Quantum Mechanics
Physics 237

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Course Announcements

- Next week, April 19: exam # 3 (Chapters 9 – 11).
  - Review session:
  - Extra office hours:
    - Monday 10 am – 12 pm: Wolfs, B&L 203A
  - QA session: Monday at 4.50 pm – 6.20 pm, Hylan 305.
- Last PHY 237 homework (# 10) is due on Friday.

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Some comments on numerical calculations.

- The extra credit problem of HW # 9 focused on the calculation of the Coulomb repulsion between the 2 electrons of the helium atom.
- Several common mistakes were made by the majority:
  - Calculating the expectation value of $1/abs(r_2-r_1)$ where r_1 and r_2 where the radial coordinates of the two electrons (scalars).
  - Using incorrect wavefunctions (either incorrect normalization or symmetry).
  - Using a full 6-dimensional integration with Mathematic which runs forever.

6. **20 points extra credit:** In Chapter 9 we discussed the effect of Coulomb repulsion on the energy levels of the Helium atom. Use Mathematica to calculate the Coulomb repulsion between the electrons in the Helium atom for the following two configurations (see Figure 9.7):

   a. The ground state of Helium ($n = 1$, $\ell = 0$, $n = 1$, $\ell = 0$)

   b. The first excited state of Helium ($n = 1$, $\ell = 0$, $n = 2$, $\ell = 0$)

   To carry out this calculation, use the following procedure:

   1. Obtained the wavefunctions for each electron from Table 7.2.
   2. Construct the appropriate total wavefunction of the state with the proper spatial symmetry.
   3. The position of electron 1 is specified by 3 spatial coordinates; the position of electron 2 is specified by 3 other spatial coordinates. The distance between the two electrons, Δr, depends on these 6 spatial coordinates.
   4. To calculate the Coulomb repulsion, determine the expectation value of $1/\Delta r$. Note: this requires and integration of over the 6 spatial coordinates.

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Some comments on numerical calculations.

- Consider the integration:

$$\int\int\int\int\int\int \psi^*(\vec{r}_1,\vec{r}_2)\frac{1}{abs(\vec{r}_1-\vec{r}_2)}\psi(\vec{r}_1,\vec{r}_2)r_1^2 r_2^2 \sin\theta_1 \sin\theta_2 dr_1 dr_2 d\theta_1 d\theta_2 d\phi_1 d\phi_2$$

- Even though correct, it may take forever to evaluate.
- Consider the following short cuts (to evaluate this integral):
  - No loss of generality occurs if we assume that electron 1 is located on the z axis.
  - With this assumption, this distance between the two electrons only depends on the polar angle of electron 2 (note: the polar angle of electron 1 is 0 degrees.
  - The wavefunctions and the distance between the two electrons do not depend on the azimuthal angles. You can thus replace the integration over these angles with 2π.
  - Change your unit of distance of a_0. The wavefunctions are proportional to $e^{-r/a0}$. Do you really need to integrate from 0 to infinity? How about integrating between 0 and 100 a_0?
  - These changes makes the difference between getting an answer or waiting for an answer forever.

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Using Mathematica to calculate the effect. It actually completes running.

```
(*
Example of calculations of the distance between two electrons in helium.
  In this example, we use the n = 0, l = 0 and the n = 1, l = 0 wavefunctions.
*)

(*
Define the constants needed.  Note: we set a0 =
 1 and thus use the Bohr radius as our unit of distance.  When we do this,
it is easy to see that we can limit the integration over r to values between
 0 and 100.
*)
a0 = 1 (* Bohr radius. *)
Z = 2 (* Charge of the helium nucleaus. *)

(* Define wavefunctions. *)
psi0[r_] := (1/Sqrt[Pi]) * (Z/a0)^1.5 * Exp[-Z * r/a0]
psi1[r_] := (1/(4 * Sqrt[2 * Pi])) * (Z/a0)^1.5 * (2 - Z * r/a0) * Exp[-Z * r/(2 * a0)]

Out[121]= 1

Out[122]= 2

In[125]:= (*
Define total
  wavefunctions. Note: we consider both symmetric and asymmetric wavefunctions. psis =
 symmetric wavefunction.  psia = asymmetric wavefunctio.
*)
psis = (1/Sqrt[2]) * (psi0[r1] * psi1[r2] + psi0[r2] * psi1[r1])
psia = (1/Sqrt[2]) * (psi0[r1] * psi1[r2] - psi0[r2] * psi1[r1])
```

