UNIVERSIDAD COMPLUTENSE DE MADRID
DEPARTAMENTO DE FISICA TEORICA I

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Estructura de la Materia

Página web de la asignatura: http://teorica/ft8/problemas.html

Los libros de donde se toman los ejercicios están indicados entre corchetes, así [Li] es Liboff, [Gri] Griffiths, [Ga] Gasiorowicz, [LLaEs] son los ejercicios que Felipe LLanes-Estrada usaba para impartir este curso, etc. Los problemas en **rojo** se proponen como ejercicios al alumno para hacerlos en casa. No hay que entregarlos. Los problemas en negro los hago yo en clase. La solución de estos problemas, si no está escrita en estas páginas, que es lo usual, me la piden y se la llevo a clase.

$$\alpha \equiv e^2/4\pi\varepsilon_0\,\hbar c = 1/137.035\,999\,11 = 7.297\,352\,568 \times 10^{-3}$$
$$a_0 = 4\pi\varepsilon_0\hbar^2/m_e e^2 = 0.529\,177\,211 \times 10^{-10}\ \text{ m}$$
$$E_1 = -m_e c^2\alpha^2/2 = 13.605\,692\,\text{eV}$$
$$E_h = e^2/4\pi\varepsilon_0 a_0 = -2E_1 = 27.211\,385,\ \text{ eV}$$
$$m_e = 0.510\,999\,9\ \text{ MeV}/c^2$$
$$N_A = L = 6.022 \times 10^{23}\,\text{mol}^{-1}, \qquad 1\ \text{Å} = 10^{-10}\ \text{ m},$$

THE ATOM OF HELIUM

1. Del átomo de Helio hemos visto en clase: 1) Primer intento de justificar la energía del estado fundamental cuyo valor experimental (o sea, el bueno) es $-79.0051\,\text{eV}$. En este primer intento se suprime la repulsión electrón-electrón (ee, de ahora en adelante) y sale una aproximación muy mala. 2) Paridad del estado fundamental del átomo de Helio. Comentario sobre los estados excitados: sólo uno de los electrones puede estar excitado, el otro no; así es el helio. 3) Segundo intento: usar teoría de perturbaciones a primer orden incluyendo la repulsión ee. El resultado se aproxima más al valor experimental, ha mejorado. 4) Tercer intento: lo mismo pero con el principio variacional de Ritz. Ya va mucho mejor. Sacamos tb Z^* efectiva igual a 1.6875. Indica que un electrón apantalla al otro no llegando a ver ninguno de los dos la carga nuclear enterita $Z = 2$ como debía ser. 4) Aunque el hamiltoniano no considera spin, el principio de exclusion de Pauli tiene mucho que decir: energías J y K, de Coulomb y de intercambio. Ambas son positivas.

THE REAL HYDROGEN ATOM. FINE STRUCTURE

2.
3. 1) Introducción: la velocidad con la que se mueve el electrón en el átomo de hidrogeno es del orden de un uno por ciento de la velocidad de la luz; es no-relativista, pequeña, sí, pero no *tan pequeña*. Vamos, que va a toda leche comparado con lo que conocemos nosotros. Orden de magnitud de la estructura fina. 2) Sumario de relaciones físicas que serán probadas después: teorema del virial para potenciales centrales, valor medio de $1/r$ en los estados estacionarios del hidrógeno, Hellmann-Feynman theorem, valor medio de $1/r^2$, etc. 3) Energy corrections due to the relativistic speed of the electron in its orbit (makes use of perturbation theory). 4) Darwin term. 5) Spin-orbit coupling; first time along the course where the hamiltonian includes spin. Uses perturbation theory too. 6) The three terms together are called the *fine structure* of the hydrogen atom. 7) Elementary theory of radiation: selection rules. Parity of a atomic

state. 8) It all applicable to hydrogen-like atoms as well (átomos hidrogenoideos). 9) Exercises.

4. [LLaEs] [Spin-orbit coupling] ¿Cuántos estados del nivel 4F del átomo de hidrógeno tienen la misma energía de Bohr E_4? Sol: 14. Evaluar el desdoblamiento spin-órbita entre los dos valores de j en el nivel 4F. ¿Qué degeneración persiste tras considerar esta interacción? Sol: 8 y 6.

5. By the name *fine structure* is understood the sum of three terms of the same order of magnitud. They refer to the energy of the electron in a hydrogen atom or H-like atom. The terms are, the energy due to relativistic corrections to the motion of the electron, Darwin term and spin-orbit interaction term. We studied each of them during the lectures. Show that the sum of the three effects gives the following expression for the energy of the electron

$$E_{nj} = E_n \Big[1 + \frac{Z^2\alpha^2}{n}\Big(\frac{2}{2j+1} - \frac{3}{4n}\Big)\Big],$$

where $E_n = Z^2 E1/n^2$ are the Bohr energies, and $E_1 = -m_e c^2\alpha^2/2$, as above. Note that this expression does not depend on l. Then $2S_{1/2}$ and $2P_{1/2}$ levels of hydronen still have the same energy.

