Quantum Mechanics I, Sheet 8, Spring 2013

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May 7, 2013 (Ecole de Physique, Auditoire Stückelberg)

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Exercises starting with (*) are optional.

I. RADIAL POTENTIALS

Consider a particle in three dimensions in a radial potential $V(r)$,

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2\mu} + V(r) = -\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\hat{\mathbf{L}}^2}{2\mu r^2} + V(r)\,,$$

where $\hat{\mathbf{p}} = -\mathrm{i}\hbar\nabla$ is the momentum operator and $\hat{\mathbf{L}} = \mathbf{x} \wedge \hat{\mathbf{p}}$ is the angular momentum operator.

A. Radial equation

1. Prove that the eigenfunctions of $\hat{H}$ are given in spherical coordinates by

   $$\psi_{\ell,m}(\mathbf{x}) = R_\ell(r) Y_{\ell,m}(\theta,\varphi)\,,$$

   where the spherical harmonics $Y_{\ell,m}$ are the eigenfunctions of the angular momentum

   $$\hat{\mathbf{L}}^2 Y_{\ell,m} = \hbar^2 \ell\,(\ell+1)\, Y_{\ell,m}\,, \qquad L_z Y_{\ell,m} = \hbar m Y_{\ell,m}\,,$$

   and R_ℓ is the radial wave function satisfying

   $$\left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2} r + \frac{\hbar^2 \ell\,(\ell+1)}{2\mu r^2} + V(r)\right) R_\ell = E\, R_\ell\,.$$

2. Determine the differential equation satisfied by the reduced wave function $u_\ell(r) = rR_\ell(r)$.
3. (*) Check that the radial differential equation admits two independent solutions, behaving like $R_\ell(r) \approx r^s$ near $r \approx 0$ respectively with $s = \ell$ and $s = -\ell - 1$. Convince yourself that only the first solution provides an eigenvector of $\hat{H}$. Therefore to the radial differential equation we have to add the boundary condition $u_\ell(0) = 0$.

   [*Hint:* Plug $R_\ell(r) \approx r^s$ into the equation and keep only the dominant term as $r \approx 0$.]

B. Hydrogen atom and harmonic oscillator

1. Write the equation for the reduced wave function for the Coulomb potential and for the harmonic potential

   $$V_{\text{coul.}}(r) = -\frac{Ze^2}{r}\,, \qquad V_{\text{harm.}}(r) = \frac{1}{2}\mu\omega^2 r^2\,.$$

2. Show that, under the transformation $u_{\text{coul.}}(r) = s^p u_{\text{harm.}}(s)$, where $s = r^q$, and with an appropriate choice of p and q, one can cast the Coulomb problem into the same form as the harmonic-oscillator problem.

   $\Big[$*Hint:* If you do not want to do the whole calculations, check this holds for $p = q = 1/2.$$\Big]$

3. Discuss the correspondence between the parameters of the two problems.

II. SYMMETRIES AND CONSERVED QUANTITIES

In quantum mechanics a symmetry is represented by a one-parameter unitary group, *i.e.* a family of unitary operator $\big(\hat{U}_\alpha\big)_{\alpha\in\mathbb{R}}$ such that

$$\hat{U}_\alpha \hat{U}_\beta = \hat{U}_{\alpha+\beta}\,.$$

The one-parameter unitary group acts on states as

$$|\psi\rangle \mapsto \hat{U}_\alpha|\psi\rangle\,.$$

Since only the brackets have physical meaning, we have

$$\langle\phi|\hat{A}|\psi\rangle = \langle\hat{U}_\alpha\phi|\hat{A}|\hat{U}_\alpha\psi\rangle = \langle\phi|\hat{U}_\alpha^\dagger\hat{A}\hat{U}_\alpha|\psi\rangle\,,$$

and therefore, the action of the group can also be viewed as the transformation of observables,

$$\hat{A} \mapsto \hat{U}_\alpha^\dagger\hat{A}\hat{U}_\alpha\,.$$

A one-parameter unitary group $\big(\hat{U}_\alpha\big)_{\alpha\in\mathbb{R}}$ is called a *symmetry of the system* if the Hamiltonian is invariant, *i.e.*

$$\hat{H} = \hat{U}_\alpha^\dagger\hat{H}\hat{U}_\alpha\,.$$

1. Show that the requirement of $\hat{U}_\alpha$ to be unitary corresponds to the conservation of the scalar product.

2. Check that $\hat{U}_\alpha$ is a symmetry if and only if

   $$\big[\hat{U}_\alpha, \hat{H}\big] = 0\,.$$

3. Show that the Schrödinger equation is invariant under the one-parameter group if and only if $\hat{U}_\alpha$ is a symmetry.

