_{R_\pm}$. Thus $H\restriction_{R_\pm}$ has only continuous spectrum,

$$R_\pm \perp \mathcal{H}_{p.p.} = \text{bound state span}$$

Expect: $R_+ = R_- = R$, $R \oplus \mathcal{H}_{pp} = \mathcal{H}$:
asymptotic completeness. Assume this from now on
(requires proof, which can be given in our situation).
R ... space of scattering states.

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(1) This implies, more formally $\quad H\Omega_\pm = \Omega_\pm H_0$

so $\quad H = \Omega_\pm H_0 \Omega_\pm^{-1}$

We have $\psi_0 = \Omega_\pm \psi_\mp$ $\qquad$ ψ_- incoming, ψ_+ outgoing

so $\Omega_+ \psi_- = \Omega_- \psi_+$

and $\psi_+ = \Omega_-^{-1} \Omega_+ \psi_-$ $\qquad$ (inverse ex. on R)

$$= \Omega_-^* \Omega_+ \psi_-$$

The operator

$$\boxed{S = \Omega_-^* \Omega_+}$$

is called S matrix. It contains all information about the scattering process.

$$S^* S = \Omega_+^* \Omega_- \Omega_-^* \Omega_+$$

$$= \Omega_+^* \underbrace{P_R \Omega_+}_{\Omega_+}$$ since $\operatorname{ran} \Omega_+ = R_+ = R$

$$= \Omega_+^* \Omega_+ = \mathbb{1}.$$

$$S S^* = \Omega_-^* \Omega_+ \Omega_+^* \Omega_-$$

$$= \Omega_-^* P_R \Omega_- = \Omega_-^* \Omega_- = \mathbb{1}$$

Thus S is a unitary operator on the space of scattering states R.

(8)

The intertwining relation implies

$$e^{itH_0} S = e^{itH_0} \Omega_-^* \Omega_+$$
$$= \left(\Omega_- e^{-itH_0}\right)^* \Omega_+$$
$$= \left(e^{-itH} \Omega_-\right)^* \Omega_+$$
$$= \Omega_-^* e^{itH} \Omega_+$$
$$= \Omega_-^* \Omega_+ e^{itH_0}$$
$$= S e^{itH_0}$$

so $[S, e^{itH_0}] = 0$ $\quad ([S, H_0] = 0)$

"S and H_0 are jointly diagonalizable".

It also implies that $\Omega_\pm$ converts generalized EV of H_0 to ones of H: $H_0 \phi = E\phi$, $(E > 0)$

$\phi_\pm = \Omega_\pm \phi$

$\rightarrow H\phi_\pm = H\Omega_\pm \phi = \Omega_\pm H_0 \phi = \Omega_\pm E\phi = E\Omega_\pm \phi = E\phi_\pm$.

