

Lecture 4

Evolution operator

Free particle

UNITARY GROUPS

L1

Def. The family of linear operators $U(t)$, $t \in \mathbb{R}$ is a strongly continuous one-parameter group of unitary oper. in \mathcal{X} if

i) $U(t)$ is a unitary op. in \mathcal{X} $\forall t \in \mathbb{R}$

one-parameter

ii) $U(t+s) = U(t)U(s)$ $\forall s, t \in \mathbb{R}$

group property

iii) $\lim_{t \rightarrow 0} \|U(t)f - f\| = 0$ $\forall f \in \mathcal{X}$

continuity in $t=0$

\Rightarrow continuity $\forall t \in \mathbb{R}$

Prop. Let $A, D(A)$ be s.e. on Z . Then $U(t) = e^{itA}$ L2

$t \in \mathbb{R}$ is a strongly cont. one-parameter group of unitary operators. Moreover $f \in D(A) \Rightarrow e^{itA} f \in D(A)$

and

$$\rightarrow \frac{d}{dt} e^{itA} f \Big|_{t=0} = \lim_{t \rightarrow 0} \frac{1}{t} (e^{itA} f - f) = iAf$$

Proof i) unitarity of $U(t) \forall t \in \mathbb{R}$

$\forall t \rightarrow \phi(\lambda) = e^{it\lambda}$ continuous & bounded
funct. calculus $\rightarrow U(t) = e^{itA}$ bounded operator

• $U(t)^* = U(-t)$ • $1 = e^{it\lambda} e^{-it\lambda} \rightarrow 1 = U(t)U(-t) = U(-t)U(t)$

$\Rightarrow U(t)^{-1} = U(-t) = U(t)^* \Leftrightarrow U(t)$ unitary

ii) group prop. $\phi_t(\lambda) = e^{it\lambda}$ L3
 $\phi_{t+s}(\lambda) = \phi_t(\lambda)\phi_s(\lambda) \Rightarrow U(t+s) = U(t)U(s)$

iii) $\| e^{itA} f - f \|^2 = \int |e^{it\lambda} - 1|^2 d(\langle E_A(\lambda) f, f \rangle)$

$\xrightarrow{t \rightarrow 0} 0$ by dominated convergence

• $\| \frac{1}{t} (e^{iAt} f - f) - iAf \|^2$

$= \int | \frac{1}{t} (e^{it\lambda} - 1) - i\lambda f |^2 d(\langle E_A(\lambda) f, f \rangle)$

$\xrightarrow{t \rightarrow 0} 0$ by dom. conv.

STONE'S THEM Given a strongly continuous one- L4
parameter group of unitary op. $U(t)$, $t \in \mathbb{R}$, $\exists!$ s.e.
operator A , $D(A)$ s.t. $U(t) = e^{itA}$,

EVOLUTION OF A STATE IN QM

Let H , $D(H)$ be the s.e. Hamiltonian of a certain system defined on \mathcal{H} . Let $\psi_0 \in \mathcal{H}$ be the initial state. Then the state at time $t > 0$ is def. by

$$\psi(t) = \underbrace{e^{-\frac{it}{\hbar} H}}_{\text{PROPAGATOR}} \psi_0$$

Exercise $H_D = -\Delta$ on $L^2(0, \pi)$

$$D(H_D) = \left\{ f : \sum_n n^4 |\langle \phi_n, f \rangle|^2 < \infty \right\}$$

$$\phi_n(x) = \sqrt{\frac{2}{\pi}} \sin nx \quad n=1, 2, \dots$$

$$\hookrightarrow \lambda_n = n^2$$

Verify

$$(e^{-itH_D} f)(x) = \sum_n \underbrace{e^{-itn^2}}_{\substack{\uparrow \\ \text{evolution of } \phi_n(x)}} \langle \phi_n, f \rangle \phi_n(x)$$

FREE PARTICLE

L7

Classical case: $H_0^d = p^2/2m \leftarrow$ travel on \mathbb{R}^d

Step 1. Construction of $\mathcal{H}, D(\mathcal{H})$ as s.e. op. on $L^2(\mathbb{R}^d)$

