Title: PSI 2018/2019 - Foundations of Quantum Mechanics - Lecture 12

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Abstract:

Quantum Foundations
Lecture 12

PSI Review Class: 22nd January 2019

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9) The Classical Limit of Quantum Theory

1) Requirements for the Classical Limit
2) Wigner-Moyal Formalism
3) Spreading of Wavepackets
4) Coherent States
5) Environmentally Induced Decoherence

9.1) Requirements of the Classical Limit

1. Disappearance of typical Quantum Phenomena
2. Actualization of Measurement Outcomes
3. Recovery of the Equations of Classical Mechanics

Disappearance of Quantum Phenomena

- In the classical limit, we expect that typical quantum phenomena should disappear or become effectively unobservable, e.g.
  - Quantum interference (except for electromagnetic fields)
  - Incompatibility of observables
  - Contextuality, nonlocality, etc.
- Taken together, this says that our experiment should be describable by classical probability theory instead of the rules of quantum theory.
- This can be understood independently of interpretation.

Actualization of Measurement Outcomes

- If we solve the first question then we will have a description of our system in terms of classical probabilities.
- How do we know that those probabilities can be interpreted in terms of classical uncertainty?
  - e.g. even if we specify $\text{Prob}(\text{cat alive}) = \text{Prob}(\text{cat dead}) = \frac{1}{2}$ and it is not practical to perform an interference experiment, how do we know that this describes a situation in which EITHER the cat is dead OR it is alive and we simply do not know which.
  - It could still be that the cat is in some kind of indefinite state until we actually observe it.
- This cannot be solved without positing an ontology for the theory, so it is definitely an interpretation dependent question.

Recovery of the Equations of Classical Mechanics

- We should be able to identify quantities that obey the equations of classical mechanics, but note that there are two options here:
  - The Liouville Limit: A probability density on phase space obeys the Liouville equation

$$\frac{\partial \rho}{\partial t} = \{H, \rho\} \quad \text{where} \quad \{H, \rho\} = \sum_{j=1}^{n} \left[\frac{\partial \rho}{\partial p_j} \frac{\partial H}{\partial q_j} - \frac{\partial \rho}{\partial q_j} \frac{\partial H}{\partial p_j} \right]$$

  - The Trajectory Limit: There exist canonically conjugate variables that obey Hamilton's equations

$$\frac{\mathrm{d}p_j}{\mathrm{d}t} = -\frac{\partial H}{\partial q_j}, \qquad \frac{\mathrm{d}q_j}{\mathrm{d}t} = \frac{\partial H}{\partial p_j}$$

Recovery of the Equations of Classical Mechanics

- In a ψ-complete theory, we should be able to derive the trajectory limit:
  - We observe classical systems travelling along definite trajectories. If the quantum state is all there is, we somehow need to derive this from the unitary evolution of a quantum state.
- In a ψ-epistemic theory, we only expect the Liouville limit:
  - The quantum state has the same status as a probability density, so we should expect it to behave as such in the classical limit. Whatever travels along trajectories is not described by standard quantum theory.
- In a ψ-ontic, but not ψ-complete, interpretation, it is completely non-obvious what to expect.
- So this is a subtly interpretation dependent question: what might be perceived as a failure of classicality on one view need not be from other points of view.

An Important Caveat

- The Newtonian limit of Special Relativity is straightforward:
  - *Any* particle travelling with $v \ll c$ will approximately obey classical equations of motion.
- Carefully engineered mesoscopic quantum systems display quantum effects and we expect this can in principle be extended to arbitrarily macroscopic systems.
  - So we only expect to obtain the classical limit for quantum states and Hamiltonians that are typically found in nature, and only with high probability.
- It is more like the derivation of thermodynamics from statistical mechanics:
  - i.e. only typical initial states give rise to the second law, only if the dynamics is sufficiently mixing, and only with high probability.

9.2) Wigner-Moyal Formalism

- Classical mechanics is formulated on phase space whereas quantum theory is formulated in Hilbert space. We need a common mathematical language to connect the two.
- We will formulate quantum theory in phase space. This leads to the *Wigner-Moyal* formalism.
- For simplicity, we will focus on the case of a single particle in one dimension without spin. The ideas can be extended to more general systems.

Pseudo-Probability Densities

- The first thing we have to do is to convert a quantum state $\rho \in \mathcal{L}(L^2(x))$ into a function $W(x,p)$ on phase space that is analogous to a probability density.
- We associate a Hermitian operator $A_{x,p}$ to each point in phase space, called a *phase point operator*.
- We then define $W(x,p) = \mathrm{Tr}(A_{x,p}\rho)$
- If we choose these operators to be (over)-complete, i.e.

$$\int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p\, A_{x,p} = I$$

then

$$\int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p\, W(x,p) = 1$$

- In this case $W(x,p)$ is called a *pseudo-probability density*. Note that it can take negative values.

Pseudo-Probability Densities

- Suppose that we further require that the phase point operators are orthonogonal

$$\mathrm{Tr}\left(A_{x,p}A_{x',p'}\right) = N\delta(x - x')\delta(p - p')$$

- Then we can recover the density operator via

$$\rho = \frac{1}{N}\int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p\, W(x,p)A_{x,p}$$

Observables

- Now consider an observable (self-adjoint operator) M. This should become a function on phase space. If we define

$$M_W(x,p) = \frac{1}{N}\mathrm{Tr}(A_{x,p}M)$$

then we will have $M = \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p\, M_W(x,p)A_{x,p}$ and hence

$$\begin{aligned}\mathrm{Tr}(M\rho) &= \frac{1}{N}\int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p \int_{-\infty}^{+\infty} \mathrm{d}x' \int_{-\infty}^{+\infty} \mathrm{d}p'\, M_W(x,p)W(x,p)\mathrm{Tr}\big(A_{x,p}A_{x',p'}\big) \\ &= \int_{-\infty}^{+\infty} \mathrm{d}x \int_{-\infty}^{+\infty} \mathrm{d}p\, M_W(x,p)W(x,p)\end{aligned}$$

so the formula for taking expectation values is the same as in classical probability.