6. [Gri, pg 243] The most prominent feature of the hydrogen spectrum in the visible region is the red Balmer line or Balmer-alpha line, coming from the transition $n = 3$ to $n = 2$. Fine structure splits this line into several closely spaced lines; the question is: *How many*, and *what is their spacing*? First determine how many sublevels the $n = 2$ level splits into, and find the fine structure energy for each of these, in eV. Then do the same for $n = 3$. Draw an energy level diagram showing all possible transitions from $n = 3$ to $n = 2$. The energy released (in the form of a photon) is $E_3 - E_2 + \Delta E$, the first part being common to all of them, and the ΔE (due to fine structure) varying from one transition to the next. Find ΔE (in eV) for each transition.

   Este mismo ejercicio lo he hecho en clase, sólo que en clase el enunciado decía: [LLaEs] Identifique todas las transiciones *dipolares eléctricas* que contribuyen a Balmer-alpha en el hidrógeno. Al imponer reglas de selección no sale la línea que el profesor Griffiths escribe de $j = 5/2$ a $j = 1/2$, esa de 54.33×10^{-6} eV. Todo lo demás nos queda igual.

7. [Gri, pg 315] [Selection rules] Calculate the lifetime (in seconds) of each of the four $n = 2$ states of hydrogen. *Hint:* You will need to evaluate matrix elements of the form $\langle\psi_{100}|x|\psi_{200}\rangle$, $\langle\psi_{100}|y|\psi_{211}\rangle$, and so on. Remember that $x = r\sin\theta\cos\varphi$, $y = r\sin\theta\sin\varphi$ and $z = r\cos\theta$. Most of these integrals are zero, so scan them before you start calculating. *Answer:* $= 1.60 \times 10^{-9}$ s for all except ψ_{200}, which is infinite.

8. [Gri, pg 318] [Selection rules involving l and l'] [This exercise is redacted in a free manner by myself. If mistakes, they are only mine, MJRPlaza] Prove the commutation relation

$$\big[\mathbf{L}^2, [\mathbf{L}^2, \mathbf{r}]\big] = 2\hbar^2\left(\mathbf{r}\mathbf{L}^2 + \mathbf{L}^2\mathbf{r}\right),$$

as follows: 1) First show that

$$[\mathbf{L}^2, z] = 2i\hbar(xL_y - yL_x - i\hbar z)$$

using

$$[L_x, z] = -i\hbar y, \quad [L_y, z] = i\hbar x, \quad [L_z, z] = 0$$

and the Leibniz rule. Observe that the first two commutators follow the right-hand rule. This rule permits to write also that

$$[L_z, x] = i\hbar y, \quad [L_x, y] = i\hbar z, \quad [L_y, z] = i\hbar x$$

and

$$[L_x, z] = -i\hbar y, \quad [L_y, x] = -i\hbar z, \quad [L_z, y] = -i\hbar x$$

without explicit calculation (but I have checked all of them!). 2) Using $\mathbf{r}\,\mathbf{L} = \mathbf{r}\,(\mathbf{r}\times\mathbf{p}) = 0$, which is $xL_x + yL_y + zL_z = 0$ and the expression for $i\hbar(xL_y - yL_x)$ as obtained in the previous point, derive that

$$\left[\mathbf{L}^2, [\mathbf{L}^2, z]\right] = 2\hbar^2(z\mathbf{L}^2 + \mathbf{L}^2 z).$$

As Griffiths says, the generalization from z to $\mathbf{r}$ is trivial.

MANY ELECTRON ATOMS

9. [Thomas-Fermi model] In 1927, L.H. Thomas and E. Fermi, independently proposed a method to characterize the electron distribution in an atom based on the statistics of a noninteracting degenerate gas. The treatment let to the formulation of the well-known nonlinear differential equation

$$y'' = \frac{y^{3/2}}{\sqrt{x}},$$

with the boundary conditions

$$y(0) = 1, \qquad y(\infty) = 0.$$

Find the simplest particular solution of this equation trying a very reasonable ansatz. You will observe that your solution satisfies $y(\infty) = 0$ but it is singular at $x = 0$. Dont worry, Sommerfeld had the same problem. Only that he persisted and found after several transformations and an asymptotic saddle point analysis the simple approximate solution (I am not asking you for this one)

$$y = \frac{1}{\left(1 + \left(\frac{x}{\sqrt[3]{144}}\right)^{3/b}\right)^b}$$

where $b \approx 3.886$. This solution can be regarded as an assymptotic expansion of the solution that you have worked.

