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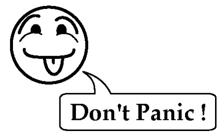

Quantum Mechanics I — Fall '98.

Quizz — Solutions (T. Hübsch)

1. Find the asymptotic behavior of the wave-function for a particle moving (in 3 dimensions) under the influence of the central potential $V(r) = \lambda r^{2n}$. [=10pt]

(Show all work below this line; use overleaf if necessary.)

The potential being independent of angles, we write the Schrödinger equation in spherical variables, and with $\psi(r,\theta,\phi) = R(r)Y_\ell^m(\theta,\phi)$. The $Y_\ell^m(\theta,\phi)$ are just the spherical harmonics, *i.e.*, the eigenfunctions of the angular momentum operator $\hat{\vec{L}}^2$ with eigenvalue $\ell(\ell{+}1)$. Since $\vec{\nabla}^2 = \frac{1}{r}\frac{\partial^2}{\partial r^2}r - \frac{1}{r^2}\hat{\vec{L}}^2$, the Schrödinger equation becomes

$$\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\big(rR(r)\big) - \Big[\frac{\ell(\ell{+}1)}{r^2} - \frac{2mE}{\hbar^2} + \frac{2m\lambda}{\hbar^2}r^{2n}\Big]R(r) = 0 \ . \tag{1}$$

For $n > 0$ and large r, we have (with the $u \stackrel{\text{def}}{=} rR(r)$ substitution)

$$u'' - \frac{2m\lambda}{\hbar^2}r^{2n}u \approx 0 \ . \tag{2}$$

This is (approximately) solved by $u \sim \exp\{-\sqrt{2m\lambda}r^{n+1}/\hbar\}$, so that

$$R(r) \sim \frac{1}{r}e^{-\sqrt{2m\lambda}r^{n+1}/\hbar} \ , \qquad r \to \infty \ . \tag{3}$$

For $n = 0$, the calculation and the result are almost the same, with $\lambda \to (\lambda{-}E)$.

Amusingly, when $n < 0$, the asymptotic behavior of the wave-function for large r no longer depends on λ. For negative n, the potential approaches zero as $r \to \infty$, while the E-term remains constant, and so dominates. Thus, for $n < 0$, $R(r) \sim \frac{1}{r}e^{-\sqrt{-2mE}r^{n+1}/\hbar}$, which is exponentially decaying for negative energies, and oscillatory for positive energies since then $\sqrt{-2mE} = i\sqrt{2m|E|}$.

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2. Find the condition(s) on the wave-functions for the operator $\hat{\vec{\mathcal{L}}} \stackrel{\text{def}}{=} \hat{\vec{r}}\times\hat{\vec{p}} = \frac{\hbar}{i}\vec{r}\times\vec{\nabla}$ to be hermitian [=10pt]

(Show all work below this line; use overleaf if necessary.)

We will prove the questioned equality below, by working on the right hand side:

$$\int_V \mathrm{d}^3\vec{r}\ \psi_i^*\hat{\vec{\mathcal{L}}}\psi_j \stackrel{?}{=} \int_V \mathrm{d}^3\vec{r}\ (\hat{\vec{\mathcal{L}}}\psi_i)^*\psi_j = \int_V \mathrm{d}^3\vec{r}\ (\frac{\hbar}{i}\vec{r}\times\vec{\nabla}\psi_i)^*\psi_j \tag{4a}$$

$$= -\frac{\hbar}{i}\int_V \mathrm{d}^3\vec{r}\ (\vec{r}\times\vec{\nabla}\psi_i^*)\psi_j = \frac{\hbar}{i}\int_V \mathrm{d}^3\vec{r}\ (\vec{\nabla}\psi_i^*)\times\vec{r}\,\psi_j \tag{4b}$$