Dynamics

- Now let's look at time evolution

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = \frac{1}{i\hbar}[H, \rho] \quad \Rightarrow \quad \frac{\mathrm{d}W(x,p)}{\mathrm{d}t} = \frac{1}{i\hbar}\mathrm{Tr}\big(A_{x,p}[H, \rho]\big)$$

$$\frac{\mathrm{d}W(x,p)}{\mathrm{d}t} = \frac{1}{Ni\hbar}\int_{-\infty}^{+\infty} \mathrm{d}x'\mathrm{d}p'\mathrm{d}x''\mathrm{d}p'' H_W(x',p')W(x'',p'')\mathrm{Tr}(A_{x,p}[A_{x',p'}, A_{x'',p''}])$$

$*$-product and Moyal Bracket

- To neaten this up, we can define a (non-commutative) product of functions

$$f * g(x,p) = \frac{1}{Ni\hbar}\int_{-\infty}^{+\infty} \mathrm{d}x'\mathrm{d}p'\mathrm{d}x''\mathrm{d}p'' f(x',p')g(x'',p'')\mathrm{Tr}(A_{x,p}A_{x',p'},A_{x'',p''})$$

and we define the *Moyal Bracket* as

$$\{\{f,g\}\} = f * g - g * f$$

- Then we will have

$$\frac{\mathrm{d}W}{\mathrm{d}t} = \{\{H_W, W\}\}$$

so we have a formal analogy with the Liouville equation $\frac{\partial \rho}{\partial t} = \{H,\rho\}$ where the Poisson bracket gets replaced with the Moyal Bracket.

Wigner Function

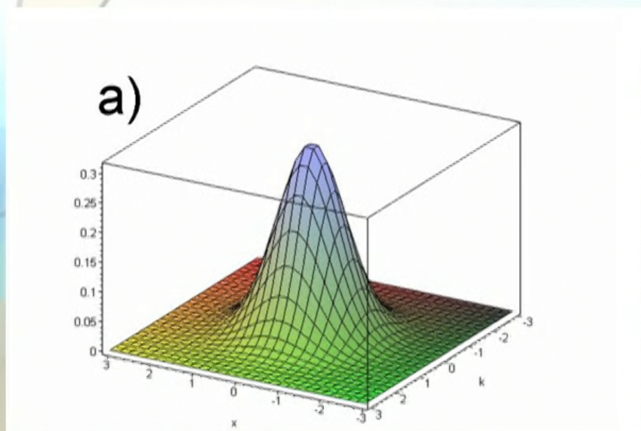
- A particular choice of pseudo-probability density is the Wigner function, where the phase-point operators are chosen to be

$$A_{x,p} = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{d}y\, e^{ipy/\hbar} \left|x+\frac{y}{2}\right\rangle\left\langle x-\frac{y}{2}\right|$$

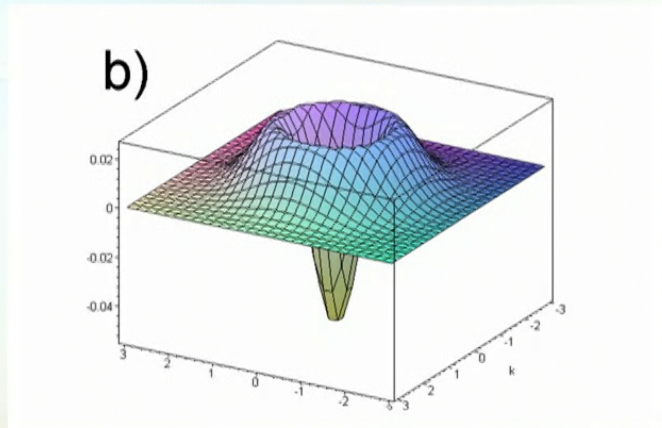
- These are orthogonal $\mathrm{Tr}\left(A_{x,p}A_{x',p'}\right) = \frac{1}{2\pi\hbar}\delta(x-x')\delta(p-p')$ and

$$W(x,p) = \frac{1}{2\pi\hbar}\int_{-\infty}^{+\infty} \mathrm{d}y\, e^{ipy/\hbar} \left\langle x-\frac{y}{2}\right|\rho\left|x+\frac{y}{2}\right\rangle$$

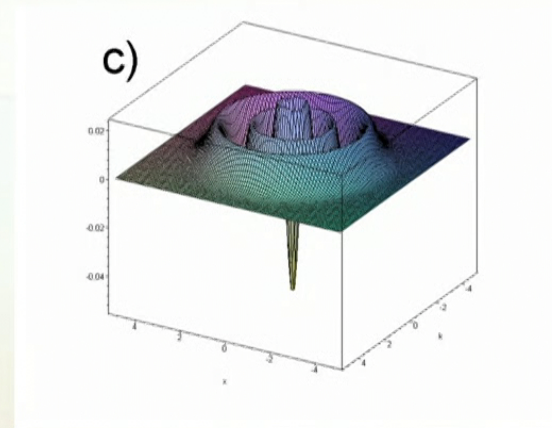
Wigner Functions for Harmonic Oscillator Energy Eigenstates



$|0\rangle$



$|1\rangle$



$|5\rangle$

Wigner Function

- The Wigner function is the unique pseudo probability density satisfying a set of natural conditions, which we won't list in full here. However, two of its useful properties are:
  - Correct marginal distributions:

$$\int_{-\infty}^{+\infty} \mathrm{d}x\, W(x,p) = \langle p|\rho|p\rangle, \qquad \int_{-\infty}^{+\infty} \mathrm{d}p\, W(x,p) = \langle x|\rho|x\rangle$$

  - Galilean Invariance:

If $\rho \to e^{-ia\hat{p}/\hbar}\rho e^{ia\hat{p}/\hbar}$ then $W(x,p) \to W(x-a,p)$

If $\rho \to e^{-ib\hat{x}/\hbar}\rho e^{ib\hat{x}/\hbar}$ then $W(x,p) \to W(x,p-b)$

Wigner-Moyal Dynamics

- We can expand the Moyal bracket as a formal power series in $\hbar$. This gives
$$\frac{\mathrm{d}W}{\mathrm{d}t} = \{\{H_W, W\}\} = \{H_W, W\} + O(\hbar^2)$$
- It looks like we have derived a Liouville limit. Quantum corrections to the Liouville equation are of order $\hbar^2$

- We can also derive the corresponding equation for observables
$$\frac{\mathrm{d}M_W}{\mathrm{d}t} = \{\{M_W, H_W\}\} = \{M_W, H_W\} + O(\hbar^2)$$

Caution!

