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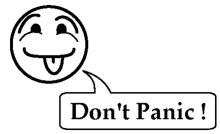

Quantum Mechanics II April '98.

2nd Midterm Exam Solutions (T. Hübsch)

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The completeness and detail presented herein were by no means expected in the Student's solutions for full credit. The additional information given here is solely for the Student's convenience and education.

1.a. The only information we have in this case is the Schrödinger equation

$$-\frac{\hbar^2}{2m}\psi''(x) + \Delta\delta(x)\psi(x) \ = \ E\psi \tag{1}$$

So, we integrate this from $-\epsilon$ to $+\epsilon$:

$$-\frac{\hbar^2}{2m}\big[\psi'(x)\big]_{-\epsilon}^{\epsilon} + \Delta\psi(0) \ = \ E\int_{-\epsilon}^{\epsilon} \mathrm{d}x \ \psi(x) \ , \tag{2}$$

where the integral cancels against one of the derivatives in the first term, and is quenched to evaluation at $x{=}0$ in the second owing to the Dirac δ-function. Thus far, we have assumed nothing about the wave-function $\psi(x)$, except that it has a single value at $x{=}0$. As the potential vanishes everywhere except at $x{=}0$, then $\psi(x)$ may be discontinuous at most at $x{=}0$—but there we already assumed it to have a single value. Hence, in fact, we have assumed that $\psi(x)$ is continuous accross $x{=}0$. Then, so must the its integral be, and taking the limit $\epsilon \to 0$, we obtain:

$$-\frac{\hbar^2}{2m}\big[\psi'(0^+) - \psi'(0^-)\big] + \Delta\psi(0) = E\lim_{\epsilon\to 0}\int_{-\epsilon}^{\epsilon} \mathrm{d}x \ \psi(x) = 0 \ . \tag{3}$$

Thus, the matching conditions are:

$$\psi(0^+) - \psi(0^-) \ = \ 0 \ , \qquad \psi'(0^+) - \psi'(0^-) \ = \ \frac{2m\Delta}{\hbar^2}\psi(0) \ . \tag{4}$$

In words, the wave-function is continuous, but not necessarily smooth: the discontinuity at $x{=}0$ in its slope is proportional to the value of the wave-function at $x{=}0$.

Note that the Schrödinger equation is symmetric with respect to $x \to -x$; the Hamiltonian commutes with the reflection operator. Then, there is a complete set of eigenfunctions of the Hamiltonian which are also eigenvalues of the reflection operator: symmetric or antisummetric. Finally, it should then be clear that the antisymmetric wave-functions are necessarily smooth.

b. Start from Park's Eq. (15.11), substitute expressions for κ_2, expand to lowest order in c and highest order in V_0:

$$\cos(2\pi n/N) \ = \cos\big(k_1 b\big)\cosh\Big(\frac{\sqrt{2m(V_0{-}E)}}{\hbar}c\Big)$$

$$
- \frac{2mE - 2m(V_0 - E)}{2\,2m\sqrt{E(V_0-E)}} \sin\big(k_1 b\big) \sinh\Big(\frac{\sqrt{2m(V_0-E)}}{\hbar} c\Big) \;, \tag{5a}
$$

$$
= \cos\big(k_1 b\big)\Big(1 + \tfrac{1}{2}\frac{\sqrt{2mV_0 c^2}}{\hbar} + \dots\Big)
$$

$$
+ \frac{V_0}{2\sqrt{EV_0}} \sin\big(k_1 b\big)\Big(\frac{\sqrt{2mV_0 c^2}}{\hbar} + \dots\Big) \;, \tag{5b}
$$

$$
= \cos\big(k_1 b\big)\Big(1 + \tfrac{1}{2}\frac{\sqrt{2m\Delta c}}{\hbar} + \dots\Big)
$$

$$
+ \frac{1}{2\sqrt{E}} \sin\big(k_1 b\big)\Big(\frac{\sqrt{2m\Delta^2}}{\hbar} + \dots\Big) \;. \tag{5c}
$$

Taking the limit $c \to 0$:

$$
\cos(2\pi n/N) = \cos\Big(\frac{\sqrt{2mE_n}}{\hbar} b\Big) + \frac{\Delta}{\hbar}\sqrt{\frac{m}{2E_n}} \sin\Big(\frac{\sqrt{2mE_n}}{\hbar} b\Big) \;, \tag{6}
$$

produces the transcendental equation which determines the (quantized) allowed values of energy E_n. This is incomparably simpler than using the matching conditions from part **a** to produce a wave-function and then sort out the energy-quantization equation above.

