February 8, 2012

The Free Particle

Abstract Method aka

Operator Method
Algebraic Method
Use the Algebra of the Operators
Basis Free Method

Go into a Basis

Solve the Differential Equation: TDSE and TISE
Freshman Physics Method to Solve Differential Equations
Standard Method to Solve Differential Equations
The eigenstates of momentum
The eigenstates of position
The eigenstates of energy
The time evolution of the eigenstates
Separation of variables
Separating time and space: TDSE => TISE

Gaussian Superposition of Eigenstates

Dispersion Relations
The Propagator
The time evolution of the position
The time evolution of the momentum
The time evolution of the energy

Fourier Transforms and Dirac Notation

Fourier transforms in space
spatial frequency: wavevector and momentum: k and p
Fourier transforms in time
temporal frequency: angular frequency and energy: ω and E

LECTURE 18 7-22-09

TODAY: SOLVE FREE PARTICLE PROBLEM

TWO WAYS

(1) ABSTRACT METHOD

$$\mathcal{H} = \frac{p^2}{2m} + V(x)$$ classical Hamiltonian

FREE $\Rightarrow$ $F = 0$ $\quad F = \frac{\partial V}{\partial x}$ $\Rightarrow$ $V = $ CONSTANT $= 0$

$$H = \frac{P_{op}^2}{2m}$$ quantum Hamiltonian

$$H \,|E_n\rangle = E_n \,|E_n\rangle$$ TISE

$$\frac{P_{op}^2}{2m} \,|E_n\rangle = E_n \,|E_n\rangle$$ TISE

$[H, P_{op}] = 0 \Rightarrow$ H AND P_{op} SHARE ALL $e\vec{v}$'s

H and p commute

$$\frac{P_{op}^2}{2m} \,|p\rangle = E \,|p\rangle$$

$$P_{op} \,|p\rangle = p \,|p\rangle \Rightarrow \frac{p^2}{2m} \,|p\rangle = E \,|p\rangle$$

$$\Rightarrow \boxed{\begin{aligned} \frac{p^2}{2m} &= E \\ p &= \pm\sqrt{2mE} \end{aligned}}$$

AKA, OPERATOR METHOD

BASIS FREE

ALGEBRA OF THE OPERATORS

$\Rightarrow$ TWO ORTHONORMAL EIGENKETS FOR EACH EIGEN ENERGY.

H_{op} IS 2-FOLD DEGENERATE

P_{op} IS NOT $|+p\rangle$ momentum eigen KETS

$|-p\rangle$

$|E, p\rangle$

$|E,+\rangle = |E, p = +\sqrt{2mE}\rangle$ energy eigen KETS

$|E,-\rangle = |E, p - \sqrt{2mE}\rangle$

SUPERPOSITION STATES

$|\psi\rangle = \alpha\,|E,+\rangle + \beta\,|E,-\rangle$ also energy eigen KETS

MEASURE H, OBTAIN E 100% OF THE TIME

MEASURE p ?

$$\text{PROB}\left(p = +\sqrt{2mE}\right) = \frac{|\langle +p|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|\alpha|^2}{|\alpha|^2 + |\beta|^2}$$

$$\text{PROB}\left(p = -\sqrt{2mE}\right) = \frac{|\langle -p|\psi\rangle|^2}{\langle\psi|\psi\rangle} = \frac{|\beta|^2}{|\alpha|^2 + |\beta|^2}$$

IF $|\psi\rangle$ IS NORMALIZED $\langle\psi|\psi\rangle = 1 = |\alpha|^2 + |\beta|^2$

$$|\psi(t)\rangle = |E,+\rangle\langle E,+|\psi(0)\rangle\, e^{-iEt/\hbar} + |E,-\rangle\langle E,-|\psi(0)\rangle\, e^{-iEt/\hbar}$$

(2) DIFF EQ METHOD (TISE) **TISE**

$$H \, | E_n \rangle = E_n | E_n \rangle$$

in-X SPACE

$$-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} \psi_n(x) = E_n \psi_n(x) \qquad \text{TISE}$$

TRIAL SOLUTION **freshman physics method**

$$\psi_n(x) = A e^{ikx} + B e^{-ikx}$$

$$-\frac{\hbar^2}{2m} (\pm i k)^2 \psi_n(x) = E_n \psi_n(x)$$

$$\boxed{E_n = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}}$$

(2') DIFF EQ METHOD TDSE

IN HILBERT SPACE: $H\,|\psi(t)\rangle = i\hbar \frac{d}{dt}\,|\psi(t)\rangle$

IN POSITION SPACE:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) = i\hbar\frac{d}{dt}\psi(x,t)$$

SECOND ORDER IN SPACE

FIRST ORDER IN TIME

freshman physics solution

TRIAL SOLUTION $\psi(x,t) = A\,e^{i(kx-\omega t)} + B\,e^{-i(kx+\omega t)}$

$ikx - i\omega t \qquad -ikx - i\omega t$

$-iE_m t/\hbar \qquad -iE_m t/\hbar$

$$-\frac{\hbar^2}{2m}(\pm ik)^2\,\psi(x,t) = i\hbar(-i\omega)\,\psi(x,t)$$

$$\boxed{\frac{\hbar^2 k^2}{2m} = \hbar\omega}$$

$p = \hbar k$

$E = \hbar\omega$

$\Rightarrow \quad \frac{p^2}{2m} = E$

separation of variables

DIFF EQ VIEW OF TDSE → TISE

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,t) = i\hbar\frac{d}{dt}\psi(x,t)$$

assume the solution factors into the the spatial dependence f(x) times the time dependence g(t)

ANSATZ $\psi(x,t) = f(x)\,g(t)$

put it in and see if it works

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\big(f(x)\,g(t)\big) = i\hbar\frac{d}{dt}\big(f(x)\,g(t)\big)$$

$$g(t)\left(-\frac{\hbar^2}{2m}\right)\frac{d^2f}{dx^2} = f(x)\,(i\hbar)\frac{dg}{dt}$$

Separates if the LHS depends only on x and the RHS depends only on t

$\frac{1}{f\cdot g}$

$$\frac{-\frac{\hbar^2}{2m}\frac{d^2f}{dx^2}}{f} = \frac{i\hbar\frac{dg}{dt}}{g}$$

LHS FCN ONLY OF X

RHS FCN ONLY OF t

HOW CAN THAT BE? = A CONSTANT = E_n

$$i\hbar\frac{dg}{dt} = E_n g$$

$$\frac{dg}{dt} = (-iE_n/\hbar)\,g \qquad g(t) = e^{-iE_nt/\hbar}$$

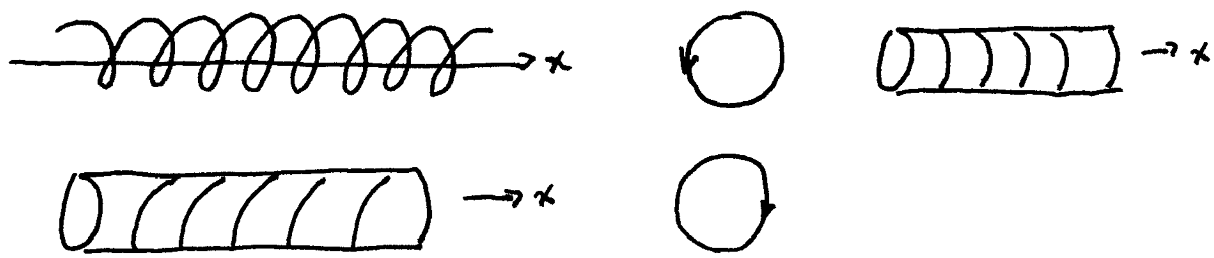
⇒ TISE $-\frac{\hbar^2}{2m}\frac{d^2\psi_n}{dx^2} = E_n\psi_n$

