

Covariant Density Functional Theory

P. Arumugam

Indian Institute of Technology Roorkee, Uttarakhand, India

- *Motivation*
- *Definitions & Basics of DFT*
- *Covariant form of field equations*
- *QHD - I*
- *Infinite matter EoS*
- *Neutron star EoS & structure*





Nuclear many-body theory



- One body problem is easier to solve, Eg. Projectile motion, $F = ma$
- Two body problem, Eg. satellite orbiting a planet, $F_{12}(x_1, x_2) = m_1 a_1$;
 $F_{12}(x_1, x_2) = m_1 a_1$
- Three body problem is complicated but solvable
- Only approximate solutions can be found for many-body systems
- The nuclear force is not known
- Average BE of least bound nucleon ~ 8 MeV, Kinetic energy $T \sim 40$ MeV
- Relativistic effect could be important but $T \ll$ nucleon mass (938 MeV)

$$v = \sqrt{\frac{2T}{m}} = c \sqrt{\frac{2T}{mc^2}} \approx 0.3 c$$

- \rightarrow Quantum effects are certainly not negligible

$$\lambda = \frac{2\pi\hbar}{mv} = \frac{2\pi(\hbar c)}{(mc^2)(v/c)} \approx 4.5 \text{ fm}$$



The quantum treatment



- Ideally we should solve the many-nucleon Schrödinger equation

$$H |\Psi_n(1, 2, \dots, A)\rangle = E_n |\Psi_n(1, 2, \dots, A)\rangle$$

$$H = \sum_{i=1}^A T_i + \frac{1}{2} \sum_{i,j=1}^A V_{ij} + \frac{1}{6} \sum_{i,j,k=1}^A V_{ijk} + \dots$$

- \rightarrow *microscopic models* \leftarrow There is no *a priori* theory for V_{ij}
- Various parametrizations are employed which are good for different purposes
- Atomic physics: QED is known, only approximations are in methods for solution
- A typical microscopic model thus depends on a nucleon-nucleon interaction which necessarily contains parameters fitted to reproduce some experimental data.
- Even microscopic approaches are *models*.
- Until the nucleon-nucleon interaction can be derived from a more fundamental theory such as quantum chromodynamics, we will have to live with this situation



Mean Field Approximation



- The many-nucleon Schrödinger equation

$$H |\Psi_n(1, 2, \dots, A)\rangle = E_n |\Psi_n(1, 2, \dots, A)\rangle$$

$$H = \sum_{i=1}^A T_i + \frac{1}{2} \sum_{i,j=1}^A V_{ij} + \frac{1}{6} \sum_{i,j,k=1}^A V_{ijk} + \dots$$

Diagram illustrating the many-body expansion of the Hamiltonian. Two curved arrows point from the V_{ijk} term to the V_{ij} term, with a '0' below each arrow, indicating that the three-body term is neglected in the mean field approximation.

- Mean Field Approximation in the independent-particle picture

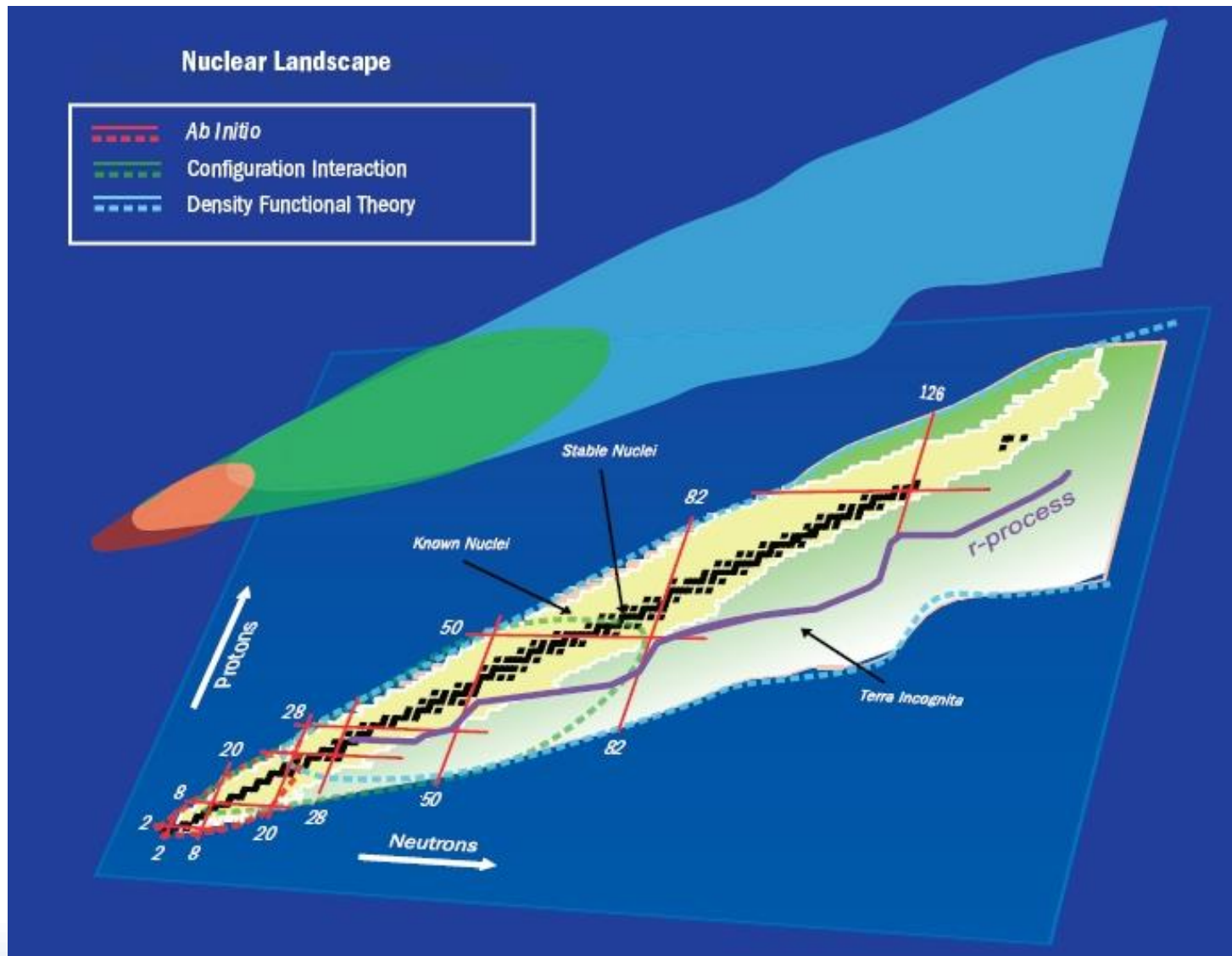
$$H = \sum_{i=1}^A (T_i + U_i) + \left(\frac{1}{2} \sum_{i,j=1}^A V_{ij} + U_i \right)$$

Diagram illustrating the Mean Field Approximation. A curved arrow points from the V_{ij} term to the U_i term, with a '0' below the arrow, indicating that the two-body interaction is approximated by a single-particle potential U_i .

- Choice of U_i is crucial



Present scenario





Motivation: Density dependence



- **Compressibility**
 - ▣ **Stiff & Soft matter – Giant resonance**
 - ▣ **BE(ρ)**
 - ▣ **Azimuthal anisotropy – RHIC data**
- **Inhomogeneous distribution**
 - ▣ **Clustering**
 - ▣ **Initial state dependence of RHI collisions**
- **Asymmetry**
 - ▣ **LDM**
 - ▣ **Neutron skin**
 - ▣ **Neutron stars**



Definitions



- Functional: A functional takes a function as input and gives a number as output. An example is: $F[f(x)] = y = \int_{-\infty}^{\infty} f(x) dx$
- ab-initio methods can be interpreted as a functional of the wavefunction, with the functional form completely known!

$$E[\Psi] = \frac{\int \Psi^*(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \hat{H} \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) d^3\vec{r}_1 d^3\vec{r}_2 \dots d^3\vec{r}_N}{\int \Psi^*(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) d^3\vec{r}_1 d^3\vec{r}_2 \dots d^3\vec{r}_N}$$

- In DFT the key variable is the electron density $n(\vec{r})$, which for a normalized Ψ is given by

$$n(\vec{r}) = N \int \Psi^*(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) d^3\vec{r}_1 d^3\vec{r}_2 \dots d^3\vec{r}_N$$

- This relation is reversible such that the GS wavefunction

$$\Psi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \Psi[n_0]$$



Hohenberg-Kohn theorem 1



The external potential (and hence the total energy), is a unique functional of the electron density.

Corollary: the ground state density uniquely determines the potential and thus all properties of the system, including the many-body wave function.

$$\Psi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \Psi[n_0]$$

Eg: The ground state properties of a many-electron system are uniquely determined by an electron density that depends on only 3 spatial coordinates.



- **The functional that delivers the ground state energy of the system, gives the lowest energy if and only if the input density is the true ground state density.**
- For any positive integer N and potential $v(\vec{r})$, a density functional $F[n]$ exists such that $E_{(v,N)}[n] = F[n] + \int v(\vec{r})n(\vec{r})d^3r$, obtains its minimal value at the ground-state density of N electrons in the potential $v(\vec{r})$.
- The minimal value of $E_{(v,N)}[n]$ is then the ground state energy of this system.
- ➔ The correct ground state electron density minimizes this energy functional.



