Lecture 3
Operator methods in quantum mechanics
Although wave mechanics is capable of describing quantum behaviour of bound and unbound particles, some properties can not be represented this way, e.g. electron spin degree of freedom.

It is therefore convenient to reformulate quantum mechanics in a framework that involves only operators, e.g. \( \hat{H} \).

Advantage of operator algebra is that it does not rely upon particular basis, e.g. for \( \hat{H} = \frac{\hat{p}^2}{2m} \), we can represent \( \hat{p} \) in spatial coordinate basis, \( \hat{p} = -i\hbar\partial_x \), or in the momentum basis, \( \hat{p} = p \).

Equally, it would be useful to work with a basis for the wavefunction, \( \psi \), which is coordinate-independent.
Dirac notation and definition of operators
2 Uncertainty principle for non-commuting operators
3 Time-evolution of expectation values: Ehrenfest theorem
4 Symmetry in quantum mechanics
5 Heisenberg representation
6 Example: Quantum harmonic oscillator
   (from ladder operators to coherent states)
Dirac notation

- Orthogonal set of square integrable functions (such as wavefunctions) form a **vector space** (cf. 3d vectors).

- In Dirac notation, state vector or wavefunction, $\psi$, is represented symbolically as a "ket", $|\psi\rangle$.

- Any wavefunction can be expanded as sum of basis state vectors, (cf. $\mathbf{v} = x\hat{e}_x + y\hat{e}_y + \cdots$)

$$|\psi\rangle = \lambda_1|\psi_1\rangle + \lambda_2|\psi_2\rangle + \cdots$$

- Alongside ket, we can define a "bra", $\langle \psi |$ which together form the **scalar product**,

$$\langle \phi | \psi \rangle \equiv \int_{-\infty}^{\infty} dx \, \phi^*(x)\psi(x) = \langle \psi | \phi \rangle^*$$
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Alongside ket, we can define a “bra”, \( \langle \psi | \) which together form the scalar product,

\[
\langle \phi | \psi \rangle \equiv \int_{-\infty}^{\infty} dx \ \phi^*(x)\psi(x) = \langle \psi | \phi \rangle^*
\]
For a complete basis set, $\phi_i$, we can define the expansion

$$|\psi\rangle = \sum_i \phi_i |i\rangle$$

where $\langle j | \psi \rangle = \sum_i \phi_i \langle j | i \rangle = \delta_{ij} \phi_j$.

For example, in the real space basis, $|\psi\rangle = \int dx \psi(x) x \rangle$.

Then, since $\langle x | x' \rangle = \delta(x - x')$,

$$\langle x' | \psi \rangle = \int dx \psi(x) \langle x' | x \rangle = \psi(x')$$

In Dirac formulation, real space representation recovered from inner product, $\psi(x) = \langle x | \psi \rangle$; equivalently $\psi(p) = \langle p | \psi \rangle$. 
An operator \( \hat{A} \) maps one state vector, \( |\psi\rangle \), into another, \( |\phi\rangle \), i.e.

\[
\hat{A}|\psi\rangle = |\phi\rangle.
\]

If \( \hat{A}|\psi\rangle = a|\psi\rangle \) with \( a \) real, then \( |\psi\rangle \) is said to be an eigenstate (or eigenfunction) of \( \hat{A} \) with eigenvalue \( a \).

e.g. plane wave state \( \psi_p(x) = \langle x|\psi_p\rangle = A e^{ipx/\hbar} \) is an eigenstate of the momentum operator, \( \hat{p} = -i\hbar \partial_x \), with eigenvalue \( p \).

For every observable \( A \), there is an operator \( \hat{A} \) which acts upon the wavefunction so that, if a system is in a state described by \( |\psi\rangle \), the expectation value of \( A \) is

\[
\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \int_{-\infty}^{\infty} dx \, \psi^*(x) \hat{A} \psi(x).
\]
An operator $\hat{A}$ maps one state vector, $|\psi\rangle$, into another, $|\phi\rangle$, i.e.

$$\hat{A}|\psi\rangle = |\phi\rangle.$$ 

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For every observable $A$, there is an operator $\hat{A}$ which acts upon the wavefunction so that, if a system is in a state described by $|\psi\rangle$, the expectation value of $A$ is

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \int_{-\infty}^{\infty} dx \, \psi^*(x) \hat{A} \psi(x).$$
Every operator corresponding to observable is **linear** and **Hermitian**, i.e. for any two wavefunctions $|\psi\rangle$ and $|\phi\rangle$, linearity implies

$$\hat{A}(\alpha|\psi\rangle + \beta|\phi\rangle) = \alpha \hat{A}|\psi\rangle + \beta \hat{A}|\phi\rangle$$

For any linear operator $\hat{A}$, the **Hermitian conjugate** (a.k.a. the **adjoint**) is defined by relation

$$\langle \phi | \hat{A} \psi \rangle = \int dx \phi^* (\hat{A} \psi) = \int dx \psi (\hat{A}^\dagger \phi)^* = \langle \hat{A}^\dagger \phi | \psi \rangle$$

Hermiticity implies that $\hat{A}^\dagger = \hat{A}$, e.g. $\hat{p} = -i\hbar \partial_x$. 
Operators

- From the definition, \( \langle \hat{A}^\dagger | \phi \rangle = \langle \phi | \hat{A} \psi \rangle \), some useful relations follow:

1. From complex conjugation, \( \langle \hat{A}^\dagger | \psi \rangle^* = \langle \psi | \hat{A}^\dagger \phi \rangle = \langle \hat{A} \psi | \phi \rangle \),

   i.e. \( \langle (\hat{A}^\dagger)^\dagger | \psi \rangle = \langle \hat{A} \psi | \phi \rangle \), \( \Rightarrow (\hat{A}^\dagger)^\dagger = \hat{A} \)

2. From \( \langle \phi | \hat{A} \hat{B} \psi \rangle = \langle \hat{A}^\dagger \phi | \hat{B} \psi \rangle = \langle \hat{B}^\dagger \hat{A}^\dagger \phi | \psi \rangle \),

   it follows that \( (\hat{A} \hat{B})^\dagger = \hat{B}^\dagger \hat{A}^\dagger \).

