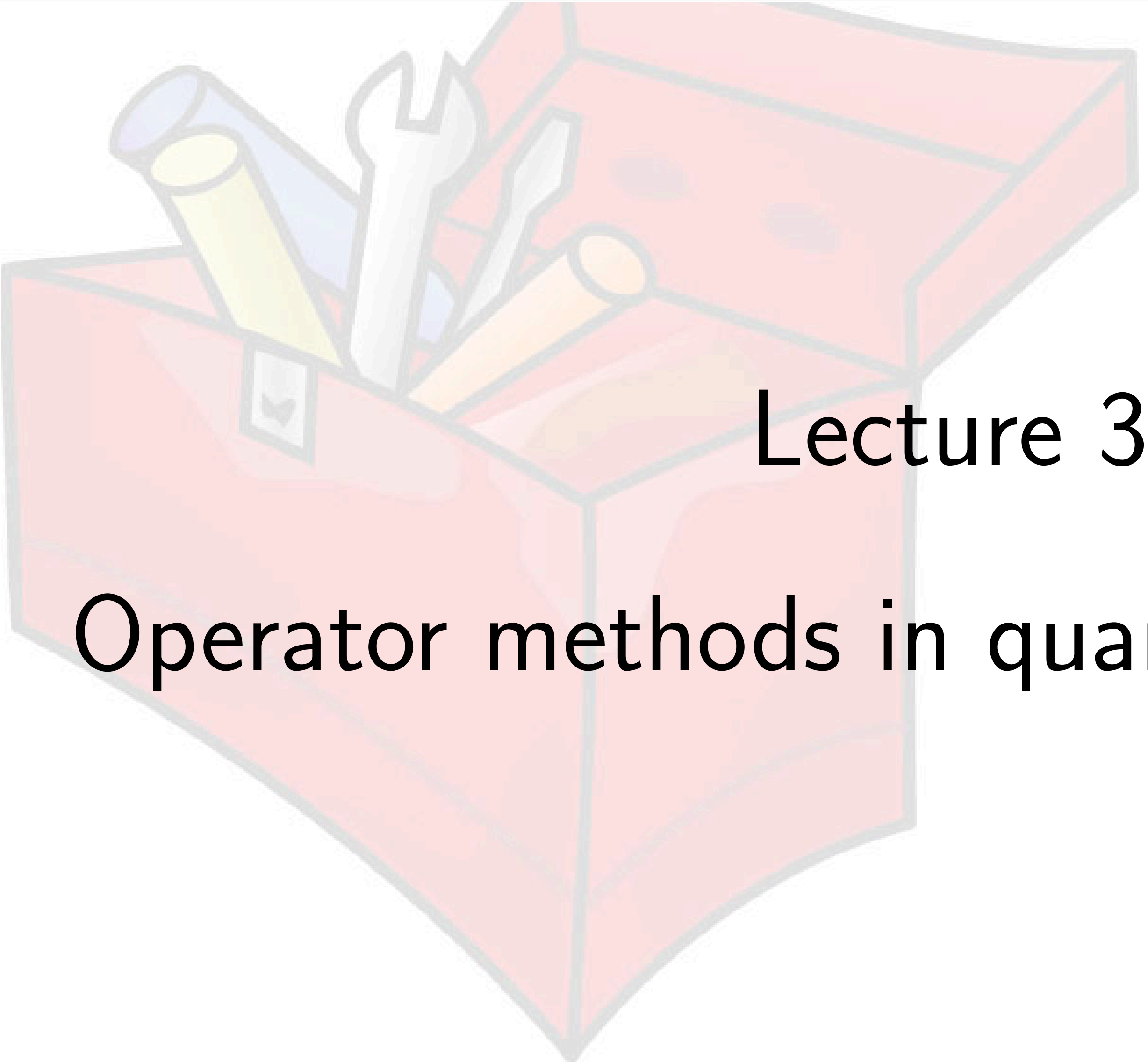

Lecture 3

Operator methods in quantum mechanics

Background

- 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 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, ψ, which is coordinate-independent.