By Weyl quantization $p_j \rightarrow \frac{\hbar}{i} \frac{\partial}{\partial x_j}$

$$\dot{H}_0 = -\frac{\hbar^2}{2m} \Delta, \quad D(\dot{H}_0) = \mathcal{S}(\mathbb{R}^d)$$

We use that \dot{H}_0
is a multiplication
operator in Fourier

is it s.e. ? if not
how to find the self-adjoint ext.?

$$(\hat{H}_0 \hat{f}^\wedge)(k) := \underbrace{(\mathcal{F} \hat{H}_0 \mathcal{F}^{-1} \hat{f}^\wedge)}_{:= \hat{H}_0}(k) = \frac{\hbar^2 k^2}{2m} \hat{f}^\wedge(k)$$

Hence

$$D(\hat{H}_0) = \left\{ f \in L^2(\mathbb{R}^d) : \int dk |k^2 \hat{f}^\wedge(k)|^2 < \infty \right\}$$

$\int d\lambda |\lambda|^2 |f(\lambda)|^2 < \infty$

We conclude

$$(H_0 f)(x) = \underbrace{(\mathcal{F}^{-1} \hat{H}_0 \mathcal{F} f)}(x) = \int \frac{d^d k}{(2\pi)^{d/2}} e^{i k \cdot x} \frac{\hbar^2 k^2}{2m} \hat{f}^\wedge(k)$$

$$D(H_0) = \left\{ f \in L^2(\mathbb{R}^d) : \int dk |k^2 \hat{f}^\wedge(k)|^2 < \infty \right\} := H^2(\mathbb{R}^d)$$

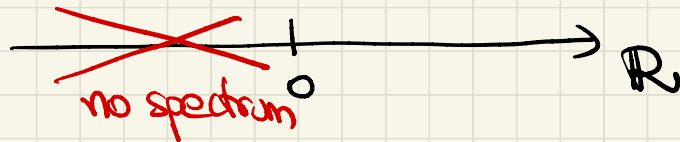
STEP 2 - Analysis of the spectrum of H_0 (H)

L9

- H_0 is s.e. $\Rightarrow \sigma(H_0) \subset \mathbb{R}$

- the resolvent in Fourier space is

$$\phi_z(\lambda) = \frac{1}{\lambda - z} \longrightarrow \frac{1}{\frac{\hbar^2 k^2}{2m} - z}$$



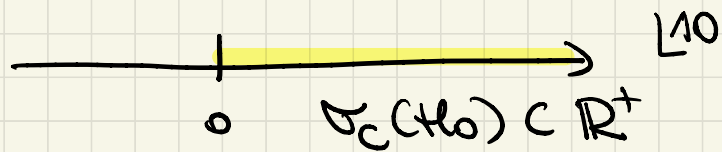
it is well defined as z bounded operator $\Leftrightarrow z < 0$

- H_0 has no eigenvalues. Assume that for $\lambda \in \mathbb{R}^+$, $\exists \phi_\lambda \in D(H_0)$ s.t. $\widehat{H}_0 \widehat{\phi}_\lambda = \lambda \widehat{\phi}_\lambda$

$$\text{then } 0 = \|(\widehat{H}_0 - \lambda)\widehat{\phi}_\lambda\|^2 = \int \left(\frac{\hbar^2 k^2}{2m} - \lambda\right)^2 |\widehat{\phi}_\lambda(k)|^2 dk$$

$$\Leftrightarrow \widehat{\phi}_\lambda = 0 \text{ a.e.} \Rightarrow \lambda \text{ is not an eigenvalue}$$

How to characterize $\sigma_c(H_0)$?



Spectral family

$$(\widehat{E}_0(\lambda) f)(k) = \chi_{(-\infty, \lambda]} \left(\frac{\hbar^2 k^2}{2m} \right) \widehat{f}(k) = \begin{cases} \widehat{f}(k) & \frac{\hbar^2 k^2}{2m} \leq \lambda \\ 0 & \text{otherwise} \end{cases}$$

$\lambda=1$

$$\langle \widehat{E}_0(\lambda) f, g \rangle = \int \chi_{(-\infty, \lambda]} \left(\frac{\hbar^2 k^2}{2m} \right) \overline{\widehat{f}(k)} \widehat{g}(k) dk$$