- Although it looks like we approximately have Liouville's equation:
  - $W(x, p)$ may have negative values, which is highly nonclassical.
  - Not all observables correspond to the functions you would expect in the Wigner-Moyal formalism.
  - If $\hat{M}$ is a Weyl-ordered polynomial in $\hat{x}$ and $\hat{p}$ then we get what we expect

$$\hat{M} = \frac{1}{3}\left(\hat{x}^2\hat{p} + \hat{x}\hat{p}\hat{x} + \hat{p}\hat{x}^2\right) \quad \text{gives} \quad M_W(x, p) = x^2 p$$

  - Other observables do not

$$\hat{M} = \hat{x}\hat{p}\hat{x} \quad \text{gives} \quad M_W(x, p) = x^2 p + \text{a complicated integral}$$

9.3) Spreading of Wavepackets

- We will now look at some examples where we get an exact Liouville limit, i.e. the $O(\hbar^2)$ term is zero.
- First consider a free particle $H = p^2/2m$ in a Gaussian state

$$\psi(x,0) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{4}} e^{-(x-a)^2/4\sigma^2}$$

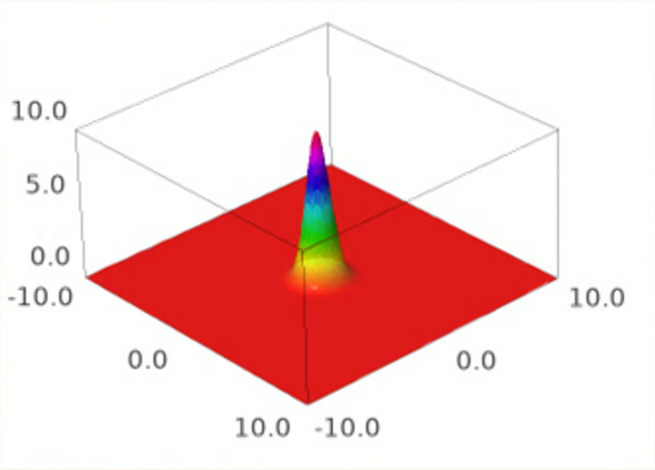
$$W(x,p,0) = \frac{1}{\pi\hbar}\exp\left[-\frac{(x-a)^2}{2\sigma^2} - \frac{2\sigma^2 p^2}{\hbar^2}\right]$$

- This has $\Delta x = \sigma$, $\Delta p = \frac{\hbar}{2\sigma}$, so is a minimum uncertainty state $\Delta x \Delta p = \frac{\hbar}{2}$.

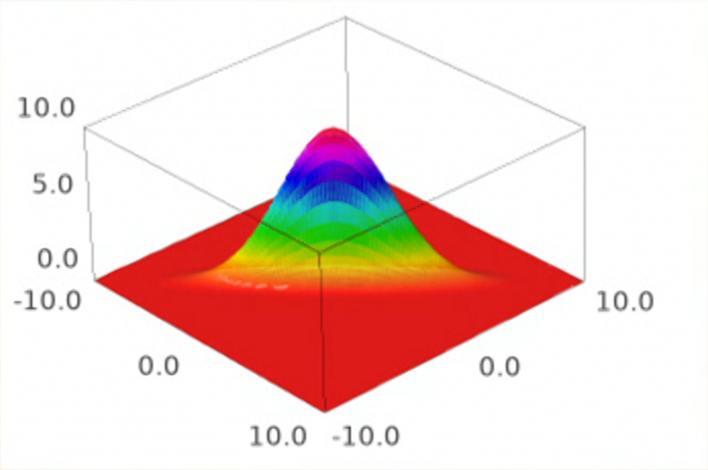
9.3) Spreading of Wavepackets

- In units $\hbar = 1$, set $\sigma = 1/\sqrt{2}$, $m = 1\text{kg}$, $a = 0$. Plot $10\pi W$

$t = 0$



$t = 0.95$ s



- We get a good Liouville limit, but not a trajectory limit.

Gaussian Quantum Mechanics

- Generally, we find that *Gaussian Quantum Mechanics* has an exact Liouville limit. If:
  - States have Gaussian distributions as their Wigner functions
  - Hamiltonians preserve Gaussianity ⇒ they are at most quadratic in the canonical variables

$$H = a + bx + cp + dx^2 + ey^2 + fxy$$

  - POVMs are represented by Gaussian functions.

then the Wigner-Moyal formalism is identical to the Liouville equation. See S. Bartlett, T. Rudolph, R. Spekkens, Phys. Rev. A 86, 012103 (2012) for proof.

- But this does not generally give a trajectory limit.

9.4) Coherent States

- To get a trajectory limit we want:
  - Wavepackets with minimal uncertainty in both position and momentum.
  - Centroids of those wavepackets obey Hamiltonian mechanics.
  - The wavepackets do not spread over time.
- Such wavepackets are called *coherent states* and they only exist for a limited class of Hamiltonians.

Coherent States of the Harmonic Oscillator

- Consider the Harmonic oscillator Hamiltonian $H = \left(a^\dagger a + \frac{1}{2}\right)\hbar\omega$
- We define a *coherent state* as an eigenstate of the lowering operator

$$a|\alpha\rangle = \alpha|\alpha\rangle$$

- Since a is not self-adjoint, its eigenvalues are complex. If we write them as

$$\alpha = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}X + i\frac{P}{\sqrt{m\omega\hbar}}\right)$$

then we can identify them with points in phase space.