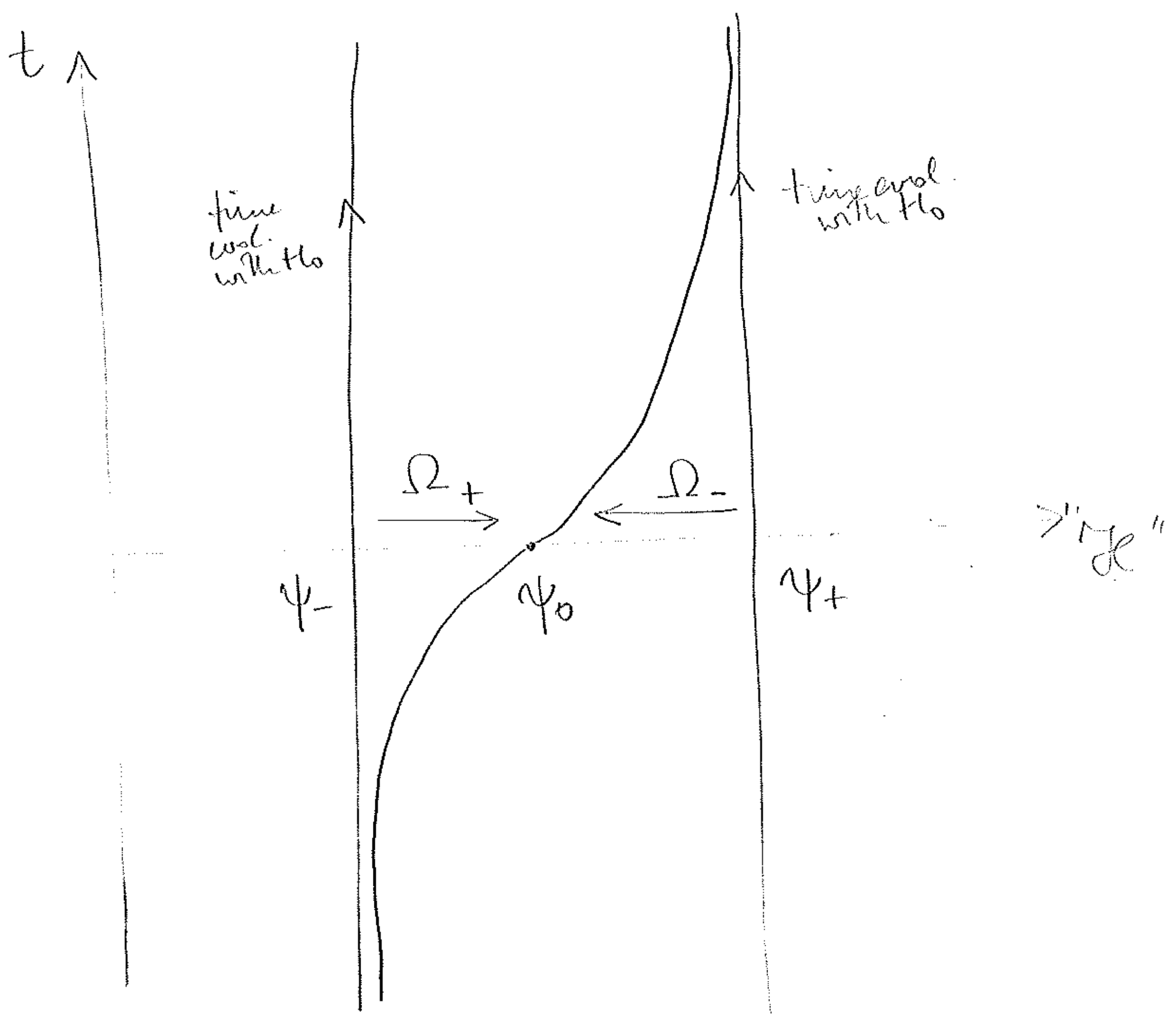
thus $\Omega_\pm$ are important by themselves for spectral theory.

<u>Summary</u>: if asymptotic completeness holds, S is unitary.

The transition probability from an initial state ψ_i to a final state ψ_f is

$$P_{fi} = |\langle \psi_f | S \psi_i \rangle|^2$$

Very schematically



(10)

An explicit proof that $\Omega_-^* \Omega_- = \mathbb{1}$.

For given ψ and $\varepsilon > 0$, there is $s > 0$ so that

$$\| (\Omega_- - e^{isH} e^{-isH_0}) \psi \| < \frac{\varepsilon}{2}$$

and $\| (\Omega_-^* - e^{isH_0} e^{-isH}) \Omega_- \psi \| < \frac{\varepsilon}{2}$.

let $\Delta = \Omega_- - e^{isH} e^{-isH_0}$

$$\Omega_-^* \Omega_- \psi = (e^{isH} e^{-isH_0} + \Delta)^* \underbrace{(e^{isH} e^{-isH_0} + \Delta)}_{\Omega_-} \psi$$

$$= \psi + \Delta^* \Omega_- \psi + e^{isH} e^{-isH_0} \Delta \psi$$

so

$$\| (\Omega_-^* \Omega_- - 1) \psi \| \leq \| \Delta^* \Omega_- \psi \| + \| \Delta \psi \| < \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon$$

Cook's method

This is a simple, but useful method. Here we use it to show the existence of the wave operators. The main idea is that

$$\frac{\partial}{\partial t}\left(e^{itH}e^{-itH_0}\right) = e^{itH}i(H-H_0)e^{-itH_0}$$

so

$$\left(e^{itH}e^{-itH_0} - e^{isH}e^{-isH_0}\right)\psi = \int_s^t e^{it'H}i(H-H_0)e^{-it'H_0}\psi\,dt' \quad (1)$$

<u>Lemma</u>: H and H_0 selfadjoint, $\mathcal{D}(H)=\mathcal{D}(H_0)$

Assume: $V=H-H_0$ satisfies $\forall\psi\in\mathcal{D}\subset\mathcal{D}(H)$ ($\mathcal{D}$ dense)

$$\int_{-\infty}^{\infty}\|Ve^{-itH_0}\psi\|\,dt<\infty \quad (2)$$

Then $\Omega_\pm$ exists.