- Operators are associative, i.e. \( (\hat{A} \hat{B}) \hat{C} = \hat{A} (\hat{B} \hat{C}) \),

  but not (in general) commutative,

\[
\hat{A} \hat{B} |\psi\rangle = \hat{A} (\hat{B} |\psi\rangle) = (\hat{A} \hat{B}) |\psi\rangle \neq \hat{B} \hat{A} |\psi\rangle.
\]
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A physical variable must have real expectation values (and eigenvalues) \( \Rightarrow \) physical operators are **Hermitian** (self-adjoint):

\[
\langle \psi | \hat{H} | \psi \rangle^* = \left[ \int_{-\infty}^{\infty} \psi^*(x) \hat{H} \psi(x) \, dx \right]^* = \int_{-\infty}^{\infty} \psi(x) (\hat{H} \psi(x))^* \, dx = \langle \hat{H} \psi | \psi \rangle
\]

i.e. \( \langle \hat{H} \psi | \psi \rangle = \langle \psi | \hat{H} \psi \rangle = \langle \hat{H}^\dagger \psi | \psi \rangle \), and \( \hat{H}^\dagger = \hat{H} \).

Eigenfunctions of Hermitian operators \( \hat{H} | i \rangle = E_i | i \rangle \) form complete orthonormal basis, i.e. \( \langle i | j \rangle = \delta_{ij} \)

For complete set of states \( | i \rangle \), can expand a state function \( | \psi \rangle \) as

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| \psi \rangle = \sum_i | i \rangle \langle i | \psi \rangle
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In coordinate representation,

\[
\psi(x) = \langle x | \psi \rangle = \sum_i \langle x | i \rangle \langle i | \psi \rangle = \sum_i \langle i | \psi \rangle \phi_i(x), \quad \phi_i(x) = \langle x | i \rangle
\]
Resolution of identity

\[ |\psi\rangle = \sum_i |i\rangle \langle i| \psi \rangle \]

- If we sum over complete set of states, obtain the (useful) resolution of identity,

\[ \sum_i |i\rangle \langle i| = \mathbb{I} \]

  i.e. in coordinate basis, \( \sum_i \phi_i^*(x)\phi_i(x') = \delta(x - x') \).

- As in 3d vector space, expansion \( |\phi\rangle = \sum_i b_i |i\rangle \) and \( |\psi\rangle = \sum_i c_i |i\rangle \)
  allows scalar product to be taken by multiplying components, \( \langle \phi | \psi \rangle = \sum_i b_i^* c_i \).
Resolution of identity

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- If we sum over complete set of states, obtain the (useful) resolution of identity,

\[ \sum_i \langle x'|i\rangle \langle i|x \rangle = \langle x'|x \rangle \]

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- As in 3d vector space, expansion \( |\phi\rangle = \sum_i b_i |i\rangle \) and \( |\psi\rangle = \sum_i c_i |i\rangle \) allows scalar product to be taken by multiplying components, \( \langle \phi|\psi \rangle = \sum_i b_i^* c_i \).
Basis states can be formed from any complete set of orthogonal states including position or momentum,

\[
\int_{-\infty}^{\infty} dx |x\rangle\langle x| = \int_{-\infty}^{\infty} dp |p\rangle\langle p| = \mathbb{I}.
\]

From these definitions, can recover Fourier representation,

\[
\psi(x) \equiv \langle x|\psi \rangle = \int_{-\infty}^{\infty} dp \langle x|p\rangle \langle p|\psi \rangle = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} dp \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \psi(p)
\]

where \(\langle x|p\rangle\) denotes plane wave state \(|p\rangle\) expressed in the real space basis.
Formally, we can evolve a wavefunction forward in time by applying time-evolution operator.

For time-independent Hamiltonian, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$, where time-evolution operator (a.k.a. the “propagator”):

$$\hat{U}(t) = e^{-i\hat{H}t/\hbar}$$

follows from time-dependent Schrödinger equation, $\hat{H}|\psi\rangle = i\hbar\partial_t|\psi\rangle$.