$\rightarrow \leq \frac{\hbar k}{\sqrt{2m}} \leq \lambda$

$$\begin{aligned} \stackrel{\text{for } \lambda > 0}{=} & \chi_{(0, \infty)}(\lambda) \int_0^{+\infty} \chi_{(0, \lambda]} \left(\frac{\hbar^2 k^2}{2m} \right) \left(\overline{\widehat{f}(k)} \widehat{g}(k) + \overline{\widehat{f}(-k)} \widehat{g}(-k) \right) dk \\ & = \chi_{(0, \infty)}(\lambda) \int_0^{\sqrt{2m\lambda}/\hbar} \left(\overline{\widehat{f}(k)} \widehat{g}(k) + \overline{\widehat{f}(-k)} \widehat{g}(-k) \right) dk \end{aligned}$$

the distr. function $\lambda \rightarrow \langle \widehat{E}_0(\lambda) f, f \rangle$ is abs. continuous w.r.t. Lebesgue

$\forall f \in L^2(\mathbb{R}) \rightarrow m_0^f$ is abs. continuous

L11

$$m_0^f((a, b]) = \langle E_0(b) f, f \rangle - \langle E_0(a) f, f \rangle$$

$$= \int_a^b \frac{d}{d\lambda} \langle E_0(\lambda) f, f \rangle d\lambda$$

Exercise: compute $\frac{d}{d\lambda} \langle E_0(\lambda) f, f \rangle$

$$\sigma(H_0) = \sigma_{ac}(H_0) = [0, +\infty)$$

Step 3 UNITARY EVOLUTION

L12

free propagator $\rightarrow U_0(t) = e^{-i \frac{t}{\hbar} H_0}$

$$(U_0(t)f)(x) = \frac{1}{(2\pi)^3} \int e^{ik \cdot x} \underbrace{e^{-i \frac{\hbar^2 k^2}{2m} t}}_{e^{-i \frac{t}{\hbar} H_0}} \hat{f}(k) dk$$

Check some result by using func. cal.

$$\langle g, U_0(t)f \rangle = \int_0^{+\infty} e^{-i \frac{t}{\hbar} \lambda} d(\langle E_0(\lambda)g, f \rangle)$$

Next step expression of $U_0(t)$ as an integral operator

Prop. Let $f \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$ then

L13

$$\left(e^{-it\frac{\Delta}{\hbar}} f \right)(x) = \left(\frac{m}{2\pi i \hbar t} \right)^{1/2} \int f(y) e^{i\frac{m}{2\hbar t} (x-y)^2} dy \quad (1)$$

Moreover, if $f \in L^2(\mathbb{R})$

$$\left(e^{-it\frac{\Delta}{\hbar}} f \right)(x) = \left(\frac{m}{2\pi i \hbar t} \right)^{1/2} \lim_{n \rightarrow \infty} \int_{|y| < n} f(y) e^{i\frac{m}{2\hbar t} (x-y)^2} dy \quad (2)$$

where the limit is in the L^2 -sense.

Rk. From (1) one obtains

$$\sup_{x \in \mathbb{R}^d} \left| \left(e^{-it\frac{\Delta}{\hbar}} f \right)(x) \right| \leq \frac{m}{2\pi\hbar} \frac{1}{|t|^{1/2}} \|f\|_2$$

DISPERSIVE
character of the
free evolution

Prop. Let $f \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$ then

$$(e^{-\frac{it}{\hbar} H_0} f)(x) = \left(\frac{m}{2\pi i \hbar t}\right)^{1/2} \int f(y) e^{i \frac{m}{2\hbar t} (x-y)^2} dy \quad (1)$$

Moreover, if $f \in L^2(\mathbb{R})$

$$(e^{-\frac{it}{\hbar} H_0} f)(x) = \left(\frac{m}{2\pi i \hbar t}\right)^{1/2} \lim_{n \rightarrow +\infty} \int_{|y| < n} f(y) e^{i \frac{m}{2\hbar t} (x-y)^2} dy \quad (2)$$

Show that (1) \Rightarrow (2). For $f \in L^2(\mathbb{R})$, take $f_n := \chi_{|y| < n} f$

then $f_n \in L^2 \cap L^1$ and (1) holds for f_n with $\int dy$

$$\rightarrow \int_{|y| < n}.$$

Now

$$\| e^{-\frac{it}{\hbar} H_0} f - e^{-\frac{it}{\hbar} H_0} f_n \| = \| f - f_n \| \xrightarrow{n \rightarrow +\infty} 0$$