b. The case $E > V_0$ is almost identical, since both ${\kappa_2}^2$ and ${k_2}^2$ limit to $2mV_0/\hbar^2$ when $V_0 \to \infty$, and to lowest nonzero order, $\sinh(x) \approx \sin(x)$ and $\cosh(x) \approx \cos(x)$. The condition would therefore be the same as (6). However, if $V_0 \to \infty$ ultimately, than it makes no sense considering $E > V_0$.

c. In the limit $\Delta \to 0$, we obtain (with $b \to L$ since $c \to 0$)

$$
\cos(2\pi n/N) = \cos\Big(\frac{\sqrt{2mE_n}}{\hbar} L\Big) \;, \tag{7}
$$

which is solved by

$$
E_n \;=\; \frac{4\pi^2\hbar^2}{2mN^2L^2}\, n^2 \;. \tag{8}
$$

This coincides with the energy spectrum of a particle in a box of size NL with periodic boundary conditions [1]: Since the opacity of the potential barriers vanishes, the particle is limited only by the periodic boundary conditions on the whole crystal.

d. In the limit $\Delta \to \infty$, (after first dividing Eq. (6) by Δ), we obtain $\sin\big(\frac{\sqrt{2mE_n}}{\hbar} L\big) = 0$, *i.e.*,

$$
E_n \;=\; \frac{\pi^2\hbar^2}{2mL^2}\, n^2 \;. \tag{9}
$$

This coincides with the energy spectrum of a particle in a box of size L, since the opacity of the potential barriers, Δ, is infinitely big, and each cell acts as a separate box.

[1] A particle in an infinite potential well has no boundary conditions on the derivative at the walls, so $kL = n\pi$ determins the enetgy levels. In contrast, with periodic boundary conditions, the derivative is also constrained, which rules out the odd-numbered wave-functions. Hence $kL = 2n\pi$ and the factor 4 in the numerator of Eq. (8).

2.a. The $\vec{B}$-field is invariant only under (real space) rotations about the z-axis. Indeed: $\big[\hat{L}_z\,,\,\vec{B}\big] = 0$. Of course, $\vec{B}$ is also invariant under spin-rotations: $\big[\hat{S}_i\,,\,\vec{B}\big] = 0$ for $i = x, y, z$, also. However, $\big[\hat{\vec{L}}^2\,,\,\vec{B}\big] \neq 0$, as can be seen by noting that $z^2 = r^2\cos^2\theta = r^2\big[\sqrt{\tfrac{16\pi}{45}}\,Y_2^0(\theta,\phi) + \sqrt{\tfrac{4\pi}{9}}Y_0^0\big]$, and the first spherical harmonic has angular momentum of $\ell = 2$ and $m = 0$. Similarly, $\big[\hat{\vec{J}}^2\,,\,\vec{B}\big] \neq 0$. So, $\vec{B}$ commutes with $\hat{L}_z, \hat{S}_i$, for $i = x, y, z$ and $\hat{\vec{S}}^2$.

Now, $\hat{H}_B = \frac{e\hbar}{2\mu}\vec{B}\cdot(\hat{\vec{L}} + 2\hat{\vec{S}}) = \frac{e\hbar B_0}{2\mu}\,z^2\,(\hat{L}_z + 2\hat{S}_z)$ is the external $\vec{B}$-field perturbation [2], and it also commutes with $\hat{S}_z$, $\hat{\vec{S}}^2$ and $\hat{L}_z$—and so also with $\hat{J}_z$, but neither with $\hat{\vec{L}}^2$ nor with $\hat{\vec{J}}^2$.

b. Since the external magnetic field is strong (spin-orbit and relativistic corrections to the energy are negligible as in the Pashen-Back effect), and we rely on the non-relativistic description of the Hydrogen atom, as in section 6.4, and in particular we'll use the states given in Table 6.1 (p.190). Recall that

$$|n,\ell,m,m_s\rangle^{(1)} = -\sum_{n',\ldots\neq n,\ldots} \frac{{}^{(0)}\langle n',\ell',m',m_s'|\hat{H}_B|n,\ell,m,m_s\rangle^{(0)}}{E_{n'}^{(0)} - E_n^{(0)}}\,|n',\ell',m,m_s\rangle^{(0)} \ .$$

Results in part **a** imply that $m_s{=}m_s'$ and $m{=}m'$, but that $|\ell{-}\ell'|{=}0,2$. However, if restricting to $n{=}n'{=}2$, the diagonal matrix elements $\langle 2,\ell,m,m_s|\hat{H}_B|2,\ell,m,m_s\rangle$ need not be considered because of the restriction in the summation!