Expressions



Ψ is a unique function of n_0 : $\Psi_0(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \Psi[n_0]$

The GS expectation value: $\mathcal{O}[n_0] = \langle \Psi[n_0] | \hat{\mathcal{O}} | \Psi[n_0] \rangle$

The GS energy: $E_0 = E[n_0] = \langle \Psi[n_0] | \hat{T} + \hat{V} + \hat{U} | \Psi[n_0] \rangle$

The contribution of the external potential $\langle \Psi[n_0] | \hat{V} | \Psi[n_0] \rangle$
$$V[n_0] = \int V(\vec{r}) n_0(\vec{r}) d^3r$$

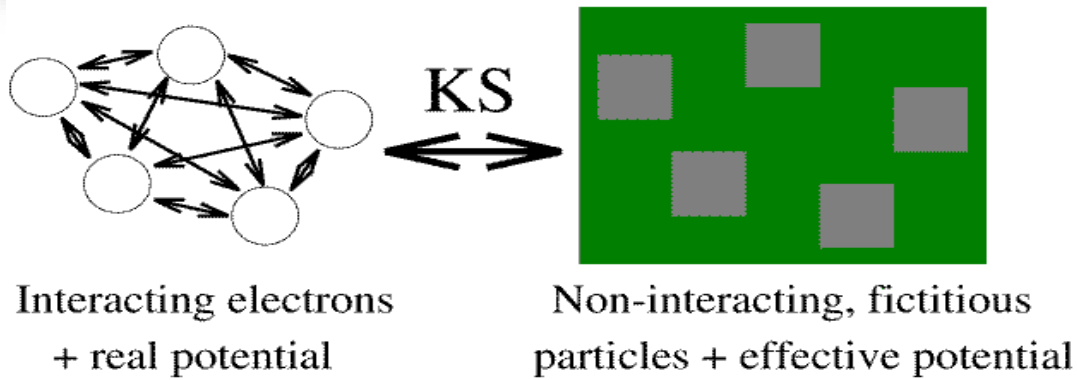
Having specified a system, i.e., having specified \hat{V} one then has to minimize the functional

$$E[n] = T[n] + U[n] + \int V(\vec{r}) n(\vec{r}) d^3r$$

with respect to $n(\vec{r})$.



KOHN –SHAM APPROACH



The system is replaced by a fictitious non-interaction system with same density as the real interacting system.

$$n(\vec{r}) \stackrel{\text{def}}{=} n_s(\vec{r}) = \sum_i^N |\phi_i(\vec{r})|^2$$

The Hamiltonian doesn't explicitly have an electron-electron interaction term:

$$H_s = T_s + V_s$$

T_s = non-interacting kinetic energy; V_s = effective potential

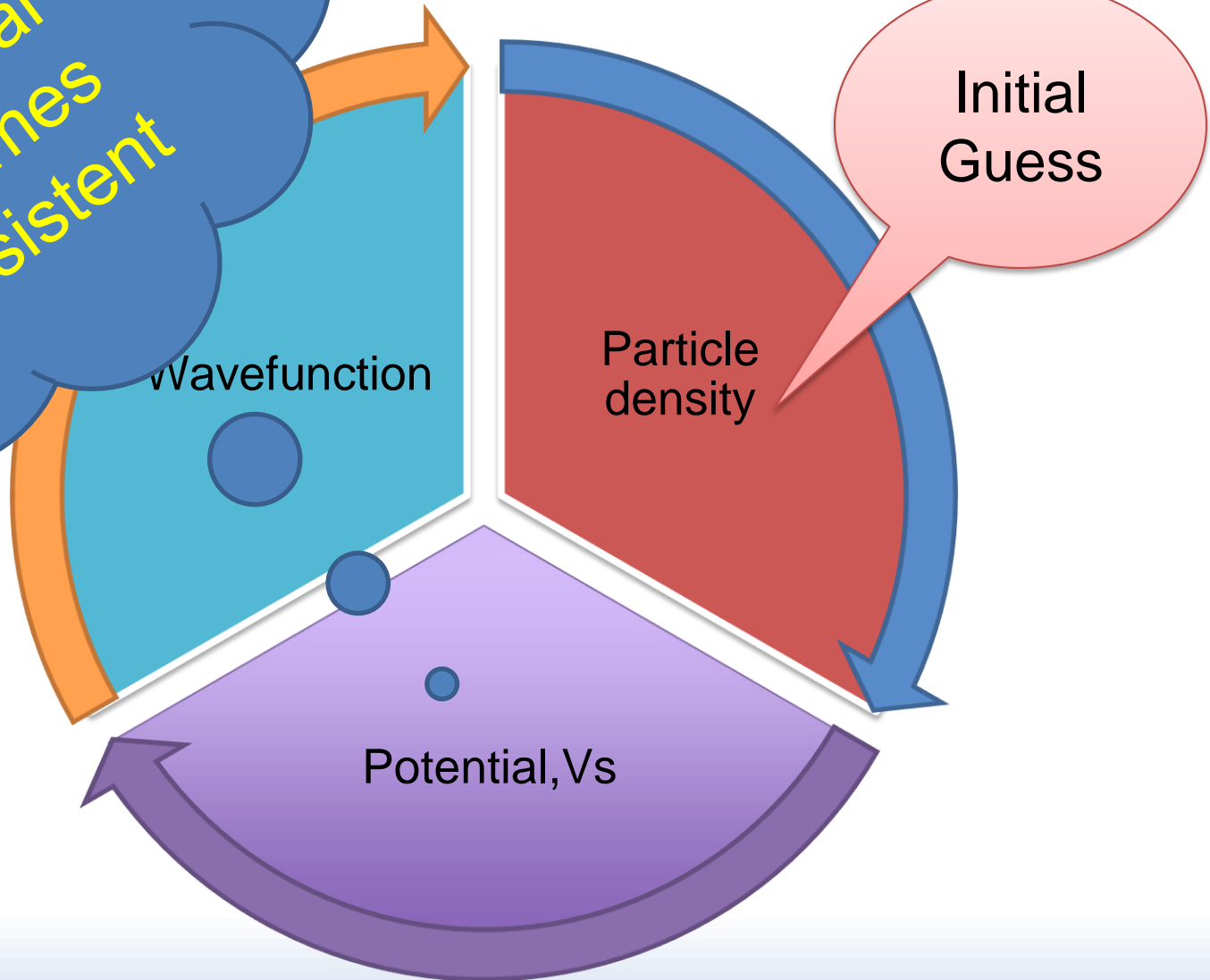
KS eqns are similar to time independent Schrodinger eqns with single particle wave functions:

$$\left[-\frac{\hbar^2}{2m} \nabla^2 + V_s(\vec{r}) \right] \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r})$$



KS eqns are solved in an iterative way

Potential
becomes
consistent





Relativistic fields



- Classical fields: space and time coordinates are treated similarly
- They are treated as parameters specifying the space-time continuum, with which the field variables are defined.
- Relativistic fields that manifests Lorentz covariance: $x'_\mu = a_\mu^\nu x_\nu$.
- Recap:

➡ Euler-Lagrange Eqn: $\frac{\partial L}{\partial q_k} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_k} = 0$ (6.5)

➡ Lagrangian density: $L = \int \mathcal{L}(\hat{x}) d^3x$, ($\hat{x}: ct, x_1, x_2, x_3$)

➡ $\frac{\partial \mathcal{L}}{\partial \psi_k} - \sum_\mu \frac{\partial}{\partial x_\mu} \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_k}{\partial x_\mu}} = 0$ (6.19)

➡ $\frac{\partial \mathcal{L}}{\partial \psi_k} - \partial_\mu \frac{\partial \mathcal{L}}{\partial (\partial_\mu \psi_k)} = 0$ (6.20)

➡ $T_{\mu\nu} = \frac{\partial \mathcal{L}}{\partial \frac{\partial \psi_k}{\partial x_\nu}} \frac{\partial \psi_k}{\partial x_\mu} - \mathcal{L} \delta_{\mu\nu}$ (6.58)



Covariant form of the KG equation



● Prove that

$$\blacksquare \mathcal{L}_{KG}(\hat{x}) = \frac{1}{2} [\partial^\mu \phi(\hat{x}) \partial_\mu \phi(\hat{x}) - m^2 \phi^2(\hat{x})] \text{ satisfies the EL eqn.} \quad (7.14)$$

$$\blacksquare H = \int T_{00} d^3x \quad (7.17)$$

● KG Equation

$$\blacksquare E^2 = c^2 p^2 + m^2 c^4$$

$$\blacksquare H^2 \psi = E^2 \psi, \quad E = i\hbar \frac{\partial \psi}{\partial t} \quad p = -i\hbar \nabla$$

$$\blacksquare \left[\nabla^2 - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \right] \psi = 0$$

$$\blacksquare \left[\square^2 - \frac{m^2 c^2}{\hbar^2} \right] \psi = 0$$

$$\blacksquare \partial^\mu = \frac{\partial}{\partial x_\mu} \rightarrow (\partial^\mu \partial_\mu + m^2) \psi = 0$$



Covariant form of the Dirac equation



$$H = c \boldsymbol{\alpha} \cdot \mathbf{p} + \beta mc^2$$

$$i\hbar \frac{\partial \psi}{\partial t} = (-i \boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + M\beta)\psi$$

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}; \quad \beta = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$$

$$\gamma^0 = \beta; \quad \boldsymbol{\gamma} = \beta \boldsymbol{\alpha} = (\gamma^1, \gamma^2, \gamma^3)$$

$$(i\gamma_\mu \partial^\mu - M)\psi = 0$$

$$\mathcal{L}_D = \bar{\psi}(i\gamma_\mu \partial^\mu - M)\psi$$

- Prove that \mathcal{L}_D satisfies Euler-Lagrange equation



The Lagrangians for various fields



- **Scalar field:** $\mathcal{L}_{KG} = \frac{1}{2} [\partial^\mu \phi \partial_\mu \phi - m^2 \phi^2]$