↑
unitarity of the group

Proof 1) $\forall g, f \in \mathcal{S}(\mathbb{R})$

$$\langle g, e^{-\frac{i\hbar}{\hbar} H_0} f \rangle = \int \overline{\hat{g}(k)} e^{-i\hbar \frac{k^2}{2m}} \hat{f}(k) dk$$

→ by density argument one extend for $f \in L^2 \cap L^1$ LS

$$= \lim_{\varepsilon \rightarrow 0} \int \overline{\hat{g}(k)} \hat{f}(k) e^{-(\varepsilon + i\hbar) k^2} dk$$

$$= \lim_{\varepsilon \rightarrow 0} \int \overline{g(x)} f(y) \int e^{-(\varepsilon + i\hbar) k^2 + ik(x-y)} dk dx dy$$

Use $\int_{-\infty}^{+\infty} dt e^{-at^2 + i\lambda t} = \sqrt{\frac{\pi}{|a|}} e^{-\frac{\lambda^2}{4a} - \frac{i}{2}\phi}$ $a = |a| e^{i\phi}$
 $\lambda \in \mathbb{R}$

$$= \lim_{\varepsilon \rightarrow 0} \frac{\sqrt{\pi}}{(2\pi)} \int \overline{g(x)} f(y) \frac{1}{(\varepsilon^2 + \hbar^2)^{1/4}} e^{-\frac{(x-y)^2}{4(\varepsilon + i\hbar)}} e^{-\frac{i}{2} \arctan(\hbar/\varepsilon)} dx dy$$

by dom. conv. $= \frac{1}{2\sqrt{\pi\hbar}} \int \overline{g(x)} f(y) e^{-\frac{(x-y)^2}{4i\hbar}} \left(e^{-\frac{i}{2} \frac{\pi}{2}} \right) = (-i)^{1/2} \star$

STEP 4 APPLICATION

L16

Prop. Asymptotic behavior For any $\phi \in L^2(\mathbb{R})$ we have, let

$$\phi_t^a(x) = \left(\frac{m}{i\hbar t}\right)^{1/2} e^{i\frac{m}{2\hbar t}x^2} \widehat{\phi}\left(\frac{mx}{\hbar t}\right), \quad \lim_{t \rightarrow \pm\infty} \left\| e^{-i\frac{t}{\hbar}H_0} \phi - \phi_t^a \right\| = 0$$

Proof fix $\phi \in L^2(\mathbb{R}) \cap L^1(\mathbb{R})$.

$$\begin{aligned} \left(e^{-i\frac{t}{\hbar}H_0} \phi \right)(x) &= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} \int \phi(y) e^{i\frac{m}{2\hbar t}(x-y)^2} dy \quad \widehat{\phi}\left(\frac{mx}{\hbar t}\right) \\ &= \left(\frac{m}{2\pi i\hbar t}\right)^{1/2} e^{i\frac{m}{2\hbar t}x^2} \int \phi(y) e^{-i\frac{m}{\hbar t}xy} e^{i\frac{m}{2\hbar t}y^2} dy \end{aligned}$$

$$:= \phi_t^a(x) + R_t(x)$$

GOAL Show $\|R_t\| \xrightarrow[t \rightarrow \pm\infty]{} 0$

$$R_t(x) = \left(\frac{m}{\hbar t}\right)^{1/2} e^{i \frac{m}{2\hbar t} x^2} \underbrace{\frac{1}{2\pi} \int \phi(y) \left(e^{i \frac{m}{2\hbar t} y^2} - 1 \right) e^{-i \frac{m}{\hbar t} xy} dy}_{\hat{h}\left(\frac{mx}{\hbar t}\right)}$$

$$\|R_t\|^2 = \frac{m}{\hbar|t|} \int dx \left| \hat{h}\left(\frac{mx}{\hbar t}\right) \right|^2$$

$$\stackrel{z = \frac{mx}{\hbar t}}{\leq} \int dz \left| \hat{h}(z) \right|^2 = \|\hat{h}\|^2$$

$$= \int \left| \phi(y) \right|^2 \left| e^{i \frac{m}{2\hbar t} y^2} - 1 \right|^2 dy \xrightarrow[t \rightarrow \pm\infty]{} 0$$

by dom. convergence

For $\phi \in L^2$ the result obtained
by a density argument.