By inserting the resolution of identity, $\mathbb{I} = \sum_i |i\rangle\langle i|$, where $|i\rangle$ are eigenstates of $\hat{H}$ with eigenvalue $E_i$,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} \sum_i |i\rangle\langle i|\psi(0)\rangle = \sum_i |i\rangle\langle i|\psi(0)\rangle e^{-iE_it/\hbar}$$
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\[
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\]
Time-evolution operator

\[ \hat{U} = e^{-i\hat{H}t/\hbar} \]

- Time-evolution operator is an example of a **Unitary operator**:
- Unitary operators involve transformations of state vectors which preserve their scalar products, i.e.

\[
\langle \phi | \psi \rangle = \langle \hat{U}\phi | \hat{U}\psi \rangle = \langle \phi | \hat{U}^\dagger \hat{U} \psi \rangle \overset{!}{=} \langle \phi | \psi \rangle
\]

i.e. \[ \hat{U}^\dagger \hat{U} = \mathbb{I} \]
For non-commuting Hermitian operators, we can establish a bound on the uncertainty in the expectation values of \( \hat{A} \) and \( \hat{B} \):

Given a state \( |\psi\rangle \), the mean square uncertainty defined as

\[
(\Delta A)^2 = \langle \psi | (\hat{A} - \langle \hat{A} \rangle)^2 | \psi \rangle = \langle \psi | \hat{U}^2 | \psi \rangle \\
(\Delta B)^2 = \langle \psi | (\hat{B} - \langle \hat{B} \rangle)^2 | \psi \rangle = \langle \psi | \hat{V}^2 | \psi \rangle
\]

where \( \hat{U} = \hat{A} - \langle \hat{A} \rangle \), \( \langle \hat{A} \rangle \equiv \langle \psi | \hat{A} | \psi \rangle \), etc.

Consider then the expansion of the norm \( ||\hat{U}|\psi\rangle + i\lambda \hat{V}|\psi\rangle||^2 \),

\[
\langle \psi | \hat{U}^2 | \psi \rangle + \lambda^2 \langle \psi | \hat{V}^2 | \psi \rangle + i\lambda \langle \hat{U} | \psi \rangle \langle \hat{V} | \psi \rangle - i\lambda \langle \hat{V} | \psi \rangle \langle \hat{U} | \psi \rangle \geq 0
\]

i.e. \( (\Delta A)^2 + \lambda^2(\Delta B)^2 + i\lambda \langle [\hat{U}, \hat{V}] | \psi \rangle \geq 0 \)

Since \( \langle \hat{A} \rangle \) and \( \langle \hat{B} \rangle \) are just constants, \( [\hat{U}, \hat{V}] = [\hat{A}, \hat{B}] \).
For non-commuting Hermitian operators, we can establish a bound on the uncertainty in the expectation values of $\hat{A}$ and $\hat{B}$:

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$$(\Delta B)^2 = \langle \psi | (\hat{B} - \langle \hat{B} \rangle)^2 | \psi \rangle = \langle \psi | \hat{V}^2 | \psi \rangle$$

where $\hat{U} = \hat{A} - \langle \hat{A} \rangle$, $\langle \hat{A} \rangle \equiv \langle \psi | \hat{A} | \psi \rangle$, etc.

Consider then the expansion of the norm $||\hat{U}|\psi\rangle + i\lambda \hat{V}|\psi\rangle||^2$,

$$\langle \psi | \hat{U}^2 | \psi \rangle + \lambda^2 \langle \psi | \hat{V}^2 | \psi \rangle + i\lambda \langle \hat{U}|\psi\rangle \langle \hat{V}|\psi\rangle - i\lambda \langle \hat{V}|\psi\rangle \langle \hat{U}|\psi\rangle \geq 0$$

i.e. $$(\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \langle [\hat{U}, \hat{V}] | \psi \rangle \geq 0$$

Since $\langle \hat{A} \rangle$ and $\langle \hat{B} \rangle$ are just constants, $[\hat{U}, \hat{V}] = [\hat{A}, \hat{B}]$. 
Uncertainty principle for non-commuting operators

\[(\Delta A)^2 + \lambda^2 (\Delta B)^2 + i\lambda \langle \psi | [\hat{A}, \hat{B}] | \psi \rangle \geq 0\]

- Minimizing with respect to \(\lambda\),

\[2\lambda (\Delta B)^2 + i\lambda \langle \psi | [\hat{A}, \hat{B}] | \psi \rangle = 0, \quad i\lambda = \frac{1}{2} \frac{\langle \psi | [\hat{A}, \hat{B}] | \psi \rangle}{(\Delta B)^2}\]

- and substituting back into the inequality,

\[(\Delta A)^2 (\Delta B)^2 \geq -\frac{1}{4} \langle \psi | [\hat{A}, \hat{B}] | \psi \rangle^2\]

- i.e., for non-commuting operators,

\[(\Delta A) (\Delta B) \geq \frac{i}{2} \langle [\hat{A}, \hat{B}] \rangle\]
Uncertainty principle for non-commuting operators

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

- For the conjugate operators of momentum and position (i.e. \([\hat{p}, \hat{x}] = -i\hbar\), recover Heisenberg's uncertainty principle,

\[(\Delta p)(\Delta x) \geq \frac{i}{2} \langle [\hat{p}, \hat{x}] \rangle = \frac{\hbar}{2}\]

- Similarly, if we use the conjugate coordinates of time and energy, \([\hat{E}, t] = i\hbar\),

\[(\Delta t)(\Delta E) \geq \frac{i}{2} \langle [t, \hat{E}] \rangle = \frac{\hbar}{2}\]
Time-evolution of expectation values

For a general (potentially time-dependent) operator \( \hat{A} \),

\[
\partial_t \langle \psi | \hat{A} | \psi \rangle = (\partial_t \langle \psi |) \hat{A} | \psi \rangle + \langle \psi | \partial_t \hat{A} | \psi \rangle + \langle \psi | \hat{A} (\partial_t | \psi \rangle)
\]