- **Dirac field:** $\mathcal{L}_D = \bar{\psi} (i\gamma_\mu \partial^\mu - M) \psi$

- **QED Lagrangian (Electromagnetic field)**

$$L = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \bar{\psi} (i\gamma^\mu \partial_\mu - m) \psi - e \bar{\psi} \gamma^\mu \psi A_\mu$$

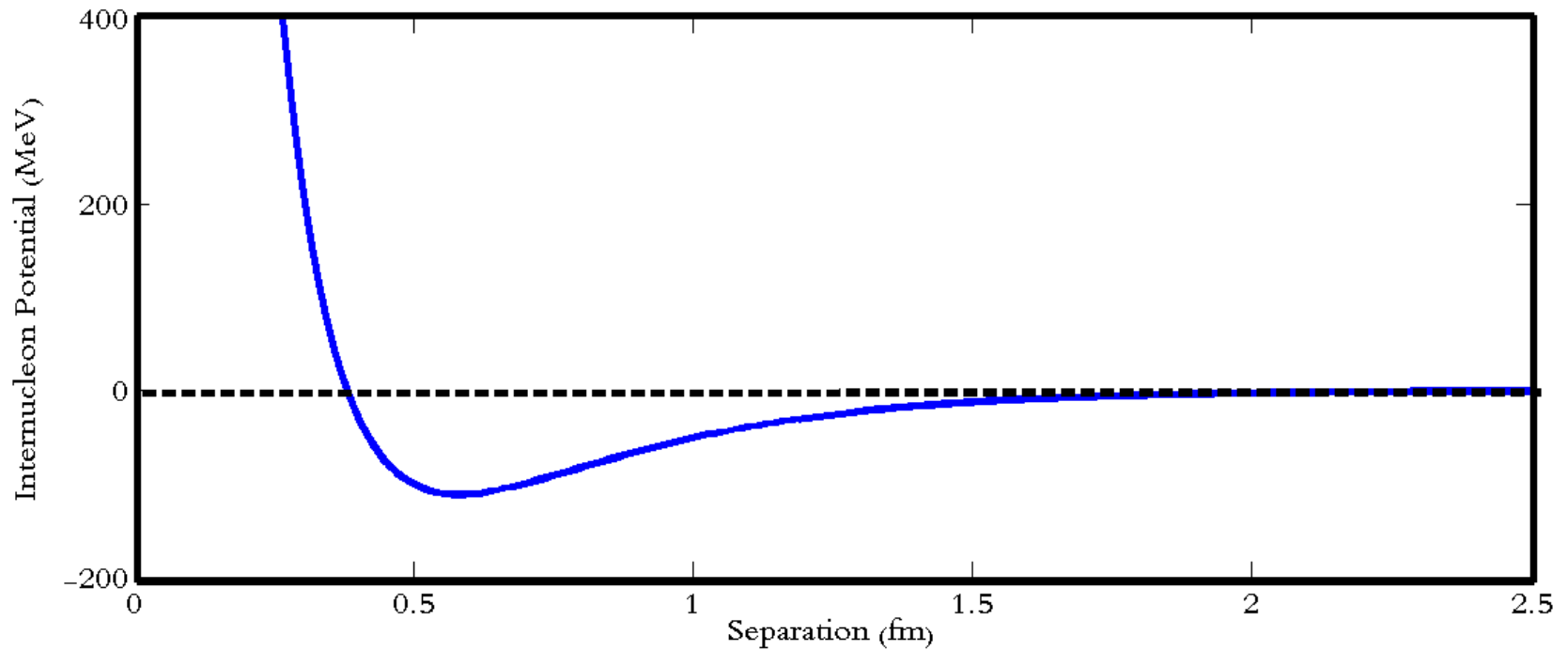
Electromagnetic field strength $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$

- **Scalar-Vector theory:**

$$L = \bar{\psi} [\gamma_\mu (i\partial^\mu - g_v V^\mu) - (M - g_s \phi)] \psi + \frac{1}{2} (\partial_\mu \phi \partial^\mu \phi - m_s^2 \phi^2) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2} m_v^2 V_\mu V^\mu$$
$$F_{\mu\nu} = \partial_\mu V_\nu - \partial_\nu V_\mu$$



- σ is a neutral scalar meson with spin parity, $J^\pi = 0^+$ and has mass of about $500 \text{ MeV}/c^2$.
- ω is neutral vector meson with spin parity, $J^\pi = 1^-$ and has mass of about $782 \text{ MeV}/c^2$.
- Thus, only vector field, V_μ (of omega mesons) and a scalar field, ϕ (of sigma mesons) are needed to describe the nuclear interaction.
- The nuclear potential is accounted by the σ & ω mesons, where the hard core repulsive part of the potential is accounted by the ω -mesons and the attractive part is accounted by the σ -mesons.
- The baryons are described by the field, ψ .



$$L = \bar{\psi}[\gamma_{\mu}(i\partial^{\mu} - g_v V^{\mu}) - (M - g_s \phi)]\psi + \frac{1}{2}(\partial_{\mu}\phi\partial^{\mu}\phi - m_s^2\phi^2) - \frac{1}{4}F_{\mu\nu}F^{\mu\nu} + \frac{1}{2}m_v^2 V_{\mu}V^{\mu}$$

$$F_{\mu\nu} = \partial_{\mu}V_{\nu} - \partial_{\nu}V_{\mu}$$



Equations of motion



$$\frac{\partial}{\partial x^\mu} \left[\frac{\partial L}{\partial (\partial q_i / \partial x^\mu)} \right] - \frac{\partial L}{\partial q_i} = 0$$

$$(\partial_\mu \partial^\mu + m_s^2) \phi = g_s \bar{\psi} \psi,$$

$$\partial_\mu F^{\mu\nu} + m_v^2 V^\nu = g_v \bar{\psi} \gamma^\mu \psi$$

$$[\gamma^\mu (i\partial_\mu - g_v V_\mu) - (M - g_s \phi)] \psi = 0$$

$$T_{\mu\nu} = -g_{\mu\nu} L + \frac{\partial q_i}{\partial x^\nu} \frac{\partial L}{\partial (\partial q_i / \partial x_\mu)}$$



Mean field theory



● Field operators \leftarrow expectation values \equiv classical fields

▣ $\phi \rightarrow \langle \phi \rangle \equiv \phi_0$

▣ $V_\mu \rightarrow \langle V_\mu \rangle \equiv \delta_{\mu 0} V_0$

● Now the field equations can be solved for constant ϕ_0 and V_0 :

▣ $\phi_0 = \frac{g_s}{m_s^2} \langle \bar{\psi} \psi \rangle = \frac{g_s}{m_s^2} \rho_s$

▣ $V_0 = \frac{g_v}{m_v^2} \langle \bar{\psi} \gamma^0 \psi \rangle = \frac{g_v}{m_v^2} \rho_B$

● With the classical meson fields the equation for Dirac field becomes linear

▣ $[i\gamma_\mu \partial^\mu - g_v \gamma^0 V_0 - (M - g_s \phi_0)]\psi = 0$



Effective mass



- $[i\gamma_\mu \partial^\mu - g_v \gamma^0 V_0 - (M - g_s \phi_0)]\psi = 0$
- Stationary state solutions for the free particles
 - ▣ $\psi = \psi(\mathbf{k}, \lambda) e^{i\mathbf{k} \cdot \mathbf{x} - i\epsilon(k)t}$
 - ▣ $\psi(\mathbf{k}, \lambda) \rightarrow$ four-component Dirac spinor, $\lambda \rightarrow$ spin index
- $(\boldsymbol{\alpha} \cdot \mathbf{k} + \beta M^*)\psi(\mathbf{k}, \lambda) = [\epsilon(k) - g_v V_0]\psi(\mathbf{k}, \lambda)$
- The effective mass M^* is defined as
 - ▣ $M^* = M - g_s \phi_0$



$$\mathcal{E} = T_{00}$$

$$P = \frac{1}{3} \langle T_{ii} \rangle \quad c_s^2 = g_s^2 \left(\frac{M^2}{m_s^2} \right) = 267.1$$

$$\mathcal{E} = \frac{g_v^2}{2m_v^2} \rho_B^2 + \frac{m_s^2}{2g_s^2} (M - M^*)^2 + \frac{\gamma}{(2\pi)^3} \int_0^{k_F} d^3k (k^2 + M^{*2})^{1/2}$$

$$P = \frac{g_v^2}{2m_v^2} \rho_B^2 - \frac{m_s^2}{2g_s^2} (M - M^*)^2 + \frac{1}{3} \frac{\gamma}{(2\pi)^3} \int_0^{k_F} d^3k \frac{k^2}{(k^2 + M^{*2})^{1/2}}$$

$$\rho_B = \frac{\gamma}{(2\pi)^3} \int_0^{k_F} d^3k = \frac{\gamma}{6\pi^2} k_F^3$$