Operator methods: outline

1. 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, ψ, is represented symbolically as a **"ket"**, $|\psi\rangle$.
- Any wavefunction can be expanded as sum of basis state vectors, (cf. $\mathbf{v} = x\hat{\mathbf{e}}_x + y\hat{\mathbf{e}}_y + \cdots$)

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

- 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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Dirac notation

- For a complete basis set, ϕ_i, we can define the expansion

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

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

- For example, in the real space basis, $|\psi\rangle = \int dx\, \psi(x)|x\rangle$.
- Then, since $\langle x|x'\rangle = \delta(x - x')$,

$$\langle x'|\psi\rangle = \int dx\, \psi(x) \underbrace{\langle x'|x\rangle}_{\delta(x-x')} = \psi(x')$$

- In Dirac formulation, real space representation recovered from inner product, $\psi(x) = \langle x|\psi\rangle$; equivalently $\psi(p) = \langle p|\psi\rangle$.

Operators

- 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

  $$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle = \int_{-\infty}^{\infty} dx\, \psi^*(x)\hat{A}\psi(x)$$

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Operators

- 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, $\langle \hat{A}^\dagger \phi | \psi \rangle = \langle \phi | \hat{A} \psi \rangle$, some useful relations follow:

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

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

  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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Operators

- 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

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

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

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  In coordinate representation,

$$\psi(x) = \langle x|\psi\rangle = \sum_i \langle x|i\rangle\langle i|\psi\rangle = \sum_i \langle i|\psi\rangle\phi_i(x), \qquad \phi_i(x) = \langle x|i\rangle$$

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, $\langle\phi|\psi\rangle = \sum_i b_i^* c_i$.

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Example: resolution of identity

- 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,

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

where $\langle x|p\rangle$ denotes plane wave state $|p\rangle$ expressed in the real space basis.

Time-evolution operator

- 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,

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Time-evolution operator

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

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

$$\langle\phi|\psi\rangle = \langle\hat{U}\phi|\hat{U}\psi\rangle = \langle\phi|\hat{U}^\dagger\hat{U}\psi\rangle \stackrel{!}{=} \langle\phi|\psi\rangle$$

i.e. $\boxed{\hat{U}^\dagger\hat{U} = \mathbb{I}}$

Uncertainty principle for non-commuting operators

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

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

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

- Since $\langle\hat{A}\rangle$ and $\langle\hat{B}\rangle$ are just constants, $[\hat{U},\hat{V}] = [\hat{A},\hat{B}]$.

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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 λ,

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

- 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**,

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

- 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,

$$\partial_t\langle\psi|\hat{A}|\psi\rangle = \frac{1}{\hbar}\langle i\hat{H}\psi|\hat{A}|\psi\rangle + \langle\psi|\partial_t\hat{A}|\psi\rangle + \frac{1}{\hbar}\langle\psi|\hat{A}|(-i\hat{H}\psi)\rangle$$

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

- For time-independent operators, $\hat{A}$, obtain **Ehrenfest Theorem**,

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

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$$\begin{aligned}\partial_t\langle\psi|\hat{A}|\psi\rangle &= \frac{1}{\hbar}\langle i\hat{H}\psi|\hat{A}|\psi\rangle + \langle\psi|\partial_t\hat{A}|\psi\rangle + \frac{1}{\hbar}\langle\psi|\hat{A}|(-i\hat{H}\psi)\rangle \\ &= \frac{i}{\hbar}\underbrace{\left(\langle\psi|\hat{H}\hat{A}|\psi\rangle - \langle\psi|\hat{A}\hat{H}|\psi\rangle\right)}_{\langle\psi|[\hat{H},\hat{A}]|\psi\rangle} + \langle\psi|\partial_t\hat{A}|\psi\rangle\end{aligned}$$

- For time-independent operators, $\hat{A}$, obtain **Ehrenfest Theorem**,

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

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 $\implies$ "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