MOMENTUM EIGENSTATES $|p\rangle \rightarrow \langle x|p\rangle =$

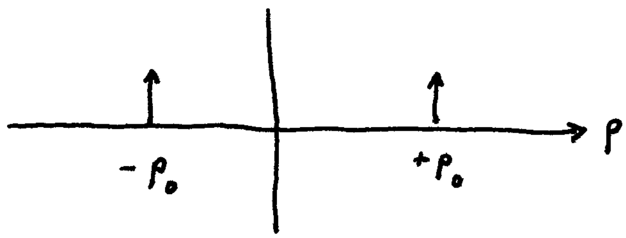
$\psi(x)$

momentum eigenstates in position space

INFINITE EXTENT HELICAL WAVES



momentum eigenstates in momentum space



$\langle p|p_0\rangle =$

$\hat{\psi}(p)$

the momentum operator is Hermitean so

ANY WAVE CAN BE EXPRESSED AS A LINEAR COMBINATION OF MOMENTUM EIGENSTATES

$$I = \int |p\rangle\langle p| \, dp$$

complete set of p states

resolution of the identity in p

$$|\psi\rangle = I|\psi\rangle = \int dp \, |p\rangle\langle p|\psi\rangle$$

$\langle x|$ both sides $\Rightarrow$ go into the x basis

$$\langle x|\psi\rangle = \int dp \, \langle x|p\rangle\langle p|\psi\rangle$$

$$\boxed{\psi(x) = \int dp \, \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \, \tilde{\psi}(p)}$$

the position space wavefunction is the Fourier transform of the momentum space wavefunction

OTHER WAY AROUND

x operator is Hermitean

$$I = \int dx \, |x\rangle\langle x|$$

complete set of states

resolution of the identity in x

dot with $\langle p|$

$$\boxed{\langle p|\psi\rangle = \int dx \, \frac{e^{-ipx/\hbar}}{\sqrt{2\pi\hbar}} \, \psi(x)}$$

the momentum space wavefunction is the Fourier transform of the position space wavefunction

THE PROPAGATOR

$$U(t) = \int dp \, |p\rangle\langle p| \, e^{-iE(p)t/\hbar}$$

$$= \int dp \, e^{-ip^2 t/2m\hbar} \, |p\rangle\langle p|$$

WE WILL USE THIS FOR THE FREE PARTICLE WAVE PACKET PROBLEM

Use the propagator to find the time evolution of superposition states, in particular that of a Gaussian superposition

FOURIER TRANSFORMS

$\boxed{\text{TIME}}$

$$F(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(t)\, e^{-i\omega t}\, dt$$

$$f(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(\omega)\, e^{i\omega t}\, d\omega$$

SYMMERIC CONVENTION

ω TEMPORAL FREQUENCY

$\boxed{\text{SPACE}}$

K SPATIAL FREQUENCY

$$F(K) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x)\, e^{-iKx}\, dx$$

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} F(K)\, e^{iKx}\, dK$$

$E = \hbar\omega$

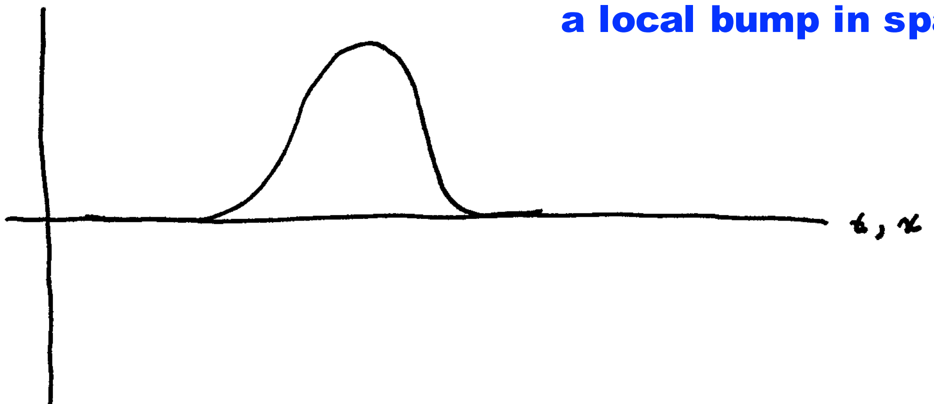
$p = \hbar K \qquad dp = \hbar\, dK$

CARTOON VERSION

a local bump in time

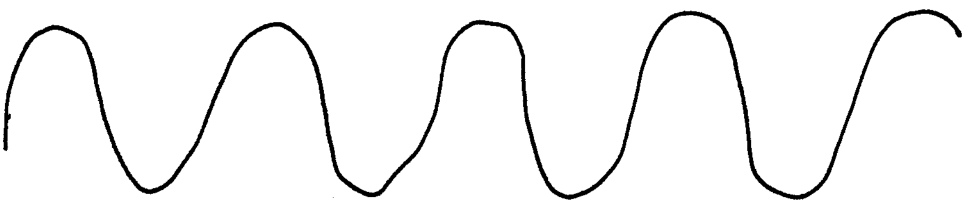
or

a local bump in space



can be expressed by a weighted integral of an infinite number of harmonic states

N.B., THESE HAVE INFINITE EXTENT



the harmonic waves have infinite extent, so although the bump looks local it really is not

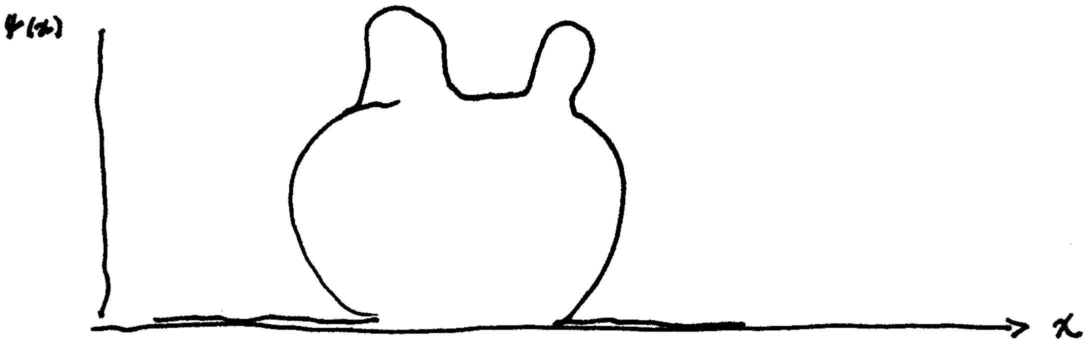
if complex => HELICIES

Essential issue in quantum mechanics is that the world is nonlocal

ANY FUNCTION?

YES

HOW ABOUT THIS WAVEFCN?