The states which differ at most in ℓ are then degenerate and we ought to use degenerate perturbation theory—in principle. However, having restricted to $n{=}n'{=}2$, $\ell < 2$, and so $|\ell{-}\ell'|{=}2$ is impossible. Therefore, the summation

$$|2,\ell,m,m_s\rangle^{(1)} = -\sum_{\ell'\neq\ell} \frac{{}^{(0)}\langle 2,\ell',m,m_s|\hat{H}_B|2,\ell,m,m_s\rangle^{(0)}}{E_2^{(0)} - E_2^{(0)}}\,|2,\ell',m,m_s\rangle^{(0)} \ .$$

is void, and the vanishing would-be denominator never occurs in our calculation: The states $|2,\ell,m,m_s\rangle$ remain unmixed (pure) to first order in perturbation theory.

c. As noted, $\hat{H}_B$ does commute with $\hat{L}_z, \hat{S}_z$, whence matrix elements will be non-zero among states of same m, m_s. Among the eight states

$$\big|2,0,0,\pm\tfrac{1}{2}\big\rangle\ ,\quad \big|2,1,0,\pm\tfrac{1}{2}\big\rangle\ ,\quad\text{and}\quad \big|2,1,\pm1,\pm\tfrac{1}{2}\big\rangle\ , \tag{10}$$

$\ell'{-}\ell| < 2$, so in fact, only diagonal matrix elements are non-zero!

The first order shift in the energy is calculated from the matrix

$$E^{(1)}_{2,\ell,m,m_s} \stackrel{\text{def}}{=} \langle 2,\ell,m,m_s|\hat{H}_B|2,\ell,m,m_s\rangle\ , \tag{11a}$$

$$= \frac{e\hbar B_0}{2\mu}\langle 2,\ell',m',m_s'|r^2\cos^2\theta(\hat{L}_z + 2\hat{S}_z)|2,\ell,m,m_s\rangle\ , \tag{11b}$$

[2] Here μ stands for the reduced mass of the electron in the Hydrogen atom; avoid using m, not to confuse with m, the eigenvalue of $\hat{L}_z$.

$$= \frac{e\hbar B_0}{2\mu}(m+2m_s)\langle 2,\ell,m|r^2\cos^2\theta|2,\ell,m\rangle \ . \tag{11c}$$

$$= \frac{e\hbar B_0}{2\mu}(m+2m_s)\int_0^\infty r^2\mathrm{d}r\ \left|R_2^\ell\right|^2 r^2 \int \mathrm{d}\Omega\ \left|Y_\ell^m\right|^2\ \cos\theta\ , \tag{11b}$$

For various ℓ, m, these matrix elements involve different integrals. For example,

$$\langle 2,0,0|r^2\ \cos^2\theta|2,0,0\rangle$$

$$= \frac{1}{8\pi a_0^3}\int_0^\infty r^4\mathrm{d}r\ (1-\frac{r}{2a_0})^2 e^{-r/a_0}\int_0^\pi \mathrm{d}\theta\sin\theta\ \cos^2\theta\int_0^{2\pi}\mathrm{d}\phi\ , \tag{12a}$$

$$= \frac{1}{6a_0^3}\int_0^\infty \mathrm{d}r\ \Big(r^4-\frac{r^5}{a_0}+\frac{r^6}{4a_0^2}\Big)e^{-r/a_0} = \frac{1}{6a_0^3}a_0^5\big[4!-5!+\tfrac{1}{4}6!\big]\ , \tag{12a}$$

So

$$E^{(1)}_{2,0,0,\pm} = \pm 7\frac{e\hbar a_0^2}{\mu}B_0\ . \tag{13}$$

Upon similar calculations,

$$E^{(1)}_{2,1,0,\pm} = \pm 7\frac{e\hbar a_0^2}{\mu}B_0\ , \qquad E^{(1)}_{2,1,m,\pm} = \frac{9}{2}\frac{e\hbar a_0^2}{\mu}B_0(m\pm 1)\ , \quad m=\pm 1\ . \tag{14}$$