Coherent States of the Harmonic Oscillator

- Calculating the Wigner function of a coherent state, we get

$$W(x,p) = \frac{1}{\pi\hbar}\exp\left[-\frac{m\omega}{\hbar}(x-X)^2 - \frac{1}{m\omega\hbar}(p-P)^2\right]$$

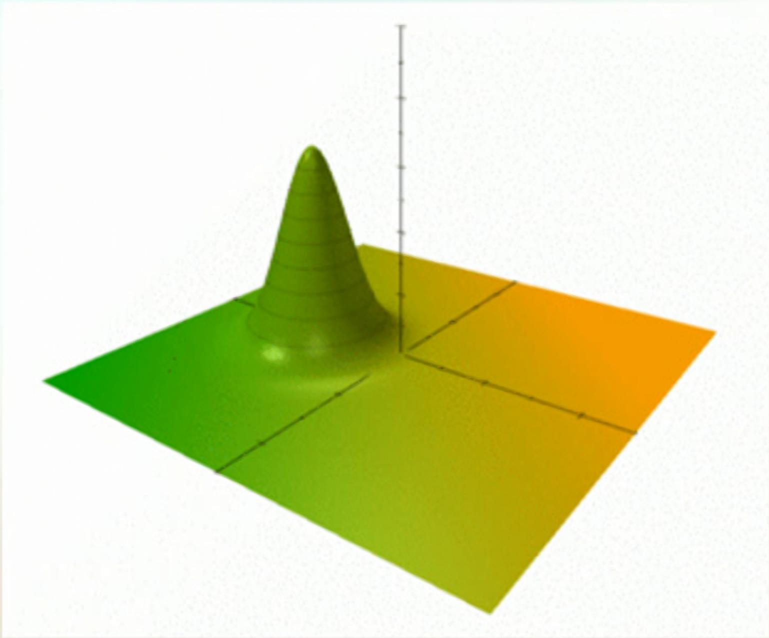
so it is a Gaussian centered at (X, P) with uncertainties

$$\Delta x = \sqrt{\frac{\hbar}{2m\omega}}, \qquad \Delta p = \sqrt{\frac{m\omega\hbar}{2}} \quad \Rightarrow \quad \Delta x \Delta p = \frac{\hbar}{2}$$

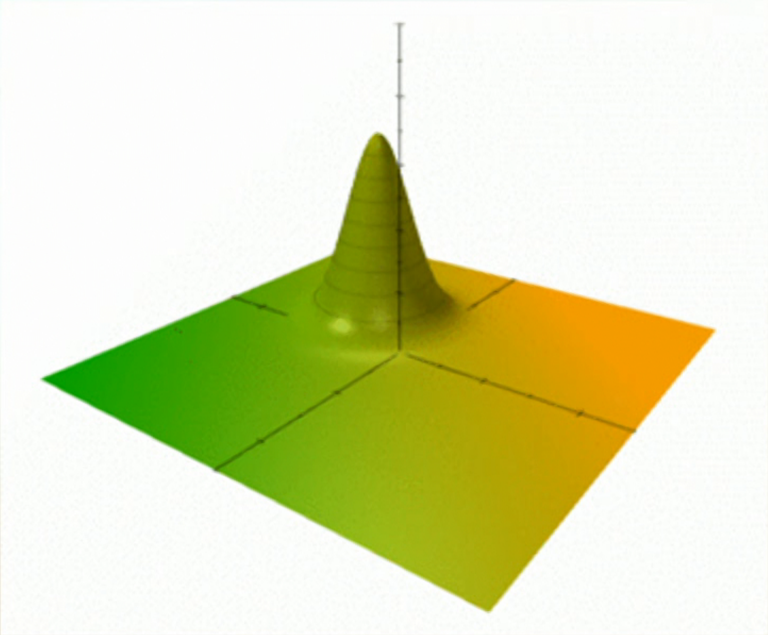
- More importantly, $W(x,p)$ maintains its form over time with

$$X(t) = A\sin(\omega t + \phi), \qquad P(t) = m\omega A\cos(\omega t + \phi)$$

Coherent States of the Harmonic Oscillator



Coherent States of the Harmonic Oscillator



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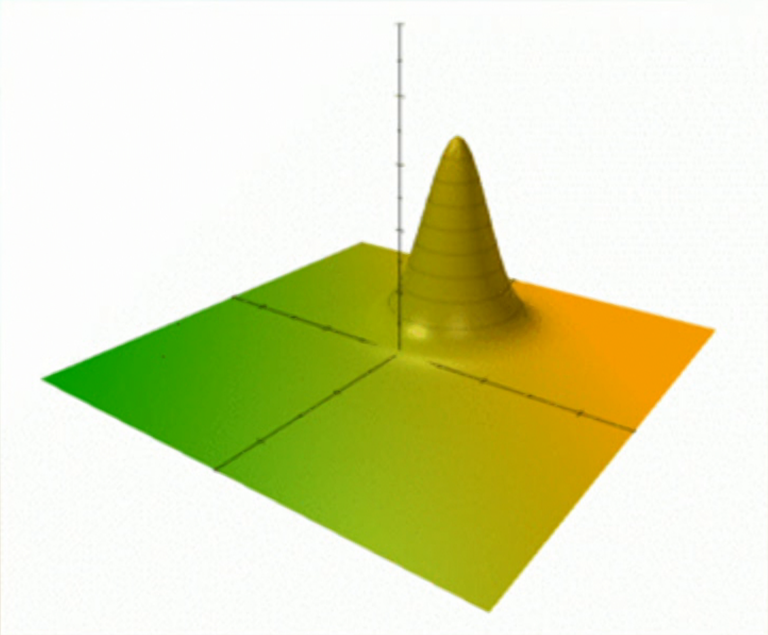