10. [Thomas-Fermi model. Baker's expansion near $x = 0$] The expansion

$$y = 1 + \frac{4}{3}x^{3/2} + \frac{1}{3}x^3 + \frac{2}{27}x^{9/2} + \frac{4}{405}x^6 + \cdots$$

is a solution of the Thomas-Fermi equation

$$x^{1/2}y'' = y^{3/2}$$

near $x = 0$ that satisfies $y(0) = 1$. However, this solution has no physical interest because does not vanish anywhere and diverges for large x. 1) Obtain it by hand as follows: start with the ansatz $y = 1 + px^n + \cdots$ and determine n and the constant p with the TF equation. You will need to use that

$$(1 + x)^{3/2} = 1 + \frac{3}{2}x + \frac{3}{8}x^2 - \frac{1}{16}x^3 + \cdots,$$

just including not as many terms as I have written but merely those to cancel the dominant contribution. You will end up with $y = 1 + \frac{4}{3}x^{3/2} + \cdots$. Repeat the algorithm with $y = 1 + \frac{4}{3}x^{3/2} + px^n + \cdots$ and so on. In this manner you will have written the first few non-zero terms of the (nonphysical) expansion. 2) Repeat now what the University of Michigan graduate student Baker did back in 1930. Try the solution

$$y = 1 + sx + \frac{4}{3}x^{3/2} + px^n + \cdots,$$

Table 1:

	H(1)							**He(2)**
1s	1.00							1.69
	Li(3)	**Be(4)**	**B(5)**	**C(6)**	**N(7)**	**O(8)**	**F(9)**	**Ne(10)**
1s	2.69	3.68	4.68	5.67	6.66	7.66	8.65	9.64
2s	1.28	1.91	2.58	3.22	3.85	4.49	5.13	5.76
2p			2.42	3.14	3.83	4.45	5.10	5.76

that introduces a slope s different from zero and determine s, p and n, same as before. Remarkably s remains free, whereas $n = 5/2$ and $p = 2s/5$. Continue (if you are tired of calculating by hand now you may use Maple, Mathematica, MATLAB) and obtain Baker's, now XYZ's (where XYZ is your name) expansion

$$y = 1 + sx + \frac{4}{3}x^{3/2} + \frac{2}{5}sx^{5/2} + \frac{1}{3}x^3 + \frac{3}{70}s^2x^{7/2} + \cdots$$

Good work.

11. [Electronic configuration] With a **periodic table** we easily find that the ground-state electronic configuration of the neon atom is $1s^2 2s^2 2p^6$. Write the ground-state electronic configuration of Ca ($Z = 20$), Rb ($Z = 37$), Cs ($Z = 55$), and TL ($Z = 81$).

12. [Hund's rules. Ground state term] The previous exercise is about how to write a configuration for a ground state of an atom. Now we determine the ground state term, i.e. $^{2s+1}L_j$. Write ground state terms $^{2s+1}L_j$ for H, He, $_3$Li, $_4$Be, $_5$B, using Pauli's principle and *Hund's rules.* Remember that fully filled shells or subshells can be excluded from consideration of the term since they have total $l = 0, s = 0$.

13. Same as before but for more interesting people $_6$C, $_7$N, $_8$O, $_9$F.

14. [Shell atomic model] 1) Estimate the total atomic binding energy of the first few atoms whose Z_{eff} are given in Table 1. These factors are the Clementi-Raimondi effective factors of nuclear charge, and can be explained by the effect of shielding in different shells and subshells. They are determined in advanced via computer calculations of atomic structure, using *self-consistent field approach* (SCF) based on Hartrees method. With these values one can quickly and easily generate an approximate energy-level diagram and estimate the size of the orbitals for any atom. Notice that the entry corresponding to the Helium, 1.69, is an approximation of $27/16 = 1.6875$, number that we already obtained with a variational principle at the beginnig of the semester.

    2) Once the energies are obtained (see the solution in a pdf file next to this one) figure if a power of Z can fit the data. Remember that in Thomas-Fermi model, the ground energy of an atom was of order $E(Z) \sim Z^{7/3}$. Perhaps here it is similar although the models are quite different.

MATHEMATICAL IDENTITIES AND PHYSICAL RELATIONS

15. Observación: junto en este apartado las matemáticas. Unas serán para el átomo de Helio, otras para el hidrógeno, otras para todo el mundo. Las pongo aquí en un principio. Luego veré si las distribuyo por sus apartados correspondientes, que será lo mejor.

16. La constante de estructura fina se define como $\alpha \equiv \dfrac{e^2}{4\pi\varepsilon_0\hbar c}$ donde $1/(4\pi\varepsilon_0) = 9.0 \times 10^9$ J m$\,$C^{-2} es la constante de la ley de Coulomb (ε_0 se conoce con el nombre de constante dieléctrica del vacío). Comprobar que α (i) es adimensional, (ii) tiene un valor aproximadamente igual a $1/137$.

