MSE 423 Fall 2024 – Week 4

CLOSE TO COLLAPSE

Last week: Postulates

- Operators, eigenvalues, eigenfunctions, expectation values $\hat{O}|\xi_i\rangle = \varepsilon_i|\xi_i\rangle$ $\varepsilon_i = \langle\xi_i|\hat{O}|\xi_i\rangle$
- Linear operators, Hermitian operators $\Rightarrow \langle\varphi|\hat{A}\psi\rangle = \langle\hat{A}\varphi|\psi\rangle$
- Products of operators, and commutators
- Commuting operators and common eigenfunctions $\Rightarrow [\hat{A},\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$
- The five postulates of quantum mechanics
  - I. **Wavefunctions** $|\psi\rangle$
  - II. **Operators**
  - III. **Measurements**
  - IV. **Expectation values, probabilities**
  - V. **…**

$|\psi\rangle = \sum_n c_n|\varphi_n\rangle = \sum_n |\varphi_n\rangle\langle\varphi_n|\psi\rangle$

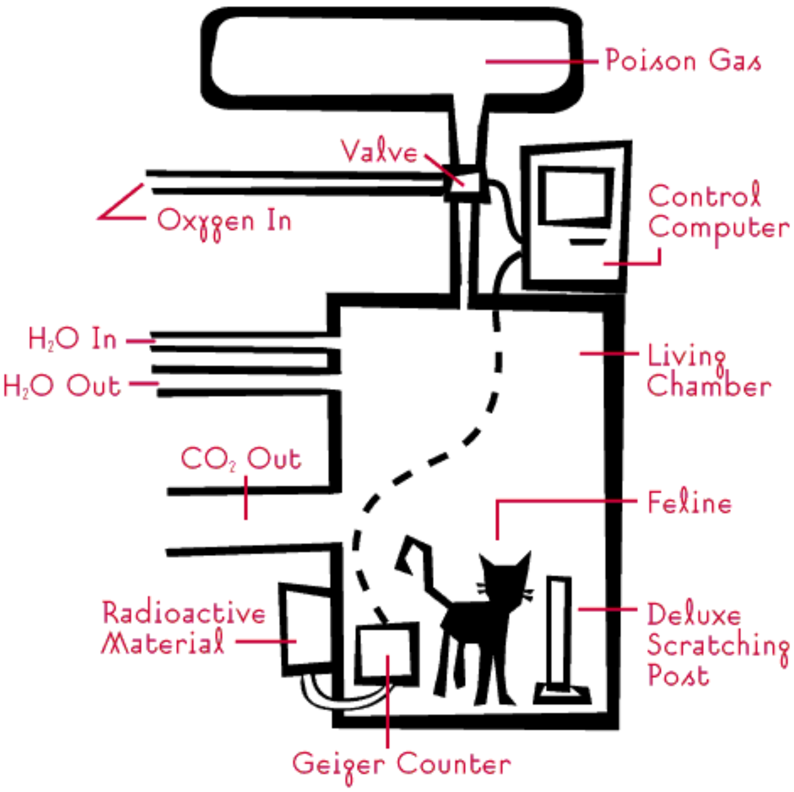
$\hat{A}|\varphi_n\rangle = a_n|\varphi_n\rangle$

$\|\langle\varphi_n|\psi\rangle\|^2$

Fifth postulate: collapse

- If the measurement of the physical quantity A gives the result a_n , the wavefunction of the system immediately after the measurement is the eigenvector $|\varphi_n\rangle$

When scientists turn bad…



Cat wavefunction

$$\left|\Psi_{cat}(t)\right\rangle = \left|\Psi_{alive}\right\rangle \left(\exp\left(-\frac{t}{\tau}\right)\right)^{\frac{1}{2}} + \left|\Psi_{dead}\right\rangle \left(1-\exp\left(-\frac{t}{\tau}\right)\right)^{\frac{1}{2}}$$

- There is not a value of the observable until it’s measured (a conceptually different “statistics” from thermodynamics)

MENU nature International journal of science

Search E-alert Submit Login

News & Comment Research

News Opinion Research Analysis Careers Books & Culture

NEWS · 18 SEPTEMBER 2018

Reimagining of Schrödinger’s cat breaks quantum mechanics — and stumps physicists

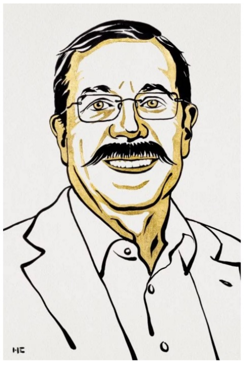
In a multi-‘cat’ experiment, the textbook interpretation of quantum theory seems to lead to contradictory pictures of reality, physicists claim.

