Lecture 4

In last lecture we discussed how one can solve the Schroedinger equation to determine the allowed energies of a particle trapped in a spherically symmetric potential. We will apply these methods to the case of neutrons and protons bound in the nucleus. First we'll discuss some properties of nuclei that pertain to our problem.

Magic Numbers

The properties of atoms show patterns. Similar chemical properties are displayed graphically in the periodic table: elements in the same column have similar chemical properties. The "magic numbers" for atomic properties are: 2, 6, 10, 14. These numbers can be understood by solving the Schroedinger equation with a spherically symmetric mean field potential derived from the Coulomb interaction. The numbers are equal to $2(2l + 1)$, where $l = 0, 1, 2, 3, \cdots$. l is the orbital angular momentum quantum number.

Nuclei also show patterns, and have their own "magic numbers". This is demonstrated on the next page. The graph is plot of the energy needed to remove a neutron versus the number of neutrons in the nucleus. The different curves correspond to the cases when the number of neutrons, N, minus the number of protons, Z, equals $1, 2, 3, \cdots$. The quantity $N - Z$ is the number of extra neutrons than protons.

From the figure, one can see that energy needed to remove a neutron drops after N equals $2, 8, 20, 28, 50, 82, \cdots$. These numbers are the "magic numbers" for nuclei. There is other experimental evidence that these numbers to bring on changes in nuclear properties. Because of the magic number phenomena, one is lead to a shell-model to describe some nuclei. The data suggest that neutrons and protons each (separately) have closed shells when their number equals the **nuclear magic numbers**:

$$2 \text{ or } 8 \text{ or } 20 \text{ or } 28 \text{ or } 50 \text{ or } 82$$
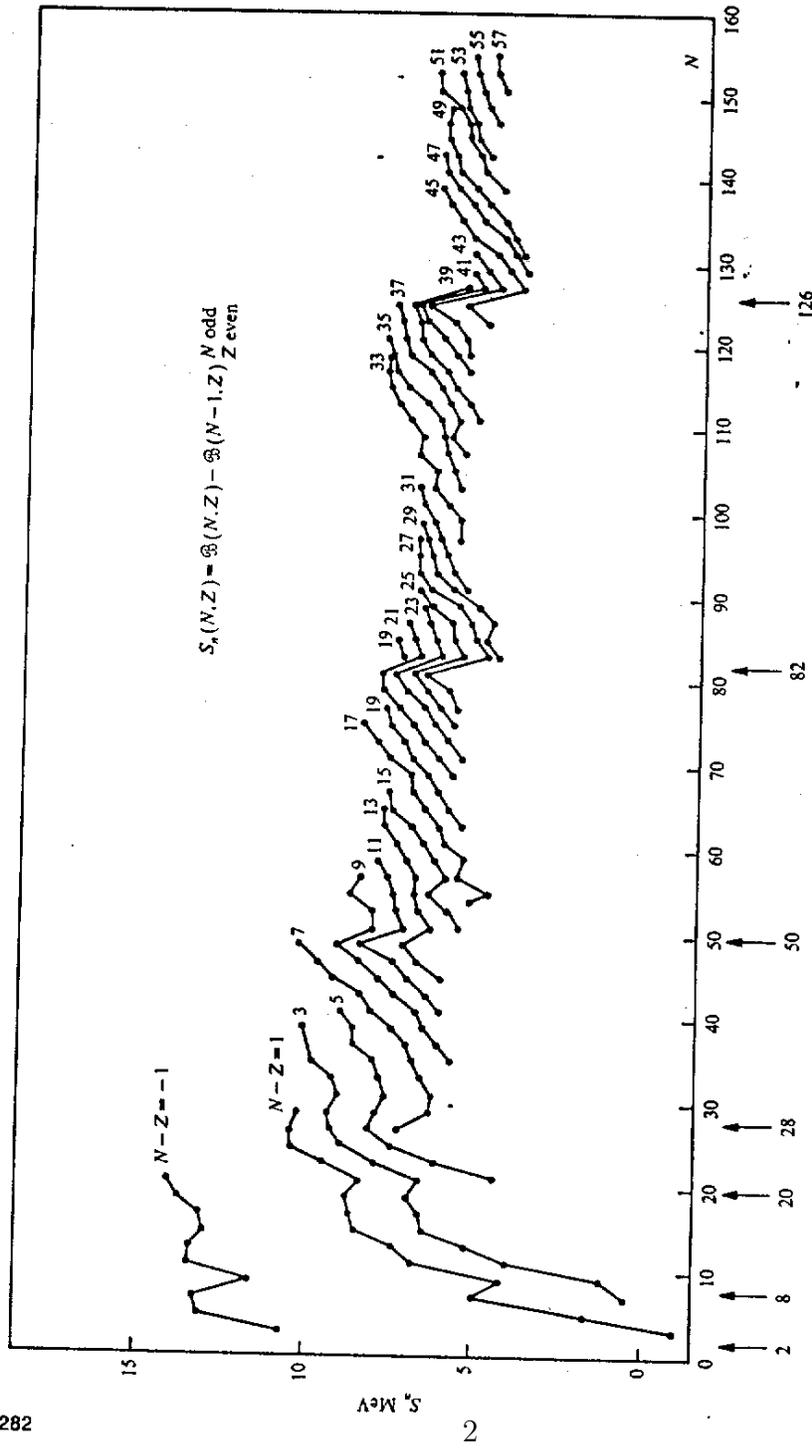
Figure 6-35 Neutron separation energies S_n taken from the compilation by J. H. E. Mattauch, W. Thiele, and A. H. Wapstra, *Nuclear Phys.*, **67**, 1 (1965).