$$= \frac{\hbar}{i}\int_V \mathrm{d}^3\vec{r}\ \vec{\nabla}\times(\psi_i^*\vec{r}\,\psi_j) - \frac{\hbar}{i}\int_V \mathrm{d}^3\vec{r}\ \psi_i^*(\vec{\nabla}\times\vec{r}\,\psi_j) \tag{4c}$$

$$= \frac{\hbar}{i}\oint_{S=\partial V} \mathrm{d}^2\vec{\sigma}\times(\psi_i^*\vec{r}\,\psi_j) - \frac{\hbar}{i}\int_V \mathrm{d}^3\vec{r}\ \psi_i^*(\vec{\nabla}\psi_j)\times\vec{r} \tag{4d}$$

$$= \frac{\hbar}{i}\oint_{S=\partial V} \mathrm{d}^2\vec{\sigma}\times(\psi_i^*\vec{r}\,\psi_j) + \frac{\hbar}{i}\int_V \mathrm{d}^3\vec{r}\ \psi_i^*(\vec{r}\times\vec{\nabla}\psi_j) \tag{4e}$$

$$= \frac{\hbar}{i}\oint_{S=\partial V} \mathrm{d}^2\vec{\sigma}\times(\psi_i^*\vec{r}\,\psi_j) + \int_V \mathrm{d}^3\vec{r}\ \psi_i^*(\hat{\vec{\mathcal{L}}}\psi_j)\ . \tag{4f}$$

Comparing the left hand side of (4a) with the right hand side of (4f), we conclude that $\hat{\vec{\mathcal{L}}}$ is hermitian if and only if

$$\frac{\hbar}{i}\oint_{S=\partial V} \mathrm{d}^2\vec{\sigma}\times(\psi_i^*\vec{r}\,\psi_j) = 0\ . \tag{5}$$

Wave-functions satisfying this boundary condition form the hermiticity domain of the operator $\hat{\vec{\mathcal{L}}}$. That is, the operator $\hat{\vec{\mathcal{L}}}$ is hermitian as long as it acts on wave-functions which satisfy the boundary condition (5).

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3. Given an unitary operator $\hat{U}$ which squares to $\mathbb{1}$, what are the possible eigenvalues? [=20pt]

If you cannot anser in general, try (for 10pts) to determine the possible eigenvalues of the "time reversal" operator, $\hat{T} : t \to -t$. (See p. 154–155.)

(Show all work below this line; use overleaf if necessary.)

Let $\hat{U}\,|n\rangle = u_n\,|n\rangle$ be the 'eigenvalue-eigenfunction' equation for the unitary operator $\hat{U}$, where n simply counts the eigenfunctions $|n\rangle$ and the corresponding eigenvalues, u_n. While it is straightforward to ensure that all $|n\rangle$ are normalized to unity, it is important to notice that the set $\{|n\rangle\}$ is not necessarily complete. Nevertheless, we can write:

$$1 = \langle n|\,\mathbb{1}\,|n\rangle \;= \langle n|\,\hat{U}^2\,|n\rangle = \langle n|\,\hat{U}\hat{U}\,|n\rangle \;, \tag{6a}$$

$$= \langle n|\,\hat{U}\big(u_n\,|n\rangle\,\big) = u_n\,\langle n|\,\hat{U}\,|n\rangle \;, \tag{6b}$$

$$= u_n\,\langle n|\,u_n\,|n\rangle = u_n^2\,\langle n|\,|n\rangle \;, \tag{6b}$$

whence there are precisely two (not fewer, not more) eigenvalues:

$$(u_n)^2 = 1\;, \qquad \Rightarrow \qquad u_1 = +1\;, \quad u_2 = -1\;. \tag{7}$$

Clearly, we can rename them into $u_\pm = \pm 1$, and write

$$\hat{U}\,|\pm\rangle = \pm\,|\pm\rangle\;. \tag{8}$$

By the same token, for an operator $\hat{\Omega}_N$ that satisfies $(\hat{\Omega}_N)^N = \mathbb{1}$, we have that precisely the N complex number of absolute value 1

$$\omega_n = e^{2in\pi/N}\;, \qquad n = 0, 1, \ldots, (N{-}1)\;. \tag{9}$$

are the eigenvalues. Of these, only $\hat{\Omega}_2$ has real eigenvalues, and so only $\hat{\Omega}_2$ is hermitian; the other $\hat{\Omega}_N$'s are not.

