Quantum Electronics

5. Eigenstates and operators

فصل ۵: حالتهای ویژه و عملگرها

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با تشکر از آقایان
امین پایان و
علی فرید

Contents: Eigenstates and operators

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۵–۱– مقدمه

❖ **مکانیک کوانتوم** یک توصیف موفق از یک سیستم در مقیاس اتم است.

❖ مکانیک کوانتوم ساده ترین توصیف ریاضی بر حسب عملگرهای خطی جابجاناپذیر است که به خوبی قابل توجه می باشد.

❖ تقارن های زیبا و به خوبی جاسازی‌شده (در این علم) و مشخصات خوشایند و مسرت بخش این علم برای بعضی از مطالعه کنندگان در این موضوع باعث توجه است.

❖ البته این توصیف ریاضی با استفاده از اصول، چهارچوب منطقی را فراهم میکند که به ایجاد یک ارتباط با نتایج اندازه گیری بینجامد.

۵-۱-۱- اصول مکانیک کوانتوم

از موارد گفته شده و بسط داده شده در فصل قبل، چهار مورد از اصول موضوعه را برای مکانیک کوانتومی در زیر ذکر می کنیم:

۵-۱-۱-۱- اصل ۱

متناسب با هر مشاهده فیزیکی، که ممکن است از نتایج اندازه گیری قابل مشاهده، نتیجه گرفته باشد، یک اپراتور $\hat{A}$ تعریف می کنیم.

- فرض می کنیم که هر اپراتور بصورت خطی از معادلات با مقادیر ویژه $\hat{A}\psi_n = a_n \psi_n$ استنتاج وتوجیه می شود، که در آن مقادیر ویژه a_n، اعداد حقیقی، و توابع ویژه ψ_n به شکل یک مجموعه متعامد کامل در فضای تابع حالت است.

- مقادیر ویژه که ممکن است بر گرفته از مقادیر گسسته یا مقادیر موجود در یک بازه زمانی باشند، پیوسته هستند که ضمانت می کنند بر حقیقی بودن آن عدد (از این رو مقادیر قابل اندازه گیری هستند) اگر اپراتور **متناظر هرمیتی** باشد.

- همچنین باید توجه کنیم که در حالت کلی توابع ویژه، مختلط هستند، بنابراین به طور مستقیم غیرقابل اندازه گیری هستند.

۵-۱-۱-۲- اصل ۲

فقط نتایج ممکن از یک اندازه‌گیری بر روی یک سیستم منفرد قابل مشاهده ی فیزیکی است که متناسب با عملگر $\hat{A}$ ، یک مقدار ویژه عملگر $\hat{A}$ است.

- در این زمینه، نتایج اندازه گیری مرتبط است با مقادیر ویژه عملگر ریاضی $\hat{A}$.
- عمل اندازه‌گیری بر روی یک سیستم با دادن یک مقادیر ویژه a_n که یک عدد حقیقی است مشخص می شود.
- تابع ویژه متناسب است با مقادیر ویژه که به صورت ایستا یا ساکن هستند.
- به عنوان یک نتیجه، بعد از اندازه گیری های انجام شده، در اندازه گیری های حالت های ویژه، حالت های از یک سیستم باقی خواهد ماند، مگر اینکه یک نیروی بر روی آن عمل کند.

۵-۱-۱-۳- اصل ۳

❖ برای هر سیستمی، همیشه یک تابع حالت ψ وجود دارد که شامل همه اطلاعاتی است که درباره سیستم می دانیم.

❖ تابع حالت ψ حاوی همه اطلاعات قابل مشاهده سیستم است.

❖ این تابع، برای یافتن احتمال نسبی مقادیر ویژه، a_n، استفاده می‌شود که با عملگر $\hat{A}$ برای یک سیستم مشخص و در زمان داده شده، متناسب است.

۵-۱-۱-۴- اصل ۴

❑ سیر تکامل زمانی ψ، توسط $i\hbar \frac{d\psi}{dt} = \hat{H}\psi$ تعیین می شود، که $\hat{H}$ عملگر همیلتونی برای سیستم است.

❑ سیر تکامل زمانی (تغییر شکل) تابع حالت را به عنوان **معادله شرودینگر** به رسمیت می شناسیم.

$$\left(\frac{-\hbar^2}{2m}\nabla^2 + V(\mathbf{r}, t)\right)\psi(\mathbf{r}, t) = i\hbar\frac{\partial}{\partial t}\psi(\mathbf{r}, t)$$

- اصول مکانیک کوانتوم، فرضیاتی اصولی و اساسی هستند که تئوری آن را می سازنند.
- آن ها فقط توجیه کننده نتایج آزمایشهای فیزیکی هستند که تناقضی وجود نداشته باشد.
- این اصول، بین جنبه های فیزیکی از یک مدل و ریاضیات مرتبط با آن ارتباط برقرار می کنند.
- توصیف یا تشریح احتمالی از اندازه‌گیری و رابطه پاشیدگی تابع حالت یک تابع ویژه، جنبه‌های فیزیکی هستند که از جنبه های قشنگ ریاضیات مکانیک کوانتوم چیزی را نمی کاهند.
- اصل تطابق (یا تناظر) (correspondence principle) این است که در آن با میل کردن $\hbar$ به سمت صفر ($\hbar \to 0$) حاوی همان نتایجی است که با محدودیت های تحمیلی توسط فیزیک از مکانیک کلاسیک می دانیم.
- در این فصل ایده اصلی، معرفی بعضی از جنبه های ریاضیات استفاده شده در مورد توصیف پدیده های کوانتومی است.
- ریاضیاتی که مجبور به یادگیری آن هستیم، جبر عملگر خطی جابجاناپذیر است.
- ما فقط قصد معرفی مفهوم را داریم و شیوه بیان این ریاضیات به صورت عملگر است.