Nuclear Shell Model

The independent particle model, or shell model, of the nucleus has been successful in understanding many properties of nuclei. In this model, the nucleons are treated as independent particles that move in an average potential (mean field) due to the other nucleons in the nucleus.

The mean field potential consists of a "strong force" part that both the neutrons and protons experience. Since the protons possess charge, they will have an electrostatic Coulomb potential in addition to the strong force.

A common potential that is used to represent the strong interaction between a nucleon and the rest of the nucleus is the "Woods-Saxon" potential:

$$V(r) = \frac{-V_0}{1 + e^{(r-c)/a}} \tag{1}$$

This potential is a smoothed out square well, and the potential strength V_0 is the same for both neutrons and protons.

For your homework exercise, you will calculate the bound state energies for neutrons and protons in various nuclei. To reduce the number of parameters, we will take use a simple model for the potential. For the strong potential **we will use a spherical square well potential** as we did for the Λ particle. For the electrostatic potential that the proton experiences, we will use the potential from a uniformly charged sphere of radius R and total charge Ze:

$$
\begin{aligned}
V_{Coulomb}(r) &= Ze^2 \frac{3R^2 - r^2}{2R^3} \qquad if \ r \leq R \\
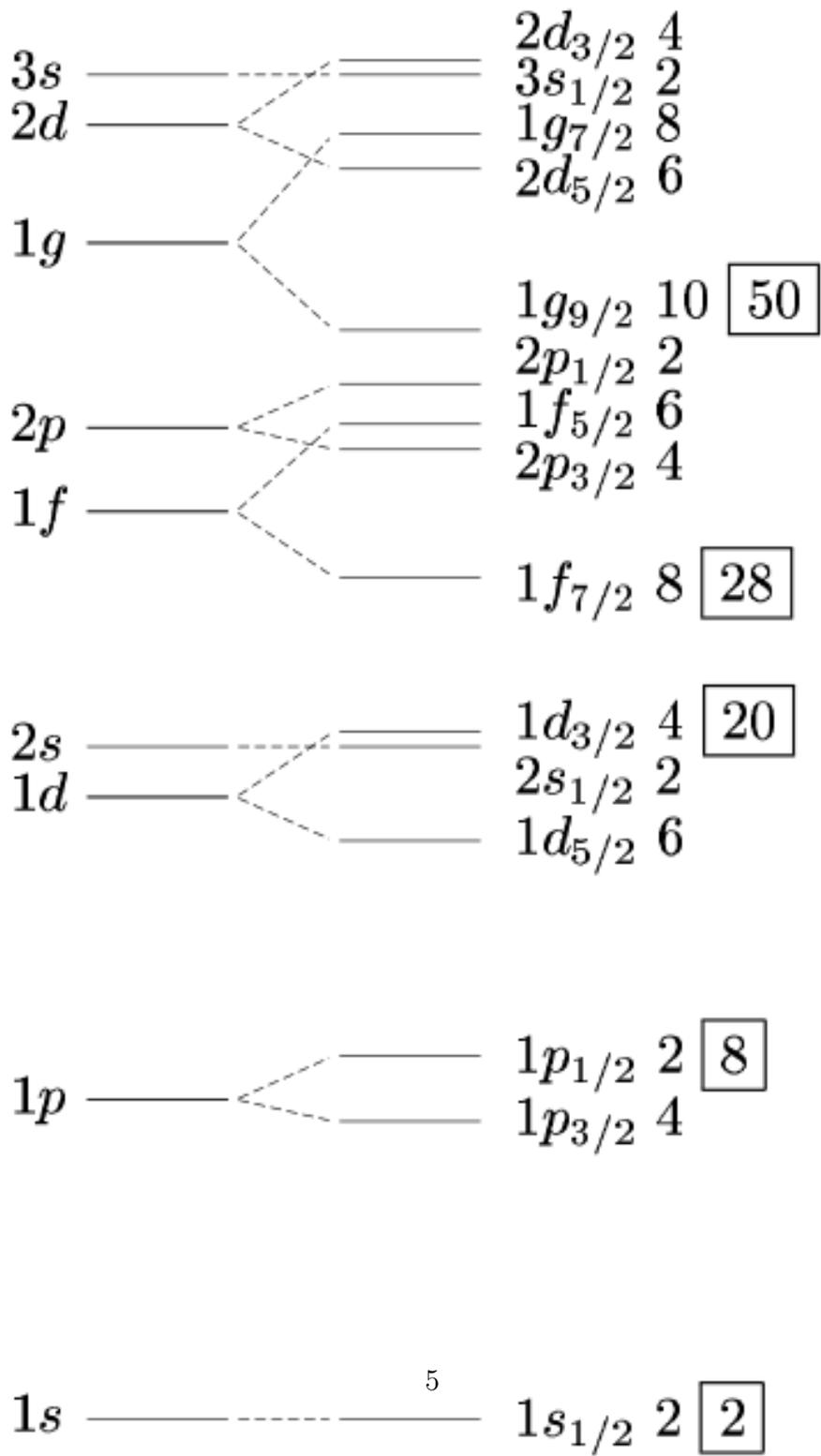&= \frac{Ze^2}{r} \qquad if \ r > R
\end{aligned}
$$

Energy levels in Nuclei

For your homework assignment, you will solve for the energy levels in a spherical square well. You will see that as the radius of the well increases, or the potential depth V_0 increases that more states are allowed in the square well. You might wonder, what is the ordering of these levels. The lowest level (ground state) will have $l = 0$, and the function $u(r)$ will have one maximum within the well. This is the same result as the ground state for the hydrogen atom. For hydrogen, the next $l = 0$ and the first $l = 1$ state have the same energy. However, the three dimensional square well will not have this property. The second $l = 0$ and the first $l = 1$ states will not have the same energy (i.e. not be degenerate). Only for a perfect $1/r$ potential will the bound state energies be independent of the orbital angular momentum quantum number l. The goal of your homework assignment is to see what the energy level spectrum for the three dimensional square well is.

On the next page, is a diagram of a calculation for the energy spectrum for a Woods-Saxon potential. You should get similar results using the 3-D square well with the levels at the extreme left.

The number of allowed states for a given orbital angular momentum is $2(2l + 1)$. There are $2l+1$ values for m_l, and an additional factor of 2 due to the electron having a spin of $1/2$.