SCATTERING

Prop Any state is a scattering state (0 diffusion state) w.r.t. the free dynamics ie \forall fixed $R > 0, \forall \phi \in L^2(\mathbb{R})$

$$\phi_t = e^{-\frac{it\hbar_0}{\hbar}} \phi \text{ is s.t.}$$

$$\lim_{t \rightarrow \pm\infty} \int_{|x| < R} |\phi_t(x)|^2 dx = 0$$

Hence

$$\mathbb{P}(x \in (-R, R); e^{-\frac{it\hbar_0}{\hbar}} \phi) = \int_{-R}^R |\phi_t(x)|^2 dx \xrightarrow{t \rightarrow \pm\infty} 0$$

INTERPRET Irresp. on the initial condition and on the choice of R after a suff. long time the particle exits $[-R, R]$ (or the ϵ -dim. ball of rad. R in higher dimensions)

Proof ($d=1$)

$$\| \chi_{<R} e^{-\frac{it}{\hbar} H_0} \phi \|$$

$$\leq \| \chi_{<R} (e^{-\frac{it}{\hbar} H_0} \phi - \phi_t^a) \| + \| \chi_{<R} \phi_t^a \|$$

$$\leq \| (e^{-\frac{it}{\hbar} H_0} \phi - \phi_t^a) \| + \underbrace{\int_{-R}^R \frac{B}{\hbar|t|} |\hat{\phi}\left(\frac{mx}{\hbar t}\right)|^2 dx}$$

\downarrow $t \rightarrow +\infty$
0

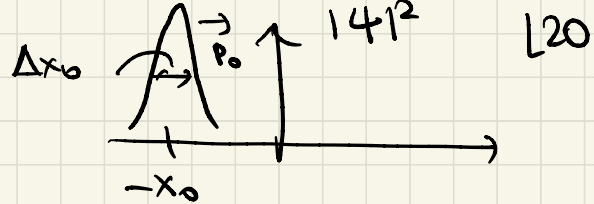
due to the asymptotic
behavior result

$$\begin{aligned} &= \int_{-\frac{mR}{\hbar t}}^{\frac{mR}{\hbar t}} |\hat{\phi}(y)|^2 dy \\ &\quad \downarrow t \rightarrow +\infty \\ &0 \end{aligned}$$

$$\phi_t^a(x) = \left(\frac{m}{i\hbar t}\right)^{\frac{1}{2}} e^{\frac{imx^2}{2\hbar t}} \hat{\phi}\left(\frac{mx}{\hbar t}\right) \quad \text{L19}$$

FREE EVOLUTION of a WAVE PACKET

Let $f \in \mathcal{V}(\mathbb{R})$, real, even, $\|f\| = 1$



$$\psi_0 = \frac{1}{\sqrt{\sigma}} f\left(\frac{x+x_0}{\sigma}\right) e^{i \frac{p_0}{\hbar} x} \quad \text{wave packet}$$

$$\Delta x_0 \Delta p_0 \geq \frac{\hbar}{2}$$

for $x_0, p_0, \sigma > 0$ given parameters

Check $\langle x \rangle(0) = -x_0$ ← f is even

$$\langle p \rangle(0) = p_0$$

$$\Delta x(0)^2 = \sigma^2 \|\hat{f}'\|_2^2$$

$$\Delta p(0)^2 = \frac{\hbar^2}{\sigma^2} \|f'\|_2^2$$

$$\Rightarrow \Delta x(0) \Delta p(0) = \hbar \|f'\| \|\hat{f}'\|$$

RK Minimal uncertainty is reached $\|f'\| = \|\hat{f}'\| = 1/\sqrt{2}$. This is the case $f(x) = e^{-x^2/2} / \pi^{1/4} \leftrightarrow \hat{f}(k) = e^{-k^2/2} / \pi^{1/4}$ GAUSSIAN WAVE PACKET

