Quantum Mechanics I, Correction Sheet 8, Spring 2013

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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. Since the potential is radial the Hamiltonian commutes with the angular momentum, and therefore we can take a basis of eigenvectors of $\hat{H}$, $\hat{\mathbf{L}}^2$ and L_z,

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

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

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

By acting with the Hamiltonian on this ansatz, we find

$$\hat{H}\psi_{\ell,m} = \left(-\frac{\hbar^2}{2\mu}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r)\right)R_\ell Y_{\ell,m}\,,$$

and therefore the Schrödinger equation $\hat{H}\psi_{\ell,m} = E\psi_{\ell,m}$ implies that the radial wave function satisfies

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

2. The change of variable $u_\ell(r) = rR_\ell(r)$, transforms the previous equation into

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

3. (*) By plugging $R_\ell(r) \approx r^s$ in the radial equation we find

$$\left(-\frac{\hbar^2 s(s+1)}{2\mu r^2} + \frac{\hbar^2\ell(\ell+1)}{2\mu r^2} + V(r) - E\right)r^s \approx 0\,.$$

Therefore by assuming that the potential is bounded by $1/r$ near $r \approx 0$, the dominant terms are the first two, so we obtain the relation

$$s\,(s+1) = \ell\,(\ell+1)\ ,$$

which has two solutions

$$s = \ell\,, \qquad\qquad s = -\ell - 1\,.$$

Consequently the second order differential equation for R_ℓ admits two independent solutions: $R_\ell(r) \approx r^\ell$ and $R_\ell(r) \approx r^{-\ell-1}$. For $\ell \geq 1$, the second solution in not square-integrable and therefore, not admissible. For $\ell = 0$, the second solution is like $1/r$, but since $\Delta(1/r) = -4\pi\delta(r)$, $\psi_{0,0}$ is not an eigenvector of the Hamiltonian. Therefore, the only physical solution is $u_\ell(r) \approx r^{\ell+1}$ which can be distinguished from the second one by adding to the radial differential equation the boundary condition $u_\ell(0) = 0$.

B. Hydrogen atom and harmonic oscillator

1. The equation for the hydrogen atom is

$$\left(\frac{\partial^2}{\partial r^2} - \frac{\ell\,(\ell+1)}{r^2} + \frac{2\mu Z e^2}{\hbar^2}\frac{1}{r} + \frac{2\mu E}{\hbar^2}\right) u_\ell = 0\,,$$

and the one for the harmonic oscillator is

$$\left(\frac{\partial^2}{\partial r^2} - \frac{\ell\,(\ell+1)}{r^2} - \frac{\mu^2\omega^2}{\hbar^2} r^2 + \frac{2\mu E}{\hbar^2}\right) u_\ell = 0\,.$$

2. By using the change of variable $u_\ell(r) = s^p v_\ell(s)$, with $s = r^q$, we have

$$\frac{\partial}{\partial r} u_\ell(r) = \frac{\partial s}{\partial r}\frac{\partial}{\partial s}\left(s^p v_\ell(s)\right) = q s^{p-1/q}\left(s\frac{\partial}{\partial s} v_\ell(s) + p v_\ell(s)\right)\ ,$$

and

$$\frac{\partial^2}{\partial r^2} u_\ell(r) = q s^{p-2/q}\left(q s^2 \frac{\partial^2}{\partial s^2} v_\ell(s) + q\,(2pq + q - 1)\, s\frac{\partial}{\partial s} v_\ell(s) + p\,(pq-1)\, v_\ell(s)\right)\ .$$

Since no first derivatives are contained in both equations, we have to set $2pq + q - 1 = 0$, *i.e.* $1/q = 1 + 2p$. That way the equation for the hydrogen atom becomes

$$\left(q^2 s^{-4p}\frac{\partial^2}{\partial s^2} + pq\,(pq-1)\, s^{-2/q} - \ell\,(\ell+1)\, s^{-2/q} + \frac{2\mu Z e^2}{\hbar^2} s^{-1/q} + \frac{2\mu E}{\hbar^2}\right) v_\ell = 0\,,$$

or equivalently

$$\left(\frac{\partial^2}{\partial s^2} - \frac{\ell\,(\ell+1)\,(1+2p)^2 + p\,(p+1)}{s^2} + \frac{2\mu Z e^2}{\hbar^2 q^2} s^{2p-1} + \frac{2\mu E}{\hbar^2 q^2}\,(1+2p)^2\, s^{4p}\right) v_\ell = 0\,.$$

By choosing $p = 1/2$, *i.e.* $q = 1/2$, this equation becomes

$$\left(\frac{\partial^2}{\partial s^2} - \frac{4\ell\,(\ell+1) + 3/4}{s^2} + \frac{8\mu E}{\hbar^2} s^2 + \frac{8\mu Z e^2}{\hbar^2}\right) v_\ell = 0\,,$$

which is similar to the equation for the harmonic oscillator.