Using \( i\hbar \partial_t | \psi \rangle = \hat{H} | \psi \rangle \), \(-i\hbar (\partial_t \langle \psi |) = \langle \psi | \hat{H} \), and Hermiticity,

\[
\partial_t \langle \psi | \hat{A} | \psi \rangle \equiv \frac{1}{\hbar} \langle i\hat{H} | \psi \rangle \hat{A} | \psi \rangle + \langle \psi | \partial_t \hat{A} | \psi \rangle + \frac{1}{\hbar} \langle \psi | \hat{A} (-i\hat{H} | \psi \rangle)
\]

\[
= \frac{i}{\hbar} \left( \langle \psi | \hat{H} \hat{A} | \psi \rangle - \langle \psi | \hat{A} \hat{H} | \psi \rangle \right) + \langle \psi | \partial_t \hat{A} | \psi \rangle
\]

For time-independent operators, \( \hat{A} \), obtain Ehrenfest Theorem,

\[
\partial_t \langle \psi | \hat{A} | \psi \rangle = \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{A}] | \psi \rangle.
\]
Time-evolution of expectation values

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  \]

- Using $i\hbar \partial_t | \psi \rangle = \hat{H} | \psi \rangle$, $-i\hbar (\partial_t \langle \psi |) = \langle \psi | \hat{H}$, and Hermiticity,
  \[
  \partial_t \langle \psi | \hat{A} | \psi \rangle = \frac{1}{\hbar} \langle i\hat{H} \psi | \hat{A} | \psi \rangle + \langle \psi | \partial_t \hat{A} | \psi \rangle + \frac{1}{\hbar} \langle \psi | \hat{A} (-i\hat{H} \psi) \rangle
  \]
  \[
  = \frac{i}{\hbar} \left( \langle \psi | \hat{H} \hat{A} | \psi \rangle - \langle \psi | \hat{A} \hat{H} | \psi \rangle \right) + \langle \psi | \partial_t \hat{A} | \psi \rangle
  \]
  \[
  = \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{A}] | \psi \rangle
  \]

- For time-independent operators, $\hat{A}$, obtain \textbf{Ehrenfest Theorem},
  \[
  \partial_t \langle \psi | \hat{A} | \psi \rangle = \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{A}] | \psi \rangle.
  \]
Ehrenfest theorem: example

\[ \partial_t \langle \psi | \hat{A} | \psi \rangle = \frac{i}{\hbar} \langle \psi | [\hat{H}, \hat{A}] | \psi \rangle. \]

- For the Schrödinger operator, \( \hat{H} = \frac{\hat{p}^2}{2m} + V(x) \),

\[ \partial_t \langle x \rangle = \frac{i}{\hbar} \langle [\hat{H}, \hat{x}] \rangle = \frac{i}{\hbar} \langle [\frac{\hat{p}^2}{2m}, x] \rangle = \frac{\langle \hat{p} \rangle}{m} \]

- Similarly,

\[ \partial_t \langle \hat{p} \rangle = \frac{i}{\hbar} \langle [\hat{H}, -i\hbar \partial_x] \rangle = -\langle (\partial_x \hat{H}) \rangle = -\langle \partial_x V \rangle \]

i.e. Expectation values follow Hamilton’s classical equations of motion.
Symmetry in quantum mechanics

- Symmetry considerations are very important in both low and high energy quantum theory:

1. Structure of eigenstates and spectrum reflect symmetry of the underlying Hamiltonian.

2. Transition probabilities between states depend upon transformation properties of perturbation \( \rightarrow \) “selection rules”.

- Symmetries can be classified as **discrete** and **continuous**, e.g. mirror symmetry is discrete, while rotation is continuous.
Symmetry in quantum mechanics

- Formally, symmetry operations can be represented by a group of (typically) unitary transformations (or operators), $\hat{U}$ such that

$$\hat{O} \rightarrow \hat{U}^\dagger \hat{O} \hat{U}$$

- Such unitary transformations are said to be **symmetries of a general operator** $\hat{O}$ if

$$\hat{U}^\dagger \hat{O} \hat{U} = \hat{O}$$

i.e., since $\hat{U}^\dagger = \hat{U}^{-1}$ (unitary), $[\hat{O}, \hat{U}] = 0$.

- If $\hat{O} \equiv \hat{H}$, such unitary transformations are said to be symmetries of the quantum system.
Continuous symmetries: Examples

- Operators $\hat{p}$ and $\hat{r}$ are **generators of space-time transformations**:

- For a constant vector $\mathbf{a}$, the unitary operator

  $$\hat{U}(\mathbf{a}) = \exp \left[ -\frac{i}{\hbar} \mathbf{a} \cdot \hat{\mathbf{p}} \right]$$

  effects **spatial translations**, $\hat{U}^\dagger(\mathbf{a})f(\mathbf{r})\hat{U}(\mathbf{a}) = f(\mathbf{r} + \mathbf{a})$.