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4. Using Ehrenfest's theorem, $\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{Q}\rangle = \langle\frac{i}{\hbar}[\hat{H},\hat{Q}]\rangle + \langle\frac{\partial\hat{Q}}{\partial t}\rangle$ and with the Hamiltonian $\hat{H} = \frac{1}{2m}\hat{p}^2 + V(x)$, derive that:

$$m\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle = \langle\hat{p}\rangle\ , \qquad \text{and} \qquad \frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = -\langle\frac{\mathrm{d}V}{\mathrm{d}x}\rangle\ .$$

(Show all work below this line; use overleaf if necessary.)

Start with $\hat{Q} = \hat{x}$ and work on the right-hand-side of Ehrenfest's theorem:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{x}\rangle = \langle\frac{i}{\hbar}[\hat{H},\hat{x}]\rangle + \langle\frac{\partial\hat{x}}{\partial t}\rangle = \frac{i}{\hbar}\langle[\frac{1}{2m}\hat{p}^2,x]\rangle + \frac{i}{\hbar}\langle[V(x),x]\rangle\ , \tag{10a}$$

$$= \frac{i}{2m\hbar}\Big[\langle\hat{p}[\hat{p},x]\rangle + \langle[\hat{p},x]\hat{p}\rangle\Big] = \frac{i}{2m\hbar}\langle 2(-i\hbar)\hat{p}\rangle = \frac{1}{m}\langle\hat{p}\rangle\ , \tag{10b}$$

where in the first line we used that $\hat{x}$ does not explicitly depend on time, and that any function of x only must commute with $\hat{x}$[1]. In the second statement, we used the commutator identity $[AB,C] = A[B,C] + [A,C]B$.

Now set $\hat{Q} = \hat{p}$, and use that neither does $\hat{p}$ depend explicitly on time:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{p}\rangle = \langle\frac{i}{\hbar}[\hat{H},\hat{p}]\rangle + \langle\frac{\partial\hat{p}}{\partial t}\rangle = \frac{i}{\hbar}\langle[\frac{1}{2m}\hat{p}^2,\hat{p}]\rangle + \frac{i}{\hbar}\langle[V(x),\hat{p}]\rangle\ , \tag{11a}$$

$$= \frac{i}{\hbar}\Big[\Big\langle\big[V(x),\frac{\hbar}{i}\frac{\mathrm{d}}{\mathrm{d}x}\big]\Big\rangle\Big] = -\Big\langle\frac{\mathrm{d}V}{\mathrm{d}x}\Big\rangle\ . \tag{11b}$$

The last line may be easiest to see if one applies the commutator $\big[V(x),\frac{\mathrm{d}}{\mathrm{d}x}\big]$ to an arbitrary function $f(x)$, so that $\big[V,\frac{\mathrm{d}}{\mathrm{d}x}\big]f = V\big(\frac{\mathrm{d}}{\mathrm{d}x}f\big) - \big(\frac{\mathrm{d}}{\mathrm{d}x}Vf\big) = -\big(\frac{\mathrm{d}}{\mathrm{d}x}V\big)f$. We have also used throughout the distributivity of the commutator with addition: $[A+B,C] = [A,C]+[B,C]$.

[1] Just expand the function into a power series and verify the statement term by term.

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5. a. Consider a system in a state described by the wave-function $\psi(x) = A\mathrm{e}^{-\alpha|x|}$ for $|x|<\infty$. Normalize the (constant) amplitude A. [=5pt.]

b. Calculate the expected measurement of the observable represented by $\hat{Q} = x^2$ in this system. [=5pt.]