The postulates of quantum mechanics

- We may write down ***four*** *assumptions or postulates for quantum mechanics*:

➢ *Postulate 1*

*Associated with every **physical observable** is a corresponding **operator** Â from which results of measurement of the observable may be deduced.*

We assume that each operator is linear and satisfies an eigenvalue equation of the form $\hat{A}\psi_n = a_n\psi_n$

✓ a_n is real

✓ Eigenfunctions ψ_n complete orthogonal set in state-function space.

The eigenvalues, which may take on discrete values or exist for a continuous range of values.

We also note that, in general, the eigenfunctions themselves are complex and hence not directly measurable.

The postulates of quantum mechanics

➢ *Postulate 2*

The result of measurement is related to the eigenvalue of the mathematical operator Â.

The act of measurement on the system gives an eigenvalue a_n, which is a real number.

The eigenfunction associated with this eigenvalue is stationary.

➢ *Postulate 3*

For every system there always exists a state-function Ψ *that contains all of the information that is known about the system.*

The state-function Ψ contains all of the information on all observables in the system. It may be used to find the relative probability of obtaining eigenvalue a_n associated with operator Â for a particular system at a given time.

The postulates of quantum mechanics

- ***Postulate 4***

The time evolution of Ψ is determined by $i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi$ where $\hat{H}$ is the Hamiltonian operator for the system.

We recognize the time evolution of the state function as Schrödinger's equation

- The postulates, which are a connection between mathematics

and the physical aspects of the model, contain the strangeness of quantum mechanics.

5.2 One-particle wave function space (1)

- Physical experience suggests that it is reasonable to assume that the total probability of finding the particle somewhere in space is unity, so that:

$$\int_{-\infty}^{\infty} |\psi(\mathbf{r}, t)|^2 d^3 r = 1$$

- The integrands for which this equation converges are square integrable functions. This is a set called l^2 by mathematicians and it has the structure of Hilbert space.
- There are analogies between an ordinary N-dimensional vector space consisting of N orthonormal unit vectors and the eigenfunction space in quantum mechanics. They are, for example, both linear spaces. However, an important difference becomes apparent when one considers scalar products.

$$\mathbf{A} = \sum_{j}^{N} a_j \mathbf{a}_j \quad \mathbf{B} = \sum_{j}^{N} b_j \mathbf{b}_j$$

$$\mathbf{A} \cdot \mathbf{B} = \sum_{j}^{N} a_j b_j$$

scalar product of the two vectors

5.2 One-particle wave function space (2)

- In quantum mechanics we have $\psi_A(\boldsymbol{r})$ and $\psi_B(\boldsymbol{r})$ and integral: $\int \psi_A^*(\boldsymbol{r})\psi_B(\boldsymbol{r})d^3\boldsymbol{r}$
- In Euclidean space for two vector A and B:

$$|A.B|^2 \leq |A|^2.|B|^2$$

- In Hilbert space for two $\psi_A(\boldsymbol{r})$ and $\psi_B(\boldsymbol{r})$:

$$\left|\int \psi_A^*(\boldsymbol{r})\psi_B(\boldsymbol{r})d^3\boldsymbol{r}\ \right|^2 \leq \int \psi_A^*(\boldsymbol{r})\psi_A(\boldsymbol{r})d^3\boldsymbol{r}\ .\int \psi_A^*(\boldsymbol{r})\psi_B^*(\boldsymbol{r})d^3\boldsymbol{r}$$

5.3 Properties of linear operators

- A linear operator $\hat{A}$:

$$\phi(\mathbf{r}) = \hat{A}\psi(\mathbf{r})$$

- A linear operator $\hat{A}$ commutes with constants and is distributive.

$$\hat{A}(\lambda_1\psi_1(\mathbf{r}) + \lambda_2\psi_2(\mathbf{r})) = \lambda_1\hat{A}\psi_1(\mathbf{r}) + \lambda_2\hat{A}\psi_2(\mathbf{r})$$

- if we assume:

$$\hat{A} = \hat{p}_x = -i\hbar\,\partial/\partial x.$$

- So

$$\phi(x) = -i\hbar\frac{\partial}{\partial x}(\lambda_1\psi_1(x) + \lambda_2\psi_2(x)) = -\lambda_1 i\hbar\frac{\partial}{\partial x}\psi_1(x) - \lambda_2 i\hbar\frac{\partial}{\partial x}\psi_2(x)$$

5.3.1 Product of operators

- The product of operators Â and B^ acting upon the function $\psi(\boldsymbol{r})$

$$(\hat{A}\hat{B})\psi(\mathbf{r}) = \hat{A}(\hat{B}\psi(\mathbf{r}))$$

- We must be know $\hat{A}\hat{B} \neq \hat{B}\hat{A}$
- To illustrate this important property. We assume :

- So: $\hat{A} = \hat{p}_x = -i\hbar\, \partial/\partial x.$ $\hat{B} = \hat{x}.$

$$\hat{A}\hat{B}\psi(x) = -i\hbar\frac{\partial}{\partial x}(x\psi(x)) = -i\hbar\psi(x) - i\hbar\hat{x}\frac{\partial}{\partial x}\psi(x)$$

- But:

$$\hat{B}\hat{A}\psi(x) = -i\hbar x\frac{\partial}{\partial x}\psi(x)$$

5.3.2 Properties of Hermitian operators

- The results of physical measurements are real numbers. This means that a physical model of reality is restricted to prediction of real numbers. Hermitian operators play a special role in quantum mechanics, because these operators guarantee real eigenvalues. Hence, a physical system described using a Hermitian operator will provide information on measurable quantities.
- The Hermitian $\hat{A}^\dagger$ of an operator $\hat{A}$ is defined by:

$$\int \psi^*(\mathbf{r})\hat{A}^\dagger\phi(\mathbf{r})d^3r = \left(\int \phi^*(\mathbf{r})\hat{A}\psi(\mathbf{r})d^3r\right)^*$$