Calculations



minimizing $\mathcal{E}(M^*)$

$$M^* = M - \frac{g_s^2}{m_s^2} \frac{\gamma}{(2\pi)^3} \int_0^{k_F} d^3k \frac{M^*}{(k^2 + M^{*2})^{1/2}}$$

$$M^* = M - \frac{g_s^2}{m_s^2} \frac{\gamma M^*}{4\pi^2} \left[k_F E_F^* - M^{*2} \ln \left(\frac{k_F + E_F^*}{M^*} \right) \right]$$

$$\text{where } E_F^* = (k_F^2 + M^{*2})^{1/2}$$

$$C_s^2 = g_s^2 \left(\frac{M^2}{m_s^2} \right) = 267.1 \qquad C_v^2 = g_v^2 \left(\frac{M^2}{m_v^2} \right) = 195.9$$

$$M = 939 \text{ MeV}, \qquad \hbar c = 197.3269631 \text{ MeV fm}$$

<http://www.wolframalpha.com> integrate $x^2/\sqrt{x^2+m^2}$

$$\int \frac{x^2}{\sqrt{x^2 + m^2}} dx = \frac{1}{2} x \sqrt{m^2 + x^2} - \frac{1}{2} m^2 \log \left(\sqrt{m^2 + x^2} + x \right) + \text{constant}$$



Solving transcendental equation: Secant method



$$x_n = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$$

$$x_n = x_{n-1} - f(x_{n-1}) \frac{x_{n-1} - x_{n-2}}{f(x_{n-1}) - f(x_{n-2})}$$

```
function func(x)
func=sin(x)
end
```

```
external func
x=secmethod(func,3.10)
print *, x
end
```

```
function secmethod(f,x00)
logical flag
x0=x00
f0=f(x0)
x1=x0+x0/100.0d0
f1=f(x1)
flag=.true.
do i=1,100
    x=x1-f1*(x1-x0)/(f1-f0)
    if(abs(x-x1).le.1e-4) then
        flag=.false.
        exit
    end if
    x0=x1
    f0=f1
    x1=x
    f1=f(x)
end do
if (flag) print *, 'No convergence'
secant=x
end
```




Solving for M^*



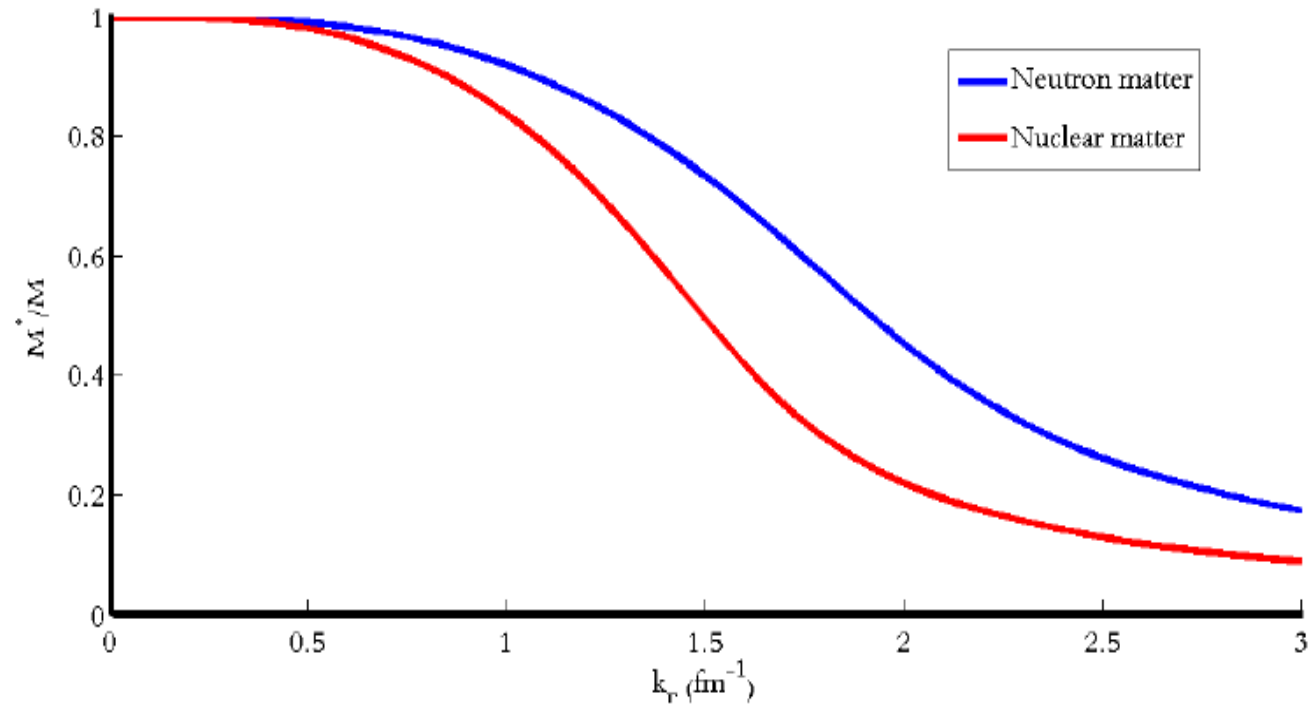
```
function rmstar(x)
common /set1/ rkf,gama,am,cs2,sv2,pi
amef=x
efef=sqrt(rkf**2+amef**2)
rmstar=COMPLETE THIS BY YOURSELF
end
```

```
external rmstar
common /set1/ rkf,gama,am,cs2,sv2,pi
read *,gama
pi=4.0*atan(1.0)
hc=197.3269804
am=939.0
cs2=267.1
cv2=195.9
amef=939.0
do i=0,50
    akf=float(i)/10.0
    rkf=hc*akf
    amef=secmethod(rmstar,amef)
    print *, akf,amef/939.0
end do
end
```

```
include 'secmethod.for'
```



Calculated M^*/M





Numerical integration: Simpson's 1/3 rule



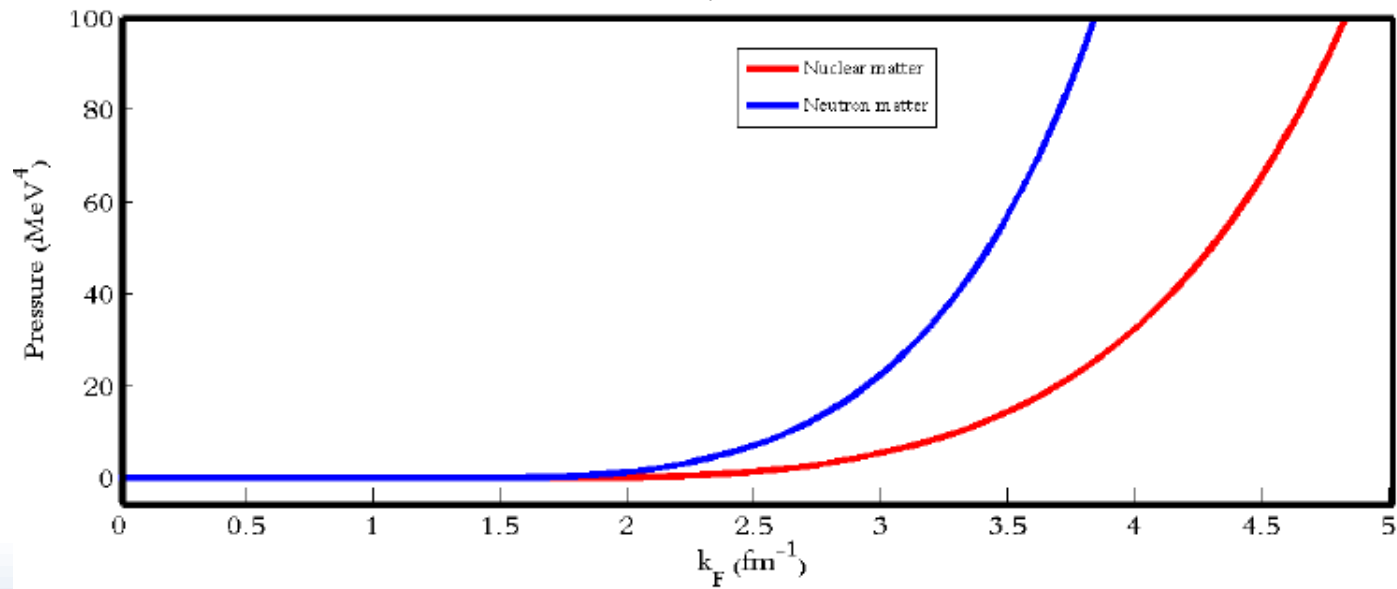
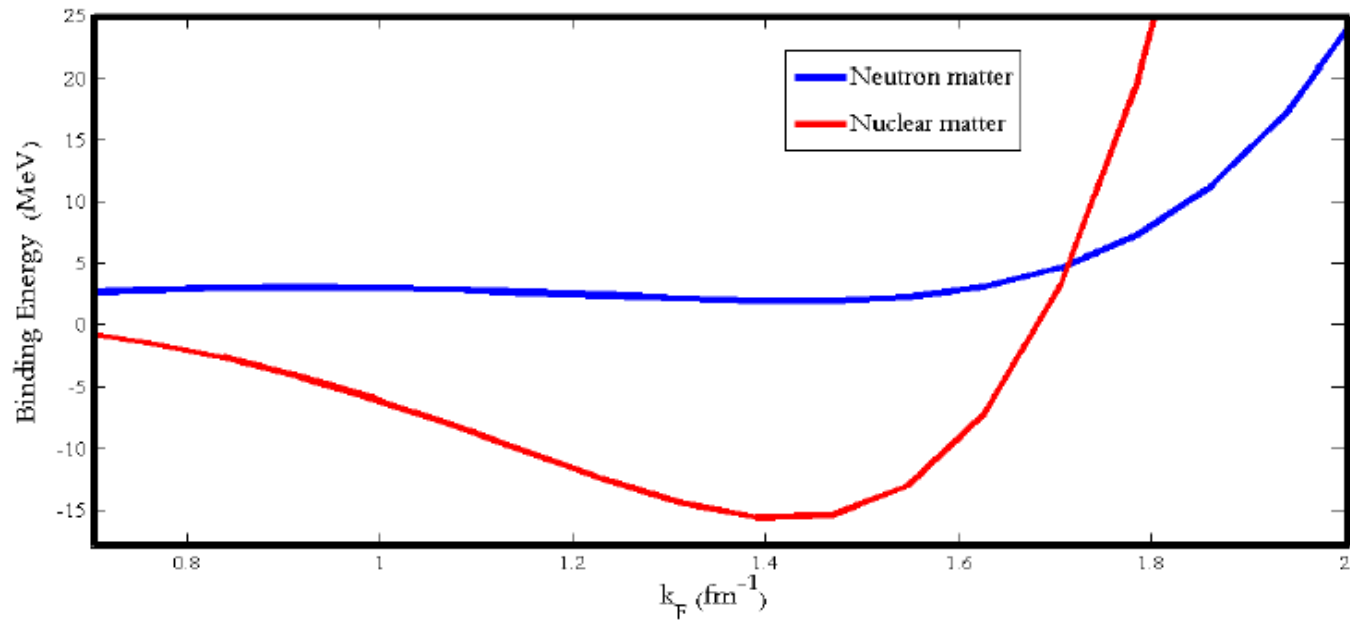
```
function simp(x,y,n)
dimension x(n),y(n)
h=abs(x(n)-x(1))/float(n-1)
sum=0.0
do i=1,n/2
    sum=sum+y(2*i-1)+4.0*y(2*i)+y(2*i+1)
end do
simp=sum*h/3.0
end
```

```
function rmstar(x)
common /set1/ rkf,gama,am,cs2,sv2,pi
parameter (nn=101)
dimension xx(nn),yy(nn)
amef=x
do i=1,nn
    xx(i)=dfloat(i-1)*rkf/dfloat(nn-1)
    efef=sqrt(xx(i)**2+amef**2)
    yy(i)=xx(i)**2*amef/efef
end do
rmstar=COMPLETE THIS BY YOURSELF
end
```