3.a. Easily, $V_0 = (\hbar c - 2Ze'^2)/R$ ensures continuity of

$$V(r) = \begin{cases} \frac{\hbar c}{R^2}r - V_0 & r<R, \\ 2Ze'^2/r & r>R. \end{cases} \tag{15}$$

For a state of energy $E>0$, the classical turning points are:

$$r_1 = \frac{R^2(E+V_0)}{\hbar c}\ , \qquad r_2 = \frac{2Ze'^2}{E}\ . \tag{16}$$

b. Since ψ is independent of angles, the Laplacian reduces to $\frac{1}{r^2}\frac{\mathrm{d}}{\mathrm{d}r}r^2\frac{\mathrm{d}}{\mathrm{d}r} = \frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}r$, and the Schrödinger equation becomes

$$\frac{1}{r}\frac{\mathrm{d}^2}{\mathrm{d}r^2}\big(r\psi\big) + \frac{2m}{\hbar^2}\Big(E - V(r)\Big)\psi = 0\ , \tag{17}$$

and on writing $\psi(r) = \frac{u(r)}{r}$, we have

$$u''(r) + \tfrac{2m}{\hbar^2}\big(E - V(r)\big)u(r) = 0\ . \tag{18}$$

c. Clearly, we need to deal with the two regions

$$u''(r) + \tfrac{2m}{\hbar^2}\Big[E + V_0 - \frac{\hbar c}{R^2}r\Big]u(r) = 0\ , \qquad \text{for } 0\le r\le R\ , \tag{19a}$$

$$u''(r) + \tfrac{2m}{\hbar^2}\Big[E - \frac{2Ze'^2}{r}\Big]u(r) = 0\ , \qquad \text{for } R\le r\le \infty\ , \tag{19b}$$

separately. For the first case, we simplify $\frac{2m}{\hbar^2}\big[\frac{\hbar c}{R^2}r - E + V_0\big] = \sqrt[3]{\frac{4m^2c^2}{\hbar^2R^4}}\rho$:

$$u''(\rho) - \rho \;=\; 0\;. \tag{20}$$

This is the Airy differential equation, encountered in the first semester when dealing with a vertically bouncing quantum ping-pong ball. The solution then quoted refers to $J_{1/3}(x^{\frac{3}{2}})$, so a transformation of both the independent variable, ρ, and also the function, u, should lead to the Bessel equation. Indeed, substituting $\rho = z^{\alpha}$ yields

$$z^2u''(z) + (1-\alpha)zu'(z) - \alpha^2z^{\alpha}u(z) \;=\; 0\;. \tag{21}$$

Letting now $u(z) = z^{\beta}f(z)$, we obtain

$$z^2f''(z) + (1{+}2\beta{-}\alpha)zf'(z) + \big[\beta(\beta-\alpha) - \alpha^2z^{3\alpha}\big]f(z) \;=\; 0\;. \tag{22}$$

For this to become the Bessel equation, we require $3\alpha{=}2$ and $1{+}2\beta{-}\alpha{=}1$, *i.e.*, $\alpha{=}\frac{2}{3}$ and $\beta{=}\frac{1}{3}$. The differential equation (19a) thus becomes

$$z^2f''(z) + zf'(z) - \Big[\big(\tfrac{3z}{2}\big)^2 + \big(\tfrac{1}{3}\big)^2\Big]f(z) \;=\; 0\;. \tag{23}$$

This is the modified Bessel equation, solved by a linear combination of $K_{\frac{1}{3}}(\frac{3z}{2})$ and $I_{\frac{1}{3}}(\frac{3z}{2})$. Recall now that $z = \rho^{\frac{3}{2}}$, so that

$$u(r) = A\sqrt{\rho}I_{\frac{1}{3}}\big(\rho^{\frac{3}{2}}\big) + B\sqrt{\rho}K_{\frac{1}{3}}\big(\rho^{\frac{3}{2}}\big)\;, \tag{24}$$

or

$$\psi(r) = \tfrac{A}{\sqrt{\rho}}I_{\frac{1}{3}}\big(\rho^{\frac{3}{2}}\big) + \tfrac{B}{\sqrt{\rho}}K_{\frac{1}{3}}\big(\rho^{\frac{3}{2}}\big)\;, \tag{25}$$