Proof. Let $\varepsilon>0$. If $\psi\in\mathcal{D}$ then by (1)

$$\|\underbrace{(e^{itH}e^{-itH_0}-e^{isH}e^{-isH_0})}_{\Delta}\psi\| \le \int_s^t\|Ve^{-it'H_0}\psi\|\,dt'$$

By (2), $\exists\ T>0$ such that for all $s,t>T$:

$$\int_s^t\|Ve^{-itH_0}\psi\|<\frac{\varepsilon}{3}.$$

Let $\phi\in\mathcal{H}$. $\mathcal{D}$ dense $\rightarrow\exists\psi\in\mathcal{D}$: $\|\phi-\psi\|<\frac{\varepsilon}{3}$,

so $\Delta\phi = \Delta(\phi-\psi)+\Delta\psi$. Obviously, $\|\Delta\|\le 2$, so

$\|\Delta\phi\|\le 2\|\phi-\psi\|+\|\Delta\psi\| < \varepsilon$. ∎

Theorem. If $H_0 = \frac{\vec{P}^2}{2m}$ and V satisfies

$\exists\, \varepsilon > 0, c > 0$ such that for all $\vec{x}$

$$|V(\vec{x})| \leq \frac{c}{(1+|\vec{x}|)^{1+\varepsilon}}$$

then the wave operators exist.

NB: As defined, the wave op's do not exist for $\varepsilon = 0$ because the time evolution does not approach the free one in the limit. However, modified wave operators exist (one has to change the comparison dynamics).

Proof see pages 13 & 14.

The Lippmann-Schwinger equation.

In the following, we show how stationary scattering theory comes out from this. The analysis will also make clear why the outgoing spherical wave comes out. The heart of the matter is the

Theorem about abelian limits.

Let $t \mapsto f(t)$ be bounded and $\lim_{t\to\infty} f(t) = a$.

Then
$$\lim_{\varepsilon \searrow 0} \varepsilon \int_0^\infty e^{-\varepsilon t} f(t)\, dt = a.$$

Proof. Let $\delta > 0$, then by hypothesis there is $T = T(\delta) > 0$ $\forall t \geq T$: $|f(t) - a| < \delta$. Because f is bounded, the integral converges, and

$$\varepsilon \int_0^\infty f(t) e^{-\varepsilon t} dt - a = \varepsilon \int_0^\infty e^{-\varepsilon t} (f(t) - a)$$

so

$$\|\cdot\| = \varepsilon \left\| \int_0^\infty e^{-\varepsilon t}(f(t) - a) \right\| \leq \varepsilon \int_0^\infty e^{-\varepsilon t} \|f(t) - a\| dt$$

$$\leq \varepsilon \int_0^T \|f(t) - a\| dt + \varepsilon \int_T^\infty e^{-\varepsilon t} \underbrace{\|f(t) - a\|}_{\leq \delta \text{ since } t \geq T} dt$$

$$\leq \varepsilon \cdot T \cdot \sup_t \|f(t) - a\| + \varepsilon \delta \int_T^\infty e^{-\varepsilon t} dt$$

$$\leq \varepsilon T \left(\sup_t \|f(t)\| + \|a\|\right) + \delta \xrightarrow[\varepsilon \to 0]{} \delta$$

$\square$

Consider now the case of an initial state ϕ_{in} given as a plane wave, $\phi_{in}(\vec{x}) = e^{i\vec{k}\cdot\vec{x}}$.
Then $H_0 \phi_{in} = E \phi_{in}$ with $E = k^2$
(we are using natural units, where the factor $\hbar^2/2m$ drops out).

Then

$$\Omega_+ \phi_{in} = \lim_{t \to -\infty} e^{itH} e^{-itH_0} \phi_{in}$$

$$= \lim_{t \to \infty} e^{-itH} e^{itH_0} \phi_{in}$$

$$= \lim_{\varepsilon \searrow 0} \varepsilon \int_0^\infty dt\, e^{-\varepsilon t - itH} \underbrace{e^{itH_0} \phi_{in}}_{e^{itE} \phi_{in}}$$

$$= \lim_{\varepsilon \searrow 0} \varepsilon \int_0^\infty dt\, e^{it(E + i\varepsilon - H)} \phi_{in}$$

$$= \lim_{\varepsilon \searrow 0} (i\varepsilon) (E + i\varepsilon - H)^{-1} \phi_{in}$$