Excercise:
Extend this code to calculate E & P



Results of QHD-I





Check the numbers

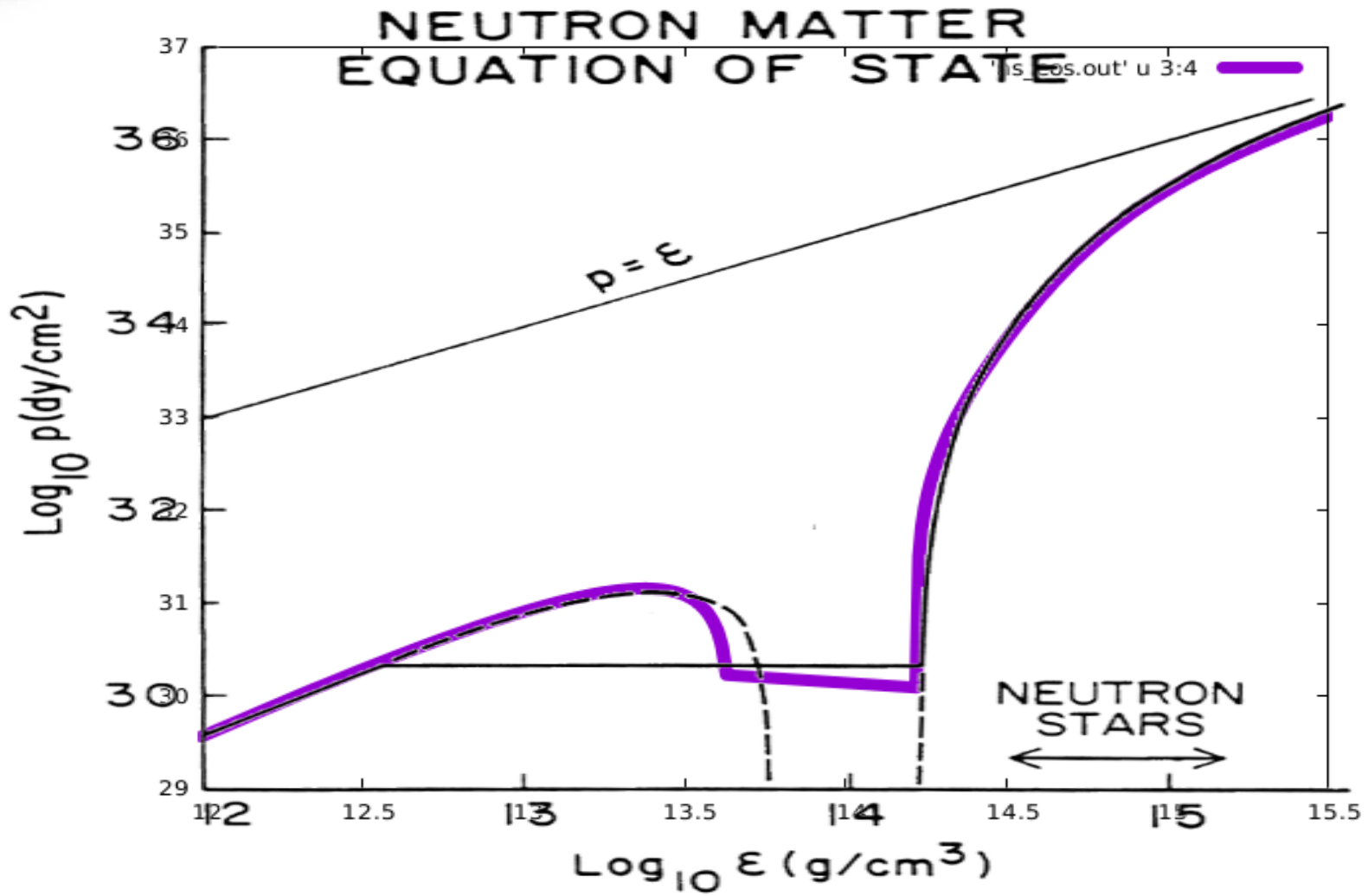


Fig. 14.6 of J.D. Walecka, Theoretical nuclear and subnuclear physics, 2e, World Scientific (2004)



Constants & conversions



- $1 \text{ erg} = 1 \text{ dyn}\cdot\text{cm} = 1 \text{ g}\cdot\text{cm}^2/\text{s}^2 = 6.241509074 \times 10^4 \text{ MeV}$
- $1 \text{ erg} = 10^{-7} \text{ J}$
- $1 \text{ eV} = 1.602176634 \times 10^{-19} \text{ J}$ (<https://physics.nist.gov/cgi-bin/cuu/Value?evj>)
- $1 \text{ eV} = 1.602176634 \times 10^{-19} \times 10^7 \text{ erg}$
- $1 \text{ MeV} = 1.602176634 \times 10^{-12} \times 10^6 \text{ erg} = 1.602176634 \times 10^{-6} \text{ erg}$
- $1 \text{ MeV}/\text{fm}^3 = 1.602176634 \times 10^{-6} / 10^{-3 \times 13} \text{ erg}/\text{cm}^3$
- $1 \text{ MeV}/\text{fm}^3 = 1.602176634 \times 10^{33} \text{ erg}/\text{cm}^3 = 1.602176634 \times 10^{33} \text{ dyn}/\text{cm}^2$
- $1 \text{ MeV}/c^2 = 1.782661921 \times 10^{-27} \text{ g}$
- $1 \text{ MeV}/\text{fm}^3 = 1.782661921 \times 10^{12} \text{ c}^2 \text{ g}/\text{cm}^3$

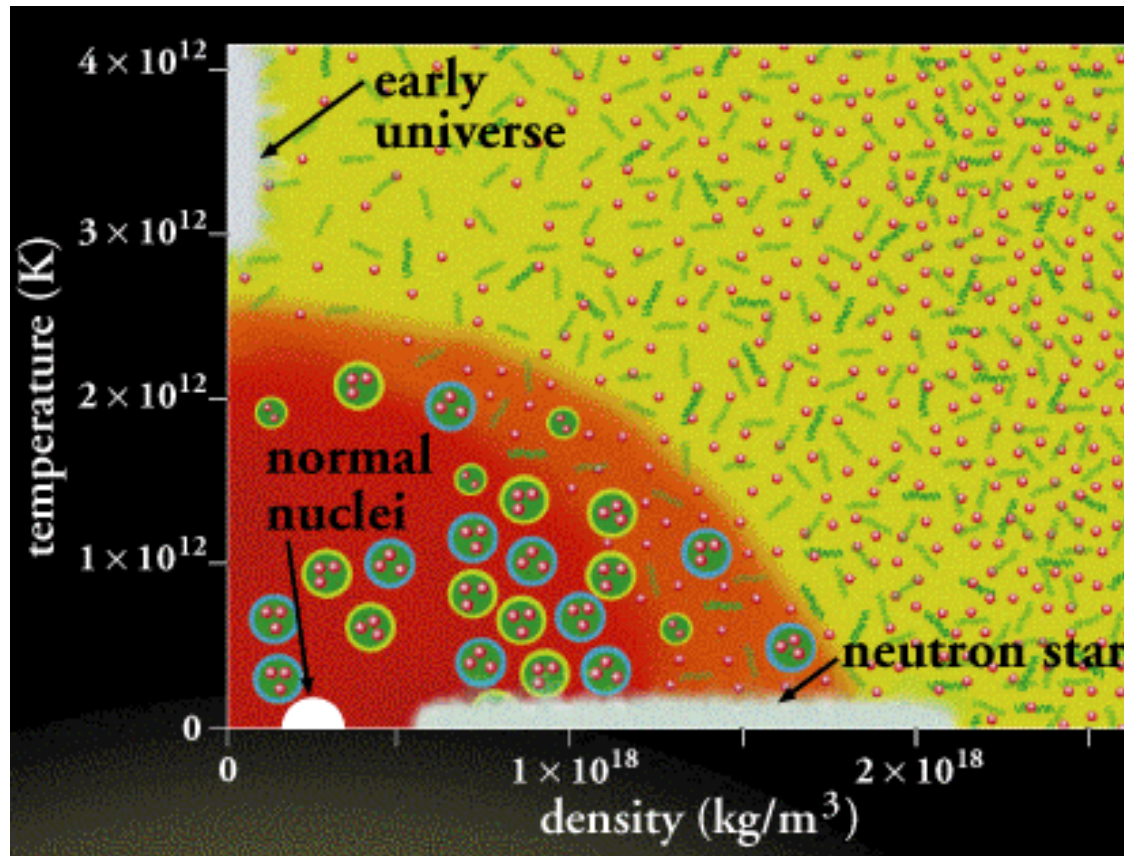
$$e = e \cdot 1.782661921 \cdot 10^{12} / hc^3$$