17. [Li, pg 640] [Fourier representation of the Coulomb potential] Often we need to operate with $\dfrac{1}{r_{12}}$, where $r_{12} = |\mathbf{r_1} - \mathbf{r_2}|$ is the distance between two particles. It is useful to know that

$$\frac{1}{r_{12}} = \frac{1}{2\pi^2}\int d^3\mathbf{k}\,\frac{e^{i\mathbf{k}\cdot\mathbf{r}_{12}}}{k^2},$$

or in general that

$$\frac{1}{r} = \frac{1}{2\pi^2}\int d^3\mathbf{k}\,\frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{k^2}, \qquad r = |\mathbf{r}|.$$

Prove any of these relations (are the same!).

18. Show that

$$\int_0^\infty dx\,\frac{\sin ax}{x} = \frac{\pi}{2}.$$

Notice that the integral is (surprisingly) independent of a. But not the integral from 0 to π, for instance, or from from 0 to a finite number, that depends on a (something that you can check with Maple). Does not depend on a when the integration interval runs to infinity.

19. •

BRIEF INTRODUCTION TO ELEMENTARY PARTICLES

20. [Conservation of energy and momentum] Some conservation laws are absolute whereas some others, parity for instance, are conserved by some of the three fundamental interactions but not all. Three means here that Gravity is excluded. Conservation of energy and momentum is absolute. This exercise is about it.

Un cuerpo de masa m_0 que se encuentra en reposo se desintegra en dos partes cuyas masas son m_1 y m_2. Demostrar que la energía de cada parte es

$$E_1 = \frac{c^2}{2m_0}\,(m_0^2 + m_1^2 - m_2^2), \qquad E_2 = \frac{c^2}{2m_0}\,(m_0^2 - m_1^2 + m_2^2).$$

21. [Lorentz tranformation] En un sistema inercial S un fotón con energía E se mueve en el plano xy formando un ángulo θ con el eje x. Demostrar que: (1) en un segundo inercial S' cuya velocidad relativa con respecto a S es v dirigida según el eje x, la energía y el ángulo del fotón están dados por

$$E' = \gamma E(1 - \beta\cos\theta), \qquad \cos\theta' = \frac{\cos\theta - \beta}{1 - \beta\cos\theta},$$

donde $\beta = v/c$ y $\gamma = (1-\beta^2)^{-1/2}$; (2) escribir E y $\cos\theta$ como funciones de E' y $\cos\theta'$. (3) Demostrar que un fotón moviéndose en la dirección x experimenta un cambio en la frecuencia dado por el factor $\sqrt{(1-\beta)/(1+\beta)}$. A este cambio se le llama *efecto Doppler relativista*. (4) A continuación considere una fuente de fotones que está en reposo en S'. Considere los fotones emitidos en la dirección hacia delante, i.e., $\cos\theta' > 0$. Demuestre que si β es muy próximo a la unidad, esos fotones se verán desde S concentrados en un estrecho cono alrededor de $\theta = 0$. Esto se conoce como *headlight effect*.

22. [French] Demostrar que los procesos que se señalan a continuación son imposibles desde un punto de vista dinámico (quiere decir que no se conserva energía-momento: o falla conservación de energía o conservación de momento o ambas):

   (a) Un fotón choca con un electrón en reposo y entrega toda su energía al electrón.

   (b) Un fotón situado en el espacio libre se transforma en un electrón y un positrón.

   (c) Un positrón rápido y un electrón en reposo se destruyen mutuamente dando lugar a un solo fotón.

   Ayuda: Si una reacción no puede tener lugar en un sistema de referencia no puede tener lugar en ningún otro sistema de referencia pues se pasa de unos a otros mediante transformaciones de Lorentz. Demostrar que en un sistema de referencia dado, el más sencillo en cada caso, la reacción planteada es imposible. Positrón: la antipartícula del electrón: misma masa y carga pero ésta positiva.

23. 1) Complete these reactions attending to lepton number conservation: a) $\pi \to \mu + \nu$, b) $\mu \to e + \nu + \nu$. 2) Why is this reaction never observed $\mu \leftarrow e + \gamma$? (look at the piece of paper I gave to you. This decay is not there). 3) Using lepton number, electron number and muon number conservation complete with $\nu_e, \bar{\nu}_e, \nu_\mu, \bar{\nu}_\mu$ the reactions: a) neutron decay, $n \to p+e+\nu$, b) pion decay, $\pi \to \mu + \nu$, c) muon decay, $\mu \to e + \nu + \nu$.

24. a) Why is the proton stable?