Out[125]= $\frac{0.450158\, e^{-r1-2\,r2}(2-2\,r1)+0.450158\, e^{-2\,r1-r2}(2-2\,r2)}{\sqrt{2}}$

Out[126]= $\frac{-0.450158\, e^{-r1-2\,r2}(2-2\,r1)+0.450158\, e^{-2\,r1-r2}(2-2\,r2)}{\sqrt{2}}$

```
In[127]:= (* Check normalization of both
  wavefunctions: should be 1. Note:
   polar and azimuthal angle instegrations increate the integral by (4Pi)^2.*)
Integrate[psis * psis * r1^2 * r2^2, {r1, 0, 100}, {r2, 0, 100}] * (4 * Pi)^2
Integrate[psia * psia * r1^2 * r2^2, {r1, 0, 100}, {r2, 0, 100}] * (4 * Pi)^2

Out[127]= 1.

Out[128]= 1.

In[129]:= (*
   Limit the range of variables.  Assume that electron 1 is on the z-
    axis (theta1 = 0 degrees).  This means: 1) we do not need to integrate
  over theta1 and the integration over phi1 and phi2 provides a multiplication
  factor of (2Pi)^2.
*)

(* For these assumptions, determine the distance between the two electrons. *)
DeltaR = Sqrt[Abs[r1^2 + r2^2 - 2 * r1 * r2 * Cos[theta2]]]
```

Out[129]= $\sqrt{\text{Abs}[r1^2+r2^2-2\, r1\, r2\, \text{Cos}[theta2]]}$

```
In[130]:= (* Get the expectation values. *)
(* Consider both wavefunctions (symmetric and astnnetric). *)
Integrate [psis * (1/DeltaR) * psis * r1^2 * r2^2 * Sin[theta2], {r1, 0, 100},
  {r2, 0, 100}, {theta2, 0, Pi}] * (2 * Pi)^2
Integrate [psia * (1/DeltaR) * psia * r1^2 * r2^2 * Sin[theta2], {r1, 0, 100},
  {r2, 0, 100}, {theta2, 0, Pi}] * (2 * Pi)^2

Out[130]= 0.231824

Out[131]= 0.187929

In[132]:=
```


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Calculating the Coulomb repulsion energy.

- These calculations show that the energy shift due to Coulomb repulsion is:
  - 6.3 eV if the electrons are in an S = 0 spin state,
  - 5.1 eV if the electrons are in an S = 1 spin state.
- This type of shift is observed in the spectrum of helium.

```
In[162]:= (* Calculte the energy shift for both cases. *)
(* Define some constans. *)
a0ToMeter = 5.29 * 10^{-11} (* Convert from a0 units to meter. *)
eCharge = 1.602 * 10^{-19} (* Charge of an electrons in Coulomb. *)
coulombsLawConstaant = 8.998 * 10^9 (* Coulomb's law constant in Nm^2/C^2. *)
fineStructureConstant = 1/137
jouleToEv = 6.242 * 10^(18) (* Convert Joule to eV *)

(* Now calculate the Coulb repulsions energy. *)
(* Start with the symmetric wvefunction (S = 0)*)
coulombsLawConstaant * eCharge^2 * Exp1OverRs * (1/a0ToMeter) * jouleToEv

(* continue with the asymmetric wvefunction (S = 1)*)
coulombsLawConstaant * eCharge^2 * Exp1OverRa * (1/a0ToMeter) * jouleToEv
```

Out[162]= $\{5.29\times10^{-11}\}$

Out[163]= $\{1.602\times10^{-19}\}$

Out[164]= 8.998×10^{9}

Out[165]= $\frac{1}{137}$

Out[166]= 6.242×10^{18}

Out[167]= {6.31682}

Out[168]= {5.12073}

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Details of helium spectrum. Good to know.

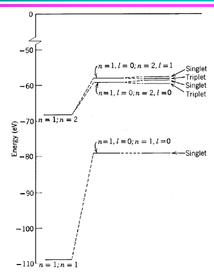

Figure 9-7 The low-lying energy levels of helium. *Left:* The levels that would be found if there were no Coulomb interaction between its electrons. *Center:* The levels that would be found if there were a Coulomb interaction but no exchange force. *Right:* The levels that would be found if there were a Coulomb interaction and an exchange force. These levels are in excellent agreement with the experimentally observed levels shown on the right in Figure 9-6.

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Back to regular programming:

Chapter 17 and our discussion of two nucleon systems.