l	number of states = 2(2l+1)
0	2
1	6
2	10
3	14

$2d_{3/2}$ 4

$3s$ .... $3s_{1/2}$ 2

$2d$ ——— $1g_{7/2}$ 8

$2d_{5/2}$ 6

$1g$ ——— $1g_{9/2}$ 10 $\boxed{50}$

$2p_{1/2}$ 2

$2p$ ——— $1f_{5/2}$ 6

$2p_{3/2}$ 4

$1f$ ——— $1f_{7/2}$ 8 $\boxed{28}$

$1d_{3/2}$ 4 $\boxed{20}$

$2s$ .... $2s_{1/2}$ 2

$1d$ ——— $1d_{5/2}$ 6

$1p_{1/2}$ 2 $\boxed{8}$

$1p$ ——— $1p_{3/2}$ 4

5

$1s$ ——— $1s_{1/2}$ 2 $\boxed{2}$

Spin Orbit interaction

Using the ordering of the levels on the left, the numbers are not magical. Since two neutrons can occupy the same level, closed shells occur when the neutron number is $2, 8, 28, 34, \cdots$. The agreement starts out OK, but fails with 34. To correct the problem, Maria Mayer and Hans Jenkens suggested that a spin-orbit correction might be strong enough to produce closed shells which match with experiment. The ordering of the nuclear levels including the spin-orbit term are shown at the right in the diagram. As you can see, the addition of the spin-orbit correction results in the correct magic numbers. In the assignment, your task is to see if the level ordering without the spin-orbit correction agrees with the left column.

To check your code, I will give you results for two nuclei: the valance neutron in ^{13}C and the valance proton in ^{13}N. Using $R = 1.28A^{1/3}$ I get

A	Z	V_0(MeV)	l	$|E|_{calculated}$(MeV)	$|E|_{experiment}$(MeV)
12	0	32.3	1	4.97	4.95
12	6	32.3	1	1.79	1.94

which match the experimental data quite well. As expected the energy levels for the proton are higher than for the neutron. This phenomena explains why neutrons are stable when they are bound in nuclei. In free space the neutron will undergo beta decay into a proton via the weak interaction:

$$n \rightarrow p + e + \bar{\nu}_e \qquad (2)$$

since the mass of the neutron is greater than the sum of the proton and electron mass. The lifetime is around 12 minutes. However, the valance neutron in ^{13}C cannot beta decay into a proton, since in the resulting ^{13}N nucleus the proton will be at an energy around 3 MeV higher than the initial neutron. Neutrons should be grateful to the Coulomb repulsion of the protons, which gives them their stability when bound in nuclei.

In the following table, I list results of a Cal Poly Pomona senior project. We used a Woods-Saxon potential, with $a = 0.6fm$, for the strong interaction and found values of V_0 and $R = r_0A^{1/3}$ that agreed with experiment for valance nucleons.

Table III.

    Experimental and calculated values for the valence nucleon. The binding energies are given in units of MeV.

Core Nucleus	l(jP)	Binding Energy of Valence Neutron	Binding Energy of Valence Proton	r_0(fm)	V_0(MeV)
He(4)	——	——	——	——	——
Li(6)	1(3/2-)	7.250	5.606	1.52	43.11
Be(8)	1(3/2-)	1.665	——	—-	——
B(10)	1(3/2-)	11.454	8.689	1.34	47.41
C(12)	1(1/2-)	4.946	1.943	1.29	35.11
N(14)	1(1/2-)	10.833	7.297	1.33	40.11
O(16)	2(5/2+)	4.144	.601	1.34	47.71
F(18)	2(1/2+)	10.432	6.412	1.36	52.64
Ne(20)	2(3/2+)	6.761	2.431	1.32	46.80
Na(22)	2(3/2+)	12.419	7.580	1.32	53.09
Mg(24)	2(5/2+)	7.331	2.271	1.29	44.91
Al(26)	2(5/2+)	13.058	7.463	1.28	51.81
Si(28)	0(1/2+)	8.473	2.748	1.28	46.54
P(30)	0(1/2+)	12.312	6.133	1.30	49.91
S(32)	2(3/2+)	8.641	2.276	1.27	41.42
Cl(34)	2(3/2+)	12.644	5.896	1.29	45.05
Ar(36)	2(3/2+)	8.789	1.857	1.27	39.29
K(38)	2(3/2+)	13.077	5.764	1.29	43.39
Ca(40)	3(7/2-)	8.363	1.085	1.29	51.62
Sc(42)	3(7/2-)	12.138	4.488	1.29	55.22
Ti(44)	3(7/2-)	9.520	1.614	1.28	51.49
V(46)	1(3/2-)	13.001	4.767	1.31	58.03
Cr(48)	3(5/2-)	10.582	2.085	1.27	51.14
Mn(50)	3(5/2-)	13.687	4.885	1.27	53.66
Fe(52)	3(7/2-)	10.683	1.599	1.25	50.11
Co(54)	3(7/2-)	14.090	4.614	1.25	53.82
Ni(56)	1(3/2-)	10.247	0.694	1.27	51.34
Cu(58)	1(3/2-)	12.763	2.887	1.28	53.16
Zn(60)	1(3/2-)	10.231	0.454	1.31	47.21
Ga(62)	1(?)	12.765	2.203	1.25	53.26