- Operator $\hat{A}$ is *anti-Hermitian* if $\hat{A}^\dagger = -\hat{A}.$
- The Hermitian adjoint of a complex number a is its complex conjugate – that is

$$a^\dagger = a^*$$

- If $\hat{A}$ is a Hermitian operator $\hat{A}^\dagger = \hat{A}$ and the expectation value is :

$$\int (\phi^*(\mathbf{r})\hat{A}\psi(\mathbf{r}))^* d^3r = \int \psi^*(\mathbf{r})\hat{A}\phi(\mathbf{r})d^3r = \int (\hat{A}\psi(\mathbf{r}))^*\phi(\mathbf{r})d^3r$$

5.3.2 Properties of Hermitian operators (2)

- or, equivalently, in matrix notation

$$\boxed{A_{nm}^* = A_{mn}}$$

- where

$$A_{nm}^* = \int (\phi_n^*(\mathbf{r}) \hat{A} \psi_m(\mathbf{r}))^* d^3 r$$

$$A_{mn} = \int \psi_m^*(\mathbf{r}) \hat{A} \phi_n(\mathbf{r}) d^3 r.$$

- It follows that for two operators $\hat{A}$ and $\hat{B}$ complex number a the following relations hold:

$$(a\hat{A})^\dagger = a^* \hat{A}^\dagger$$

$$(\hat{A}^\dagger)^\dagger = \hat{A}$$

$$(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger$$

5.3.2 Properties of Hermitian operators (3)

- To show that the eigenvalues of a Hermitian operator are real and that the associated eigenfunctions are orthogonal.
- We start by :

$$\hat{A}\phi_n = a_n \phi_n$$

- If we multiply both sides of previous Eq by ψ_m^* and integrate over all space we obtain:

$$\int \phi_m^* \hat{A} \phi_n d^3 r = a_n \int \phi_m^* \phi_n d^3 r$$

- Similarly, interchanging the subscripts m and n, we have:

$$\int \phi_n^* \hat{A} \phi_m d^3 r = a_m \int \phi_n^* \phi_m d^3 r$$

- which can be

$$\int (\hat{A}\phi_n)^* \phi_m d^3 r = a_m \int \phi_n^* \phi_m d^3 r$$

5.3.2 Properties of Hermitian operators (4)

- If now one takes the complex conjugate, this gives:

$$\int \phi_m^* \hat{A} \phi_n d^3 r = a_m^* \int \phi_m^* \phi_n d^3 r$$

- Subtracting previous equation and first equation gives:

$$0 = (a_n - a_m^*) \int \phi_m^* \phi_n d^3 r$$

- For the case when n = m, we have:

$$0 = (a_n - a_n^*) \int \phi_n^* \phi_n d^3 r$$

- Since $|\phi_n|^2$ is finite : $a_n = a_n^*$
- For the case in which $n \neq m$, then the integral is zero provided $a_n \neq a_m$. Hence the nondegenerate eigenfunctions of Hermitian operators are *orthogonal* to each other

$$0 = \int \phi_m^* \phi_n d^3 r$$

for $n \neq m$.

5.3.3 Normalization of eigenfunctions

- Because eigenvalue equations involve linear operators, we may specify eigenfunctions to within an arbitrary constant. It is convention that the constant is chosen in such a way that the integral over all space is unity. This means that the eigenfunctions are normalized to unity. Eigenfunctions that are orthogonal and normalized are called *orthonormal*. The orthonormal properties of Hermitian operator eigenfunctions can be expressed as

$$\int \phi_n^* \phi_m d^3 r = \delta_{nm}$$

where the Kronecker delta $\delta_{nm} = 0$ if $n \neq m$ and $\delta_{nm} = 1$ if $n = m$.

5.3.4 Completeness of eigenfunctions

- The completeness property of eigenfunctions $\phi_n(\boldsymbol{r})$ we consider means they can be used to expand an *arbitrary function* $\psi(\boldsymbol{r})$

$$\boxed{\psi(\mathbf{r}) = \sum_n a_n \phi_n(\mathbf{r})}$$

- Multiply both sides of the equation by $\phi_m^*(\boldsymbol{r})$:

$$\int \phi_m^*(\mathbf{r})\psi(\mathbf{r})d^3r = \sum a_n \int \phi_m^*(\mathbf{r})\phi_n(\mathbf{r})d^3r$$

- We know that :

$$\int \phi_m^*(\mathbf{r})\phi_n(\mathbf{r})d^3r = \delta_{mn}.$$

- So

$$\int \phi_m^*(\mathbf{r})\psi(\mathbf{r})d^3r = a_m$$

5.3.5 Commutator algebra

- The commutator for the pair of operators $\hat{A}$ and $\hat{B}$

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$$

- If we have $\hat{A} = \hat{p}_x = -i\hbar\partial/\partial x$ and $\hat{B} = \hat{x}$. so:

$$[\hat{p}_x, \hat{x}] = -i\hbar$$

- Interchange two operators $\hat{A}$ and $\hat{B}$ we obtain that:

$$[\hat{x}, \hat{p}_x] = i\hbar$$

- So: $$[\hat{A}, \hat{B}] = -[\hat{B}, \hat{A}]$$

5.3.5 Commutator algebra (2)

- other useful relationships:

$$[\hat{A}, \hat{B}+\hat{C}+\hat{D}+\cdots] = [\hat{A}, \hat{B}]+[\hat{A}, \hat{C}]+[\hat{A}, \hat{D}]+\cdots$$

- The distributive nature of linear operators requires:

$$\begin{aligned}[\hat{A}, \hat{B}\hat{C}] &= \hat{A}\hat{B}\hat{C} - \hat{B}\hat{C}\hat{A} \\ &= (\hat{A}\hat{B} - \hat{B}\hat{A})\hat{C} + \hat{B}(\hat{A}\hat{C} - \hat{C}\hat{A}) \\ &= \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}\end{aligned}$$