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What states can be occupied by a nucleon pair?

- 2n and 2p systems must obey the Pauli exclusion principle.
- np systems do not need to obey the Pauli exclusion principle.
- Consider the following states:
  - $^3S_1$: $l = 0$, $s = 1$, and $j = 1$. Wave function is symmetric: in principle ok for np systems but not ok for 2n and 2p systems.
  - $^1P_1$: $l = 1$, $s = 0$, and $j = 1$. Wave function is symmetric: in principle ok for np systems but not ok for 2n and 2p systems.
  - $^3P_{0,1,2}$: $l = 1$, $s = 1$, and $j = 0,1,2$. Wave function is asymmetric: in principle ok for np, 2n, and 2p systems.
  - $^1D_2$: $l = 2$, $s = 0$, and $j = 2$. Wave function is asymmetric: in principle ok for np, 2n, and 2p systems.
  - $^3D_{1,2,3}$: $l = 2$, $s = 1$, and $j = 1,2,3$. Wave function is symmetric: ok for np systems but not ok for 2n and 2p systems.

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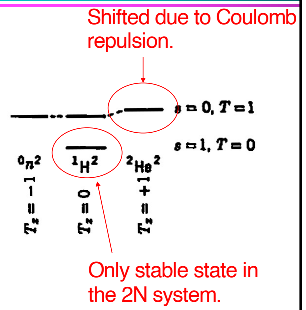
Isospin. N = 2 system.

- Since the nucleon force is independent of nuclear charge, we consider the proton and the neutron to be two different forms of the same particle with different "isospin T" parameters.
- Protons and neutrons are isospin ½ particles with different values of T_z.
  - Protons: $T_z = + ½$.
  - Neutrons: $T_z = - ½$.
- Since protons and neutrons have different values of T_z, they are distinguishable.



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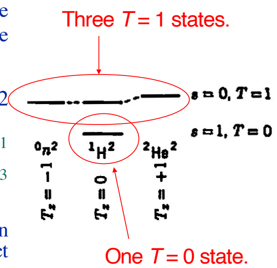
Isospin. N = 2 system.

- Isospin can be used to relate energy levels in nuclei with the same number of nucleons.
- In the example of the N = 2 system we see:
  - T = 0: expect to see $(2T + 1) = 1$ state.
  - T = 1: expect to see $(2T + 1) = 3$ states.
- Since each proton/neutron carries a fixed T_z, we expect that the total charge of a system depends on the total T_z.



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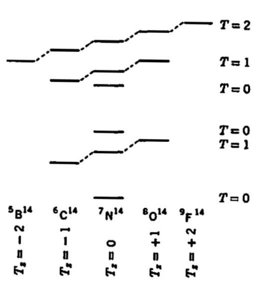
Isospin. N = 14 system.

- The total T_z of a nucleon system is equal to $(Z–N)/2$.
- For the N = 14 system we see:
  - B: $T_z = -2$
  - C: $T_z = -1$
  - N: $T_z = 0$
  - O: $T_z = +1$
  - F: $T_z = +2$
- Energy levels observed in the N = 14 system can be grouped according to total isospin: $T = 0$, $T = 1$, and $T = 2$.



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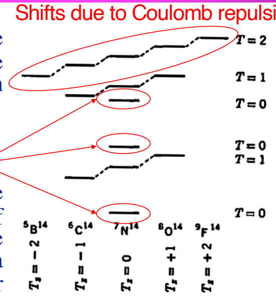
Isospin. N = 14 system.

Shifts due to Coulomb repulsion.

- The grouping of the energy levels for the N = 14 system is shown in the figure.



- When we look at the states that are part of the $T = 2$ group, we expect them to have a similar nuclear structure.

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Wavefunctions for the two-nucleon wave function.

- The total wavefunction of the two-nucleon system is the product of a spatial wavefunction, a spin wavefunction, and an isospin wavefunction:

$$\psi = \psi_\ell \psi_s \psi_T$$

- Since the two nucleons are fermions, the total wavefunction must be asymmetric.
- Consider $l = 0$ states.
  - The spatial wavefunction is symmetric.
  - If the system is in a spin singlet state, the isospin state must be symmetric ($s = 0$, $T = 1$).
  - If the system is in a spin triplet state, the isospin state must be asymmetric ($s = 1$, $T = 0$).