(Show all work below this line; use overleaf if necessary.)

By definition, $\int \mathrm{d}x\ |\psi(x)|^2 = 1$, so we calculate:

$$\int \mathrm{d}x\ |\psi(x)|^2 = \int_{-\infty}^{\infty} \mathrm{d}x\ A^* \mathrm{e}^{-\alpha^*|x|} A\mathrm{e}^{-\alpha|x|} = \int_{-\infty}^{\infty} \mathrm{d}x\ |A|^2 \mathrm{e}^{-2\,\Re e(\alpha)|x|} \tag{12a}$$

$$= 2|A|^2 \int_0^{\infty} \mathrm{d}x\ \mathrm{e}^{-2\,\Re e(\alpha)|x|} = 2|A|^2 \frac{\Gamma(\frac{0+1}{1})}{1\,[2\,\Re e(\alpha)]^{0+1}} \tag{12b}$$

$$= 2|A|^2 \frac{\Gamma(1)}{2\,\Re e(\alpha)} = \frac{|A|^2}{\Re e(\alpha)} \stackrel{!}{=} 1\ , \tag{12b}$$

whereby $|A| = \sqrt{\Re e(\alpha)}$. Note that the (complex) phase of A cannot be determined.

For the expectation value,

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} \mathrm{d}x\ A^* \mathrm{e}^{-\alpha^*|x|}\, x^2\, A\mathrm{e}^{-\alpha|x|} = \Re e(\alpha) \int_{-\infty}^{\infty} \mathrm{d}x\ x^2 \mathrm{e}^{-2\,\Re e(\alpha)|x|} \tag{13a}$$

$$= 2\,\Re e(\alpha) \int_0^{\infty} \mathrm{d}x\ x^2 \mathrm{e}^{-2\,\Re e(\alpha)|x|} = 2\,\Re e(\alpha) \frac{\Gamma(\frac{2+1}{1})}{1\,[2\,\Re e(\alpha)]^{2+1}} \tag{13b}$$

$$= 2\,\Re e(\alpha) \frac{\Gamma(3)}{8[\Re e(\alpha)]^3} = \frac{2!}{4[\Re e(\alpha)]^2} = \frac{1}{2[\Re e(\alpha)]^2}\ . \tag{13b}$$

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6. Let ψ satisfy the Schrödinger equation, $i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + (V + i\hat{\Sigma})\psi$, where V and $\hat{\Sigma}$ are real. Defining as usual $\rho \stackrel{\text{def}}{=} |\psi|^2$ and $\vec{\jmath} \stackrel{\text{def}}{=} \frac{\hbar}{2im}[\psi^*\vec{\nabla}\psi - (\vec{\nabla}\psi^*)\psi]$, derive the modified 'continuity equation' and interpret $\hat{\Sigma}$. [=10pt]

(Show all work below this line; use overleaf if necessary.)

The continuity equation involves the time derivative of ρ, so that's what we start with:

$$\begin{aligned}
\frac{\partial\rho}{\partial t} &= \frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t}\ , \\
&= -\frac{1}{i\hbar}\Big[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi^* + (V - i\hat{\Sigma})\psi^*\Big]\psi + \psi^*\frac{1}{i\hbar}\Big[-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi + (V + i\hat{\Sigma})\psi\Big]\ , \\
&= \frac{\hbar}{2im}\Big[(\vec{\nabla}^2\psi^*)\psi - \psi^*(\vec{\nabla}^2\psi)\Big] + \frac{2}{\hbar}\psi^*\hat{\Sigma}\psi; \\
&= \frac{\hbar}{2im}\vec{\nabla}\cdot\Big[(\vec{\nabla}\psi^*)\psi - \psi^*(\vec{\nabla}\psi)\Big] + \frac{2}{\hbar}\psi^*\hat{\Sigma}\psi;
\end{aligned} \tag{14}$$