- so that if $\hat{B} = \hat{C}$

$$[\hat{A}, \hat{B}^2] = \hat{B}[\hat{A}, \hat{B}] + [\hat{A}, \hat{B}]\hat{B}$$

5.3.5 Commutator algebra (3)

- The Jacobi identity: $[\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] = 0$
- follows since

$$\begin{aligned}
[\hat{A}, [\hat{B}, \hat{C}]] &= [\hat{A}, \hat{B}\hat{C}] - [\hat{A}, \hat{C}\hat{B}] \\
&= \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C} - \hat{C}[\hat{B}, \hat{A}] - [\hat{A}, \hat{C}]\hat{B} \\
&= [\hat{B}, [\hat{A}, \hat{C}]] + [[\hat{A}, \hat{B}], \hat{C}] \\
&= -[\hat{B}, [\hat{C}, \hat{A}]] - [\hat{C}, [\hat{A}, \hat{B}]]
\end{aligned}$$

If operators $\hat{A}$ and $\hat{B}$ are Hermitian then $\hat{A}^\dagger = \hat{A}$, $\hat{B}^\dagger = \hat{B}$

$$[\hat{A}, \hat{B}]^\dagger = (\hat{A}\hat{B} - \hat{B}\hat{A})^\dagger = \hat{B}^\dagger\hat{A}^\dagger - \hat{A}^\dagger\hat{B}^\dagger = -(\hat{A}\hat{B} - \hat{B}\hat{A}) = -[\hat{A}, \hat{B}]$$

so that the commutator of two Hermitian operators is anti-Hermitian.

5.4 Dirac notation

- single particle quantum systems using wave functions $\psi(\boldsymbol{r}, t)$This is a real space representation. If we take the Fourier transform to obtain $\psi(\boldsymbol{k}, t)$. we have a momentum space representation.
- the physical state of the system should be independent of the coordinate representation.
- In the basis independent notation introduced by Dirac, state vectors,ψ are called ket vectors and depicted by the symbol $|\psi\rangle$
- They are elements of a linear Hilbert space.
- Complex conjugate ψ is ψ^*a shown by the bra symbol$\langle\psi|$.
- $(\phi, \psi) = \int \phi^*(\mathbf{r}, t)\psi(\mathbf{r}, t)d^3r$ is represented by $\langle\phi(\mathbf{r}, t)|\psi(\mathbf{r}, t)\rangle$
- And so:

$$\int \phi^*(\mathbf{r}, t)\psi(\mathbf{r}, t)d^3r \equiv \langle\phi(\mathbf{r}, t)|\psi(\mathbf{r}, t)\rangle = \langle\psi(\mathbf{r}, t)|\phi(\mathbf{r}, t)\rangle^*$$

5.4 Dirac notation (2)

- In Dirac notation the time-independent Schrödinger equation is: $\hat{H}|n\rangle = E_n|n\rangle$
- the set $\{|n\rangle\}$ is the Hilbert-space basis.
- The time-dependence of the state vector is:
- the Schrödinger equation which describes the t $|n, t\rangle = |n\rangle e^{-iE_n t/\hbar}$ ıtum state $|\psi\rangle$

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

For every ket there is an associated bra such that $|\psi'\rangle = \hat{A}|\psi\rangle$ and $\langle\psi'| = \langle\psi|\hat{A}^\dagger$. If we use this with the property of a scalar product $\langle\psi'|\phi\rangle = \langle\phi|\psi'\rangle^*$ then $\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\psi'|\phi\rangle = \langle\phi|\psi'\rangle^* = \langle\phi|\hat{A}|\psi\rangle^*$ which can then be used to define the Hermitian adjoint $\hat{A}^\dagger$ of an operator $\hat{A}$.

The Hermitian adjoint $\hat{A}^\dagger$ of an operator $\hat{A}$ is defined by

$$\langle\psi|\hat{A}^\dagger|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$$

Alternatively, noting that $|\hat{A}\psi\rangle = \hat{A}|\psi\rangle = |\psi'\rangle$ and $\langle\hat{A}\psi| = \langle\psi|\hat{A}^\dagger = \langle\psi'|$ we may then use the fact that $(\hat{A}^\dagger)^\dagger = \hat{A}$ so that $\langle\hat{A}^\dagger\phi| = \langle\phi|(\hat{A}^\dagger)^\dagger = \langle\phi|\hat{A}$ and we have $\langle\hat{A}^\dagger\phi|\psi\rangle = \langle\phi|\hat{A}\psi\rangle$ which can also be used to define a Hermitian adjoint.

The operator $\hat{A}$ is Hermitian when it is its own Hermitian adjoint $\hat{A}^\dagger$, that is, $\hat{A}^\dagger = \hat{A}$ or $\langle\psi|\hat{A}|\phi\rangle = \langle\phi|\hat{A}|\psi\rangle^*$ or $\langle\psi|\hat{A}\phi\rangle = \langle\hat{A}\psi|\phi\rangle$

5.4 Dirac notation (3)

- The orthonormal condition is expressed as:

$$\int \phi_n^*(\mathbf{r})\phi_m(\mathbf{r})d^3r = \langle \phi_n|\phi_m\rangle = \langle n|m\rangle = \delta_{nm}$$

- The projection of $\psi(\boldsymbol{r})$ on $\phi_m(\boldsymbol{r})$ is expressed as:

$$a_m = \langle \phi_m|\psi\rangle$$

- and the expansion of an arbitrary state-function $|\psi\rangle$ is $|\psi\rangle = \sum_n b_n|n\rangle$
- If $|\phi_i\rangle$ forms an orthonormal set then the operator :

$$\sum_i |\phi_i\rangle\langle\phi_i| = \hat{1}$$

- is a unit operator ^1 since: $\sum_i |\phi_i\rangle\langle\phi_i|\phi_j\rangle = \sum_i |\phi_i\rangle\delta_{ij} = |\phi_j\rangle$

- The Schwarz inequality for states $|\psi\rangle$ and $|\phi\rangle$ is $|\langle\phi|\psi\rangle|^2 \leq \langle\phi|\phi\rangle\langle\psi|\psi\rangle$
- the average or expectation value of the observable A associated with operator Â is:

$$\int \phi^*(\mathbf{r}, t)\hat{A}\psi(\mathbf{r}, t)d^3r = \langle \phi(\mathbf{r}, t)|\hat{A}|\psi(\mathbf{r}, t)\rangle = \langle A\rangle$$

5.5 Measurement of real numbers

- In quantum mechanics, each type of physical observable is associated with a Hermitian operator. Hermitian operators ensure that any eigenvalue is a real quantity. In this way, the result of a measurement is a real number that corresponds to one of the set of continuous or discrete eigenvalues for the system:

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

where $\hat{A}$ is a Hermitian operator, $|n\rangle$ is an eigenfunction, and a_n is its eigenvalue.