3. The correspondence between the parameters of the two problems is given by

$$\ell_{\text{harm.}} = 2\ell_{\text{coul.}} + \frac{1}{2}\,, \qquad E_{\text{harm.}} = 4Ze^2\,, \qquad \mu\omega^2 = -8E_{\text{coul.}}\,,$$

and therefore the roles of the coupling constants and of the energy eigenvalues are interchanged. It is important to notice that this correspondence is not totally exact from a physical point of view since both physical problems have integers ℓ, but the relation between $\ell_{\text{harm.}}$ and $\ell_{\text{coul.}}$ does not implies that. In fact this peculiar relation between the Coulomb potential and the harmonic potential comes from the fact that there are the only two radial potentials which have an "hidden symmetry" called a dynamical symmetry. In addition to angular momentum, a second independent quantity is conserved for these two potentials: the Lenz vector. Intuitively this symmetry is related to the fact that in classical mechanics orbits are closed with the two potentials in consideration.

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 act on states as

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

Since only 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 as symmetry of the system if the Hamiltonian is invariant, *i.e.*

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

1. The action of the symmetry on the scalar product is given by

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

which shows that the requirement of $\hat{U}_\alpha$ to be unitary correspond to the conservation of the scalar product.

2. By multiplying the definition of a symmetry by $\hat{U}_\alpha$ we obtain

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

which proves that $\hat{U}_\alpha$ is a symmetry if and only if

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

3. The action of the one-parameter group on the Schrödinger equation is given by
$$\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \hat{H}\right)|\psi\rangle \mapsto \left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \hat{H}\right)\hat{U}_\alpha|\psi\rangle = \hat{U}_\alpha\left(\mathrm{i}\hbar\frac{\partial}{\partial t} - \hat{U}_\alpha^\dagger\hat{H}\hat{U}_\alpha\right)|\psi\rangle\,,$$
and so the Schrödinger equation is invariant if and only if $\hat{U}_\alpha^\dagger\hat{H}\hat{U}_\alpha = \hat{H}$, *i.e.* 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. By taking the derivative with respect to α, and evaluating at $\alpha = 0$, we directly find that
$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}\alpha}\hat{U}_\alpha = \hat{Q}\hat{U}_\alpha\,, \qquad\qquad \hat{U}_0 = \hat{I}\,.$$
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. If $\hat{U}_\alpha$ is a symmetry, then
$$\big[\hat{Q},\hat{H}\big] = \mathrm{i}\hbar\Big[\frac{\mathrm{d}}{\mathrm{d}\alpha}\hat{U}_\alpha\bigg|_{\alpha=0},\hat{H}\Big] = \mathrm{i}\hbar\,\frac{\mathrm{d}}{\mathrm{d}\alpha}\big[\hat{U}_\alpha,\hat{H}\big]\bigg|_{\alpha=0} = 0\,,$$
and reciprocally if $\big[\hat{Q},\hat{H}\big] = 0$, then
$$\big[\hat{U}_\alpha,\hat{H}\big] = \big[\mathrm{e}^{-\mathrm{i}\alpha\hat{Q}/\hbar},\hat{H}\big] = 0\,.$$
In particular there exists a basis of the Hilbert space formed from eigenvectors common to $\hat{H}$ and $\hat{Q}$.

6. By using Ehrenfest theorem, we obtain that $\langle\hat{Q}\rangle$ is a conserved quantity,
$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{Q}\rangle = \frac{1}{\mathrm{i}\hbar}\Big\langle\big[\hat{Q},\hat{H}\big]\Big\rangle = 0\,.$$
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. The set $\big(\hat{T}_\alpha\big)_{\alpha\in\mathbb{R}}$ is a one-parameter group because
$$\hat{T}_\alpha\hat{T}_\beta|\psi(x)\rangle = \hat{T}_\alpha|\psi(x-\beta)\rangle = |\psi(x-\beta-\alpha)\rangle = \hat{T}_{\alpha+\beta}|\psi(x)\rangle\,.$$
Since
$$\langle\phi(x)|\psi(x)\rangle = \langle\phi(x-\alpha)|\psi(x-\alpha)\rangle = \langle\hat{T}_\alpha\phi(x)|\hat{T}_\alpha\psi(x)\rangle = \langle\phi(x)|\hat{T}_\alpha^\dagger\hat{T}_\alpha|\psi(x)\rangle\,,$$
we obtain that $\hat{T}_\alpha^\dagger\hat{T}_\alpha = \hat{I}$. Since $\hat{T}_\alpha^{-1} = \hat{T}_{-\alpha}$ this prove that $\hat{T}_\alpha$ is surjective, so $\hat{T}_\alpha\hat{T}_\alpha^\dagger = \hat{I}$ and therefore $\hat{T}_\alpha$ is unitary.