- Proof: Using the Baker-Hausdorff identity (exercise),

  $$e^{\hat{A}}\hat{B}e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \cdots$$

  with $e^{\hat{A}} = \hat{U}^\dagger = e^{\mathbf{a} \cdot \nabla}$ and $\hat{B} = f(\mathbf{r})$, it follows that

  $$\hat{U}^\dagger(\mathbf{a})f(\mathbf{r})\hat{U}(\mathbf{a}) = f(\mathbf{r}) + a_i (\nabla_i f(\mathbf{r})) + \frac{1}{2!} a_i a_j (\nabla_i \nabla_j f(\mathbf{r})) + \cdots$$

  $$= f(\mathbf{r} + \mathbf{a}) \quad \text{by Taylor expansion}$$
Continuous symmetries: Examples

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- For a constant vector $\mathbf{a}$, the unitary operator
  
  $\hat{U}(\mathbf{a}) = \exp \left[ -\frac{i}{\hbar} \mathbf{a} \cdot \hat{p} \right]$

  effects spatial translations, $\hat{U}^\dagger(\mathbf{a}) f(\mathbf{r}) \hat{U}(\mathbf{a}) = f(\mathbf{r} + \mathbf{a})$.

- Proof: Using the Baker-Hausdorff identity (exercise),
  
  $e^{A}B e^{-A} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \cdots$

  with $e^{\hat{A}} \equiv \hat{U}^\dagger = e^{\mathbf{a} \cdot \nabla}$ and $\hat{B} \equiv f(\mathbf{r})$, it follows that
  
  $\hat{U}^\dagger(\mathbf{a}) f(\mathbf{r}) \hat{U}(\mathbf{a}) = f(\mathbf{r}) + a_{i_1}(\nabla_{i_1} f(\mathbf{r})) + \frac{1}{2!} a_{i_1} a_{i_2}(\nabla_{i_1} \nabla_{i_2} f(\mathbf{r})) + \cdots$

  $= f(\mathbf{r} + \mathbf{a})$ by Taylor expansion
Continuous symmetries: Examples

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- For a constant vector \( \mathbf{a} \), the unitary operator 

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\hat{U}(\mathbf{a}) = \exp \left[ -\frac{i}{\hbar} \mathbf{a} \cdot \hat{p} \right]
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effects **spatial translations**, \( \hat{U}^\dagger(\mathbf{a}) f(\mathbf{r}) \hat{U}(\mathbf{a}) = f(\mathbf{r} + \mathbf{a}) \).

- Therefore, a quantum system has spatial translation symmetry iff 

\[
\hat{U}(\mathbf{a}) \hat{H} = \hat{H} \hat{U}(\mathbf{a}), \quad \text{i.e.} \quad \hat{p} \hat{H} = \hat{H} \hat{p}
\]

i.e. (sensibly) \( \hat{H} = \hat{H}(\hat{p}) \) must be independent of position.

- Similarly (with \( \hat{L} = \mathbf{r} \times \hat{p} \) the angular momentum operator),

\[
\begin{align*}
\hat{U}(\mathbf{b}) &= \exp \left[ -\frac{i}{\hbar} \mathbf{b} \cdot \hat{r} \right] \\
\hat{U}(\theta) &= \exp \left[ -\frac{i}{\hbar} \theta \hat{e}_n \cdot \hat{L} \right] \\
\hat{U}(t) &= \exp \left[ -\frac{i}{\hbar} \hat{H} t \right]
\end{align*}
\]

- \( \hat{U}(\mathbf{b}) \): momentum translations
- \( \hat{U}(\theta) \): spatial rotations
- \( \hat{U}(t) \): time translations
Continuous symmetries: Examples

- Operators $\hat{p}$ and $\hat{r}$ are generators of space-time transformations:
- For a constant vector $\mathbf{a}$, the unitary operator
  \[ \hat{U}(\mathbf{a}) = \exp \left[ -\frac{i}{\hbar} \mathbf{a} \cdot \hat{p} \right] \]
effects spatial translations, $\hat{U}^\dagger(\mathbf{a}) f(r) \hat{U}(\mathbf{a}) = f(r + \mathbf{a})$.
- Therefore, a quantum system has spatial translation symmetry iff
  \[ \hat{U}(\mathbf{a}) \hat{H} = \hat{H} \hat{U}(\mathbf{a}) \], i.e. $\hat{p} \hat{H} = \hat{H} \hat{p}$
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  \end{align*} \right\} \\
  \left\{ \begin{align*}
  \quad &\quad \text{spatial rotations} \\
  \quad &\quad \text{time translations} \\
  \right\} 
\]
The parity operator, $\hat{P}$, involves a sign reversal of all coordinates,

$$\hat{P}\psi(r) = \psi(-r)$$

discreteness follows from identity $\hat{P}^2 = 1$.

- Eigenvalues of parity operation (if such exist) are $\pm 1$.
- If Hamiltonian is invariant under parity, $[\hat{P}, \hat{H}] = 0$, parity is said to be conserved.

Time-reversal is another discrete symmetry, but its representation in quantum mechanics is subtle and beyond the scope of course.
Consequences of symmetries: multiplets

- Consider a transformation $\hat{U}$ which is a symmetry of an operator observable $\hat{A}$, i.e. $[\hat{U}, \hat{A}] = 0$.