Davide Castelvecchi

Top Three List

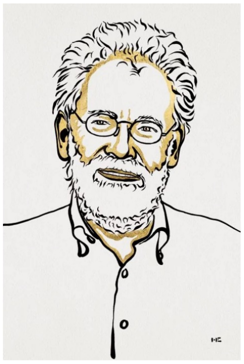
- ***Albert Einstein:*** *"Gott wurfelt nicht!" [God does not play dice!]*
- ***Werner Heisenberg*** *"I myself . . . only came to believe in the uncertainty relations after many pangs of conscience. . ."*
- **Erwin Schrödinger:** *"Had I known that we were not going to get rid of this damned quantum jumping, I never would have involved myself in this business!"*

The Nobel Prize in Physics 2022



Ill. Niklas Elmehed © Nobel Prize Outreach
Alain Aspect
Prize share: 1/3

Ill. Niklas Elmehed © Nobel Prize Outreach
John F. Clauser
Prize share: 1/3



Ill. Niklas Elmehed © Nobel Prize Outreach
Anton Zeilinger
Prize share: 1/3

The Nobel Prize in Physics 2022 was awarded jointly to Alain Aspect, John F. Clauser and Anton Zeilinger "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

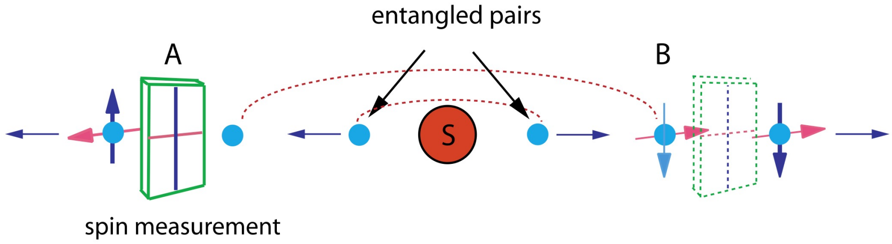
MAY 15, 1935 PHYSICAL REVIEW VOLUME 47

Can Quantum-Mechanical Description of Physical Reality Be Considered Complete?

A. EINSTEIN, B. PODOLSKY AND N. ROSEN, *Institute for Advanced Study, Princeton, New Jersey*

(Received March 25, 1935)

In a complete theory there is an element corresponding to each element of reality. A sufficient condition for the reality of a physical quantity is the possibility of predicting it with certainty, without disturbing the system. In quantum mechanics in the case of two physical quantities described by non-commuting operators, the knowledge of one precludes the knowledge of the other. Then either (1) the description of reality given by the wave function in quantum mechanics is not complete or (2) these two quantities cannot have simultaneous reality. Consideration of the problem of making predictions concerning a system on the basis of measurements made on another system that had previously interacted with it leads to the result that if (1) is false then (2) is also false. One is thus led to conclude that the description of reality as given by a wave function is not complete.



https://www.nobelprize.org/uploads/2022/10/advanced-physicsprize2022.pdf

Uncertainties, and Heisenberg's Indetermination Principle

variance ψ $\langle\psi|\hat{A}|\psi\rangle$

$$\underbrace{(\Delta A)^2}_{\text{variance}} = \langle (\hat{A} - \langle \hat{A} \rangle)^2 \rangle = \langle \hat{A}^2 \rangle - \langle \hat{A} \rangle^2$$