Now, note that $\rho = 0$ occurs at $r_1 = \frac{(E+V_0)R^2}{\hbar c}$ — the first turning point. For negative ρ, imaginary z, *i.e.*, $0 \le r \le r_1$ (in the classically allowed region within the linear well), the modified Bessel Equation reverts to the usual Bessel equation, solved by a linear combination of $J_{\frac{1}{3}}(\frac{3z}{2})$ and $N_{\frac{1}{3}}(\frac{3z}{2})$. However, $N_{\frac{1}{3}}(\frac{3z}{2})$ and $K_{\frac{1}{3}}(\frac{3z}{2})$ blow up at $z = 0$, *i.e.*, at $r{=}r_1$ and should not be used. Furthermore, $I_{\nu}(x) = e^{-\nu\pi i/2}J_{\nu}(xe^{i\pi/2})$.

So, for $0{\le}r{\le}R$ (in the classically allowed inside region), the solution may be written entirely in terms of $I_{\frac{1}{3}}(\rho^{\frac{3}{2}})$, understanding that in the classically allowed region, for $0{\le}r{\le}r_1$, it in face becomes the oscillatory $J_{\frac{1}{3}}(\rho^{\frac{3}{2}})$:

$$\psi(\rho) \;=\; \frac{A}{\sqrt{\rho}}I_{\frac{1}{3}}\big(\rho^{\frac{3}{2}}\big)\;, \qquad 0 \le r \le R\;. \tag{26}$$

No such transformation to the Bessel equation can be found for the second part, in Eq. (19b), but we can solve it in analogy with the H-atom.

Consider first the $E < 0$ case. For $r \to \infty$, the $1/r$ term in (19b) may be neglected, and we see that $u(r) \sim e^{-kr}$ where $k^2 = 2m|E|/\hbar^2$ as usual, discarding the e^{+kr} solutions as unnormalizable. The full solution is then sought in the form $u(r) = e^{-kr}f(r)$, which we insert into (19b) and obtain the differential equation for $f(r)$:

$$rf''(r) - 2krf'(r) - af(r) \;=\; 0\;, \qquad a = \tfrac{4mZe'^2}{\hbar^2}\;. \tag{27}$$

After rescaling $\xi = 2kr$, this yields

$$\xi f''(\xi) - \xi f'(\xi) - \tfrac{a}{2k} f(\xi) \;=\; 0 \;, \tag{28}$$

a special case of the confluent hypergeometric equation [Arfken, § 13.6], with $c = 0$. For this case, the 'second' solution is given as $f = \xi \; {}_1F_1\big(\genfrac{}{}{0pt}{}{1+a/2k}{2}; \xi\big)$, so

$$\psi_2(\xi) = Be^{-kr} {}_1F_1\big(\genfrac{}{}{0pt}{}{1+a/2k}{2}; 2kr\big) \;. \tag{29}$$

Owing to the relationship between the confluent hypergeometric functions and the Laguerre polynomials,

$${}_1F_1\big(\genfrac{}{}{0pt}{}{1+a/2k}{2}; \xi\big) \;=\; -\tfrac{1}{a} L^1_{-(1+a/2k)}(\xi) \;. \tag{30}$$

Thus, the wave-function $\psi_2(\rho) = Be^{ikr} {}_1F_1\big(\genfrac{}{}{0pt}{}{1+a/2k}{2}; 2kr\big)$ is simply the repulsive potential analytic continuation of the usual Hydrogen-like wave-function. Furthermore, using the relationship between Bessel and confluent hypergeometric functions, we can write

$$\psi_1(\rho) = A' e^{-\rho^{3/2}} {}_1F_1\big(\genfrac{}{}{0pt}{}{5/6}{5/3}; \rho^{\frac{3}{2}}\big) \;. \tag{31}$$

For $E > 0$, the above analysis holds with only minor changes. The asymptotic solution, for $\rho \to \infty$, is now a linear combination of e^{ikr} (the outgoing wave, for α-decay) and e^{-ikr} (the incomng wave, for α-capture). Now we write $u(r) = e^{\pm ikr} F_\pm(r)$. Upon the rescaling $r \to \eta = \mp 2ikr$, we find that $F(\eta)$ must satisfy