NO MICKEY MOUSE WAVEFCNS!

$$\hat{q}(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} q(x)\, e^{-ipx/\hbar}\, dx$$

$$q(x) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \hat{q}(p)\, e^{ipx/\hbar}\, dp$$

similar for E and omega

FT OF DELTA FCNS

$$\hat{f}(k) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \delta(x - x')\, e^{-ikx}\, dx$$

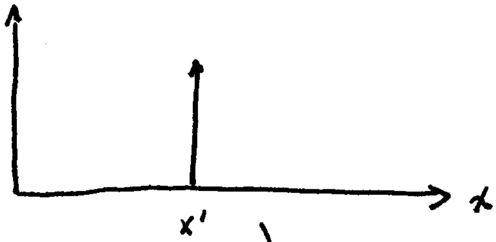
$$= (2\pi)^{-1/2}\, e^{-ikx'}$$

$$f(x) = (2\pi)^{-1/2} \int_{-\infty}^{\infty} \delta(k - k')\, e^{ikx}\, dk$$

$$= (2\pi)^{-1/2}\, e^{ik'x}$$

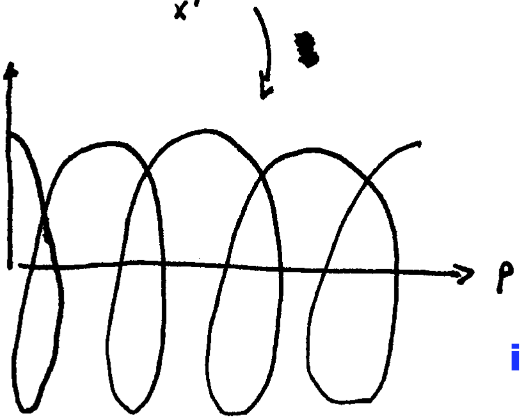
the integral of any function with a delta function, is the value of the function evaluated at the position of the delta function

eigenfunction of the position operator



$\delta(x-x')$

in position space

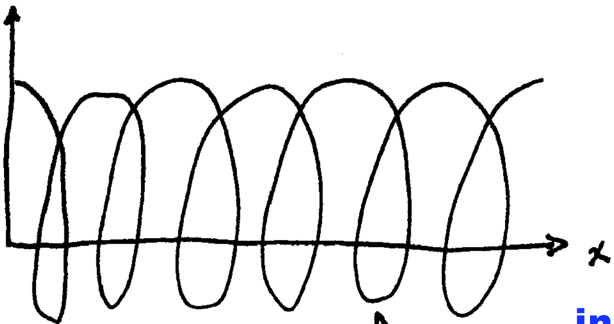


$e^{-ipx'/\hbar}$

$e^{-ikx'}$

in momentum space

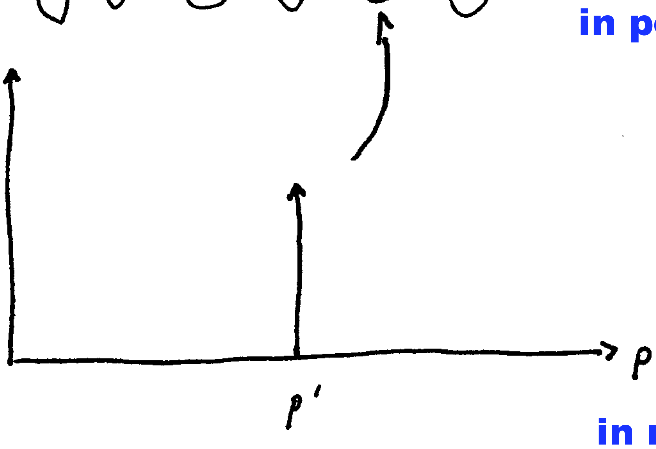
eigenfunction of the momentum operator



$e^{ip'x/\hbar}$

$e^{ik'x}$

in position space



$\delta(p-p')$

in momentum space

CONVOLUTION THM

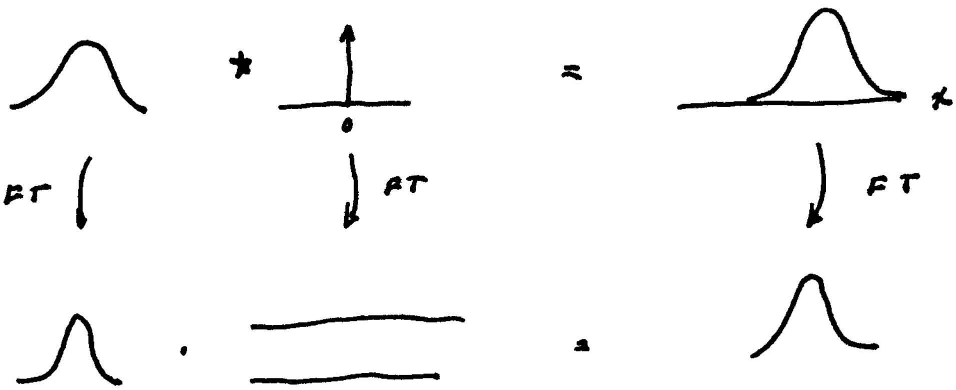
The Convolution Theorem

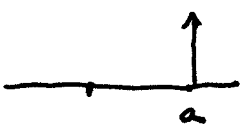
CONVOLUTION IN ONE SPACE $\Longleftrightarrow$ MULTIPLICATION IN THE OTHER SPACE

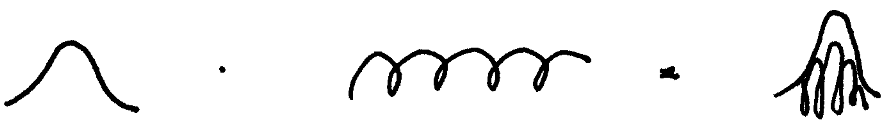
$f \star q$ $\qquad\qquad$ $\hat{f} \cdot \hat{q}$

$f \cdot q$ $\qquad\qquad$ $\hat{f} \star \hat{q}$

$$FT\{ f(x) \star q(x) \} = \hat{f}(k) \cdot \hat{q}(k)$$

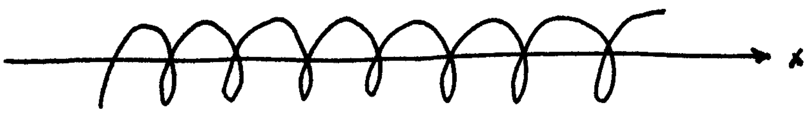




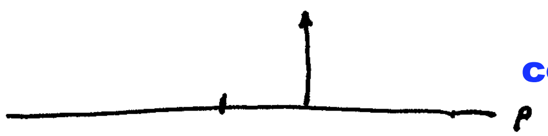


CONVOLUTION INTEGRAL

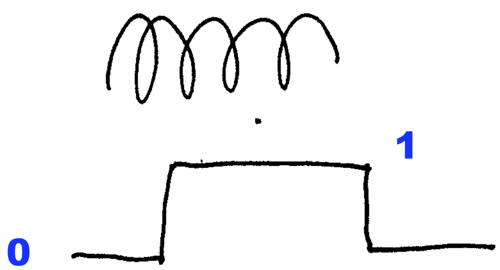
$$h(x) = \int_{-\infty}^{\infty} f(u)\, g(x-u)\, du$$



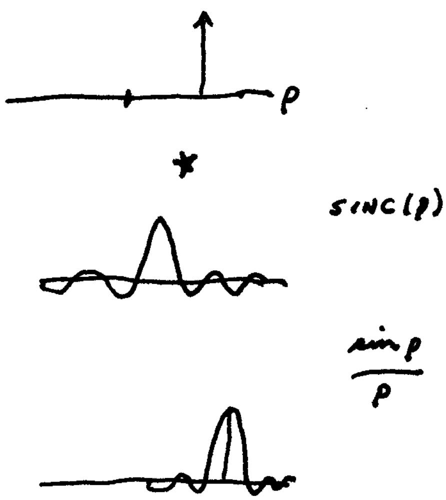
FT



convolving with a delta function puts a copy of the function centered on the position of the delta function



in position space multiply the helix by a square window



in momentum space convolve the delta function with the sinc function

FTs AND DIRAC NOTATION

$$|q\rangle = |q\rangle$$

$$= I\,|q\rangle$$ INSERT A COMPLETE SET OF STATES

$$= \int dk\; |k\rangle\langle k|q\rangle$$

insert a complete set of k states

$$= \int dk\; |k\rangle \;\hat{q}(k)$$

dot with x bra

$$\langle x|q\rangle = \langle x| \int dk\; |k\rangle\, \hat{q}(k)$$

$$q(x) = \int \underbrace{\langle x|k\rangle}_{(2\pi)^{-1/2} e^{ikx}} \hat{q}(k)\; dk$$