Time evol

$$\psi_t = e^{-\frac{i}{\hbar} t H_0} \psi_0^{x_0, p_0, \sigma}$$

L21

$$\bullet \langle p \rangle(t) = \int dx \overline{\psi_t(x)} \frac{\hbar}{i} \frac{d}{dx} \psi_t(x) = \hbar \int dk k |\widehat{\psi}_t(k)|^2 = \langle p \rangle(0)$$

$$|\widehat{\psi}_0(k)|^2$$

the momentum is a constant of motion for the free particle evol.

$$= p_0$$

$$\langle \Delta p \rangle(t) = \langle \Delta p \rangle(0)$$

$$\widehat{\psi}_t(k) = e^{-\frac{i \hbar t}{2m} k^2} \widehat{\psi}_0(k)$$

$$\bullet \langle x \rangle(t) = \int dk \widehat{\psi}_t(k) i \frac{d}{dk} \widehat{\psi}_t(k)$$

$$= \int dk \widehat{\psi}_0(k) \left(\frac{\hbar t}{m} k + i \frac{d}{dk} \widehat{\psi}_0(k) \right)$$

$$= \frac{p_0}{m} t - x_0$$

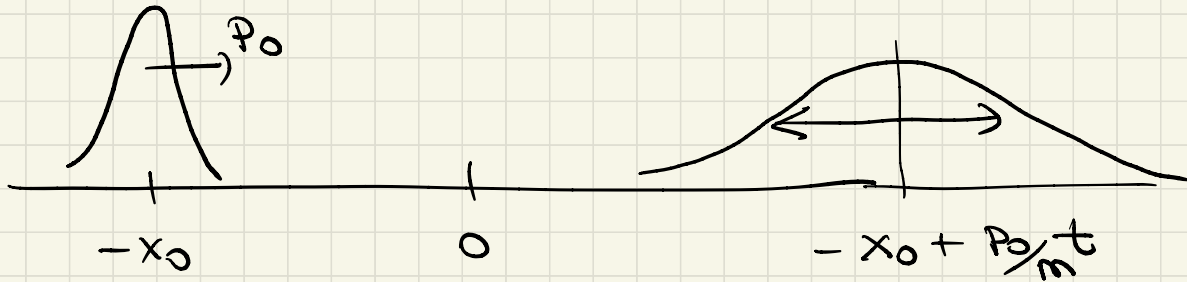
the mean value is moving with uniform velocity p_0/m towards the right, starting from $-x_0$

For a gaussian wave packet an explicit comput. gives:

L22

$$\Delta x(t)^2 = \underbrace{\left(\frac{t}{m}\right)^2 \Delta p(0)^2}_{\text{increase in time}} + \Delta x(0)^2$$

increase in time: the wave packet is going to diffuse as time goes on



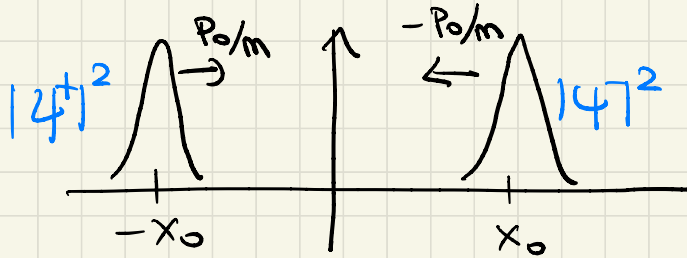
→ we lost information on the position of the particle.

INTERFERENCE of two wave packets

[23

Consider the one particle state

$$\psi_0 = \underbrace{c}_{\substack{\text{normalization} \\ \text{constant}}} \left[\underbrace{\frac{1}{\sqrt{\sigma}} f\left(\frac{x+x_0}{\sigma}\right)}_{\psi^+(x)} e^{i\frac{p_0 x}{\hbar}} + \frac{1}{\sqrt{\sigma}} f\left(\frac{x-x_0}{\sigma}\right) e^{-i\frac{p_0 x}{\hbar}} \right]$$



$\frac{\sigma}{x_0} \ll 1$ well separated bumps

Evolved state

$$\psi_t(x) = c \left[e^{-i\frac{t}{\hbar} E_0} \psi^+(x) + e^{-i\frac{t}{\hbar} E_0} \psi^-(x) \right]$$

Question what happens at time t : $\frac{p_0}{m} t = x_0$, ie when the centers of the two bumps reach the origin.