so that

$$\frac{\partial\rho}{\partial t} = \vec{\nabla}\cdot\vec{\jmath} + \frac{2}{\hbar}\psi^*\hat{\Sigma}\psi \tag{15}$$

is the modified continuity equation. Integrated over a volume V, this becomes:

$$\frac{\mathrm{d}}{\mathrm{d}t}P_V = \oint_{S=\partial V}\mathrm{d}\vec{\sigma}\cdot\vec{\jmath} + \frac{2}{\hbar}\langle\psi|\hat{\Sigma}|\psi\rangle_V\ , \tag{16}$$

where $\langle\psi|\Sigma|\psi\rangle_V \stackrel{\text{def}}{=} \int_V \mathrm{d}^3\vec{r}\,\psi^*\hat{\Sigma}\psi$ is the expectation value of $\hat{\Sigma}$, restricted however to the volume V and $P_V \stackrel{\text{def}}{=} \langle\psi|\mathbf{1}|\psi\rangle$ is the probability of finding the particle inside volume V; S is the surface bounding the volume V.

Thus, the rate of change of the probability of finding the particle inside the volume V equals the flux of the probability current through the bounding surface S, plus the restricted expectation value of the operator $\hat{\Sigma}$. If positive; $\langle\psi|\hat{\Sigma}|\psi\rangle_V$ would be deemed a source of such particles; if negative, $\langle\psi|\hat{\Sigma}|\psi\rangle_V$ would act as a sink (absorber).

7. For the wave-function $\psi = C\,z\,e^{-\beta r}$, with $z = r\cos\theta$, (**a**) find the eigenvalues of $\hat{L}_z$ and $\hat{L}^2$, and (**b**) determine the normalization constant.

a. As given in class, and also found in the appendix 3 on p.569, $\hat{L}_z = -i\frac{\partial}{\partial\varphi}$. Since ψ is independent of φ, the $\hat{L}_z$-eigenvalue must vanish; $m = 0$. Another way to see this is to use Cartesian variables where $\hat{L} = -i(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x})$. Now, z is manifestly a constant with respect to this first order derivative operator. That $e^{-\beta r}$ is also a constant follows from the fact that $\hat{L}_z$ generates rotations about the z-axis, while r and so $e^{-\beta r}$ is a scalar and so does not transform under rotations.

Now, as for $\hat{L}^2$, we can again use the expression on spherical coordinates (p.569):

$$\hat{L}^2 = -\Big[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}\Big] \;,$$

where again the $\frac{\partial^2}{\partial\varphi^2}$-term contributes nothing as ψ is independent of φ. The first term produces

$$\begin{aligned}
\hat{L}^2\;C\,z\,e^{-\beta r} &= -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}C\,z\,e^{-\beta r} \;= -C\,e^{-\beta r}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta}r\cos\theta \;,\\
&= -C\,r\,e^{-\beta r}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta(-\sin\theta) \;= C\,r\,e^{-\beta r}\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin^2\theta) \;,\\
&= 2C\,r\,e^{-\beta r}\frac{1}{\sin\theta}\sin\theta\cos\theta \;= 2C\,r\cos\theta\,e^{-\beta r} \;=\; 2\psi
\end{aligned}$$

so that the $\hat{L}^2$-eigenvalue is 2, and $\ell = 1$. Another way is to use that $\hat{L}^2 = \sum_i \hat{L}_i{}^2$ in Cartesian coordinates. Again, on the scalar $e^{-\beta r}$, $\hat{L}^2$ gives zero. As discussed and derived in class $[\hat{L}_j, x^k] = (\hat{L}_j\,x^k) = i\epsilon_{jkl}x^l$, so that[2]