$$= (2\pi)^{-1/2} \int \underbrace{\hat{q}(k)}_{G(k)}\; e^{ikx}\; dk$$

EXERCISE:

$$I = \int dx\; |x\rangle\langle x|$$

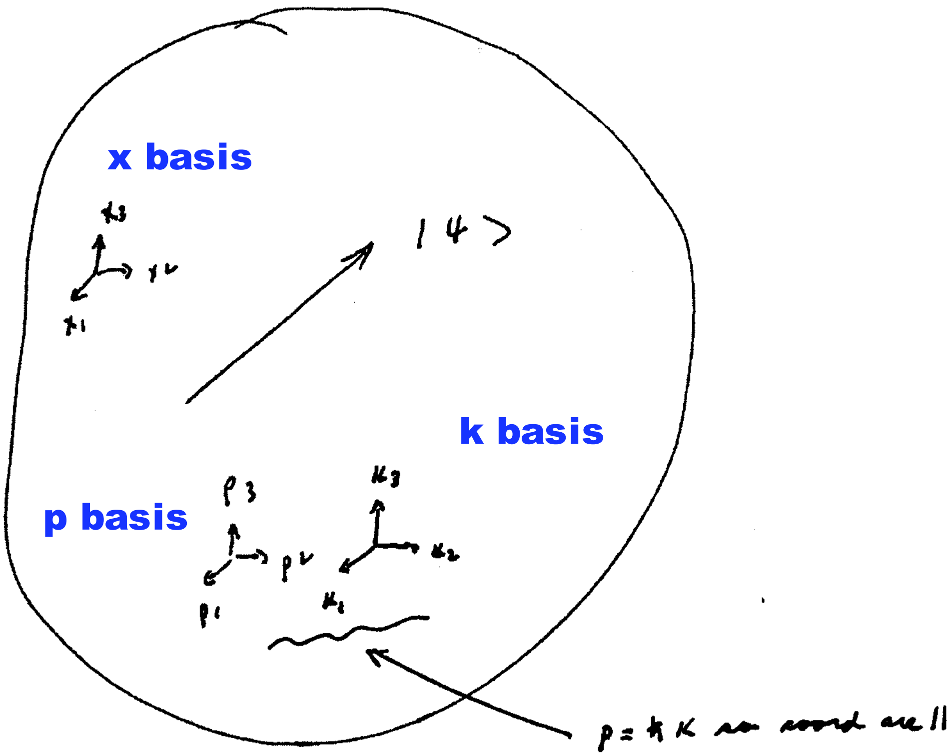
$$\hat{q}(k) = (2\pi)^{-1/2} \int q(x)\, e^{-ikx}\, dx$$

remember that

$\langle k | x \rangle = \langle x | k \rangle^*$

In Quantum Mechanics, Fourier transforms are just a change of basis

FOURIER TRANSFORMS ARE JUST A CHANGE OF BASIS



$$\langle x|\psi\rangle = \psi(x)$$
$$\langle k|\psi\rangle = \hat{\psi}(k)$$
$$\langle p|\psi\rangle = \hat{\psi}(p)$$
$$\langle E|\psi\rangle = \tilde{\psi}(E)$$

all have all of the info

precisely the same info

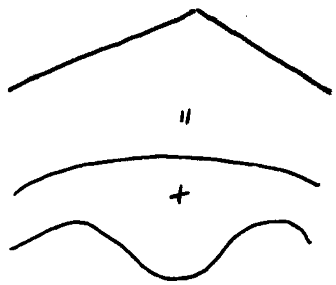
$|\psi\rangle$ is the real thing

FT's are just a change in basis in QM!

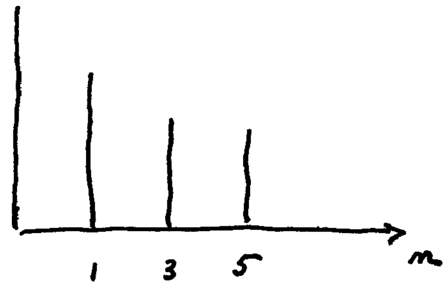
ALL OBSERVABLES ...

Time evolution of superposition states

FOR THE SQUARE WELL



FOURIER SERIES

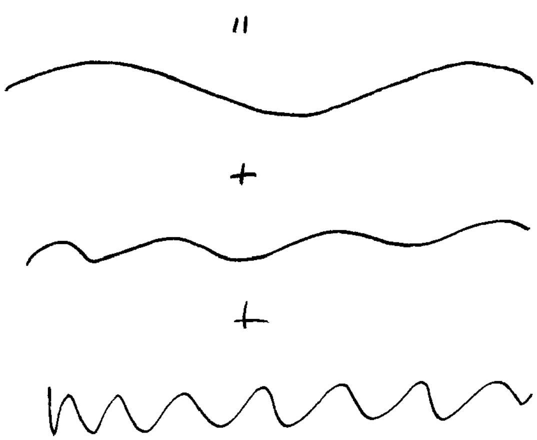


a_m's are the FOURIER SERIES EXPANSION COEFFS! DISCRETE

http://www.st-andrews.ac.uk/~qmanim/animations_2/Expansion_Eigenstates_V3.swf

FOR THE FREE PARTICLE

Gaussian



FOURIER TRANSFORM

Gaussian

a_m's are given by the Fourier transform coeffs

CONTINUOUS

SHOW MOVIES HERE!?

EIGENSTATES FOR THE FREE PARTICLE

$$\Psi(x,t) \quad A \, e^{\pm i K x} \; e^{-i E_K t/\hbar}$$

$$E_K = \frac{\hbar^2 K^2}{2m} \qquad\qquad E_p = \frac{p^2}{2m}$$

$|E\rangle$ ARE 2-FOLD DEGENERATE

$$|\Psi\rangle = \alpha\,|+p\rangle + \beta\,|-p\rangle$$

MEASURE MOMENTUM

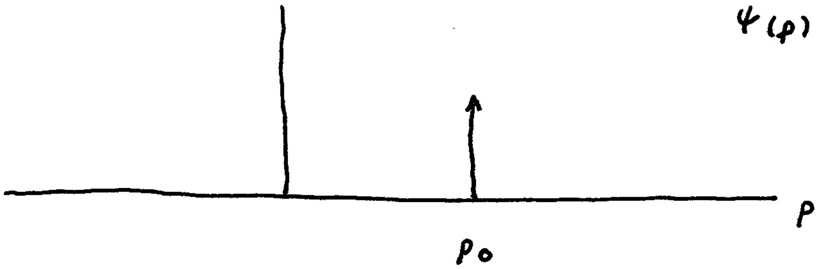
$+p \qquad |\alpha|^2$

$-p \qquad |\beta|^2$

MEASURE ENERGY

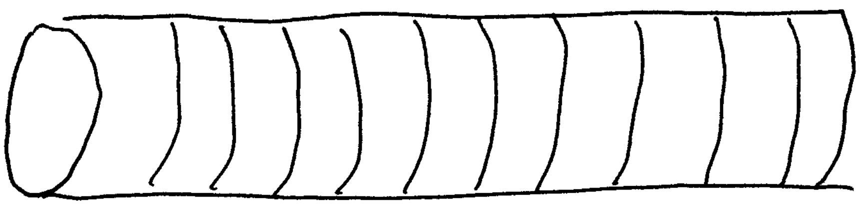
$E = \dfrac{p^2}{2m}$ 100% of the time

IN MOMENTUM SPACE



$$\hat{\psi}(p) = \delta(p - p_0)$$

IN X-SPACE $\quad \psi(x) = e^{i p_0 x/\hbar} = e^{i k_0 x}$



RH HELIX

PITCH = k_0 SPATIAL WAVELENGTH

EIGENSTATE OF p : "INFINITE PLANE WAVE"

PLANE WAVE OF INFINITE SPATIAL EXTENT

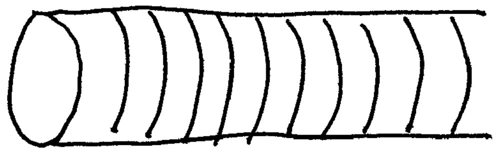
EIGENSTATE OF E : PLANE WAVE WITH INFINITE TEMPORAL EXTENT

OBVIOUSLY IDEALIZATIONS!