- there are two different physical observables with eigenvalues a_n and b_n with two operators $\hat{A}$ and $\hat{B}$

5.5 Measurement of real numbers (2)

- If the measurements interfere with each other, then the commutator

$$[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} \neq 0$$

- Measurement of position and momentum are good examples of measurements that interfere with each other. $\hat{B}\hat{A} = \hat{A}\hat{B}$
- If measurements do not interfere with each other, then the commutator
- And also $\hat{A}\hat{B}\phi_B = \hat{B}\hat{A}\phi_B = \hat{A}b\phi_B = b\hat{A}\phi_B$
- If there is only one eigenfunction of $\hat{B}$ associated with eigenvalue b, then

$$\hat{A}\phi_B = c\phi_B$$

- where c is a constant, so that ϕ_B is an eigenfunction of $\hat{A}$

5.5.1 Expectation value of an operator

- $\psi^*(r)\psi(r)d^3r$ is the probability of finding the particle in volume element d^3r at position **r**. the integral over all space is unity.
- so the expectation of finding the particle somewhere is unity.
- Consider the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\mathbf{r}) + V(\mathbf{r})\psi(\mathbf{r}) = E\psi(\mathbf{r})$$

- Multiplying by $\psi^*(r)$ and integrating over all space gives

$$\frac{\hbar^2}{2m}\int \psi^*(\mathbf{r})\nabla^2\psi(\mathbf{r})d^3r + \int \psi^*(\mathbf{r})V(\mathbf{r})\psi(\mathbf{r})d^3r = E\int \psi^*(\mathbf{r})\psi(\mathbf{r})d^3r$$

↓ Local Kinetic energy — ↓ local Potential energy — ↓ position

5.5.1 Expectation value of an operator (2)

- We are weighting the kinetic energy operator and potential operator at position **r** with the probability that the particle is at position **r**. We then integrate over all space to get the average value or *expectation value*.

$$\langle T\rangle = \langle\psi|\hat{T}|\psi\rangle = -\frac{\hbar^2}{2m}\int \psi^*(\mathbf{r})\nabla^2\psi(\mathbf{r})d^3r$$

$$\langle V\rangle = \langle\psi|\hat{V}|\psi\rangle = \int \psi^*(\mathbf{r})V(\mathbf{r})\psi(\mathbf{r})d^3r$$

$$\langle \mathbf{r}\rangle = \langle\psi|\hat{\mathbf{r}}|\psi\rangle = \int \psi^*(\mathbf{r})\mathbf{r}\psi(\mathbf{r})d^3r$$

- This measure of average value is most useful if the distribution is symmetric and strongly peaked.
- Given that we have defined an average value for the result of a measurement, it is natural to consider the time evolution of the expectation value as well as the spread or deviation from the average value when a measurement is performed separately on many identically prepared systems

5.5.2 Time dependence of expectation value

- To find the time dependence of an expectation value, we start by writing down the expectation value of the observable A associated

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle$$

- The time dependence of this equation can be expressed in terms of the Schrödingerequation

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

- We now find the time derivative. using the chain rule

$$\frac{d}{dt}\langle A \rangle = \langle \frac{\partial \psi}{\partial t} | \hat{A} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle + \langle \psi | \hat{A} | \frac{\partial \psi}{\partial t} \rangle$$

$$\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar} \langle \hat{H} \psi | \hat{A} | \psi \rangle - \frac{i}{\hbar} \langle \psi | \hat{A} \hat{H} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle$$

$$\frac{d}{dt}\langle A \rangle = \frac{i}{\hbar} \langle \psi | \hat{H} \hat{A} | \psi \rangle - \frac{i}{\hbar} \langle \psi | \hat{A} \hat{H} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle$$

$$= \frac{i}{\hbar} \langle \psi | \hat{H} \hat{A} - \hat{A} \hat{H} | \psi \rangle + \langle \psi | \frac{\partial}{\partial t} \hat{A} | \psi \rangle$$

5.5.2 Time dependence of expectation value (2)

- where we used the Hermitian property of $\hat{H}$ such that $\langle \hat{H}\psi|\phi\rangle = \langle\psi|\hat{H}\phi\rangle$. Hence,

$$\boxed{\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{A}]\rangle + \langle\frac{\partial}{\partial t}\hat{A}\rangle}$$

- If the operator $\hat{A}$ has no explicit time dependence, then $\langle\frac{\partial}{\partial t}\hat{A}\rangle = 0$ and

$$\frac{d}{dt}\langle A\rangle = \frac{i}{\hbar}\langle[\hat{H}, \hat{A}]\rangle$$

- *Time dependence of position operator of particle moving in free space*
- To check this result, consider a particle of mass m moving in free space in such a way that the Hamiltonian describing motion in the x direction is

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

5.5.2 Time dependence of expectation value (3)

- To evaluate the time dependence of the expectation value of the observable x associated with the position operator.

$$\frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle[\hat{H},\hat{x}]\rangle$$