- If $\hat{A}$ has eigenvector $|a\rangle$, it follows that $\hat{U}|a\rangle$ will be an eigenvector with the same eigenvalue, i.e.

$$\hat{A}U|a\rangle = \hat{U}\hat{A}|a\rangle = aU|a\rangle$$

- This means that either:
  - $|a\rangle$ is an eigenvector of both $\hat{A}$ and $\hat{U}$ (e.g., $|p\rangle$ is eigenvector of $\hat{H} = \frac{p^2}{2m}$ and $\hat{U} = e^{i\theta \hat{L}/\hbar}$), or
  - eigenvalue $a$ is degenerate: linear space spanned by vectors $\hat{U}^n|a\rangle$ ($n$ integer) are eigenvectors with same eigenvalue.
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E.g. next lecture, we will address central potential where \( \hat{H} \) is invariant under rotations, \( \hat{U} = e^{i\theta \hat{L}_z/\hbar} \) - states of angular momentum, \( \ell \), have \( 2\ell + 1 \)-fold degeneracy generated by \( \hat{L}_z \).
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**Schrödinger representation:** time-dependence of quantum system carried by wavefunction while operators remain constant.

However, sometimes useful to transfer time-dependence to operators: For observable $\hat{B}$, time-dependence of expectation value,

$$\langle \psi(t) | \hat{B} | \psi(t) \rangle = \langle e^{-i\hat{H}t/\hbar} \psi(0) | \hat{B} | e^{-i\hat{H}t/\hbar} \psi(0) \rangle$$

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Quantum harmonic oscillator

- The harmonic oscillator holds priviledged position in quantum mechanics and quantum field theory.

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 x^2 \]

- It also provides a useful platform to illustrate some of the operator-based formalism developed above.

- To obtain eigenstates of \( \hat{H} \), we could seek solutions of linear second order differential equation,

\[ \left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \right] \psi = E \psi \]

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\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2x^2 \]

- Form of Hamiltonian suggests that it can be recast as the “square of an operator”: Defining the operators (no hats!)

\[ a = \sqrt{\frac{m\omega}{2\hbar}} \left( x + i \frac{\hat{p}}{m\omega} \right), \quad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}} \left( x - i \frac{\hat{p}}{m\omega} \right) \]

we have \( a^\dagger a = \frac{m\omega}{2\hbar}x^2 + \frac{\hat{p}^2}{2\hbar m\omega} - i \frac{\hbar}{2\hbar} [\hat{p}, x] = \frac{\hat{H}}{\hbar\omega} - \frac{1}{2} \)

- Together with \( aa^\dagger = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2} \), we find that operators fulfil the commutation relations

\[ [a, a^\dagger] \equiv aa^\dagger - a^\dagger a = 1 \]
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- Setting \( \hat{n} = a^\dagger a \), \( \hat{H} = \hbar\omega (\hat{n} + 1/2) \)

- Since operator \( \hat{n} = a^\dagger a \) positive definite, eigenstates have energies \( E \geq \hbar\omega/2 \).
Quantum harmonic oscillator

\[ \hat{H} = \hbar \omega (a^\dagger a + 1/2) \]

- **Ground state** \( |0\rangle \) identified by finding state for which

\[ a|0\rangle = \sqrt{\frac{m\omega}{2\hbar}} \left( x + i \frac{\hat{p}}{m\omega} \right) |0\rangle = 0 \]

- In coordinate basis,

\[ \langle x|a|0\rangle = 0 = \int dx' \langle x|a|x'\rangle \langle x'|0\rangle = \left( x + \frac{\hbar}{m\omega} \partial_x \right) \psi_0(x) \]

i.e. ground state has energy \( E_0 = \hbar \omega/2 \) and

\[ \psi_0(x) = \langle x|0\rangle = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} e^{-m\omega x^2/2\hbar} \]

N.B. typo in handout!
Quantum harmonic oscillator

$$\hat{H} = \hbar \omega (a^{\dagger} a + 1/2)$$

- **Excited states** found by acting upon this state with \( a^{\dagger} \).
  
  Proof: using \([a, a^{\dagger}] \equiv a a^{\dagger} - a^{\dagger} a = 1\), if \( \hat{n}|n\rangle = n|n\rangle \),

  \[
  \hat{n}(a^{\dagger}|n\rangle) = a^{\dagger} \underbrace{a a^{\dagger}}_{a^{\dagger} a + 1} |n\rangle = (a^{\dagger} a a + a^{\dagger})|n\rangle = (n + 1)a^{\dagger}|n\rangle \]

  equivalently, \([\hat{n}, a^{\dagger}] = \hat{n}a^{\dagger} - a^{\dagger}\hat{n} = a^{\dagger}\).

- Therefore, if \( |n\rangle \) is eigenstate of \( \hat{n} \) with eigenvalue \( n \), then \( a^{\dagger}|n\rangle \) is eigenstate with eigenvalue \( n + 1 \).

- Eigenstates form a “tower”; \( |0\rangle, |1\rangle = C_1 a^{\dagger}|0\rangle, |2\rangle = C_2 (a^{\dagger})^2|0\rangle, \ldots \), with normalization \( C_n \).
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Quantum harmonic oscillator

\[ \hat{H} = \hbar \omega (a^\dagger a + 1/2) \]

- **Normalization**: If \( \langle n|n \rangle = 1 \), \( \langle n|a a^\dagger|n \rangle = \langle n|\hat{n} + 1|n \rangle = (n + 1) \), i.e. with \( |n + 1 \rangle = \frac{1}{\sqrt{n + 1}} a^\dagger |n \rangle \), state \( |n + 1 \rangle \) also normalized.

\[ |n \rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0 \rangle, \quad \langle n|n' \rangle = \delta_{nn'} \]

are eigenstates of \( \hat{H} \) with eigenvalue \( E_n = (n + 1/2)\hbar \omega \) and

\[ a^\dagger |n \rangle = \sqrt{n + 1} |n + 1 \rangle, \quad a |n \rangle = \sqrt{n} |n - 1 \rangle \]

- \( a \) and \( a^\dagger \) represent **ladder operators** that lower/raise energy of state by \( \hbar \omega \).
Quantum harmonic oscillator

- In fact, operator representation achieves something remarkable and far-reaching: the quantum harmonic oscillator describes motion of a single particle in a confining potential.