Make localized wave packets

FREE WAVE PACKETS

PLANE WAVE $e^{ip_0 x/\hbar}$

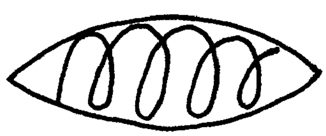


INFINITE EXTENT $\Rightarrow$ $\Delta x = \infty$

$$\Delta x \, \Delta p \geq \frac{\hbar}{2} \Rightarrow \Delta p = 0$$

an idealization since the universe is finite

to represent a localized particle in position space, we make a localized packet



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position space

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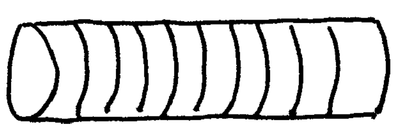
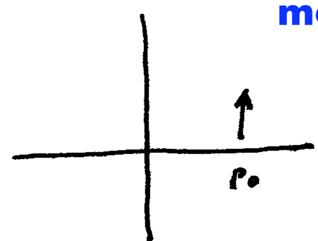


momentum space



X

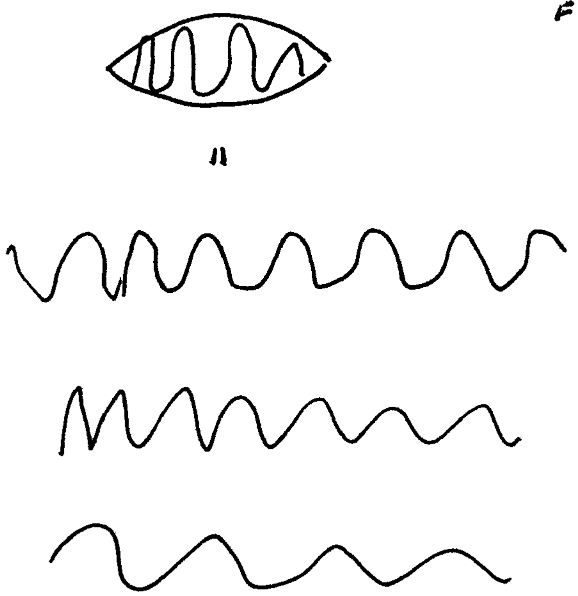
$\otimes$

$\Longleftrightarrow$

we cut out a Gaussian shaped piece of an infinite helical (plane) wave

in momentum space convolution theorem multiply Gaussian times delta fcn

SPREADING OF THE WAVEPACKET



FINITE PACKET

FT

INTEGRAL OVER INFINITE EXTENT WAVES

different frequency waves travel with different velocities

=> packet changes with time

can spread or contract

expand or compress

if component waves move at the same velocity, then ~~waves~~ packet stays together

LIGHT IN VACUUM

light in vacuum is not dispersive

if component waves move with different velocities, then packet disperses

LIGHT IN A PRISM

ELECTRONS IN A VACUUM

electrons in vacuum are dispersive

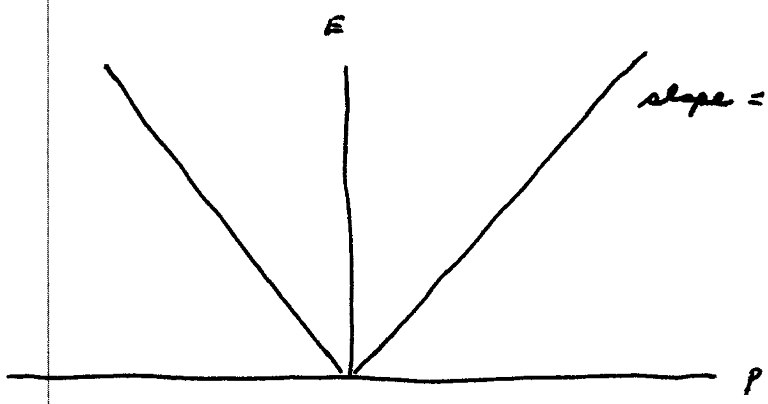
EMPTY SPACE IS DISPERSIVE FOR MATTER WAVES

" " " NON- " " EM WAVES

Dispersion Relations

Linear Dispersion: light in vacuum

LIGHT $E = pc$ LINEAR



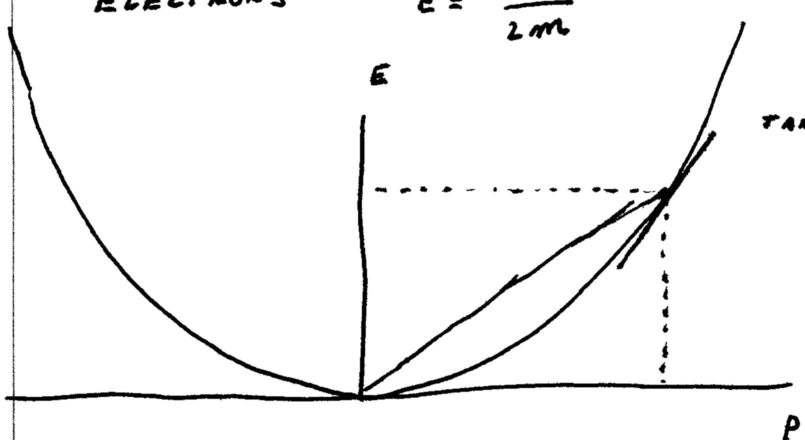
$E(p)$ $E = \hbar\omega$ $p = \hbar k$

$\omega(k)$

FUNCTIONS are called dispersion relation

Parabolic Dispersion: electrons in vacuum

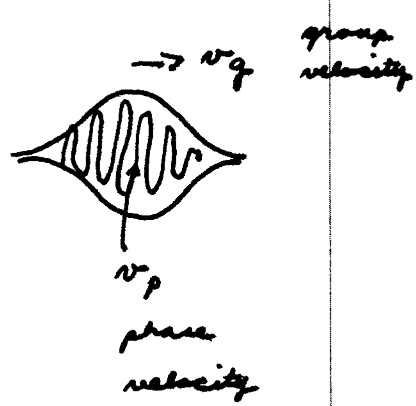
ELECTRONS $E = \frac{p^2}{2m}$ PARABOLIC



slope of the tangent line

TANGENT LINE

$$\text{slope} = \frac{dE}{dp} = \frac{2p}{2m} = v$$



slope of the chord

CHORD

$$\text{slope} = \frac{E}{p} = \frac{\frac{p^2}{2m}}{p} = \frac{1}{2}\frac{p}{m} = \frac{1}{2}v$$