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

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

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

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

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

Continuous symmetries: Examples

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

$$\begin{aligned}\hat{U}^\dagger(\mathbf{a})f(\mathbf{r})\hat{U}(\mathbf{a}) &= f(\mathbf{r}) + a_{i_1}(\nabla_{i_1}f(\mathbf{r})) + \frac{1}{2!}a_{i_1}a_{i_2}(\nabla_{i_1}\nabla_{i_2}f(\mathbf{r})) + \cdots \\ &= f(\mathbf{r}+\mathbf{a}) \qquad \text{by Taylor expansion}\end{aligned}$$

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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

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

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

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

$$\left\{\begin{array}{l} \hat{U}(\mathbf{b}) = \exp[-\frac{i}{\hbar}\mathbf{b}\cdot\hat{\mathbf{r}}] \\ \hat{U}(\theta) = \exp[-\frac{i}{\hbar}\theta\hat{\mathbf{e}}_n\cdot\hat{\mathbf{L}}] \\ \hat{U}(t) = \exp[-\frac{i}{\hbar}\hat{H}t] \end{array}\right. \text{ effects } \left\{\begin{array}{l} \text{momentum translations} \\ \text{spatial rotations} \\ \text{time translations} \end{array}\right.$$

Continuous symmetries: Examples

- Operators $\hat{\mathbf{p}}$ and $\hat{\mathbf{r}}$ 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**, $\hat{U}^\dagger(\mathbf{a})f(\mathbf{r})\hat{U}(\mathbf{a}) = f(\mathbf{r}+\mathbf{a})$.
- Therefore, a quantum system has spatial translation symmetry iff

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

  i.e. (sensibly) $\hat{H} = \hat{H}(\hat{\mathbf{p}})$ must be independent of position.
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Discrete symmetries: Examples

- The **parity** operator, $\hat{P}$, involves a sign reversal of all coordinates,

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

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

- Eigenvalues of parity operation (if such exist) are ± 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:
  1. $|a\rangle$ is an eigenvector of both $\hat{A}$ and $\hat{U}$ (e.g. $|\mathbf{p}\rangle$ is eigenvector of $\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m}$ and $\hat{U} = e^{i\mathbf{a}\cdot\hat{\mathbf{p}}/\hbar}$), or
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Heisenberg representation

- **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,

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

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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,

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

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

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

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

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

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1$$

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

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

  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"; $|0\rangle$, $|1\rangle = C_1 a^\dagger|0\rangle$, $|2\rangle = C_2(a^\dagger)^2|0\rangle$, ..., with normalization C_n.

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

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

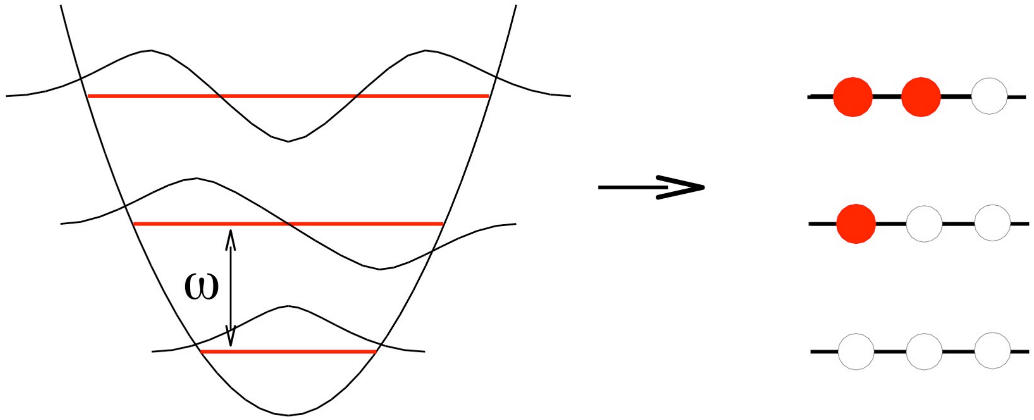
are eigenstates of $\hat{H}$ with eigenvalue $E_n = (n+1/2)\hbar\omega$ and

$$a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \qquad a|n\rangle = \sqrt{n}|n-1\rangle$$

- a and $a^\dagger$ represent **ladder operators** that lower/raise energy of state by $\hbar\omega$.