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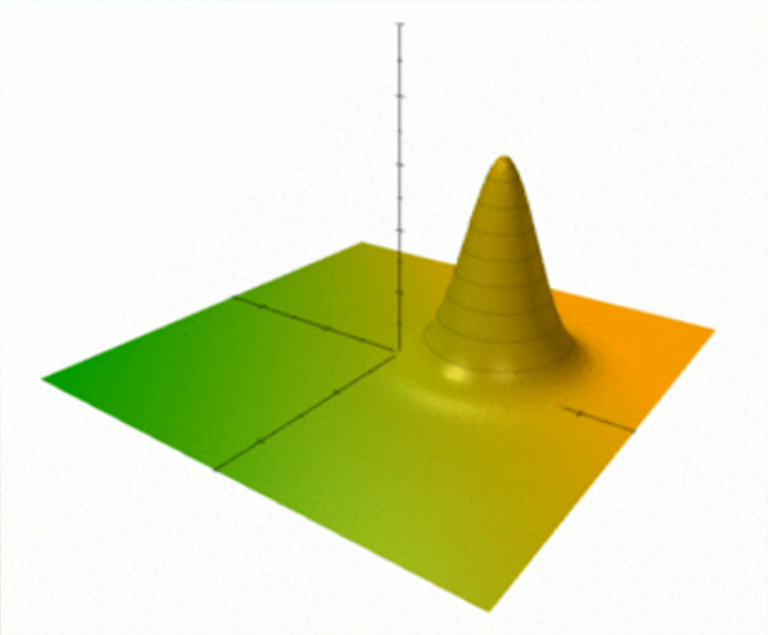

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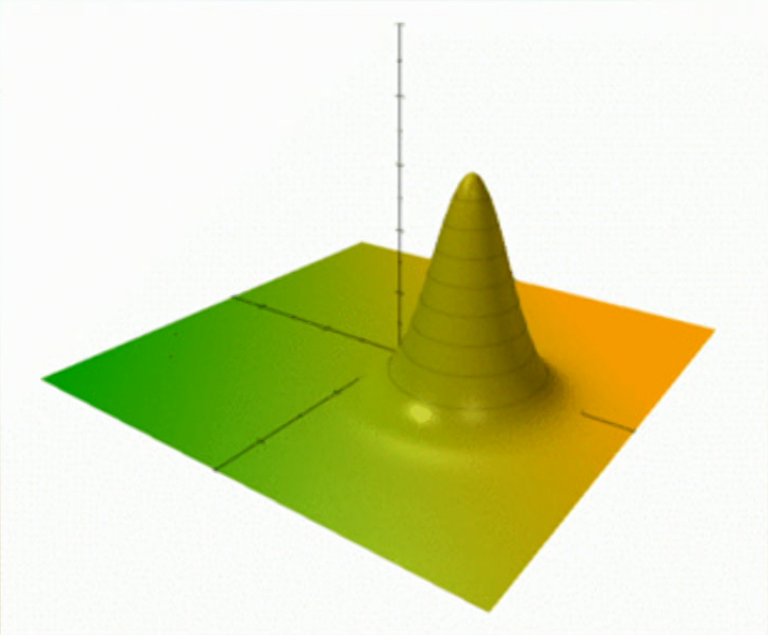

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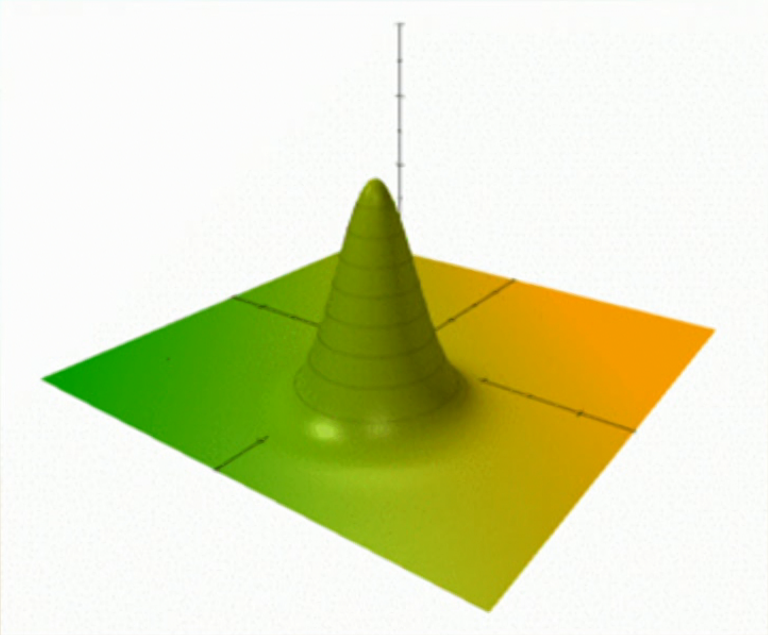

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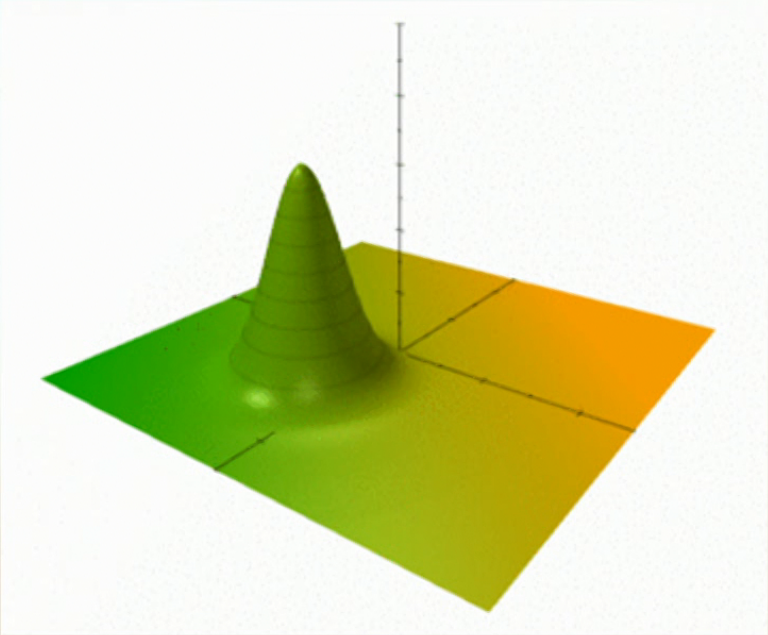