Electrostatic Potential for a uniformly charged sphere

Let's remind ourselves how we can obtain the electrostatic potential for a uniformly charged sphere of charge. Let the total charge be Q, and the radius of the sphere be R. Let's first find the electric field everywhere, then integrate to find the potential.

We can determine the electric field for $r > R$ by applying Gauss's Law to a spherical surface of radius $r > R$:

$$\int \vec{E} \cdot d\vec{S} = \frac{Q_{inside}}{\epsilon_0}$$

$$4\pi r^2 |E| = \frac{Q}{\epsilon_0}$$

$$|E| = \frac{kQ}{r^2}$$

where $k = 1/(4\pi\epsilon_0)$.

Using a surface within the charged sphere, where $r < R$, we have:

$$\oint \vec{E} \cdot d\vec{S} = \frac{Q_{inside}}{\epsilon_0}$$

$$4\pi r^2 |E| = \frac{Q}{\epsilon_0}\left(\frac{r^3}{R^3}\right)$$

$$|E| = \frac{kQr}{R^3}$$

since the fraction of the charge that lies within a radius r is (r^3/R^3).

Now we can find the potential from the electric field. Using as a reference $V(\infty) \equiv$ 0, we have for $r > R$:

$$
\begin{aligned}
V(r) - V(\infty) &= \int_r^\infty \frac{kQ}{r^2} dr \\
V(r) - 0 &= -\frac{kQ}{r} \\
V(r) &= \frac{kQ}{r}
\end{aligned}
$$

for $r > R$. Now for $r < R$, we have:

$$
\begin{aligned}
V(r) - V(R) &= \int_r^R \frac{kQr}{R^3} dr \\
V(r) - \frac{kQ}{R} &= \frac{kQ}{2R^3}(R^2 - r^2) \\
V(r) &= \frac{kQ}{R}\left(\frac{3R^2 - r^2}{2R^2}\right)
\end{aligned}
$$

Summarizing, the electrostatic potential due to a uniformly charged sphere of radius R, charge Q, is

$$
\begin{aligned}
V(r) &= \frac{kQ}{r} & for\ r \geq R \\
&= \frac{kQ}{R}\left(\frac{3R^2 - r^2}{2R^2}\right) & for\ r < R
\end{aligned}
$$

For our application, Z equals the total number of protons in the nucleus minus 1.

```
psi[0] = 0.0;
psi[1] = 1.0;
del = 0.01;
 for (i=1; i<imax; i++)
 {
   r[i] = i*del;
   fac = -z*fsc/r[i];
   if (r[i]<c) fac=v0-z*fsc*(3/c-r[i]*r[i]/c/c/c)/2.0;
   psi[i+1] = 2*psi[i] - psi[i-1] + psi[i]*del*del*l*(l+1)/r[i]/r[i]
        + del*del*psi[i]*2*mc2/hc/hc*(e-fac);
 }
```

Other methods for solving Differential Equations

For our exercise I have shown one rather simple method of solving differential equations. There are other algorithms that one can use which can give better convergence to the function. I'll briefly mention some of them here to make you aware of other possibilities.

These algorithms are usually designed to find solutions to the following first order differential equation:

$$\frac{dx}{dt} = f(t, x) \tag{3}$$

where $x(t)$ is a function of t. Notice that in general x can appear on the right side of the equation.