$$p = p \cdot 1.602176634 \cdot 10^{33} / hc^3$$

`write(*, '(2x, 4e14.5)') akf, amef/939.0, log10(e), log10(p)`

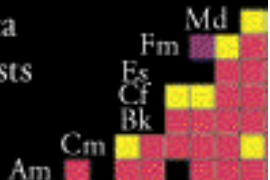


Neutron Star: Another Probe



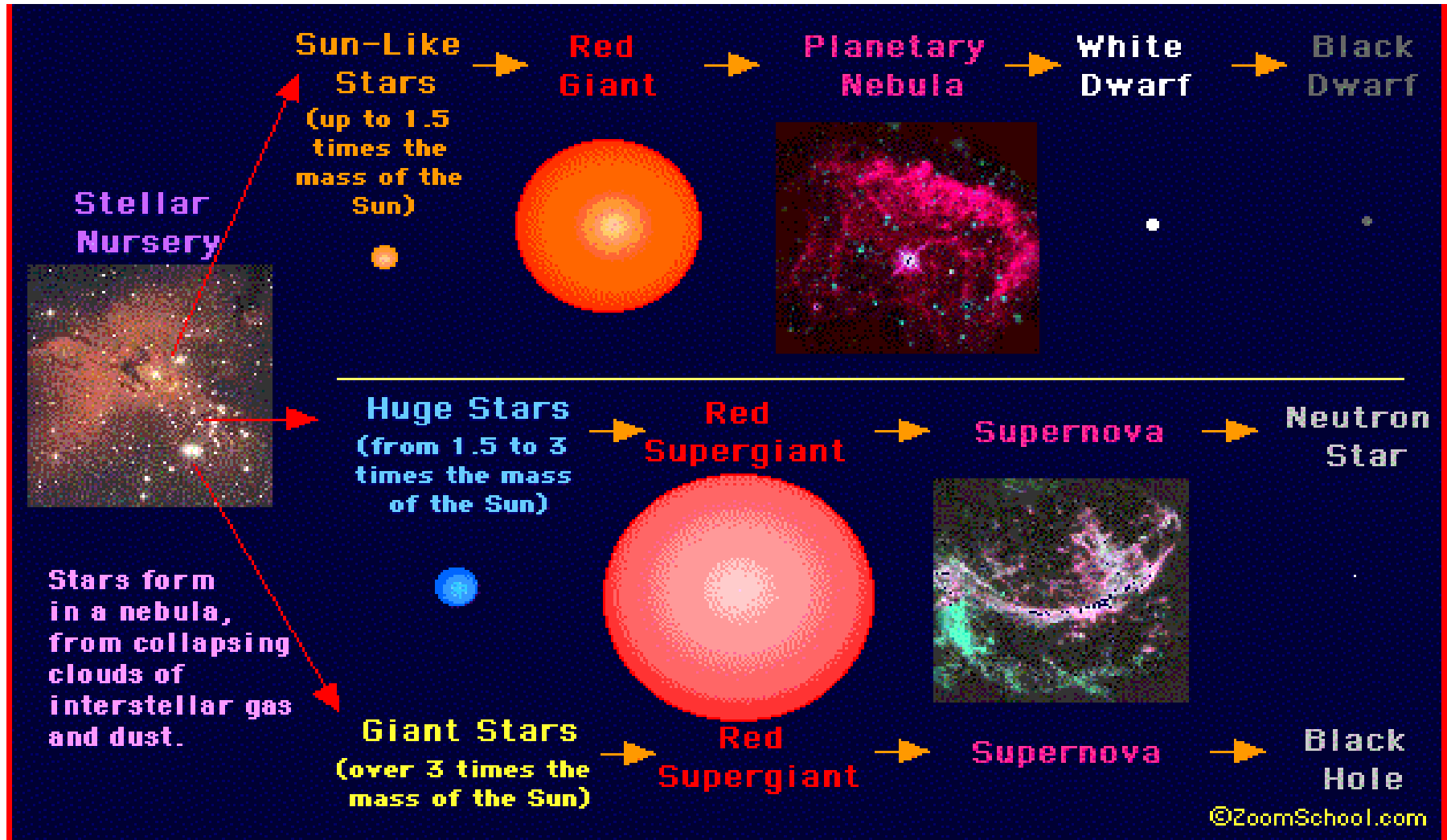
Phases of Nuclear Matter

Nuclear matter can exist in several phases. When collisions excite nuclei, individual protons and neutrons may evaporate from the nuclear fluid. At sufficiently high temperature or density, a gas of nucleons (red background) forms. At even more extreme conditions, individual nucleons may cease to have meaningful identities, merging into the quark-gluon plasma (yellow background). Current data provide hints that physicists have glimpsed the quark-gluon plasma.