$$\begin{aligned}
\sum_{j=1}^{3}\hat{L}_j{}^2 x^k &= \sum_{j=1}^{3}\big(\hat{L}_j(\hat{L}_j\,x^k)\big) \;=\; \sum_{j=1}^{3}\Big[\hat{L}_j\,,\,\big[\,\hat{L}_j\,,\,x^k\big]\Big] \;=\; \sum_{j=1}^{3}\big[\hat{L}_j\,,\,(i\epsilon_{jkl}x^l)\big] \;,\\
&= \sum_{j=1}^{3} i\epsilon_{jkl}\big[\hat{L}_j\,,\,x^l\big] \;=\; \sum_{j,l=1}^{3} i\epsilon_{jkl}(i\epsilon_{jlm}x^m) \;=\; -\sum_{j,l=1}^{3}\epsilon_{jkl}\epsilon_{jlm}\,x^m \;,\\
&= -\Big(\sum_{j,l=1}^{3}(-\epsilon_{jlk})\epsilon_{jlm}\Big)\,x^m \;=\; (2\delta^k_m)\,x^m \;=\; 2x^k.
\end{aligned}$$

Therefore, $\hat{L}^2\psi = Ce^{-\beta r}\hat{L}^2 z = Ce^{-\beta r}(2z) = 2\psi$, so $\ell = 1$.

Note in particular, that (with $\hat{D}$ *any* linear and first order differential operator):

$$\begin{aligned}
\hat{D}^2 f(x) = \Big(\hat{D}\big(\hat{D}\,f(x)\big)\Big) &= \;\Big[\,\hat{D}\,,\,\big[\,\hat{D}\,,\,f(x)\,\big]\,\Big] \;,\\
&\neq\; \big[\,\hat{D}^2\,,\,f(x)\,\big] = \;\Big(\hat{D}\big(\hat{D}\,f(x)\big)\Big) + 2\big(\hat{D}\,f(x)\big)\hat{D} \;,
\end{aligned}$$

b. Normalization is straightforward:

$$\begin{aligned}
1 \stackrel{!}{=} \int \mathrm{d}^3\vec{r}\;|\psi|^2 = |C|^2\int_0^\infty r^2\mathrm{d}r\int_0^\pi \sin\theta\mathrm{d}\theta\int_0^{2\pi}\mathrm{d}\varphi\;r^2\cos^2\theta e^{-2\beta r} \;,\\
= |C|^2\int_0^\infty \mathrm{d}r\;r^4 e^{-2\beta r}\int_{-1}^{1}\mathrm{d}(\cos\theta)\cos^2\theta\int_0^{2\pi}\mathrm{d}\varphi \;,\\
= |C|^2\Big[\frac{\Gamma(5)}{(2\beta)^5}\Big]\Big[\frac{u^3}{3}\Big]_{-1}^{1}\Big[2\pi\Big] \;= |C|^2\Big[\frac{4!}{32\beta^5}\Big]\Big[\frac{2}{3}\Big]\Big[2\pi\Big] \;= |C|^2\Big[\frac{\pi}{\beta^5}\Big] \;,
\end{aligned}$$

[2] Summation is implied over subscript–superscript index pairs.

whence $C = \sqrt{\beta^5/\pi}$. Here, we used the standard trick in evaluating the θ-integrals: the volume integral measure contains $\sin\theta \mathrm{d}\theta = -\mathrm{d}(\cos\theta)$, which suggests the change of variables $u = \cos\theta$, whereupon the integral is a table one[3]. The radial integral is a special case of the frequently used Γ-function integral found on p.558 of the text, under "Some Useful Integrals". Note that

$$\int_0^\infty \mathrm{d}x\; x^n e^{-(ax)^m} \;=\; \frac{\Gamma(\frac{n+1}{m})}{m\, a^{\frac{n+!}{m}}}$$

is in fact an analytic function of a, m, n except: (**1**) when $m = 0$, (**2**) when $a^{\frac{n+1}{m}} = 0$, and (**3**) when $\frac{n+1}{m}$ is a negative integer. Many of the "radial" integrals are of this type, or can be reduced to this.

[3] Be careful with the limits of integration; $u(\theta{=}0) = 1$ and $u(\theta{=}\pi) = -1$.