Euler Algorithm

For our example, we have been using an algorithm similar to as "the Euler algorithm". In the Euler Algorithm, the derivative is replaced by its finite difference approximation. Defining $x_i \equiv x(t_i)$, we have

$$\frac{dx}{dt} \approx \frac{x_{i+1} - x_i}{\delta} \tag{4}$$

Substituting into the differential equation gives:

$$\frac{x_{i+1} - x_i}{\delta} \approx f(t_i, x_i) \tag{5}$$

Solving for x_{i+1} yields

$$x_{i+1} \approx x_i + \delta f(t_i, x_i) \tag{6}$$

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If the initial condition is such that x_0 is known, the above equation can be used to find x_1. Then the equation can be used again to find x_2, etc.

The Euler algorithm is equivalent to including only the first term in the Taylor expansion. The Taylor expansion for $x(t + \delta)$ about $x(t)$ is given by

$$
\begin{aligned}
x(t + \delta) &= x(t) + \delta x'(t) + \frac{\delta^2}{2} x''(t) + \cdots \\
x(t + \delta) &= x(t) + \delta f(t, x) + \frac{\delta^2}{2} f'(t, x) + \cdots
\end{aligned}
$$

Neglecting terms or order δ^2 or greater gives the approximation

$$
x(t + \delta) \approx x(t) + \delta f(t, x) \tag{7}
$$

which is the Euler algorithm.

Runge-Kutta Methods

The Euler algorithm is conceptually easy to understand. To improve accuracy, one can decrease the step size and increase the number of iteration points. However, the computation time increases with the number of iteration points. As you might guess, there are a more efficient algorithms for increasing accuracy. We will describe one such method first, the Second-Order Runge-Kutta algorithm, then "prove" why it is more accurate.

We want the best estimate of $x(t+\delta)$, with the knowledge of $x(t)$ and $f(t, x)$. The Euler algorithm uses the first two terms of the Taylor expansion, with the derivative evaluated at x at time t. From the mean-value theorum, there is a value of $x = x'$ and $t = t'$ such that

$$
x(t + \delta) = x(t) + \delta f(x', t') \tag{8}
$$

A simple improvement over the Euler method is to choose values $x' = x_m$, where x_m is half way between $x(t)$ and $x(t + \delta)$. We don't know x_m exactly, but we can use the Euler algorithm to approximate it. The two step process would be as follows:

$$
\begin{aligned}
x_m &\approx x(t) + (\delta/2) * f(x(t), t) \\
t_m &\approx t + \delta/2 \\
x(t + \delta) &\approx x(t) + \delta * f(x_m, t_m)
\end{aligned}
$$

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Note that x_m is determined via the Euler algorithm, but with a step size of $\delta/2$. The results are still approximate, but as we will show are accurate to order δ^2. The above method is a type of second-order Runge-Kutta algorithm.

Derivation of Runge-Kutta Forms

The approach in second-order Runge-Kutta methods is to use only first derivative information to best estimate the change in x(t) for one step size. A good method to accomplish this is to use a combination of two terms: one with derivative information at the start of the interval $f(t_0, x_0)$ and a second term which uses derivative information somewhere in the interval $f(t_0 + \alpha\delta, x_0 + \beta\delta f(t_0, x_0))$. Here α and β are constants, and the interval starts at time t_0 and $x_0 \equiv x(t_0)$. The ansatz for this approach is

$$x(t_0 + \delta) = x(t_0) + w_1\delta f(t_0, x_0) + w_2\delta f(t_0 + \alpha\delta, x_0 + \beta\delta f(t_0, x_0)) \qquad (9)$$

where w_1 is the weighting for the derivative at the start of the interval, and w_2 is the weighting for the derivative somewhere in the interval. The argument x_0 means $x(t_0)$. Note, that the Euler algorithm is obtained if $w_1 = 1$ and $w_2 = 0$.