- Eigenvalues turn out to be equally spaced, cf. ladder of states.

- Although we can find a coordinate representation $\psi_n(x) = \langle x | n \rangle$, operator representation affords a second interpretation, one that lends itself to further generalization in quantum field theory.

- Quantum harmonic oscillator can be interpreted as a simple system involving many fictitious particles, each of energy $\hbar \omega$. 
In new representation, known as the **Fock space** representation, vacuum $|0\rangle$ has no particles, $|1\rangle$ a single particle, $|2\rangle$ has two, etc.

Fictitious particles created and annihilated by raising and lowering operators, $a^{\dagger}$ and $a$ with commutation relations, $[a, a^{\dagger}] = 1$.

Later in the course, we will find that these commutation relations are the hallmark of **bosonic** quantum particles and this representation, known as **second quantization** underpins the quantum field theory of relativistic particles (such as the photon).
Quantum harmonic oscillator: “dynamical echo”

- How does a general wavepacket $|\psi(0)\rangle$ evolve under the action of the quantum time-evolution operator, $\hat{U}(t) = e^{-i\hat{H}t/\hbar}$?

- For a general initial state, $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$. Inserting the resolution of identity on the complete set of eigenstates,

$$|\psi(t)\rangle = e^{-i\hat{H}t/\hbar} \sum_n |n\rangle \langle n|\psi(0)\rangle = \sum_n |n\rangle \langle n|\psi(0)\rangle e^{-iE_n t/\hbar}$$

- For the harmonic oscillator, $E_n = \hbar\omega(n + 1/2)$.

- Therefore, at times $t = \frac{2\pi}{\omega} m$, $m$ integer, $|\psi(t)\rangle = e^{-i\omega t/2} |\psi(0)\rangle$ leading to the coherent reconstruction (echo) of the wavepacket.

- At times $t = \frac{\pi}{\omega}(2m + 1)$, the “inverted” wavepacket

$\psi(x, t) = e^{-i\omega t/2} \psi(-x, 0)$ is perfectly reconstructed (exercise).
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Therefore, making use of the identity, \( [\hat{H}, a] = -\hbar \omega a \) (exercise),

\[
\partial_t a = -i\omega a, \quad \text{i.e. } a(t) = e^{-i\omega t} a(0)
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Combined with conjugate relation \( a^\dagger(t) = e^{i\omega t} a^\dagger(0) \), and using

\[
x = \sqrt{\frac{\hbar}{2m\omega}} (a^\dagger + a), \quad \hat{p} = -i \sqrt{\frac{m\hbar \omega}{2}} (a - a^\dagger) \quad \text{(exercise)}
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\hat{p}(t) = \hat{p}(0) \cos(\omega t) - m\omega \hat{x}(0) \sin(\omega t)
\]

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i.e. operators obey equations of motion of the classical harmonic oscillator.

But how do we use these equations...?
Quantum harmonic oscillator: time-dependence

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- Consider dynamics of a (real) wavepacket defined by \( \phi(x) \) at \( t = 0 \). Suppose we know expectation values, \( p_0^2 = \langle \phi|\hat{p}^2|\phi \rangle \), \( x_0^2 = \langle \phi|x^2|\phi \rangle \), and we want to determine \( \langle \phi(t)|\hat{p}^2|\phi(t) \rangle \).

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and similarly \( \langle \phi | \hat{x}^2(t) | \phi \rangle = x_0^2 \cos^2(\omega t) + \frac{p_0^2}{(m\omega)^2} \sin^2(\omega t) \)
\[ \hat{p}(t) = \hat{p}(0) \cos(\omega t) - m\omega \hat{x}(0) \sin(\omega t) \]
\[ \hat{x}(t) = \hat{x}(0) \cos(\omega t) + \frac{\hat{p}(0)}{m\omega} \sin(\omega t) \]

Consider dynamics of a (real) wavepacket defined by \( \phi(x) \) at \( t = 0 \). Suppose we know expectation values, \( p_0^2 = \langle \phi | \hat{p}^2 | \phi \rangle \), \( x_0^2 = \langle \phi | x^2 | \phi \rangle \), and we want to determine \( \langle \phi(t) | \hat{p}^2 | \phi(t) \rangle \).

In Heisenberg representation, \( \langle \phi(t) | \hat{p}^2 | \phi(t) \rangle = \langle \phi | \hat{p}^2(t) | \phi \rangle \) and
\[ \hat{p}^2(t) = \hat{p}^2(0) \cos^2(\omega t) + (m\omega x(0))^2 \sin^2(\omega t) \]
\[ - m\omega (x(0)\hat{p}(0) + \hat{p}(0)x(0)) \]

Since \( \langle \phi | (x(0)\hat{p}(0) + \hat{p}(0)x(0)) | \phi \rangle = 0 \) for \( \phi(x) \) real, we have
\[ \langle \phi | \hat{p}^2(t) | \phi \rangle = p_0^2 \cos^2(\omega t) + (m\omega x_0)^2 \sin^2(\omega t) \]
and similarly \( \langle \phi | \hat{x}^2(t) | \phi \rangle = x_0^2 \cos^2(\omega t) + \frac{p_0^2}{(m\omega)^2} \sin^2(\omega t) \)
Coherent states

- The ladder operators can be used to construct a wavepacket which most closely resembles a classical particle – the coherent or Glauber states.