The Lifecycle of Stars





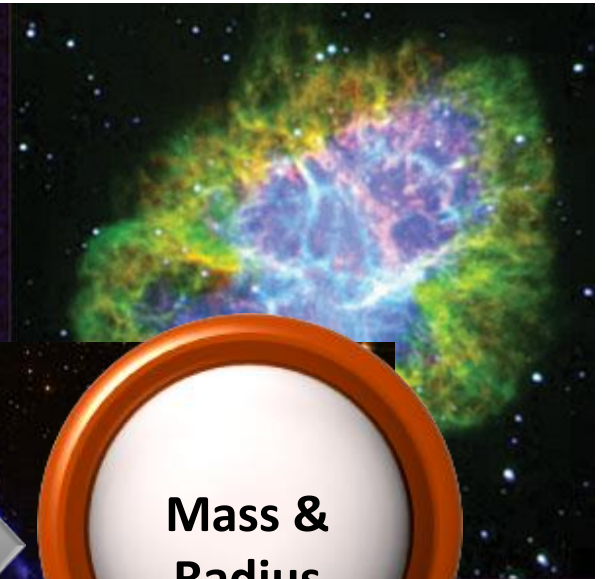
Neutron Star Observables



**Thermal
Spectra**



**Gravitational
Red Shift**

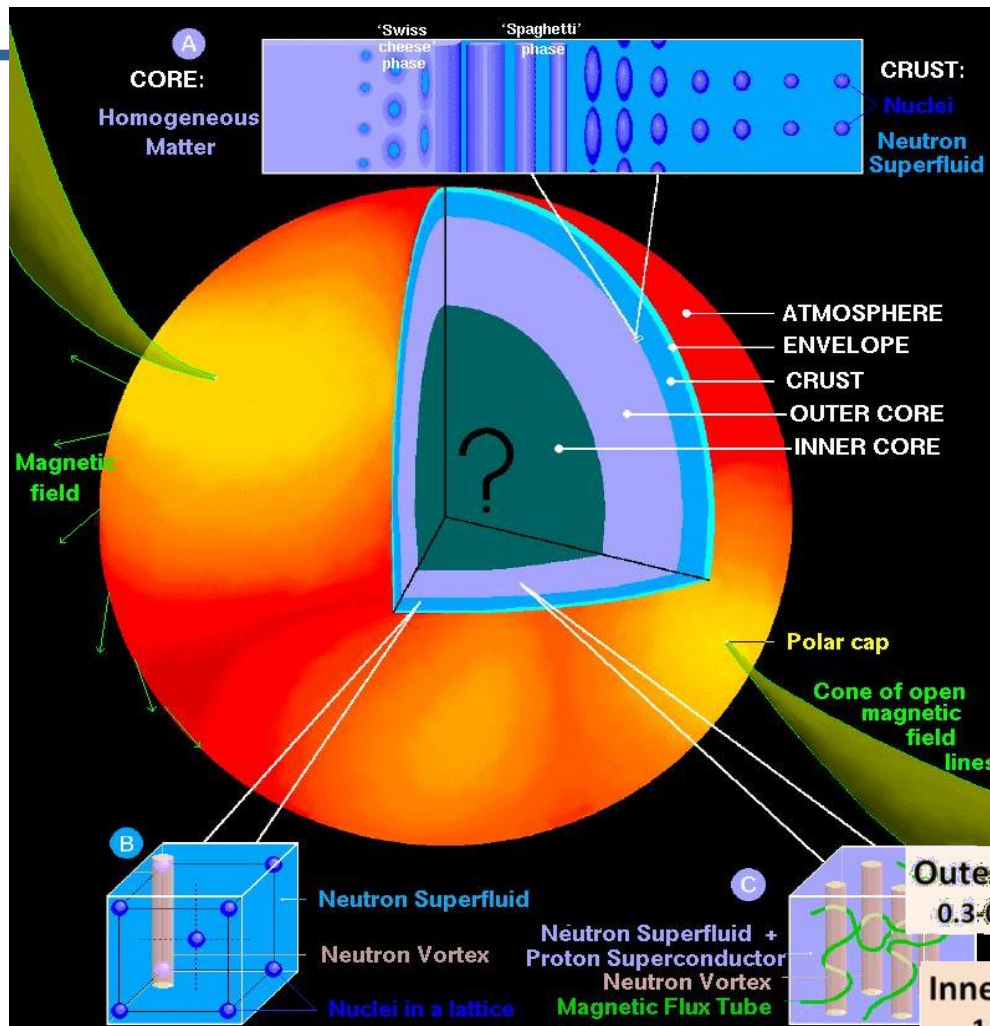


**Mass &
Radius**

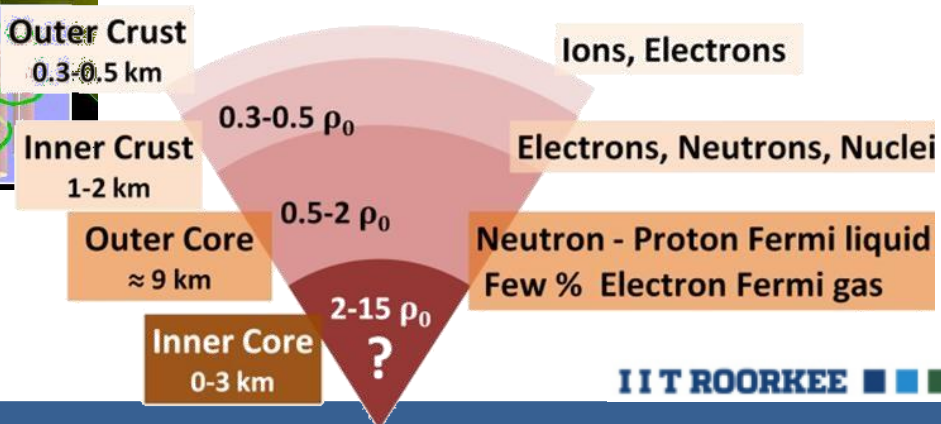




A Neutron Star: Surface and Interior

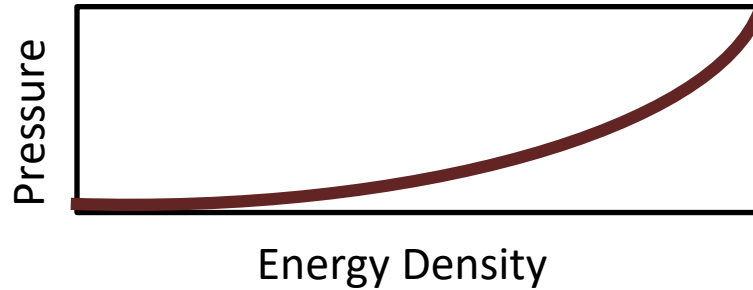


Lattimer & Prakash ,
Science 304, 536 (2004)





Neutron Star Calculations



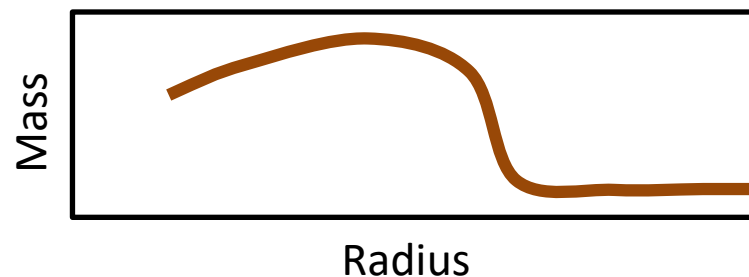
$$\frac{dP}{dr} = -(\mathcal{E} + P) \frac{m + 4\pi r^3 P}{r(r - 2m)}$$

$$\frac{dm}{dr} = 4\pi r^2 \mathcal{E}$$

$m(r)$ is the total integrated mass out to a radial distance r

R. C. Tolman, Phys. Rev. **55**, 364 (1939),

J. R. Oppenheimer and G.M. Volkoff, Phys. Rev. **55**, 374 (1939).





Solving ODE: Runge-Kutta method



$$\frac{dy}{dx} = f(x, y)$$

Given (x_0, y_0) , the solutions are $(x_1, y_1), (x_2, y_2) \dots (x_N, y_N)$

$$k_1 = hf(x_n, y_n)$$

$$k_2 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}\right)$$

$$k_3 = hf\left(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}\right)$$

$$k_4 = hf(x_n + h, y_n + k_3)$$

$$y_{n+1} = y_n + \frac{k_1}{6} + \frac{k_2}{3} + \frac{k_3}{3} + \frac{k_4}{6} + O(h^5)$$

```
external f
dimension vx(100),vy(100)
call rk4(f,0.0,1.0,10.0,100,vx,vy)
do i=1,100,10
    write(*,'(2x,f4.1,f10.5,e12.4)')
&        vx(i),vy(i),vy(i)
&        -(4.0+vx(i)*vx(i))*2/16.0
end do
end
```

```
subroutine rk4(f,x0,y0,xn,n,ax,ay)
dimension ax(n),ay(n)
h=(xn-x0)/float(n)
ax(1)=x0
ay(1)=y0
do i=2,n
    x=ax(i-1)
    y=ay(i-1)
    yk1=h*f(x,y)
    yk2=h*f(x+0.5*h,y+0.5*yk1)
    yk3=h*f(x+0.5*h,y+0.5*yk2)
    yk4=h*f(x+h,y+yk3)
    ax(i)=x+h
    ay(i)=y+(yk1+2.0*(yk2+yk3)+yk4)/6.0
end do
end

function f(x,y)
    f=x*sqrt(y)
end
```

$$\frac{dy}{dx} = x\sqrt{y}$$

Wolfram: $y'-x*\sqrt{y} = 0$

$$y(x) = \frac{1}{16} (4c_1 x^2 + 4c_1^2 + x^4)$$



II order ODE: Two coupled I order ODEs



$$\frac{d^2y}{dx^2} + q(x)\frac{dy}{dx} = r(x)$$

$$\frac{dy}{dx} = z(x)$$

$$\frac{dz}{dx} = r(x) - q(x)z(x)$$

$$m \frac{d^2x}{dt^2} = F(x)$$

$$\frac{dx}{dt} = v$$

$$\frac{dv}{dt} = F(x)/m$$

$$\frac{dy_i(x)}{dx} = f_i(x, y_1, \dots, y_N)$$

```
subroutine rk4(x0,y10,y20,xn,n,ax,ay1,ay2,f1,f2)
implicit real*8 (a-h,o-z)
dimension ax(0:n),ay1(0:n),ay2(0:n)
```

```
h=(xn-x0)/dfloat(n)
ax(0)=x0
ay1(0)=y10
ay2(0)=y20
```

```
do i=1,n
```

```
  x=ax(i-1)
  y1=ay1(i-1)
  y2=ay2(i-1)
```

```
  y1k1=h*f1(x,y1,y2)
  y2k1=h*f2(x,y1,y2)
```

```
  y1k2=h*f1(x+0.5d0*h,y1+0.5d0*y1k1,y2+0.5d0*y2k1)
  y2k2=h*f2(x+0.5d0*h,y1+0.5d0*y1k1,y2+0.5d0*y2k1)
```

```
  y1k3=h*f1(x+0.5d0*h,y1+0.5d0*y1k2,y2+0.5d0*y2k2)
  y2k3=h*f2(x+0.5d0*h,y1+0.5d0*y1k2,y2+0.5d0*y2k2)
```

```
  y1k4=h*f1(x+h,y1+y1k3,y2+y2k3)
  y2k4=h*f2(x+h,y1+y1k3,y2+y2k3)
```

```
  ax(i)=x+h
  ay1(i)=y1+(y1k1+y1k2+y1k2+y1k3+y1k3+y1k4)/6.0d0
  ay2(i)=y2+(y2k1+y2k2+y2k2+y2k3+y2k3+y2k4)/6.0d0
```

```
end do
end
```



II order ODE: Exercises



- Projectile motion
- Rutherford scattering
- Solving Schrodinger equation with boundary conditions
 - ▣ Particle in an infinite square well potential
 - ▣ Particle in a harmonic oscillator potential
 - ▣ Particle in finite potentials
- Continuity equation



Solving the TOV equations



```
real*8 function f1(x,y1,y2)
implicit real*8 (a-h,o-z)
common/cons/ams,ecf,c2,gc,g,ak,pi
f1 = -(gc/(x**2*c2))
&      *(eps(y1) + y1)
&      *(y2 + (4.0d0*pi*x**3*y1)/c2)
&      /(1.0d0 - 2.0d0*gc*y2/(x*c2))
end
```

```
real*8 function f2(x,y1,y2)
implicit real*8 (a-h,o-z)
common/cons/ams,ecf,c2,gc,g,ak,pi
f2 = 4.0d0*pi*x**2*eps(y1)/c2
end
```

$$P = K\varepsilon^\gamma \qquad \varepsilon = \left(\frac{P}{K}\right)^{1/\gamma}$$

```
real*8 function eps(p)
implicit real*8 (a-h,o-z)
common/cons/ams,ecf,c2,gc,g,ak,pi
eps = ecf*(p/(ecf*ak))**(1.0/g)
end
```

```
implicit real*8 (a-h,o-z)
external f1,f2
dimension ax(0:2000),ap(0:2000),am(0:2000)
common/cons/ams,ecf,c2,gc,g,ak,pi
ak=8.876746957d-4
g = 5.0d0/3.0d0
ams = 1.989d33
ecf = 1.6022d33
c2 = 8.987551787d20
gc = 6.67408d-8
pi = 4.0d0*datan(1.0d0)
np=2000
open(1,file='tov.out',status='unknown')
do j=1,40
  p0 = 10**((dfloat(j)/10.0)*ecf)
  call rk4(1.d0,p0,0.d0,20.d5,np,ax,ap,am,f1,f2)
  do i=0,np
    if((ap(i).ne.ap(i)).or.(ap(i).le.0)) exit
  enddo
  write(1,'(2x,2f12.4)')ax(i-1)/1.0d5,am(i-1)/ams
enddo
end
```