$\langle\psi|(\hat{A}-\langle\hat{A}\rangle)^2|\psi\rangle = \langle\psi|\hat{A}\cdot\hat{A}-2\hat{A}\cdot\langle\hat{A}\rangle+\langle\hat{A}\rangle^2|\psi\rangle$

$$\Delta A \Delta B \geq \frac{1}{2}\left|\langle [A,B] \rangle\right|$$

$f = i\hbar f$

$$\left[x, -i\hbar\frac{d}{dx}\right] = i\hbar$$

Linewidth Broadening

PHYSICAL REVIEW A **62** 063404

$$\Delta E \Delta t \geq \frac{\hbar}{2}$$

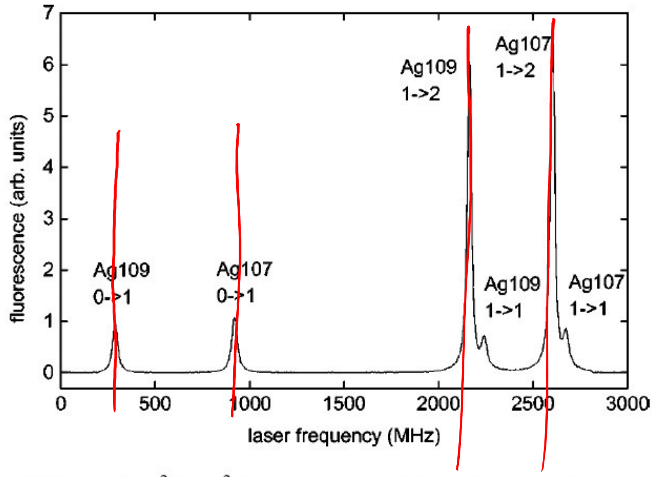


FIG. 2. The $^2S_{1/2}$–$^2P_{3/2}$ spectrum, obtained with a frequency-doubled diode laser aligned perpendicular to the thermal atomic beam.

Good Quantum Numbers

$\hat{H}|\Psi\rangle = i\hbar \frac{\partial}{\partial t}|\Psi\rangle$

$$\frac{d\langle \hat{A} \rangle}{dt} = \frac{d\langle \Psi | \hat{A} | \Psi \rangle}{dt} = \frac{1}{i\hbar}\langle [\hat{A}, \hat{H}] \rangle \Rightarrow \begin{cases} 0 & \text{Good} \\ \text{Not Good} \\ \neq 0 & \text{BAD} \end{cases}$$

If $\hat{A}$ commutes with the Hamiltonian, and it does not depend on time, its expectation value does not change with time (it's a constant of motion – if we are in an eigenstate, that quantum number will remain constant)

Variational Principle

FUNCTIONAL OF Ψ

$$E\left[\Psi\right]=\frac{\left\langle\Psi\middle|\hat{H}\middle|\Psi\right\rangle}{\left\langle\Psi\middle|\Psi\right\rangle} = \frac{\int \psi^* \hat{H} \psi}{\int \|\psi\|^2}$$

Variational Principle

$$E\left[\Psi\right]=\frac{\left\langle\Psi\middle|\hat{H}\middle|\Psi\right\rangle}{\left\langle\Psi\middle|\Psi\right\rangle}$$

$$E\left[\Psi\right]\geq E_0$$

If $E\left[\Psi\right]=E_0$, then Ψ is the ground state wavefunction, and viceversa…

$$|\Psi\rangle = \sum_n c_n \underbrace{|\varphi_n\rangle}_{\text{COMPLETE STATE OF EIGENSTATES}}$$

ARBITRARY

$$\hat{H}|\varphi_n\rangle = \varepsilon_n|\varphi_n\rangle$$

$$\underbrace{\sum_m c_m^* \overbrace{\langle\varphi_m|\varphi_n\rangle}^{\delta_{mn}}}_{c_m^*\delta_{mn}}$$

$$\frac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\langle\Psi|\hat{H}(\sum_n c_n|\varphi_n\rangle)}{\langle\Psi|(\sum_n c_n|\varphi_n\rangle)} =$$

$$= \frac{\sum_n c_n\langle\Psi|\hat{H}|\varphi_n\rangle}{\sum_n c_n\langle\Psi|\varphi_n\rangle} = \frac{\sum_n c_n\varepsilon_n\langle\Psi|\varphi_n\rangle}{\sum_n c_n\langle\Psi|\varphi_n\rangle} =$$

$$= \frac{\sum_n c_n\varepsilon_n(\sum_m c_m^*\delta_{mn})}{\sum_n c_n(\sum_m c_m^*\delta_{mn})} = \frac{\sum_\ell c_\ell c_\ell^*\varepsilon_\ell}{\sum_j c_j c_j^*} =$$