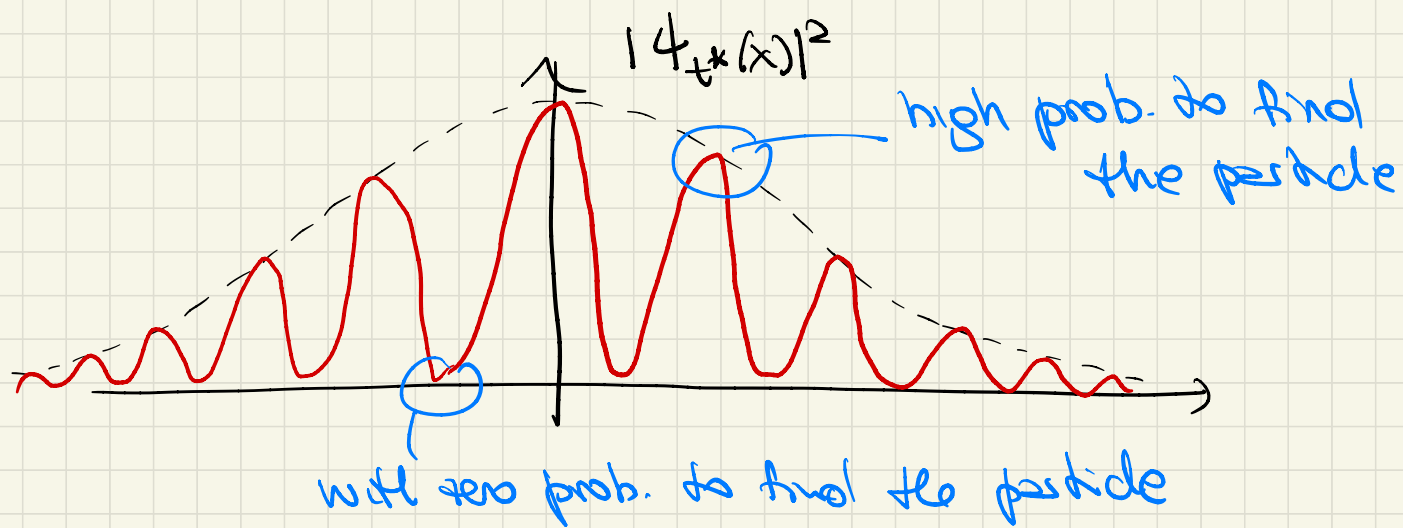
Compute $\psi_t(x) |_{t^* = m x_0 / p_0}$. In the gaussian case L24
 one finds

$$|\psi_{t^*}(x)|^2 = \underbrace{\frac{4c^2}{\sqrt{\pi} \sigma \sqrt{1+\alpha^2}}}_{\text{gaussian bump}} e^{-\frac{x^2}{\sigma^2(1+\alpha^2)}} \underbrace{\cos^2\left(\frac{p_0}{\hbar} x\right)}_{\text{modulation factor which oscillates over space}}$$

with $\alpha = \frac{\hbar x_0}{\sigma^2 p_0} \gg 1$
 gaussian bump
 with variance
 $\sigma \sqrt{1+\alpha^2} \gg \sigma$
 (expected)

RR zero of $\cos^2(\cdot) \Leftrightarrow x_k^0 = (2k+1) \frac{\pi}{2} \frac{\hbar}{p_0} \quad k \in \mathbb{Z}$

zeros in $|x| < \sigma \sqrt{1+\alpha^2} \Leftrightarrow |2k+1| \frac{\pi}{2} \frac{\hbar}{p_0} < \sigma \sqrt{1+\alpha^2}$ lots of zeros in there
 $\Leftrightarrow |2k+1| < \frac{2}{\pi} \frac{p_0}{\hbar} \sigma \frac{\hbar x_0}{\sigma^2 p_0} \sqrt{1+\alpha^2} \sim \frac{x_0}{\sigma} \gg 1$ where $1+\alpha^2 \neq 0$



When the 2 packets overlap we have an INTERFERENCE figure - with no classical counterpart!

→ TWO SLIT EXPERIMENT

RK you cannot interpret $\psi_0(x)$ with two bumps by saying that the particle is to the right with some probability or to the left with complementary prob.

References

Propagator of the quantum evolution

Sec. 4.9 Tetz's book

Free particle

Sec 6.1-6.4 Tetz's book