- The commutator operating on the wave function

$$\frac{i}{\hbar}[\hat{H},\hat{x}]\psi = -\frac{\hbar^2}{2m}\frac{i}{\hbar}\left(\frac{d}{dx}\left(\frac{d}{dx}\hat{x}\psi\right) - \hat{x}\frac{d}{dx}\left(\frac{d}{dx}\psi\right)\right)$$

$$= \frac{-i\hbar}{2m}\left(\frac{d}{dx}\psi + \frac{d}{dx}\left(\hat{x}\frac{d}{dx}\psi\right) - \hat{x}\frac{d}{dx}\left(\frac{d}{dx}\psi\right)\right)$$

$$\frac{i}{\hbar}[\hat{H},\hat{x}]\psi = \frac{-i\hbar}{2m}\left(\frac{d}{dx}\psi + \frac{d}{dx}\psi + \hat{x}\frac{d}{dx}\left(\frac{d}{dx}\psi\right) - \hat{x}\frac{d}{dx}\left(\frac{d}{dx}\psi\right)\right) = \frac{-i\hbar}{m}\frac{d}{dx}\psi$$

5.5.2 Time dependence of expectation value (4)

- The Hamiltonian does not commute with the position operator. Using the fact that the wave function of a free particle moving in the x direction is of the form $\psi = e^{i(k_x x - \omega t)}$, we may conclude that

$$\frac{d}{dt}\langle x \rangle = \frac{\hbar k_x}{m}$$

- As expected, this is just the x component of momentum divided by the mass or, equivalently, the speed of the particle in the x direction


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5.5.3 Uncertainty of expectation value

- Here we want to establish a measure of the deviation of the result of a measurement from the mean value.
- Let A^ be an operator corresponding to an observable A when the system is in state r The mean (expectation) value of the observable A is:

$$\langle A\rangle = \int \psi^*(\mathbf{r}, t)\hat{A}\psi(\mathbf{r}, t)d^3r$$

5.5.3 Uncertainty of expectation value

$$\langle A \rangle = \int \psi^*(\mathbf{r},t)\hat{A}\psi(\mathbf{r},t)d^3r$$

$$(\Delta A)^2 = \langle(\hat{A} - \langle A\rangle)^2\rangle = \langle \hat{A}^2 + \langle A\rangle^2 - 2\hat{A}\langle A\rangle\rangle$$

$$= \langle A^2\rangle + \langle A\rangle^2 - 2\langle A\rangle\langle A\rangle$$

$$\Delta A^2 = \langle A^2\rangle - \langle A\rangle^2$$

We can also express this in integral form:

$$\Delta A^2 = \int \psi^*(\mathbf{r},t)\hat{A}^2\psi(\mathbf{r},t)d^3r - \left(\int \psi^*(\mathbf{r},t)\hat{A}\psi(\mathbf{r},t)d^3r\right)^2$$

$\langle A \rangle$ ➡ The average value of many observations on the system

ΔA ➡ Spread in the values of the measurement

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

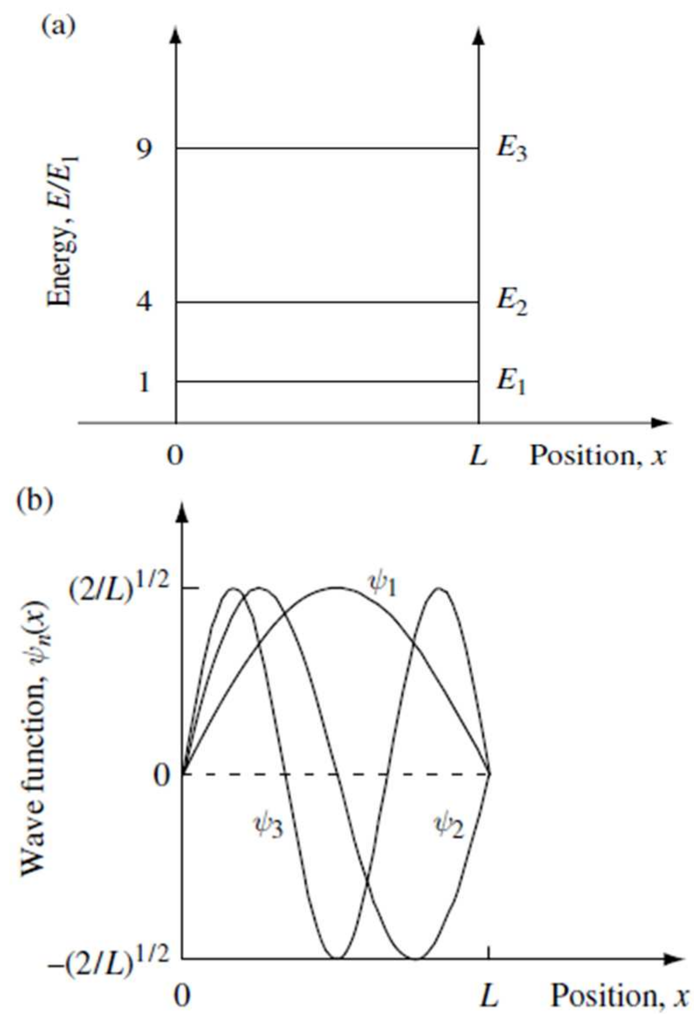
- As usual, we start out by defining the potential in which the particle moves.
- we choose the position x = 0 to be the left-hand boundary of the potential:

$$
\begin{cases} V(x) = 0 & 0 < x < L \\ V(x) = \infty & \text{elsewhere.} \end{cases}
$$

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

- (a) Sketch of a one-dimensional, rectangular potential well with infinite barrier energy showing the energy eigenvalues E1, E2, and E3.

- (b) Sketch of the eigenfunctions 1, 2, and 3 for the potential shown in (a).