REAL NUM. REAL NUMB.

$$\varepsilon_0, \varepsilon_1, \varepsilon_2, \varepsilon_3$$

$$E[\Psi] = \frac{\sum_\ell c_\ell c_\ell^* \varepsilon_\ell}{\sum_j c_j c_j^*} \geq \frac{\varepsilon_0 c_0 c_0^* + \overset{\varepsilon_0}{\cancel{\varepsilon_1}} c_1 c_1^* + \overset{\varepsilon_0}{\cancel{\varepsilon_2}} c_2 c_2^* \ldots}{\sum_j c_j c_j^*}$$

$$= \frac{\varepsilon_0 \cancel{\sum_\ell c_\ell c_\ell^*}}{\cancel{\sum_j c_j c_j^*}} = \varepsilon_0$$

$$\left(|\Psi\rangle = \sum_n c_n|\varphi_n\rangle\right)$$
$$\left(= c_0|\varphi_0\rangle\right)$$

?

$$|\Psi\rangle = a_1|\varphi_1\rangle + \cdots\cdots |a_{10}\rangle|\varphi_{10}\rangle$$

→ SIMPLE

$$E[\Psi] = f(a_1, \ldots, a_{10})$$

Matrix Formulation (I)

VECTOR IN ∞-DIM HILBERT

ONE EQ.

$$\boxed{\hat{H}|\psi\rangle = E|\psi\rangle}$$

DIFF. EQ. (ANY)

$$|\psi\rangle \cong \sum_{n=1,10} c_n |\varphi_n\rangle \qquad \{|\varphi_n\rangle\} \text{ orthoNORMAL}$$

$$\langle\varphi_m|\hat{H}|\psi\rangle = E\langle\varphi_m|\psi\rangle$$

10 EQUATIONS

$$\sum_{n=1,10} c_n \underbrace{\langle\varphi_m|\hat{H}|\varphi_n\rangle}_{H_{mn}} = Ec_m$$

$$\langle\varphi_m|\sum_{n=1,10} c_n|\varphi_n\rangle = \sum_n \underbrace{\langle\varphi_m|\varphi_n\rangle}_{\delta_{mn}} c_n = c_m$$

Matrix Formulation (II)

$$\sum_{n=1,k} H_{mn}c_n = Ec_m$$

$\langle\varphi_m|\hat{H}|\varphi_n\rangle$

$\forall m$ 1 eq.

$$\begin{pmatrix} H_{11}-E & \dots\dots & & H_{1k} \\ . & H_{22}-E & & . \\ . & & H_{33}-E & . \\ . & & \ddots & . \\ H_{k1} & \dots\dots & & H_{kk}-E \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ . \\ . \\ . \\ c_k \end{pmatrix} = E \begin{pmatrix} c_1 \\ . \\ . \\ . \\ c_k \end{pmatrix} \quad 0$$

Matrix Formulation (III)

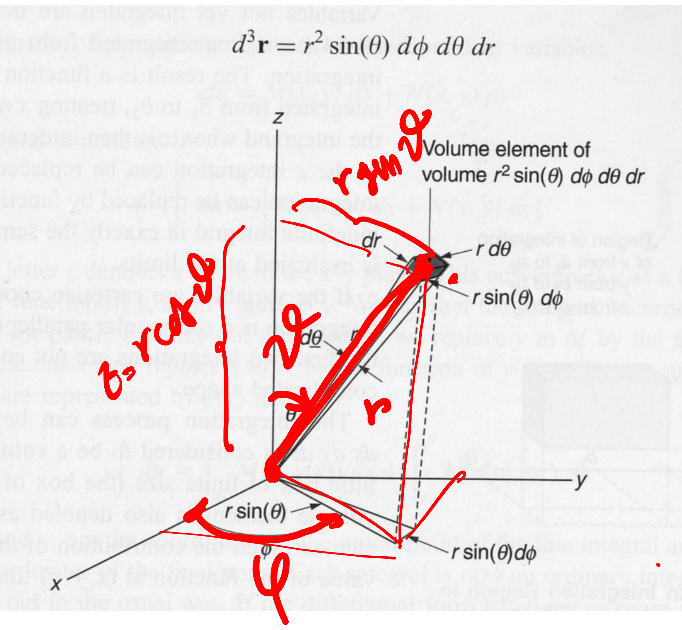
$$
\det\begin{pmatrix}
H_{11}-E & \ldots\ldots & & H_{1k} \\
. & H_{22}-E & & . \\
. & & & . \\
. & & & . \\
H_{k1} & \ldots\ldots & & H_{kk}-E
\end{pmatrix} = 0
$$