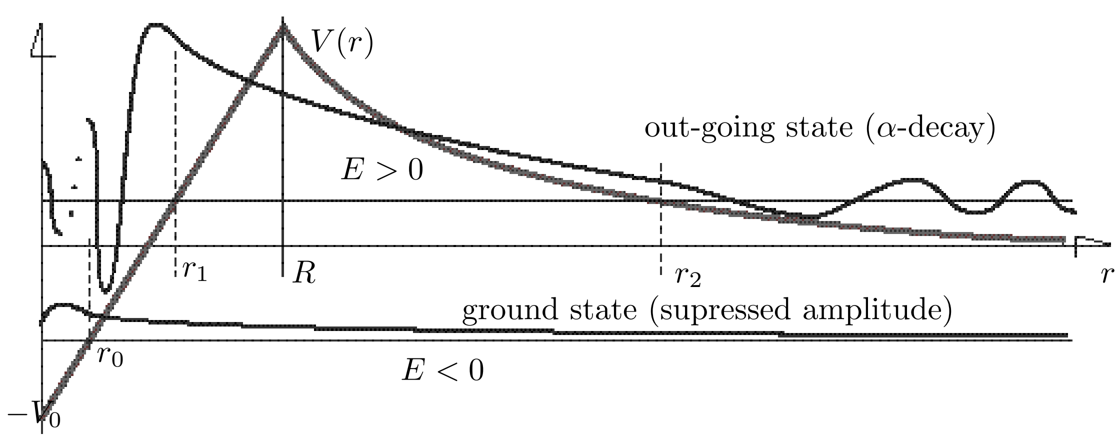
$$\eta F''_\pm(\eta) - \eta F'_\pm(\eta) \mp \tfrac{ai}{2k} F_\pm(\eta) \;=\; 0 \;, \tag{32}$$

This again is solved by $F_\pm(\eta) = {}_1F_1\big(\genfrac{}{}{0pt}{}{1\pm ai/2k}{2}; \eta\big)$

d. We now have to equate $\psi_1(\rho)$ and $\psi_2(\rho)$ and their derivatives at $r = R$. These two conditions determine the energy level and the relative ratio A/B, leaving one overall constant to be determined from normalization. This task is somewhat simplified owing to the conveinent property

$$\frac{\mathrm{d}}{\mathrm{d}x} {}_1F_1\big(\genfrac{}{}{0pt}{}{a}{c}; x\big) = \frac{a}{c} {}_1F_1\big(\genfrac{}{}{0pt}{}{a+1}{c+1}; x\big) \;. \tag{33}$$

Still the calculations are messy and do not provide any additional insight and we content ourselves with the sketch below.



e. The equation of continuity states that the rate of change of the probability of finding the particle within the radius r_2 equals the probability current flowing through the spherical surface of radius r_2. Now, if the potential well is sufficiently deep (V_0 sufficiently big) so that $E_0 < 0$, the ground state cannot decay. However, if this is not true, and $E_0 > 0$, the ground state indeed can decay. Nevertheless, for any particular state, $\frac{\mathrm{d}}{\mathrm{d}t}\int_{r<r_2} \left|\psi_n(r)\right|^2 = 0$, if $\psi_n(r)$ is the stationary state. To obtain a nonzero probability current flux through the 'Gaussian' surface of radius r_1, we should calculate not with the whole wave function, but with its 'in-coming' or 'out-going' traveling wave. The former would correspond to α-decay, and the latter to α-capture.

f. The integral $\sigma \stackrel{\text{def}}{=} \frac{1}{\hbar}\int_{r_1}^{r_2} \mathrm{d}r \sqrt{2m(E-V(r))}$ is straightforward. The two parts of

$$\sigma = \frac{\sqrt{2E}}{\hbar}\int_{r_1}^{R} \mathrm{d}r\, \sqrt{E - \tfrac{\hbar c}{R^2}r + V_0} + \frac{\sqrt{2E}}{\hbar}\int_{R}^{r_2} \mathrm{d}r\, \sqrt{E - 2Z\frac{e'^2}{r}} \tag{34}$$

are evaluated using the general formulae

$$\int \mathrm{d}x\sqrt{a-bx} = -\tfrac{2}{3b}\sqrt{(a-bx)^3}\ ,$$

$$\int \mathrm{d}x\sqrt{a-\tfrac{b}{x}} = x\sqrt{a-\tfrac{b}{x}} - \tfrac{b}{2\sqrt{a}}\ln\left(2ax - b + 2\sqrt{a}x\sqrt{a-\tfrac{b}{x}}\right)\ .$$

The limits r_1, r_2 and V_0 have been determined above and the substitutions are left to the student. Although no particular simplification ensues, the point was to show that the result is calculable exactly.