Coherent States in General

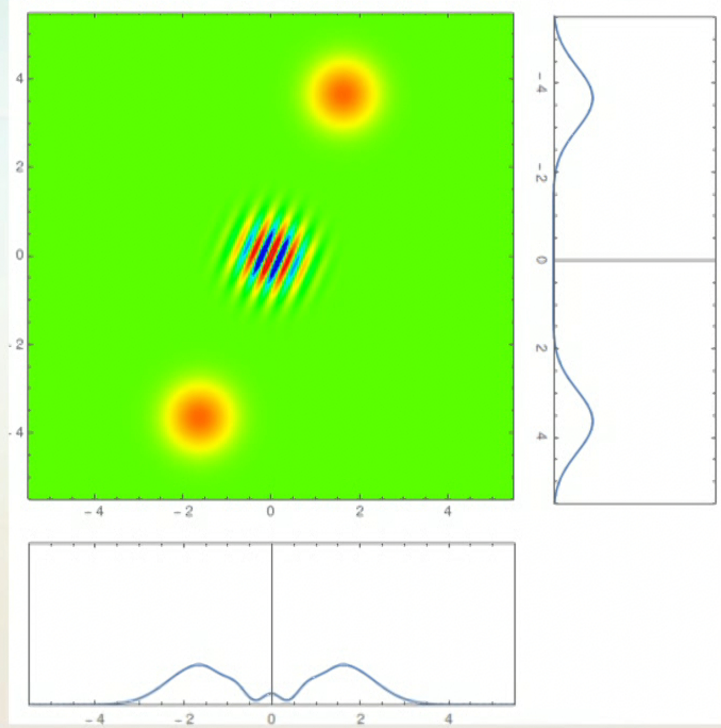
- Most bosonic fields in nature have (approximate) coherent states
- Example: Electromagnetic field. Ignoring photon-photon interactions (which are order g^4) the EM field has coherent states that are approximately localized around specific values of $\vec{E}$ and $\vec{B}$. These obey the free-field Maxwell equations.
- So long as the photons do not scatter off a charged particle (which would cause entanglement) we can take these as a model for coherent light travelling in free space, e.g. a laser beam.

Summary So Far

- Gaussian quantum mechanics has a well defined Liouville limit.
- Coherent states have a trajectory limit.
  - Both of these are severe restrictions on the class of states and Hamiltonians we can deal with.
  - As soon as we introduce interactions, the EM field Hamiltonian is no longer quadratic.
  - Even superpositions of two Gaussian states have negative Wigner functions.
  - If we want a trajectory limit, we can't even have all Gaussian states and quadratic Hamiltonians due to spreading in phase space.

Example: Schrödinger Cat State

- Superposition of two coherent states of a harmonic oscillator.
- The Wigner function is negative at some points (blue regions). This is responsible for interference.
- As the two components are moved further apart, there is less negativity, but it is always there and can be amplified by moving them together.
- We need to get rid of the negativity to model this as a classical particle that is in one of two states.



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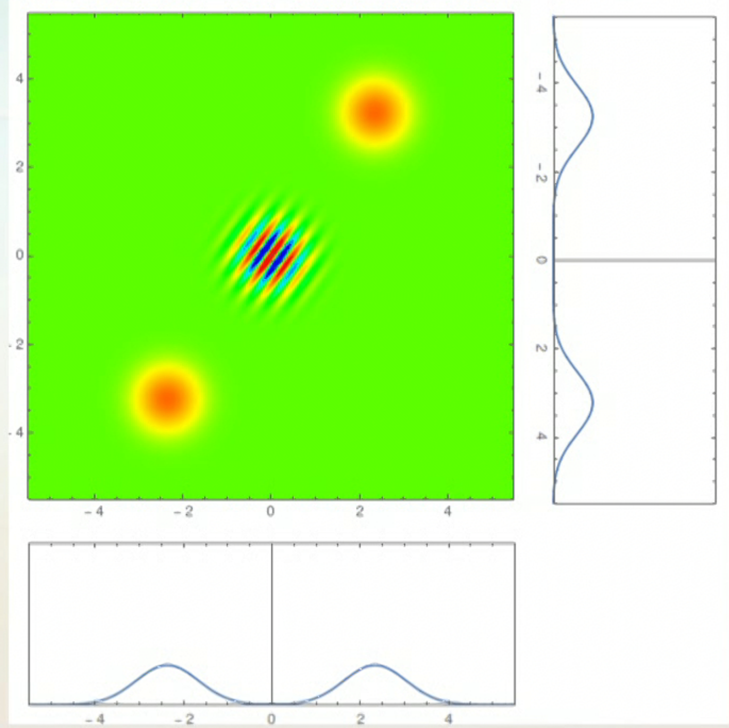

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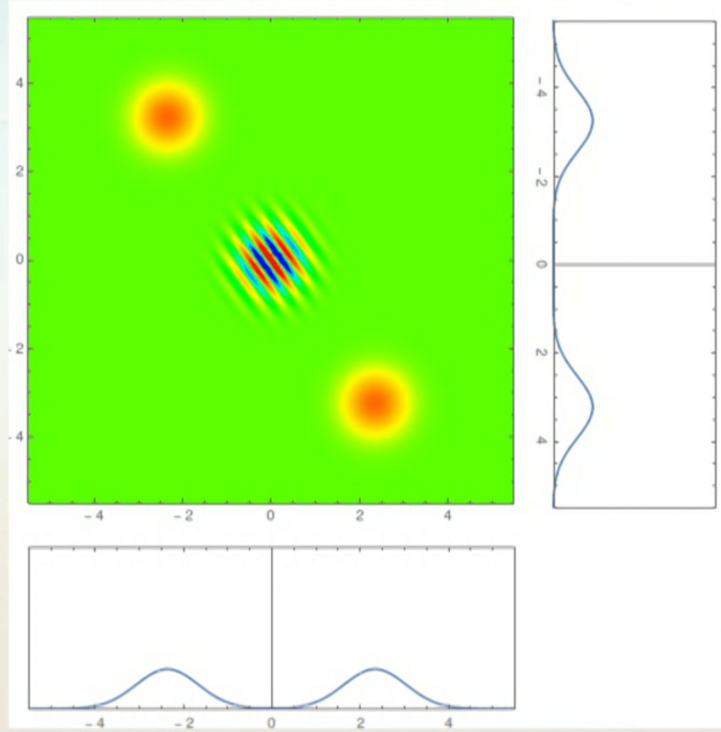