$$
\det\begin{pmatrix} H_{11}-E & H_{12} \\ H_{21} & H_{22}-E \end{pmatrix} = (H_{11}-E)(H_{22}-E) - H_{12}H_{21} = 0
$$

$$
\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} f(x,y,z)\,dx\,dy\,dz =
$$

Spherical Coordinates

$$
= \int_0^{+\infty} dr \int_0^{\pi} d\theta \int_0^{2\pi} d\varphi
$$



$$x = r\sin\theta\cos\varphi$$

$$y = r\sin\theta\sin\varphi$$

$$z = r\cos\theta$$

$$dx\,dy\,dz = r^2 \sin\theta\, dr\, d\theta\, d\varphi$$

Angular Momentum

Classical

$$\vec{L} = \vec{r} \times \vec{p}$$

$\vec{r} \rightarrow r$, $\vec{p} \rightarrow -i\hbar\vec{\nabla}$

$L_x = y p_z - z p_y$

$L_y = z p_x - x p_z$

$L_z = x p_y - y p_x$

Quantum

$\hat{L} = \vec{r} \times (-i\hbar\vec{\nabla}) =$

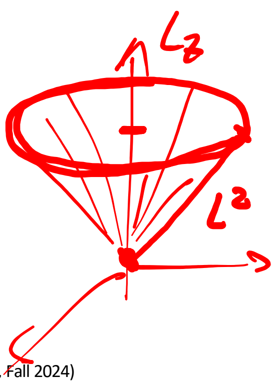
$\hat{L}_x = \hat{y}\left(-i\hbar \frac{d}{dz}\right) - \hat{z}\left(i\hbar \frac{d}{dy}\right)$

Commutation Relation

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

$$\left[\hat{L}^2, \hat{L}_x\right] = \left[\hat{L}^2, \hat{L}_y\right] = \left[\hat{L}^2, \hat{L}_z\right] = 0$$

$$\left[\hat{L}_x, \hat{L}_y\right] = i\hbar\hat{L}_z \neq 0$$



Angular Momentum in Spherical Coordinates

$$[\hat{L}_z, \hat{L}^2] = 0$$

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$$

$$\hat{L}^2 = -\hbar^2 \left(\underbrace{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)}_{\vartheta} + \underbrace{\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}}_{\vartheta,\,\varphi} \right)$$

Simultaneous eigenfunctions of $\hat{L}^2$, $\hat{L}_z$

$$\hat{L}_z Y_\ell^m(\vartheta,\varphi) = m\hbar\, Y_\ell^m(\vartheta,\varphi)$$

$$-\ell \leq m \leq \ell$$

$\ell = 0 \Rightarrow m = 0$

$\ell = 1 \Rightarrow m = -1,\ m = 0,\ m = 1$

$\ell = 2 \Rightarrow m = -2, -1, 0, 1, 2$

$$\hat{L}^2 Y_\ell^m(\vartheta,\varphi) = \hbar^2 \ell(\ell+1) Y_\ell^m(\vartheta,\varphi)$$

$\ell = 0, 1, 2, 3, \ldots$

$\hat{L}^2$ EIGENV = 0, $2\hbar^2$, $6\hbar^2$, $12\hbar^2$ ....