the group velocity of an electron = its classical velocity

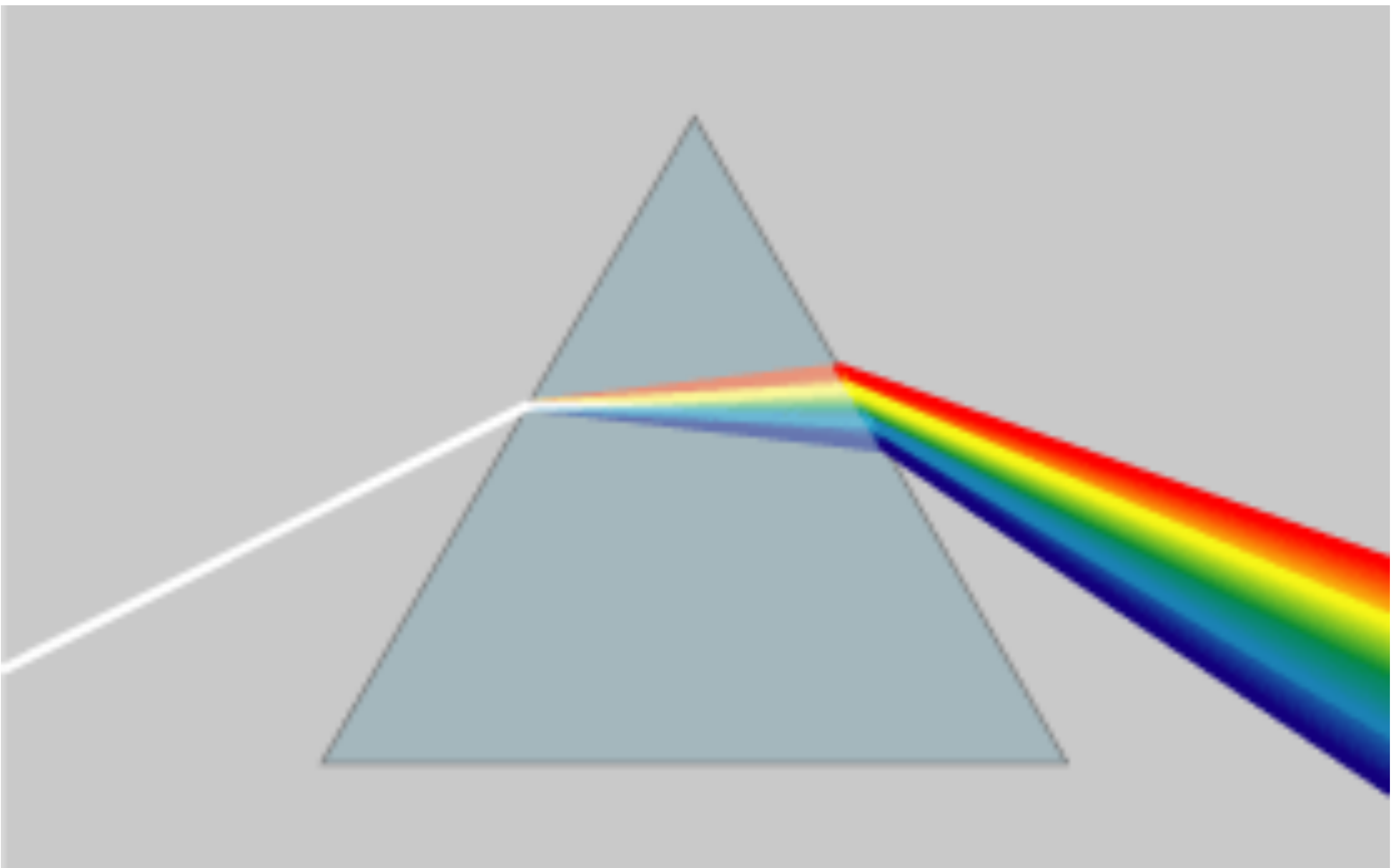
the phase velocity of an electron = 0.5 times its classical velocity