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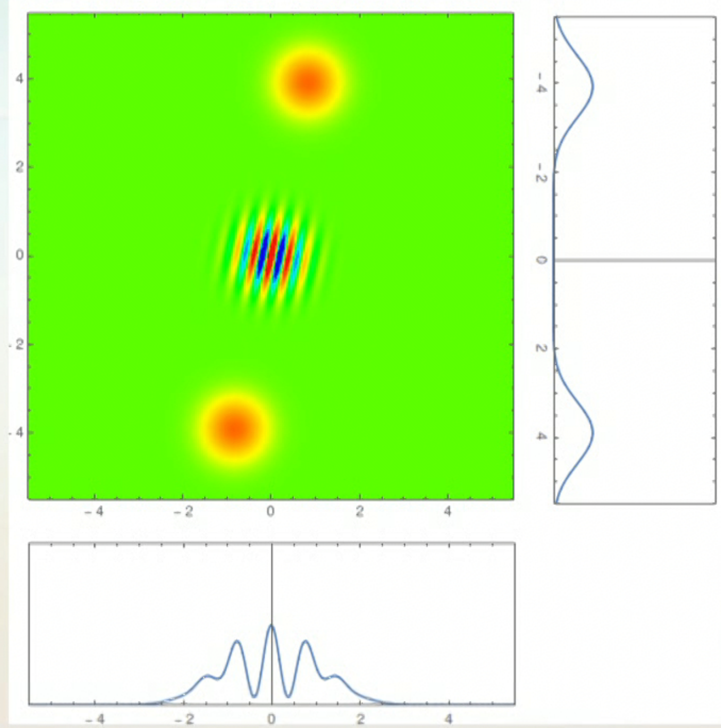

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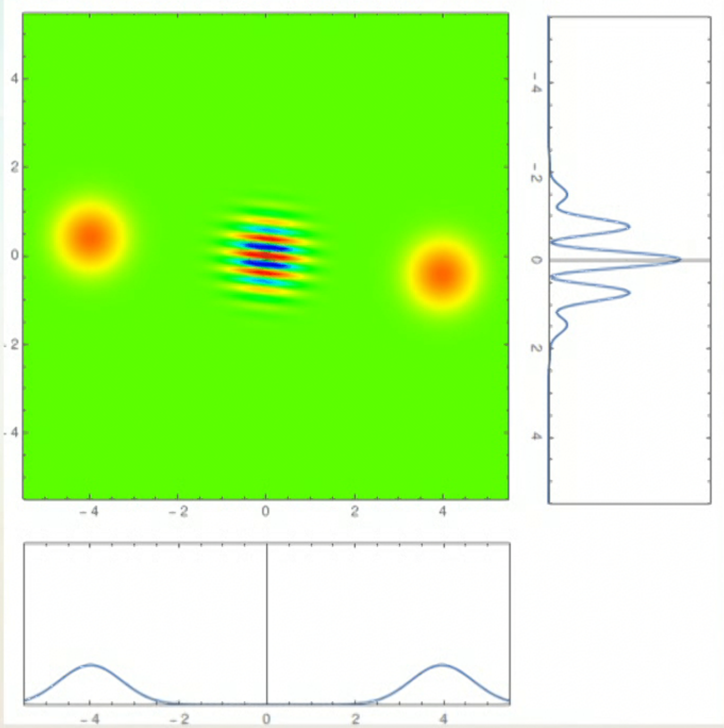

9.5) Environmentally Induced Decoherence

- Suppose we have a system in a superposition of two macroscopically distinct (approximately) orthogonal states
$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle$$
e.g. $|\psi_1\rangle = |\text{cat alive}\rangle$, $|\psi_2\rangle = |\text{cat dead}\rangle$ or $|\psi_j\rangle$ = a large object at two different locations.
- The system is interacting with the environment all the time, e.g. photons and air molecules scatter off it.
- Suppose the system is initially uncorrelated with the scattering particle
$$|\psi\rangle|\chi_0\rangle$$
- The scattered particle gets correlated (not necessarily a lot) with the system, but the interaction hardly perturbs the system.
$$|\psi_j\rangle|\chi_0\rangle \rightarrow |\psi_j\rangle|\chi_j\rangle \quad \text{with} \quad |\langle\chi_1|\chi_2\rangle| \text{ not necessarily} = 0.$$

9.5) Environmentally Induced Decoherence

- After one scattering event, the joint state will be

$$\alpha|\psi_1\rangle|\chi_1\rangle + \beta|\psi_2\rangle|\chi_2\rangle$$

and the reduced density operator of the system will be

$$\rho = |\alpha|^2|\psi_1\rangle\langle\psi_1| + |\beta|^2|\psi_2\rangle\langle\psi_2| + \alpha\beta^*\langle\chi_2|\chi_1\rangle|\psi_1\rangle\langle\psi_2| + \beta\alpha^*\langle\chi_1|\chi_2\rangle|\psi_2\rangle\langle\psi_1|$$

- After N scattering events, we will have

$$\alpha|\psi_1\rangle|\chi_1\rangle^{\otimes N} + \beta|\psi_2\rangle|\chi_2\rangle^{\otimes N}$$

and

$$\rho = |\alpha|^2|\psi_1\rangle\langle\psi_1| + |\beta|^2|\psi_2\rangle\langle\psi_2| + \alpha\beta^*\langle\chi_2|\chi_1\rangle^N|\psi_1\rangle\langle\psi_2| + \beta\alpha^*\langle\chi_1|\chi_2\rangle^N|\psi_2\rangle\langle\psi_1|$$

9.5) Environmentally Induced Decoherence

- If the average time between scattering events is τ then after time t there will be $N \approx t/\tau$ such events
- The modulus of the off-diagonal elements of the density operator will be

$$|\alpha\beta^*||\langle\chi_2|\chi_1\rangle|^{t/\tau}$$

i.e. they decrease exponentially in t.