5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

- We wish to find the expectation value of the particle position and the uncertainty in the position when the particle is in the n-th energy state:

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V(x)\right)\psi_n(x)=E_n\psi_n(x)$$

$\psi_n(x)=0$ at $x=0$ and $x=L$. $\Rightarrow$ $\psi_n = A_n \sin(k_n x)$

$k_n = n\pi/L$, $n = 1, 2, 3, \ldots$ $\Rightarrow$

$$\int_{x=0}^{x=L}\psi_n^*(x)\psi_n(x)dx = A_n^2\int_{x=0}^{x=L}\sin^2(k_n x)dx = 1$$

$$\frac{1}{A_n^2}=\int_{x=0}^{x=L}\left(\frac{1}{2}-\frac{1}{2}\cos(2k_n x)\right)dx=\left[\frac{x}{2}+\frac{1}{4k_n}\sin(2k_n x)\right]_0^L=\frac{L}{2}+0$$

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

- To find the expectation value of x, we must solve the integral

$$\langle x_n \rangle = \int \psi_n^*(x) x \psi_n(x) dx = A_n^2 \int x \ \sin^2(k_n x) dx = A_n^2 \int x \left(\frac{1}{2} - \frac{1}{2}\cos(2k_n x)\right) dx$$

$$\Downarrow$$

$$\langle x_n \rangle = \frac{L}{2}$$

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

- In classical mechanics, the particle in the potential well moves at constant velocity, and traverses the well in time

$\tau = L/v.$ The average position is given by:

$$\langle x \rangle_{\text{classical}} = \int_{t=0}^{t=\tau} \frac{vtdt}{\tau} = \frac{1}{2} v \frac{\tau^2}{\tau} = \frac{1}{2} v\tau = \frac{1}{2} v \frac{L}{v} = \frac{L}{2}$$

which is quite satisfying, since it is the same as the quantum result.

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

To find the expectation value of the observable x^2 associated with the quantum mechanical operator $\hat{x}^2$ we must solve

$$\langle x_n^2 \rangle = A_n^2 \int x^2 \sin^2(k_n x) dx = A_n^2 \int \left(\frac{x^2}{2} - \frac{x^2}{2} \cos(2k_n x) \right) dx$$

$$\langle x_n^2 \rangle = A_n^2 \left(\left[\frac{x^3}{6} - \frac{x^2}{2} \frac{1}{2k_n} \sin(2k_n x) \right]_0^L + \int \frac{x}{2k_n} \sin(2k_n x) dx \right)$$

$$\langle x_n^2 \rangle = A_n^2 \left(\left[\frac{x^3}{6} - \frac{x^2}{2} \frac{1}{2k_n} \sin(2k_n x) + \frac{x}{2k_n} \left(-\frac{1}{2k_n} \right) \cos(2k_n x) \right]_0^L \right.$$

$$\left. + \int \frac{1}{4k_n^2} \cos(2k_n x) dx \right)$$

$$\langle x_n^2 \rangle = A_n^2 \left[\frac{x^3}{6} - \frac{x^2}{4k_n} \sin(2k_n x) + \frac{x}{4k_n^2} \cos(2k_n x) + \frac{1}{8k_n^3} \sin(2k_n x) \right]_0^L$$

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

- Then:

$$\langle x_n^2 \rangle = \frac{L^2}{3} - \frac{L^2}{2n^2\pi^2}$$

- The uncertainty in the position of the particle in the n-th state is given by the standard deviation $\Delta x_n = (\langle x_n^2 \rangle - \langle x_n \rangle^2)^{1/2}$

, which we calculate:

$$\Delta x_n^2 = \frac{L^2}{12}\left(1 - \frac{6}{n^2\pi^2}\right)$$

5.5.3.1 A particle confined by one-dimensional, infinite, rectangular potential

- in the limit of very high-energy eigenvalues $(n \rightarrow \infty)$

  the standard deviation in particle position approaches the classical result

$$\Delta x_{\text{classical}} = L/\sqrt{12}.$$

5.5.4 The generalized uncertainty relation

- We consider the specific example of finding the expectation value and uncertainty in particle position in a one-dimensional, rectangular potential well with infinite barrier energy.
- In quantum mechanics, links the uncertainty in results of measurement between a given pair of associated noncommuting operators.
- The spread in results of one set of measurements associated with one operator is related to the spread in measured values of the associated noncommuting operator.

5.5.4 The generalized uncertainty relation

$$\langle \hat{A}\hat{A}^\dagger \rangle = \langle \psi | \hat{A}^\dagger \hat{A} | \psi \rangle = \langle \hat{A}\psi | \hat{A}\psi \rangle \geq 0$$

from the definition of Hermitian conjugate. Or, in terms of integrals

$$\langle \hat{A}\hat{A}^\dagger \rangle = \int \psi^* (\hat{A}^\dagger \hat{A}\psi) d^3r = \int (\hat{A}\psi)^* (\hat{A}\psi) d^3r = \int (\hat{A}\psi)^2 d^3r \geq 0$$

We can create a linear combination

$$\langle \hat{A} + i\hat{B} \rangle = \langle \hat{A} \rangle + i \langle \hat{B} \rangle$$

$$\langle (\hat{A} + i\lambda\hat{B})(\hat{A} + i\lambda\hat{B})^\dagger \rangle = \langle (\hat{A} + i\lambda\hat{B})(\hat{A}^\dagger - i\lambda\hat{B}^\dagger) \rangle \geq 0$$

$$\langle A^2 \rangle + \lambda^2 \langle B^2 \rangle - i\lambda \langle \hat{A}\hat{B} - \hat{B}\hat{A} \rangle \geq 0$$

5.5.4 The generalized uncertainty relation

- If $\hat{A}$ and are Hermitian: $(\hat{A} + i\hat{B})^{\dagger} = \hat{A} - i\hat{B}$
- If one now considers an operator ^A +i ^ B, where is real and and $\hat{A}$are Hermitian operators

$$\langle(\hat{A} + i\lambda\hat{B})(\hat{A} + i\lambda\hat{B})^{\dagger}\rangle = \langle(\hat{A} + i\lambda\hat{B})(\hat{A}^{\dagger} - i\lambda\hat{B}^{\dagger})\rangle \geq 0$$

$$\langle A^2\rangle + \lambda^2\langle B^2\rangle - i\lambda\langle\hat{A}\hat{B} - \hat{B}\hat{A}\rangle \geq 0$$