Call $R_H(z) = (z - H)^{-1}$ $\quad (z \notin \sigma(H))$
(resolvent of H). Then

$$\Omega_\pm \phi_{in} = \lim_{\varepsilon \searrow 0} (\pm i\varepsilon) R_H(E \pm i\varepsilon) \phi_{in}.$$

The operator eqs.

$$(A-B)^{-1} - A^{-1} = A^{-1}(A-(A-B))(A-B)^{-1}$$
$$= A^{-1} B (A-B)^{-1}$$

implies with $A = z - H_0$, $B = V$
the resolvent equation

$$R_H(z) = R_{H_0}(z) + R_{H_0}(z) V R_H(z).$$

Thus

$$\Omega_\pm \phi_{in} = \lim_{\varepsilon \searrow 0} (\pm i\varepsilon)\left[R_{H_0}(E \pm i\varepsilon) - R_{H_0}(E\pm i\varepsilon) V R_H(E\pm i\varepsilon)\right]\phi_{in}$$

Because $H_0 \phi_{in} = E\phi_{in}$

$$(\pm i\varepsilon) R_{H_0}(E \pm i\varepsilon)\phi_{in} = \frac{(\pm i\varepsilon)}{(\pm i\varepsilon)}\phi_{in} = \phi_{in}$$

and
$$\phi_0 = \Omega_+ \phi_{in}$$
satisfies the Lippmann-Schwinger equation

$$\phi_0 = \phi_{in} + R_{H_0}(E + i\varepsilon) V \phi_0$$

$$\Leftrightarrow (1 - R_{H_0}(E+i\varepsilon)V)\phi_0 = \phi_{in},$$

(18) With $\langle \vec{x} | \phi_0 \rangle = \phi_0(\vec{x})$ etc, have

$$\phi_0(\vec{x}) = e^{i\vec{k}\cdot\vec{x}} - \int G_0(\vec{x},\vec{y})\, V(\vec{y})\, \phi_0(\vec{y})\, d\vec{y}$$

where

$$G_0(\vec{x},\vec{y}) = \langle \vec{x} | R_{H_0}(E+i0) \underbrace{\,}_{\int d^3p\, |\vec{p}\rangle\langle\vec{p}|} \vec{y} \rangle$$

$$= \lim_{\varepsilon \downarrow 0} \int d^3p\; e^{i\vec{p}(\vec{x}-\vec{y})} \cdot \left(E + i\varepsilon - p^2 \right)^{-1}$$

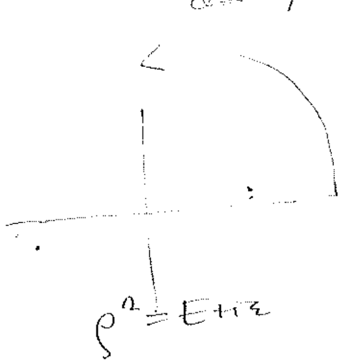
$\langle \vec{x} | \vec{p} \rangle = e^{i\vec{p}\cdot\vec{x}}$

To calculate G_0, we use polar coord. (ρ, θ, φ) for $\vec{p}$ such that $\vec{p}\cdot(\vec{x}-\vec{y}) = \rho \cdot |\vec{x}-\vec{y}| \cdot \cos\theta$.

Call $|\vec{x}-\vec{y}| = r$, then:

$$G_0(\vec{x},\vec{y}) = \frac{1}{(2\pi)^3} \cdot 2\pi \int_0^\infty \rho^2 d\rho \underbrace{\int_0^\pi \sin\theta\, d\theta\, e^{i\rho r\cos\theta}}_{\frac{e^{i\rho r} - e^{-i\rho r}}{i\rho r}} \frac{1}{E+i\varepsilon-\rho^2},$$

r > 0: close in upper plane



$$= \frac{1}{2\pi r} \cdot \frac{1}{2\pi i} \int_0^\infty \rho\, d\rho \left(e^{i\rho r} - e^{-i\rho r} \right) \frac{1}{E+i\varepsilon-\rho^2}$$

$$= \frac{1}{2\pi r} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \rho\, d\rho\, \frac{e^{i\rho r}}{E+i\varepsilon-\rho^2}$$

$$= \frac{1}{2\pi r} \sqrt{E+i\varepsilon}\; \frac{e^{i\sqrt{E+i\varepsilon}\, r}}{2\sqrt{E+i\varepsilon}}$$

$$\xrightarrow[\varepsilon \downarrow 0]{} \frac{1}{4\pi r} e^{ikr} \quad \text{since } \sqrt{E} = k.$$