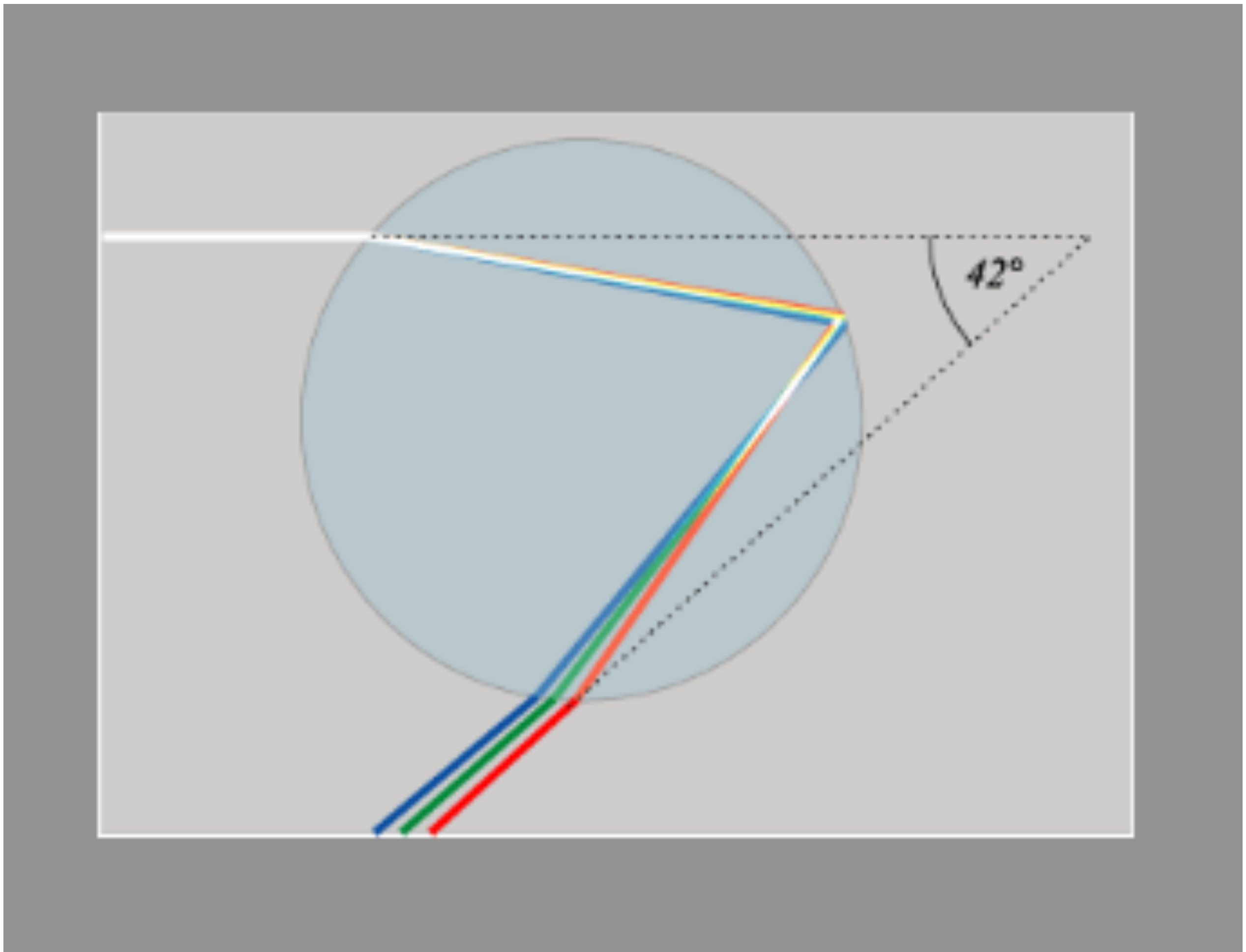
Dispersion

http://paws.kettering.edu/~drussell/Demos/Dispersion/dispersion.html

http://www.csupomona.edu/~ajm/materials/animations/packets.html

http://gregegan.customer.netspace.net.au/APPLETS/20/20.html

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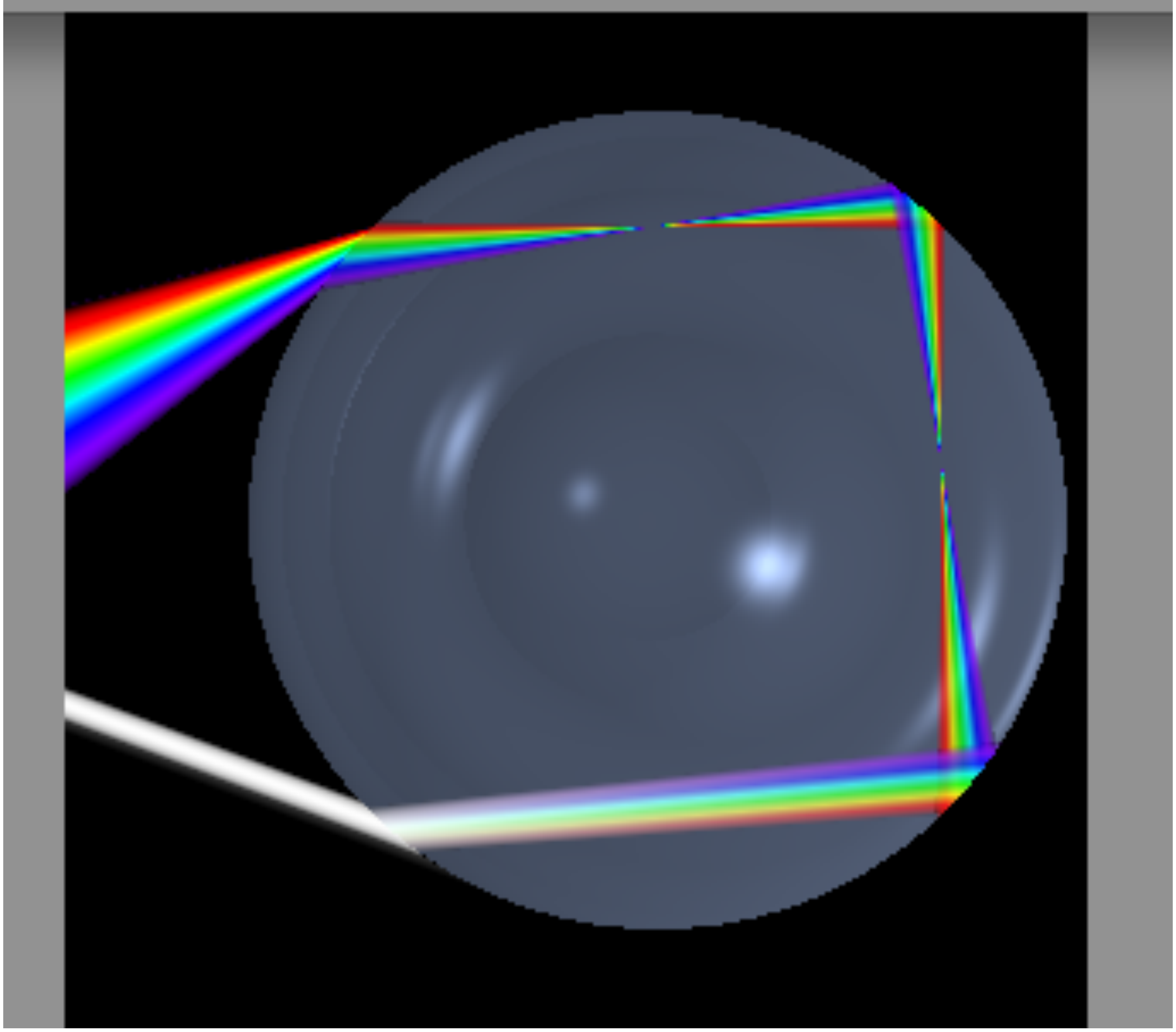

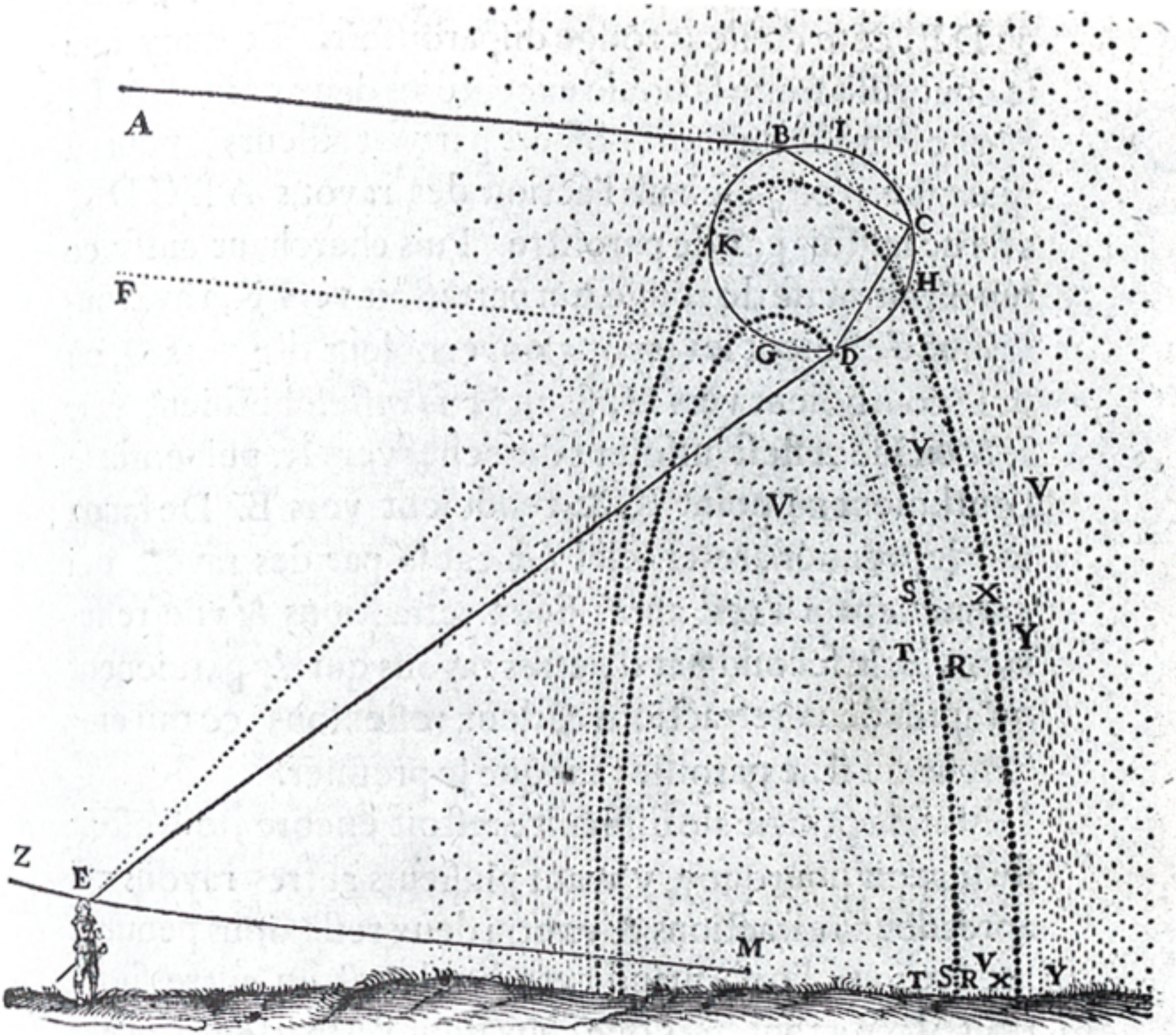

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FEYNMAN'S RAINBOW

A
SEARCH
FOR
BEAUTY
IN
PHYSICS
AND IN
LIFE

LEONARD MLODINOW

Feynman was gazing at a rainbow. As if he had never seen one before. Or maybe as if it might be his last.

I approached him cautiously and joined him in staring at the rainbow. It wasn't something I normally did—in those days.

"Do you know who first explained the true origin of the rainbow?" I asked.