- Such states have numerous applications in quantum field theory and quantum optics.

- The coherent state is defined as the eigenstate of the annihilation operator,

\[
|\beta\rangle = \beta |\beta\rangle
\]

Since \(a\) is not Hermitian, \(\beta\) can take complex eigenvalues.

- The eigenstates are constructed from the harmonic oscillator ground state by action of the unitary operator,

\[
|\beta\rangle = \hat{U}(\beta)|0\rangle, \quad \hat{U}(\beta) = e^{\beta a^\dagger - \beta^* a}
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- The proof follows from the identity (problem set I),
  \[ a\hat{U}(\beta) = \hat{U}(\beta)(a + \beta) \]
i.e. \( \hat{U} \) is a translation operator, \( \hat{U}^\dagger(\beta)a\hat{U}(\beta) = a + \beta \).
- By making use of the Baker-Campbell-Hausdorff identity
  \[ e^{\hat{X}}e^{\hat{Y}} = e^{\hat{X}+\hat{Y}+\frac{1}{2}[\hat{X},\hat{Y}]} \]
valid if \([\hat{X},\hat{Y}]\) is a c-number, we can show (problem set)
\[ \hat{U}(\beta) = e^{\beta a^\dagger - \beta^* a} = e^{-|\beta|^2/2} e^{\beta a^\dagger} e^{-\beta^* a} \]
i.e., since \( e^{-\beta^* a}|0\rangle = |0\rangle \),
\[ |\beta\rangle = e^{-|\beta|^2/2} e^{\beta a^\dagger} |0\rangle \]
Coherent states

\[ a|\beta\rangle = \beta|\beta\rangle, \quad |\beta\rangle = e^{-|\beta|^2/2} e^{\beta a^\dagger} |0\rangle \]

- Expanding the exponential, and noting that \(|n\rangle = \frac{1}{\sqrt{n!}} (a^\dagger)^n |0\rangle\), \(|\beta\rangle\) can be represented in number basis

\[ |\beta\rangle = \sum_{n=0}^{\infty} \frac{(\beta a^\dagger)^n}{n!} |0\rangle = \sum_n e^{-|\beta|^2/2} \frac{\beta^n}{\sqrt{n!}} |n\rangle \]

i.e. Probability of observing \(n\) excitations is

\[ P_n = |\langle n|\beta\rangle|^2 = e^{-|\beta|^2} \frac{|\beta|^{2n}}{n!} \]

a Poisson distribution with average occupation, \(\langle \beta | a^\dagger a | \beta \rangle = |\beta|^2\).
coherent states

\[ a|\beta\rangle = \beta|\beta\rangle, \quad |\beta\rangle = e^{-|\beta|^2/2} e^{\beta a^\dagger} |0\rangle \]

Furthermore, one may show that the coherent state has minimum uncertainty \( \Delta x \Delta p = \frac{\hbar}{2} \).

In the real space representation (problem set I),

\[ \psi_\beta(x) = \langle x|\beta\rangle = N \exp \left[ - \frac{(x - x_0)^2}{4(\Delta x)^2} - \frac{i}{\hbar} p_0 x \right] \]

where \( (\Delta x)^2 = \frac{\hbar}{2m\omega} \) and

\[ x_0 = \sqrt{\frac{\hbar}{2m\omega}} (\beta^* + \beta) = A \cos \varphi \]

\[ p_0 = i \sqrt{\frac{\hbar m\omega}{2}} (\beta^* - \beta) = m\omega A \sin \varphi \]

where \( A = \sqrt{\frac{2\hbar}{m\omega}} \) and \( \beta = |\beta| e^{i\varphi} \).
Coherent States: dynamics

\[ a|\beta\rangle = \beta|\beta\rangle, \quad |\beta\rangle = \sum_n e^{-|\beta|^2/2} \frac{\beta^n}{\sqrt{n!}} |n\rangle \]

- Using the time-evolution of the stationary states,
  \[ |n(t)\rangle = e^{-iE_n t/\hbar} |n(0)\rangle, \quad E_n = \hbar \omega (n + 1/2) \]
  it follows that
  \[ |\beta(t)\rangle = e^{-i\omega t/2} \sum_n e^{-|\beta|^2/2} \frac{\beta^n}{\sqrt{n!}} e^{-i\omega t} |n\rangle = e^{-i\omega t/2} e^{-i\omega t |\beta\rangle} \]

- Therefore, the form of the coherent state wavefunction is preserved in the time-evolution, while centre of mass and momentum follow that of the classical oscillator,
  \[ x_0(t) = A \cos(\varphi + \omega t), \quad p_0(t) = m\omega A \sin(\varphi + \omega t) \]
Operator methods provide a powerful formalism in which we may bypass potentially complex coordinate representations of wavefunctions.

Operator methods allow us to expose the symmetry content of quantum systems – providing classification of degenerate submanifolds and multiplets.

Operator methods can provide insight into dynamical properties of quantum systems without having to resolve eigenstates.

Quantum harmonic oscillator provides example of “complementarity” – states of oscillator can be interpreted as a confined single particle problem or as a system of fictitious non-interacting quantum particles.

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