- The minimum value of λ found by taking the derivative with respect to such tλat

$$0 = \frac{d}{d\lambda}(\langle A^2\rangle + \lambda^2\langle B^2\rangle - i\lambda\langle\hat{A}\hat{B} - \hat{B}\hat{A}\rangle)$$

$$0 = 2\lambda_{\min}\langle B^2\rangle - i\langle\hat{A}\hat{B} - \hat{B}\hat{A}\rangle = 2\lambda_{\min}\langle B^2\rangle - i\langle[\hat{A},\hat{B}]\rangle$$

$$\lambda_{\min} = \frac{i}{2}\frac{\langle[\hat{A},\hat{B}]\rangle}{\langle B^2\rangle}$$

5.5.4 The generalized uncertainty relation

$$\lambda_{\min} = \frac{i}{2}\frac{\langle[\hat{A},\hat{B}]\rangle}{\langle B^2\rangle} \Rightarrow \langle A^2\rangle + \lambda^2\langle B^2\rangle - i\lambda\langle\hat{A}\hat{B} - \hat{B}\hat{A}\rangle \geq 0$$

$$\langle A^2\rangle\langle B^2\rangle \geq -\frac{\langle[\hat{A},\hat{B}]\rangle^2}{4}$$

5.5.4 The generalized uncertainty relation

- The product of the square of a Hermitian operator with the square of another has a minimum value that is proportional to the square of the commutator of the two operators. To show that this applies to the standard deviation we create a new set of operators.

$$\hat{A} \rightarrow \hat{A} - \langle A \rangle \equiv \delta \hat{A}$$

$$\hat{B} \rightarrow \hat{B} - \langle B \rangle \equiv \delta \hat{B}$$

$$\langle (\delta A)^2 \rangle = \langle (\hat{A} - \langle A \rangle)^2 \rangle = \langle A^2 \rangle - \langle 2\hat{A}\langle A \rangle \rangle + \langle A \rangle^2$$

$$= \langle A^2 \rangle - \langle A \rangle^2 = \Delta A^2$$

- ΔA is the standard deviation.

5.5.4 The generalized uncertainty relation

$$[\delta\hat{A}, \delta\hat{B}] = \hat{A}\hat{B} - \hat{A}\langle B\rangle - \langle A\rangle\hat{B} + \langle A\rangle\langle B\rangle$$
$$-\hat{B}\hat{A} + \langle B\rangle\hat{A} + \hat{B}\langle A\rangle - \langle B\rangle\langle A\rangle$$

$$[\delta\hat{A}, \delta\hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A} = [\hat{A}, \hat{B}]$$

$$\langle A^2\rangle\langle B^2\rangle \geq -\langle[\hat{A}, \hat{B}]\rangle^2/4$$

$$\Delta A^2 \Delta B^2 \geq -\langle[\hat{A}, \hat{B}]\rangle^2/4$$

$$\langle\delta A^2\rangle\langle\delta B^2\rangle \geq -\langle[\hat{A}, \hat{B}]\rangle^2/4$$

Using $\langle\delta A^2\rangle = \Delta A^2$

$$\Delta A \Delta B \geq \frac{i}{2}\langle[\hat{A}, \hat{B}]\rangle$$

5.5.4 The generalized uncertainty relation

$$\Delta A \Delta B \geq \frac{i}{2}\langle[\hat{A},\hat{B}]\rangle$$

- This relationship between a conjugate pair of noncommuting linear operators may be considered a consequence of the mathematics that is built into our description of quantum phenomena.
- It arises from the linear algebra of noncommuting Hermitian operators.

5.5.4 The generalized uncertainty relation

- from the commutation relation

$$\langle[\hat{p}_x, \hat{x}]\rangle \equiv [\hat{p}_x, \hat{x}] = -i\hbar$$

$$\Delta A \Delta B \geq \frac{i}{2}\langle[\hat{A}, \hat{B}]\rangle$$

$$\Delta p_x \Delta x \geq \frac{i}{2}\langle[\hat{p}_x, \hat{x}]\rangle = \frac{-i}{2} i\hbar$$

$$\Delta p_x \Delta x \geq \frac{\hbar}{2}$$

5.6 The no cloning theorem

- When we discussed secure quantum communication in we made use of the fact that nonorthogonal states can never be precisely copied.
- This is called the no cloning theorem and is a basic feature that arises due to the linear algebra of quantum mechanics.
- To prove the no cloning theorem we suppose one can make a copy of a pure state

$$|\psi_1\rangle \to |\psi_1\rangle|\psi_1\rangle$$

$$|\psi_2\rangle \to |\psi_2\rangle|\psi_2\rangle$$

5.6 The no cloning theorem

- In each case we used the information contained in the wave function describing the particle to create an additional independent, identical, particle.
- The resulting two particle wave function is a product of the independent particle wave functions. If we now try to copy a new state

$$|\psi\rangle = a_1|\psi_1\rangle + a_2|\psi_2\rangle$$

- near combination

$$|\psi\rangle \rightarrow a_1|\psi_1\rangle|\psi_1\rangle + a_2|\psi_2\rangle|\psi_2\rangle$$

5.6 The no cloning theorem

$$|\psi\rangle \rightarrow (a_1|\psi_1\rangle + a_2|\psi_2\rangle)(a_1|\psi_1\rangle + a_2|\psi_2\rangle)$$
$$= a_1^2|\psi_1\rangle|\psi_1\rangle + a_2^2|\psi_2\rangle|\psi_2\rangle + a_1a_2(|\psi_1\rangle|\psi_2\rangle + |\psi_2\rangle|\psi_1\rangle)$$

- It follows that we can only copy pure orthogonal states and not nonorthogonal linear superposition states.
- The no cloning theorem highlights the fact that quantum information is different from classical information.
- For example, it is not possible to make precise backup copies of quantum information contained in nonorthogonal states.

5.6 The no cloning theorem قضیه غیر همسانه سازی

- The same idea showed up when we considered secure quantum communication in Section 2.1.4.
- Because an eavesdropper cannot make a precise copy of the non-orthogonal quantum state carrying the information, there is always some signature of the eavesdropper's presence impressed on the signal that can subsequently be detected.