- For sufficiently long t, we will have

$$\rho \approx |\alpha|^2|\psi_1\rangle\langle\psi_1| + |\beta|^2|\psi_2\rangle\langle\psi_2|$$

so it will be indistinguishable from a mixture. The timescale on which this happens is usually extremely short.

The General Framework

- Suppose the system is described by Hilbert space $\mathcal{H}_S$ and the environment by $\mathcal{H}_E$ so that the joint space is $\mathcal{H}_S \otimes \mathcal{H}_E$. Write the Hamiltonian as

$$H = H_S \otimes I_E + I_S \otimes H_E + H_{\text{int}}$$

- We define a *pointer state* as a state of the system that does not get entangled with the environment in the course of this evolution

$$|\psi_P(0)\rangle_S|\chi(0)\rangle_E \to |\psi_P(t)\rangle_S|\chi(t)\rangle_E$$

- A sufficient condition for a pointer state is

$$[H_{\text{int}}, |\psi_P\rangle\langle\psi_P| \otimes I_S] = 0$$

which is known as *Zurek's commutation condition*.

The General Framework

- Exact pointer states need not exist for all Hamiltonians, but for physically realistic Hamiltonians, we can usually find approximate pointer states

$$[H_{\text{int}}, |\psi_P\rangle\langle\psi_P| \otimes I_S] = \epsilon$$

for some small ϵ. These do not get entangled very much with the environment.

The Measurement Limit

- Suppose the typical timescale (energy gap) of H_{int} is large compared with H_S. Then we can set $H_S \approx 0$.
- Let $H_{\text{int}} = A_S \otimes B_E$. Then, the pointer states will be the eigenstates of A_S.
- We can think of this interaction as measuring the observable A_S. An initial state $|\psi\rangle_S = \sum_j \alpha_j \left|a_j\right\rangle_S$ will quickly evolve into

$$\rho_S \approx \sum_j \left|\alpha_j\right|^2 |a_j\rangle\langle a_j|$$

The "Quantum" Limit

- Suppose the typical timescale (energy gap) of H_{int} is small compared with H_S.
- Then, the pointer states will be eigenstates of H_S, i.e. energy eigenstates.
- Explains why microscopic systems that are well-isolated from the environment are typically found in energy eigenstates, e.g. the hydrogen atom.

The Intermediate Regime

- The intermediate regime is the most interesting (and most difficult mathematically). Exact pointer states do not usually exist, but for typical interactions we often get coherent states as approximate pointer states.
- So, our Schrödinger cat state

$$\frac{1}{\sqrt{2}}(|\alpha_1\rangle + |\alpha_2\rangle)$$

would evolve to $\approx \frac{1}{2}(|\alpha_1\rangle\langle\alpha_1| + |\alpha_2\rangle\langle\alpha_2|)$

- The negativity in the Wigner function would disappear and the evolution would look like a mixture of two Gaussians under Liouville dynamics.

The Intermediate Regime

- This regime is also important if you want to get a trajectory limit in cases where the Wigner function spreads out over phase space.
- If you start with a coherent state $|\alpha\rangle$, after a time t the state will be a superposition of coherent states
$$\int \mathrm{d}\alpha\ f(\alpha)|\alpha\rangle$$
Note, this is not unique as coherent states form an overcomplete basis.
- But this will quickly decohere to
$$\rho_S \approx \int \mathrm{d}\alpha |f(\alpha)|^2 |\alpha\rangle\langle\alpha|$$
- The centroids of each component will obey Hamilton's equations, but they will also spread and decohere into a mixture again.
- If you track the mod-squared amplitude of these branches, the overwhelming weight of probability will be on paths that are approximately classical trajectories in phase space.

What about chaotic systems?

- If H_S is a Hamiltonian that exhibits chaos (exponential divergence of nearby trajectories in phase space) then decoherence may not act quickly enough to localize the Wigner function in phase space.
- This is a problem if you think we must always obtain a trajectory limit.
- However, even classically you cannot predict the exact trajectory if you have even a tiny amount of uncertainty about the initial conditions. Therefore, the predictions of Liouville mechanics for minimal uncertainty initial states are indistinguishable from those of Hamiltonian mechanics in practice.
- For this reason, it is fine to only get a Liouville limit for chaotic systems.

How Do Other Quantum Effects Disappear?

- We have mostly been talking about interference, but why don't we typically see nonlocality, contextuality, etc. in the classical limit?
- These effects depend on being able to make a choice among measuring different incompatible observables on the system.
- When we observe a macroscopic system, we typically do so by intercepting a small fraction of the environment of the system.
  - e.g. you are intercepting a small fraction of the photons that have scattered off me.
- We can only measure information about the system that is encoded in that small fraction of the environment.

How Do Other Quantum Effects Disappear?

- For example, consider the scattering state
$$\alpha|\psi_1\rangle|\chi_1\rangle^{\otimes N} + \beta|\psi_2\rangle|\chi_2\rangle^{\otimes N}$$
- If you make any quantum measurement on $k \ll N$ of the environment systems then you can determine the effective measurement you have performed on the system (as in the quantum steering Homework problem).
- As $N \rightarrow \infty$ you will find that all of these measurements are *compatible*, i.e. there exists a POVM you could have done directly on the system that gives you the correct outcome probabilities for all of them.
- Zurek's *quantum Darwinism* says that classical information is that which is redundantly encoded in the environment. This will be a compatible set of measurements in the limit.

Summary

- Some systems look classical in the Wigner-Moyal formalism
  - Gaussian quantum mechanics has a Liouville limit
  - Coherent states give a trajectory limit
- In other cases we need environmental decoherence to get a limit
  - Explains the disappearance of interference
  - Explains how Wigner functions become positive
  - Explains why observables become compatible
  - Gives an effective equivalence to an ensemble of trajectories obeying Hamiltonian mechanics.
- Decoherence works for the reduced density operator of the system. State of the universe is still a pure entangled state, so it is not clear that this solves actualization of measurement outcomes.