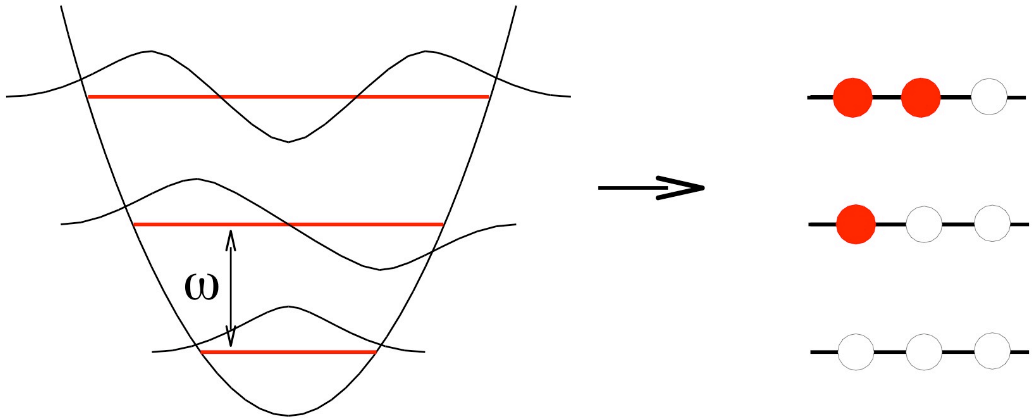
Quantum harmonic oscillator

- 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 $\hbar\omega$.

Quantum harmonic oscillator



- 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,

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

- 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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Quantum harmonic oscillator: time-dependence

- In Heisenberg representation, we have seen that $\partial_t \hat{B} = \frac{i}{\hbar}[\hat{H}, \hat{B}]$.
- Therefore, making use of the identity, $[\hat{H}, a] = -\hbar\omega a$ (exercise),

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- Combined with conjugate relation $a^\dagger(t) = e^{i\omega t} a^\dagger(0)$, and using $x = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$, $\hat{p} = -i\sqrt{\frac{m\hbar\omega}{2}}(a - a^\dagger)$ (exercise)

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

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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 $\langle\phi(t)|\hat{p}^2|\phi(t)\rangle$.
- 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,

$$a|\beta\rangle = \beta|\beta\rangle$$

  Since a is not Hermitian, β can take complex eigenvalues.
- The eigenstates are constructed from the harmonic oscillator ground state the by action of the unitary operator,

$$|\beta\rangle = \hat{U}(\beta)|0\rangle, \qquad \hat{U}(\beta) = e^{\beta a^\dagger - \beta^* a}$$

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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

$$a|\beta\rangle = \beta|\beta\rangle, \qquad |\beta\rangle = e^{-|\beta|^2/2} e^{\beta a^\dagger}|0\rangle$$

- 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

$$a|\beta\rangle = \beta|\beta\rangle, \qquad |\beta\rangle = e^{-|\beta|^2/2} e^{\beta a^\dagger}|0\rangle$$

- 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

$$a|\beta\rangle = \beta|\beta\rangle, \qquad |\beta\rangle = \sum_n e^{-|\beta|^2/2}\frac{\beta^n}{\sqrt{n!}}|n\rangle$$

- Using the time-evolution of the stationary states,

$$|n(t)\rangle = e^{-iE_n t/\hbar}|n(0)\rangle, \qquad E_n = \hbar\omega(n+1/2)$$

  it follows that

$$|\beta(t)\rangle = e^{-i\omega t/2}\sum_n e^{-|\beta|^2/2}\frac{\beta^n}{\sqrt{n!}}e^{-in\omega t}|n\rangle = e^{-i\omega t/2}|e^{-i\omega t}\beta\rangle$$

- 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,

$$x_0(t) = A\cos(\varphi+\omega t), \qquad p_0(t) = m\omega A\sin(\varphi+\omega t)$$

Summary: operator methods

- 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.

This last point is subtle but the implications are very far-reaching!

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