2. By writing the exponential as a series, and using the Taylor expansion, we obtain

$$\mathrm{e}^{-\mathrm{i}\alpha\hat{P}/\hbar}|\psi(x)\rangle = \mathrm{e}^{-\alpha\partial_x}|\psi(x)\rangle = \sum_{n=0}^{\infty}(-\alpha\partial_x)^n\,|\psi(x)\rangle = |\psi(x-\alpha)\rangle = \hat{T}_\alpha|\psi(x)\rangle\,,$$

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

3. By Ehrenfest theorem, if the Hamiltonian is invariant under translation, then the momentum $\langle\hat{P}\rangle$ is conserved.

4. By considering a particle in a periodic potential $V(x+a) = V(x)$ of period a, the Hamiltonian is invariant under $\hat{T}_a$. Since $\hat{T}_a$ is unitary, the eigenvalue λ corresponding to an eigenvector $|\psi(x)\rangle$ of $\hat{T}_a$ is normalized, so we choose $\lambda = \mathrm{e}^{-\mathrm{i}ka}$, with $k \in \mathbb{R}$. Therefore,

$$|\psi(x-a)\rangle = \hat{T}_a|\psi(x)\rangle = \lambda|\psi(x)\rangle = \mathrm{e}^{-\mathrm{i}ka}|\psi(x)\rangle\,,$$

and the wavefunction $|\psi(x)\rangle$ is not a-periodic, but can be written as

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

where u is periodic of period a. This is the Bloch theorem. Then the Schrödinger equation becomes

$$\left(-\frac{\hbar^2}{2m}\partial_x^2 + V(x) - E\right)|\psi(x)\rangle = \mathrm{e}^{\mathrm{i}kx}\left(-\frac{\hbar^2}{2m}\left(\partial_x + \mathrm{i}k\right)^2 + V(x) - E\right)u(x)\,,$$

and can be solved with a Fourier series, because $u(x)$ is periodic.

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, we have

$$\mathrm{e}^{-\mathrm{i}\alpha\hat{H}/\hbar}|\psi(t)\rangle = \mathrm{e}^{\alpha\partial_t}|\psi(t)\rangle = \sum_{n=0}^{\infty}(\alpha\partial_t)^n\,|\psi(t)\rangle = |\psi(t+\alpha)\rangle\,.$$

2. By defining the Hamiltonain as the generator of the time-invariance unitary group, by Stone's theorem we have that $\hat{H}$ is an hermitian operator and that

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

We already prove that

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

which is equivalent to the Schrödinger equation.

C. (*) Rotation invariance

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

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

where R_α is the following rotation matrix

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

1. The generator of the rotation symmetry is defined by

$$\hat{L}_z = \mathrm{i}\hbar \, \frac{\mathrm{d}}{\mathrm{d}\alpha} \hat{R}_\alpha \bigg|_{\alpha=0} \,.$$

   First of all we define the infinitesimal rotation generator,

$$A_z = \frac{\mathrm{d}}{\mathrm{d}\alpha} R_\alpha \bigg|_{\alpha=0} = \frac{\mathrm{d}}{\mathrm{d}\alpha} \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix} \bigg|_{\alpha=0} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \,.$$

   So by acting on a state and using the chain rule we obtain

$$\begin{aligned} \hat{L}_z |\psi(\mathbf{x})\rangle &= \mathrm{i}\hbar \, \frac{\mathrm{d}}{\mathrm{d}\alpha} \hat{R}_\alpha |\psi(\mathbf{x})\rangle \bigg|_{\alpha=0} = \mathrm{i}\hbar \, \frac{\mathrm{d}}{\mathrm{d}\alpha} |\psi(R_\alpha \mathbf{x})\rangle \bigg|_{\alpha=0} \\ &= \mathrm{i}\hbar \, \frac{\mathrm{d}}{\mathrm{d}\alpha} R_\alpha \mathbf{x} \bigg|_{\alpha=0} \cdot \nabla |\psi(\mathbf{x})\rangle = \mathrm{i}\hbar \, (A_z \mathbf{x}) \cdot \nabla |\psi(\mathbf{x})\rangle \\ &= -\,(A_z \mathbf{x}) \cdot \hat{\mathbf{p}} |\psi(\mathbf{x})\rangle = (x \hat{p}_y - y \hat{p}_x) \, |\psi(\mathbf{x})\rangle \,. \end{aligned}$$

   This proves that the generator of the rotation symmetry in the angular momentum

$$\hat{L}_z = x \hat{p}_y - y \hat{p}_x \,.$$

2. In three dimensions the rotation of angle α around the axis $\mathbf{n}$, is generated by the angular momentum $\hat{\mathbf{L}}$ along $\mathbf{n}$, *i.e.* $\mathbf{n} \cdot \hat{\mathbf{L}}$,

$$\hat{R}_{\mathbf{n},\alpha} = \mathrm{e}^{-\mathrm{i}\alpha \mathbf{n} \cdot \hat{\mathbf{L}}/\hbar} \,.$$

   Therefore, an Hamiltonian which is invariant under the rotation along $\mathbf{n}$ induces the conserved quantity $\langle \mathbf{n} \cdot \hat{\mathbf{L}} \rangle$.