Simultaneous eigenfunctions of L^2, L_z

$$Y_l^m(\theta,\varphi)=\begin{cases}(-1)^m\sqrt{\dfrac{2l+1}{4\pi}\dfrac{(l-m)!}{(l+m)!}}P_l^m(\cos\theta)e^{im\varphi} & m\geq 0\\ \sqrt{\dfrac{2l+1}{4\pi}\dfrac{(l+m)!}{(l-m)!}}P_l^{-m}(\cos\theta)e^{im\varphi} & m<0\\ l=0,1,2\ldots \quad m=-l,-l+1,\ldots,-1,0,1,\ldots,l-1,l\end{cases}$$

$$Y_0^0(\theta,\phi)=\frac{1}{(4\pi)^{1/2}}$$

$$Y_1^0(\theta,\phi)=\left(\frac{3}{4\pi}\right)^{1/2}\cos\theta$$

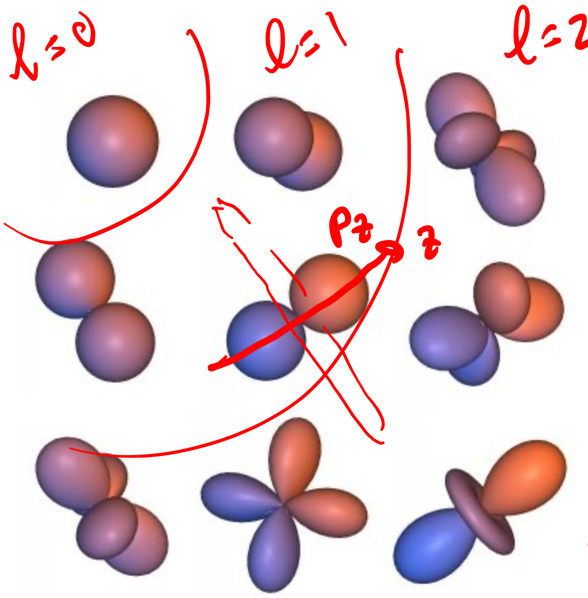
$$Y_1^{\pm1}(\theta,\phi)=\left(\frac{3}{8\pi}\right)^{1/2}\sin\theta\, e^{\pm i\phi}$$

$$Y_2^0(\theta,\phi)=\left(\frac{5}{16\pi}\right)^{1/2}\left(3\cos^2\theta-1\right)$$

$$Y_2^{\pm1}(\theta,\phi)=\left(\frac{15}{8\pi}\right)^{1/2}\sin\theta\cos\theta\, e^{\pm i\phi}$$

$$Y_2^{\pm2}(\theta,\phi)=\left(\frac{15}{32\pi}\right)^{1/2}\sin^2\theta\, e^{\pm 2i\phi}$$

Spherical Harmonics in Real Form



l=1

$$p_x=\frac{1}{\sqrt{2}}\left(Y_1^1+Y_1^{-1}\right)=\sqrt{\frac{3}{4\pi}}\sin\theta\cos\phi$$

$$p_y=\frac{1}{\sqrt{2}\,i}\left(Y_1^1-Y_1^{-1}\right)=\sqrt{\frac{3}{4\pi}}\sin\theta\sin\phi$$

$$p_z=Y_1^0=\sqrt{\frac{3}{4\pi}}\cos\theta$$

l=2

$$d_{z^2}=Y_2^0=\sqrt{\frac{5}{16\pi}}\left(3\cos^2\theta-1\right)$$

$$d_{xz}=\frac{1}{\sqrt{2}}\left(Y_2^1+Y_2^{-1}\right)=\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\cos\phi$$

$$d_{yz}=\frac{1}{\sqrt{2}\,i}\left(Y_2^1-Y_2^{-1}\right)=\sqrt{\frac{15}{4\pi}}\sin\theta\cos\theta\sin\phi$$

$$d_{x^2-y^2}=\frac{1}{\sqrt{2}}\left(Y_2^2+Y_2^{-2}\right)=\sqrt{\frac{15}{16\pi}}\sin^2\theta\cos 2\phi$$

$$d_{xy}=\frac{1}{\sqrt{2}\,i}\left(Y_2^2-Y_2^{-2}\right)=\sqrt{\frac{15}{16\pi}}\sin^2\theta\sin 2\phi$$