4. By the Stone's theorem, every one-parameter unitary group can be written as

   $$\hat{U}_\alpha = \mathrm{e}^{-\mathrm{i}\alpha\hat{Q}/\hbar}\,,$$

   where $\hat{Q}$ is an hermitian operator, which is called the generator of the symmetry. Show that the one-parameter group satisfies the differential equation

   $$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}\alpha}\hat{U}_\alpha = \hat{Q}\hat{U}_\alpha\,, \qquad\qquad \hat{U}_0 = \hat{I}\,.$$

   In particular the generator of the symmetry is given by

   $$\hat{Q} = \mathrm{i}\hbar\,\frac{\mathrm{d}}{\mathrm{d}\alpha}\hat{U}_\alpha\bigg|_{\alpha=0}\,.$$

5. Show that $\hat{U}_\alpha$ is a symmetry if and only if

$$\big[\hat{Q}, \hat{H}\big] = 0\,.$$

In particular there exists a basis of the Hilbert space formed from eigenvectors common to $\hat{H}$ and $\hat{Q}$.

6. Using the Ehrenfest theorem, check that $\big\langle\hat{Q}\big\rangle$ is a conserved quantity. This result is the quantum analog of the Noether's theorem which relates symmetries to conserved quantities.

A. Translation invariance

The translation operator is defined as

$$\hat{T}_\alpha|\psi(x)\rangle = |\psi(x-\alpha)\rangle\,.$$

1. Check that $\big(\hat{T}_\alpha\big)_{\alpha\in\mathbb{R}}$ is a one-parameter unitary group.

2. Show that the translation operator can be written as

$$\hat{T}_\alpha = \mathrm{e}^{-\mathrm{i}\alpha\hat{P}/\hbar}\,,$$

where $\hat{P} = -\mathrm{i}\hbar\partial_x$ is the momentum operator.

[*Hint:* Write the exponential as a series and recognize the Taylor expansion.]

3. Conclude that if the Hamiltonian is invariant under translation, then the momentum $\big\langle\hat{P}\big\rangle$ is conserved.

4. By considering a particle in a periodic potential $V(x+a) = V(x)$ of period a, the Hamiltonian is invariant under $\hat{T}_a$. Show that in a basis where $\hat{H}$ and $\hat{T}_a$ are diagonal, we have

$$|\psi(x)\rangle = \mathrm{e}^{\mathrm{i}kx}u(x)\,,$$

where $k\in\mathbb{R}$ and u is periodic of period a. This is called the Bloch theorem.

[*Hint:* The eigenvalues of a unitary operator are normalized, so we can choose $\lambda = \mathrm{e}^{-\mathrm{i}ka}$.]

B. Time invariance

The time-translation operator or evolution operator is given by

$$\hat{U}_\alpha|\psi(t)\rangle = |\psi(t+\alpha)\rangle\,.$$

1. By using the Schrödinger equation, show that the evolution operator is given by

$$\hat{U}_\alpha = \mathrm{e}^{\alpha\partial_t} = \mathrm{e}^{-\mathrm{i}\alpha\hat{H}/\hbar}\,,$$

where $\hat{H}$ is the Hamiltonian of the system.

2. Convince yourself that we can define the Hamiltonian as the generator of the time-invariance unitary group, and that with this definition the Schrödinger equation is a consequence of the Stone's theorem, has well has the fact that the Hamiltonian is an hermitian operator.

C. (*) Rotation invariance

In two dimensions $\mathbf{x} = (x, y)$, the operator associated to a rotation of angle α is given by

$$\hat{R}_\alpha |\psi(\mathbf{x})\rangle = |\psi(R_\alpha^{-1}\mathbf{x})\rangle \,,$$

where R_α is the following rotation matrix

$$R_\alpha = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \,.$$

1. Prove that the generator of the rotation symmetry is the angular momentum $\hat{L}_z = \hat{x}\hat{p}_y - y\hat{p}_x$.
   $\Big[$*Hint:* Take the derivative with respect to α in the definition of $\hat{R}_\alpha$ and then evaluate at $\alpha = 0.\Big]$
2. Therefore the conserved quantity associated to the rotation invariance with respect to the axis z is $\hat{L}_z$. What is the analog result in three dimensions?