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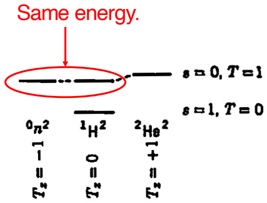
Additional conclusions, based on the observed properties of the two-nucleon system.

- The observation that the $T = 1$ states in $^0n^2$ and $^1H^2$ occur at the same energy confirms that the nucleon force does not depend on T_z.

Same energy.



- The observed shift in the $T = 1$ state in $^2He^2$ is consistent with the Coulomb repulsion between the two protons.

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Conservation of isospin.

- T is conserved:
  - This is observed in various nuclear reactions. For example:

$$^{1}H^{2} + {}^{8}O^{16} \rightarrow {}^{7}N^{14} + {}^{2}He^{4}$$

T = 0 ground states.
Total initial isospin is 0.

T = 0 ground state.
High-lying first
excited state.

T = 0 ground state.
T = 1 first excited state.
Expect that N is in the ground state.

- T_z is conserved:
  - Conservation of electric charge.

3 Minute 19 Second Intermission.

- Since paying attention for 1 hour and 15 minutes is hard when the topic is physics, let's take a 3 minute 19 second intermission.

- You can:
  - Stretch out.
  - Talk to your neighbors.
  - Ask me a quick question.
  - Enjoy the fantastic music.

Why does the nucleon force has a short range.

- Forces act via the exchange of force carriers.

- The nucleon force is due to an exchange of pions.
- The electric force is due to an exchange of photons.
- Differences in the range of the forces are due to differences in the mass of the force carriers.

- A nucleon can create virtual pion pairs.
- The Heisenberg uncertainty principle allows the nucleon to "borrow" the energy required to create the virtual pion pair for a short amount of time. The heavier the pion, the shorter the amount of time.
- During this time, the pion can travel a certain distance before it has to "return" to the nucleon to disappear before Heisenberg gets upset.

Why does the nucleon force has a short range?

- Since the pion has a mass, the energy required to create a virtual pion depend on its mass.

$$\Delta E = m_\pi c^2$$

- The time during which the virtual pion pair can exist can be determine using Heisenberg's uncertainty principle:

$$\Delta t = \frac{\hbar}{2\Delta E} = \frac{\hbar}{2m_\pi c^2}$$

- The maximum distance the pion can travel away from the nucleon, assuming it travels with the speed of light, defines the range of the nuclear force:

$$\text{Range} = \frac{1}{2}\left(c\Delta t\right) = \frac{\hbar}{4m_\pi c}$$

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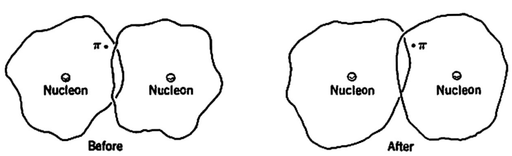
The nuclear force: a results of pion exchange.

- When another nucleon is within the range *R*, the virtual pion may be absorbed by that nucleon: that nucleon feels the nuclear force due to the nucleon that created the virtual pion.
- The nucleons feel their mutual nuclear force when their virtual pion clouds overlap.



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From virtual to real.

- The theory of pion exchange was proposed before the pion was know to exist.
- Based on the known range of the nuclear force, the estimated mass of the pion was between 25 MeV and 100 MeV.
- The pion was discovered in 1947 and found to have come in three different forms:

$$m_{\pi^+}c^2 = m_{\pi^-}c^2 = 140 \text{ MeV}$$

$$m_{\pi^0}c^2 = 135 \text{ MeV}$$

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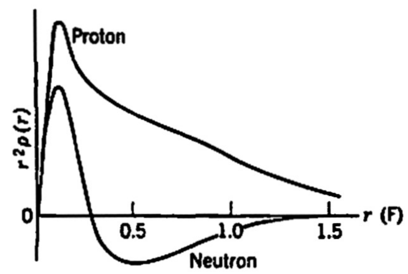
Charge distribution of nucleons.



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Force carriers.

- We know believe that all forces are the result of an exchange of force carriers.
- The heavier the force carrier, the shorter the range of the force.
- The electromagnetic force is carried by virtual photons. Since photons are massless, their range is infinite and this is why the electromagnetic force has an infinite range.
- The weak force is a result of the exchange of W and Z bosons with a mass of between 80,000 MeV/c^2 – 91,000 MeV/c^2. The weak force has thus a much shorter range than the nuclear force.
- Why do you expect all force carriers to be bosons?

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ENOUGH FOR TODAY?

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