Utilizing a tabulated EoS: Linear interpolation

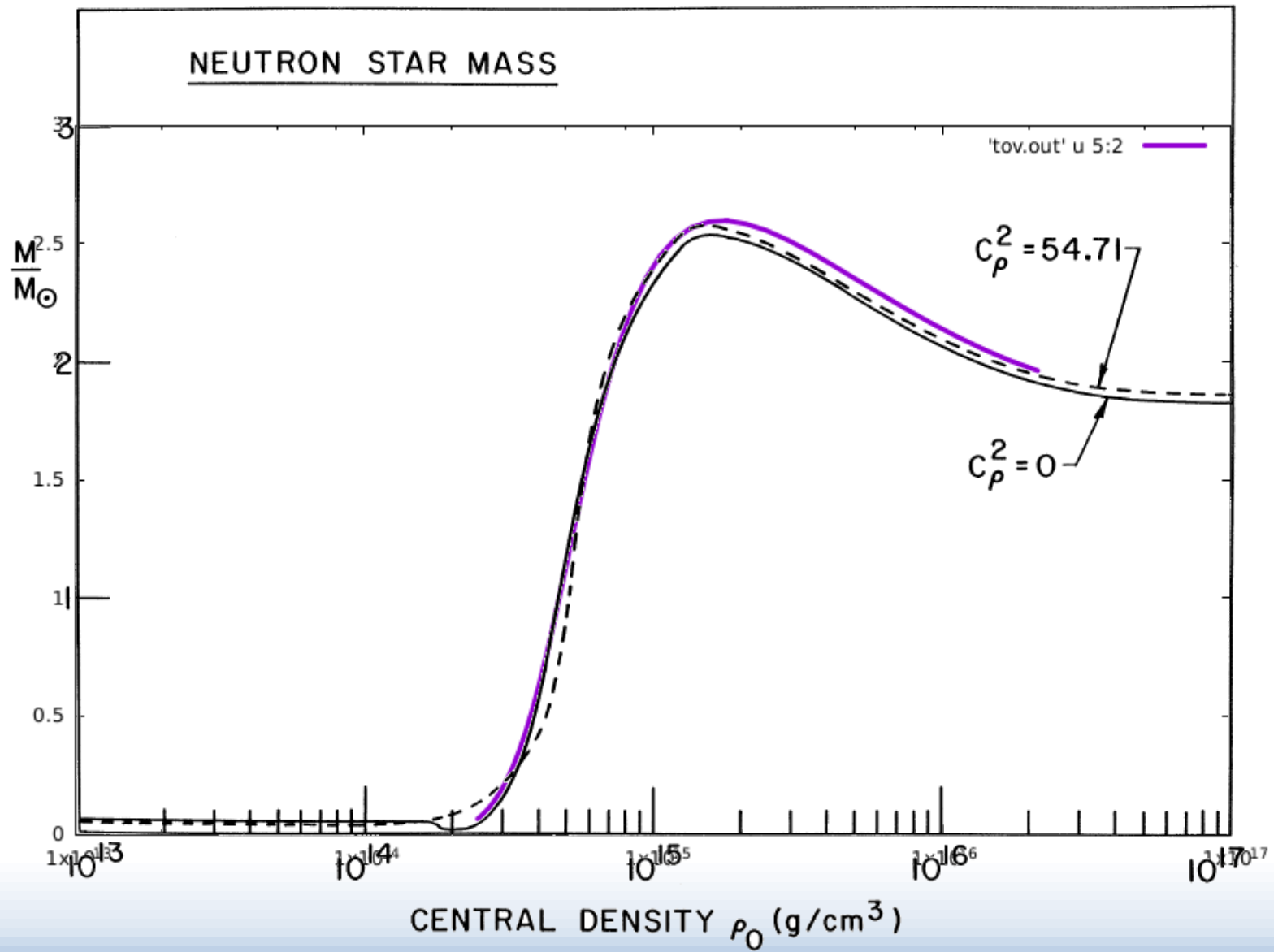


```
real*8 function lineint(x,xi,yi,ni)
implicit real*8 (a-h,o-z)
dimension xi(ni),yi(ni)
if(x.lt.xi(1))then
    n=1
else
    if(x.gt.xi(ni))then
        n=ni-1
    else
        do i=2,ni
            if(x.le.xi(i))then
                n=i-1
                exit
            endif
        end do
    endif
    100
endif
lineint=(x-xi(n))*(yi(n+1)-yi(n))/(xi(n+1)-xi(n))+yi(n)
end
```

```
real*8 function eps(p)
implicit real*8 (a-h,o-z)
common/cons/ams,ecf,c2,gc,g,ak,pi
common/eos/xi(1000),yi(1000),ni
real*8 lineint
eps = ecf*lineint(p/ecf,xi,yi,ni)
end

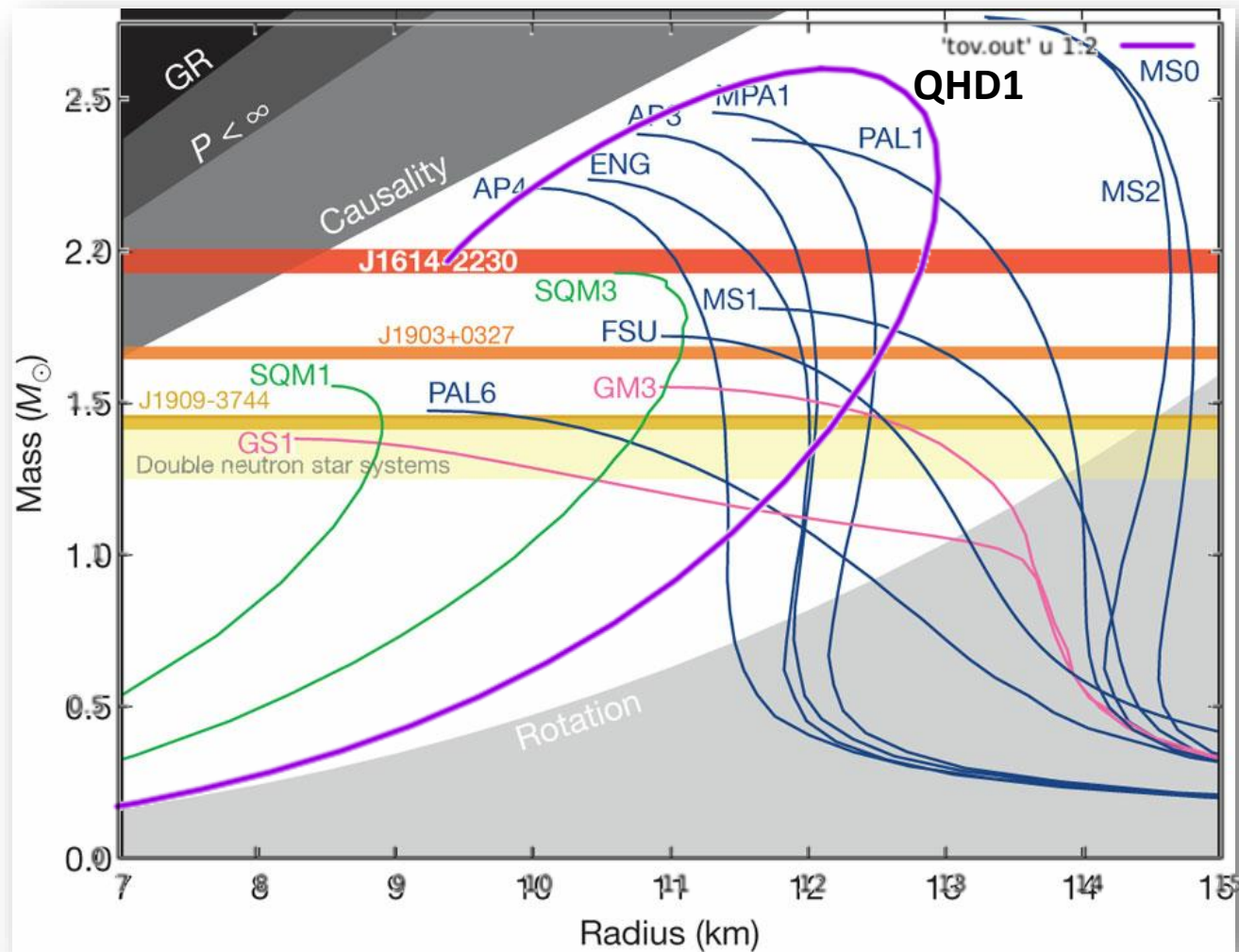
open(4,file='eos.dat',status='unknown')
i=1
do while (.true.)
    read(4,*,end=100)yi(i),xi(i)
    print *,i,xi(i),yi(i)
    i=i+1
enddo
ni=i-1

e0=eps(p0)
d0=e0/c2
write(*,*) ax(i-1)/1.0d5,am(i-1)/ams,d0
```



The 2 Solar Mass NS



P.B. Demorest, T. Pennucci, S.M. Ransom, M.S.E. Roberts, and J. W. T. Hessels, *Nature* **467**, 1081 (2010)

Thank You