"It was Descartes," he said. After a moment he looked me in the eye. "And what do you think was the salient feature of the rainbow that inspired Descartes's mathematical analysis?" he asked.

"I give up. What would you say inspired his theory?"

"I would say his inspiration was that he thought rainbows were beautiful..."

—From FEYNMAN'S RAINBOW

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Poets say science takes away from the beauty of the stars — mere globs of gas atoms. Nothing is "mere". I too can see the stars on a desert night, and feel them. But do I see less or more? The vastness of the heavens stretches my imagination — stuck on this carousel my little eye can catch one-million-year-old light. A vast pattern — of which I am a part. What is the pattern or the meaning or the why? It does not do harm to the mystery to know a little more about it. For far more marvelous is the truth than any artists of the past imagined it. Why do the poets of the present not speak of it? What men are poets who can speak of Jupiter [Roman God] if he were a man, but if he is an immense spinning sphere of methane and ammonia must be silent?

“I have a friend who's an artist and has sometimes taken a view which I don't agree with very well. He'll hold up a flower and say "look how beautiful it is," and I'll agree. Then he says "I as an artist can see how beautiful this is but you as a scientist take this all apart and it becomes a dull thing," and I think that he's kind of nutty. First of all, the beauty that he sees is available to other people and to me too, I believe. Although I may not be quite as refined aesthetically as he is ... I can appreciate the beauty of a flower. At the same time, I see much more about the flower than he sees. I could imagine the cells in there, the complicated actions inside, which also have a beauty. I mean it's not just beauty at this dimension, at one centimeter; there's also beauty at smaller dimensions, the inner structure, also the processes. The fact that the colors in the flower evolved in order to attract insects to pollinate it is interesting; it means that insects can see the color. It adds a question: does this aesthetic sense also exist in the lower forms? Why is it aesthetic? All kinds of interesting questions which the science knowledge only adds to the excitement, the mystery and the awe of a flower. It only adds. I don't understand how it subtracts.”

-Richard Feynman

http://www.youtube.com/watch?v=zSZNsIFID28

Newton versus Goethe

http://en.wikipedia.org/wiki/Theory_of_Colours

http://zebu.uoregon.edu/2000/ph102/lec19.html

The Newtonian deconstruction of the rainbow is said to have provoked John Keats to lament in his 1820 poem "Lamia":

Do not all charms fly
At the mere touch of cold philosophy?
There was an awful rainbow once in heaven:
We know her woof, her texture; she is given
In the dull catalogue of common things.
Philosophy will clip an Angel's wings,
Conquer all mysteries by rule and line,
Empty the haunted air, and gnomed mine –
Unweave a rainbow

In contrast to this is Richard Dawkins; talking about his book Unweaving the Rainbow: Science, Delusion and the Appetite for Wonder:

"My title is from Keats, who believed that Newton had destroyed all the poetry of the rainbow by reducing it to the prismatic colours. Keats could hardly have been more wrong, and my aim is to guide all who are tempted by a similar view, towards the opposite conclusion. Science is, or ought to be, the inspiration for great poetry."

In the seventeenth century, Newton published his famous experimentum crucis, in which he claimed that light is heterogeneous and is composed of (colored) rays with different refrangibilities. Experiments, especially a crucial experiment, were important for justifying Newton’s theory of light, and eventually his theory of color. Goethe conducted a series of experiments on the nature of color, especially in contradistinction to Newton, and he defended his research with a methodological principle formulated in “Der Versuch als Vermittler.” Goethe’s principle included a series of experiments and resultant higher empirical evidence as mediator between the objective (natural phenomena) and the subjective (theory or hypothesis). Although the notion of experimentum crucis became popular among scientists, even until today, in reconstructing experimental research and for justifying theories, especially for rhetorical purposes, I propose that Newton’s justification of his theory of light and color is best reconstructed in terms of Goethe’s methodological principle. Finally, Goethe’s principle has important consequences for the contemporary philosophical underdetermination thesis.

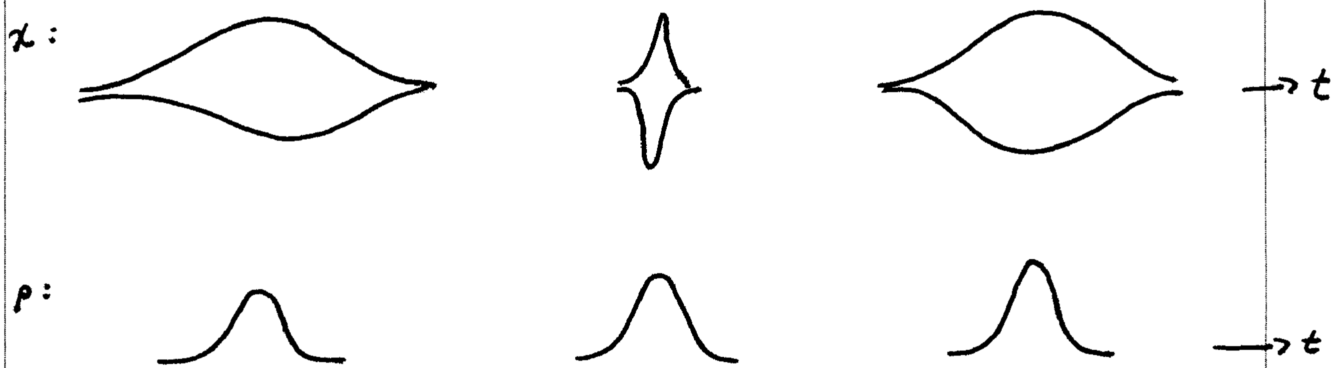
Dispersion

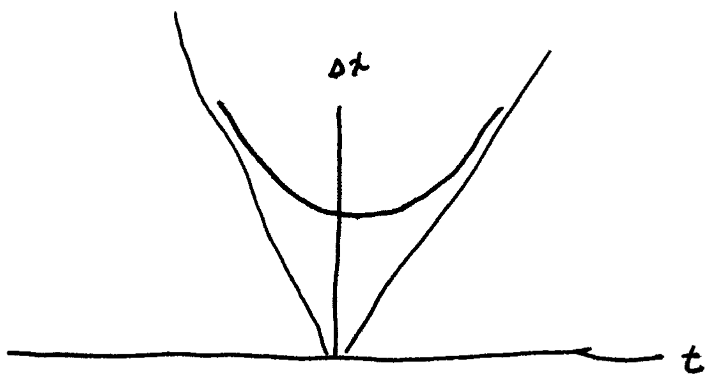
http://paws.kettering.edu/~drussell/Demos/Dispersion/dispersion.html

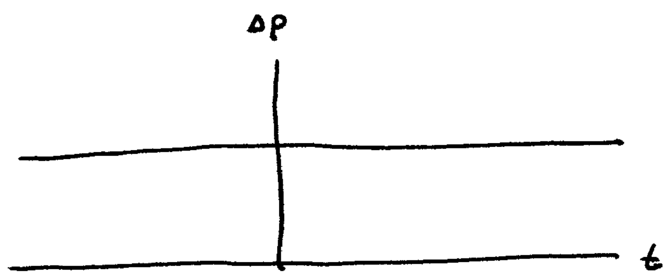
http://www.csupomona.edu/~ajm/materials/animations/packets.html

http://gregegan.customer.netspace.net.au/APPLETS/20/20.html

Cartoon Version of the Free Particle







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http://www.st-andrews.ac.uk/~qmanim/embed_item_3.php?anim_id=1

http://www.physics.nus.edu.sg/einstein/lect14/applets/propa.html

http://www.brainflux.org/java/classes/Schrodinger1D.html

http://demonstrations.wolfram.com/WavepacketForAFreeParticle/

http://demonstrations.wolfram.com/EvolutionOfAGaussianWavePacket/