To compare with the Taylor expansion, we can expand the right side of the equation about $x(t_0)$. Expanding $f(t_0 + \alpha\delta, x_0 + \beta\delta f(t_0, x_0))$ we have

$$f(t_0 + \alpha\delta, x_0 + \beta\delta f(t_0, x_0)) = f(t_0, x_0) + \alpha\delta\frac{\partial f}{\partial t} + \beta\delta f\frac{\partial f}{\partial x} + \cdots \qquad (10)$$

to order δ^2. Note that the derivative are evaluated at $x = x_0$ and $t = t_0$. Substituting into Eq. 12, yields

$$x(t_0 + \delta) = x(t_0) + w_1\delta f(t_0, x_0) + w_2\delta(f(t_0, x_0) + \alpha\delta\frac{\partial f}{\partial t} + \beta\delta f\frac{\partial f}{\partial x} + \cdots) \quad (11)$$

$$x(t_0 + \delta) = x(t_0) + (w_1 + w_2)\delta f(t_0, x_0) + \alpha w_2\delta^2\frac{\partial f}{\partial t} + w_2\beta\delta^2 f\frac{\partial f}{\partial x} + \cdots \quad (12)$$

to order δ^2. We need to compare this expression with that of the Taylor expansion of $x(t)$. The Taylor expansion of $x(t_0 + \delta)$ about $x(t_0)$ is given by

$$x(t_0 + \delta) = x(t_0) + \delta\frac{dx}{dt} + \frac{\delta^2}{2}\frac{d^2x}{dt^2} + \cdots \qquad (13)$$

to order δ^2. The first derivative of $x(t)|_{t_0}$ equals $f(t_0, x_0)$. The second derivative of $x(t)$ with respect to t equals the first derivative of f with respect to t: $d^2x/dt^2 = df/dt$. f has an implicit and explicite time dependance:

$$\frac{df}{dt} = \frac{\partial f}{\partial t} + \frac{\partial f}{\partial x}\frac{dx}{dt}$$
$$\frac{d^2x}{dt^2} = \frac{\partial f}{\partial t} + f\frac{\partial f}{\partial x}$$

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Substituting this expression for the second derivative into the Taylor expansion yields:

$$x(t_0 + \delta) = x(t_0) + \delta f(x_0, t_0) + \frac{\delta^2}{2}\frac{\partial f}{\partial t} + \frac{\delta^2}{2}f\frac{\partial f}{\partial x} + \cdots \tag{14}$$

to order δ^2, where we have used $dx/dt|_{t_0} = f(x_0, t_0)$. Comparing Eq. 15 with Eq. 17, we see that if w_1, w_2, α and β satisfy the following conditions:

$$w_1 + w_2 = 1 \qquad\qquad \alpha w_2 = 1/2 \qquad\qquad \beta w_2 = 1/2$$

then the expansion agrees with the Taylor expansion to order δ^2. This is one order of δ better than the Euler algorithm.

There is not a unique solution to these three equations. They do constrain α to equal β, and $w_2 = 1 - w_1$. However, w_1 can take on any value between 0 and 1. One of the simplest choices is $w_1 = 0$. This choice gives $w_2 = 1$, and $\alpha = \beta = 1/2$, and is the choice we presented in these notes:

$$x(t_0 + h) = x(t_0) + \delta f(t_0 + \delta/2, x_0 + (\delta/2)f(t_0, x_0)) \tag{15}$$

This equation is more clearly expressed as we did before:

$$
\begin{aligned}
x_m &\approx x(t_0) + (\delta/2) * f(t_0, x_0)) \\
t_m &\approx t_0 + \delta/2 \\
x(t_0 + \delta) &\approx x(t_0) + \delta * f(t_m, x_m)
\end{aligned}
$$

The Taylor expansion analysis allows us to determine the accuracy of the algorithms. For the Euler algorithm, $x(t + \delta)$ is exact up to first order in δ. That is, the errors decrease with order δ^2. If the step size δ is divided by N, then the error for $x(t + \delta/N)$ is $1/N^2$ as large as the error for $x(t + \delta)$. However, with $1/N$ the step size, one needs N steps to reach $x(t + \delta)$, so the overall gain is a decrease of $1/N$ in the error.

For the second-order Runge-Kutta algorithm, the errors decrease with order δ^3. If δ is decreased by a factor of N, then the error for $x(t + \delta/N)$ decreases by a factor of $1/N^3$ from the error of $x(t + \delta)$. Since N steps are needed, the overall gain is a decrease of $1/N^2$ in the error. However, since the second-order Runge-Kutta requires $5/3$ the computing time per δ/N step as the Euler algorithm, there is often only a marginal gain in accuracy per computing time.