4/21/03

So we've seen that the leading order effective action with an auxiliary field σ leads to an energy functional.

- Before trying to generalize this result in an effective field theory version of density functional theory we'll take a look at some practical nuclear phenomenology for finite nuclei with the Skyrme interaction.
- This is also relevant background for upcoming discussions of the nuclear shell model.

- If we can cast the problem into the form of independent particles (ie., no explicit interactions between them) bound by a potential like $\sigma_c(\vec{x})$ [which we call a single-particle potential] what would that potential look like and what can we say about the single-particle wave functions.

- Let's consider spherically symmetric nuclei first.
  $\Rightarrow$ what quantum numbers specify the single-particle levels?

- In anticipation of the importance of a spin-orbit potential, we consider eigenstates of
  - orbital angular momentum $\vec{l}^2 \Rightarrow l(l+1)$
  - spin $\vec{s}^2 \Rightarrow s(s+1)$ with $s = 1/2$
  - total angular momentum $\vec{j}^2 = (\vec{l}+\vec{s})^2 \Rightarrow j(j+1)$
  - z-component of $\vec{j} \Rightarrow j_z \Rightarrow m_j$
  - isospin $\vec{t} \Rightarrow t(t+1)$ with $t = 1/2$
  - component of $\vec{t}$: $m_t = +1/2$ for proton, $-1/2$ for neutron

$\Rightarrow$ $\boxed{|\alpha\rangle \equiv |n\, l\, \tfrac{1}{2}\, j\, m_j\, ;\, \tfrac{1}{2}\, m_t\rangle}$ in second-quantized form

or $\boxed{\varphi(\vec{r})_{nsljm_j} = \langle \vec{r}\,|n\, l\, s\, j\, m_j\rangle = \varphi_{nlj}(r) \sum_{m_l m_s} \langle l\, m_l\, \tfrac{1}{2}\, m_s | j\, m_j \rangle Y_{lm_l}(\theta,\varphi)\, \chi_{m_s}}$

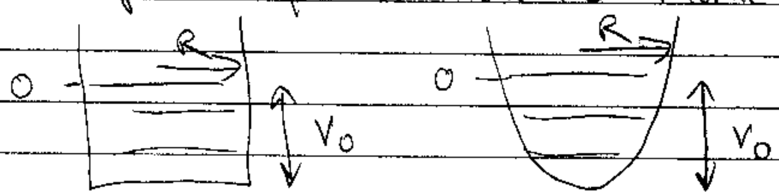
(where we've suppressed the isospinor).

4/21/03

- Note that $\boxed{j = |l \pm \tfrac{1}{2}|}$ and the parity of a state is $\boxed{(-1)^l}$

- The principle quantum number $n = 1, 2, 3, \ldots$ orders the wave function in terms of the number of radial nodels.

- The "empirical" single-particle potential (that is, a shape that reproduces observed properties of nuclei is an interpolation between two familiar, analytically solvable, potentials: the 3-d spherical square well and the harmonic oscillator:



- Note that we do not put the zero of the potential at the bottom.

- Let's recall the solutions to these central potential problems.

- Square well of radius R:
  - eigenfunctions: $\boxed{\Psi_{nlm_l}(\vec{r}) = N_{nl}\, j_l(kr)\, Y_{lm_l}(\Omega_r)}$ (regular at origin)

  with energy eigenvalues $\boxed{\epsilon = \frac{\hbar^2 k^2}{2m} - V_0}$
  - The eigenvalue spectrum follows from the vanishing of the wave function at the boundary $\boxed{j_l(kR) = 0}$

$$\Rightarrow \boxed{k_{nl} R = x_{nl}} \qquad \left(\text{so } \boxed{\epsilon_{nl} = \frac{\hbar^2 k_{nl}^2}{2m} - V_0}\right)$$

where x_{nl} is the n^{th} interior zero of the l^{th} spherical Bessel function (how would you find these?).

- The normalization factor is $\boxed{N_{nl}^2 = \frac{2}{R^3} \frac{1}{j_{l+1}^2(x_{nl})}}$

4/21/03

Harmonic Oscillator:

$$\boxed{V(r) = -V_0\left[1-\left(\frac{r}{R}\right)^2\right] = -V_0 + \frac{1}{2}m\omega^2 r^2} \quad \text{with} \quad \boxed{\frac{V_0}{R^2} = \frac{1}{2}m\omega^2}$$

The eigenfunctions take the form

$$\boxed{\Psi_{n\ell m}(\vec{r}) = \frac{u_{n\ell}(r)}{r} Y_{\ell m}(\Omega_r)}$$

where $u_{n\ell}(r)$ is a solution to

$$\boxed{\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{1}{2}m\omega^2 r^2 + \frac{\hbar^2}{2m}\frac{\ell(\ell+1)}{r^2} - (\epsilon_{n\ell}+V_0)\right]u_{n\ell}(r) = 0}$$

which can be written $\boxed{u_{n\ell}(q) = N_{n\ell}\, q^{\ell+1} e^{-\frac{1}{2}q^2} L^{\ell+1/2}_{n-1}(q^2)}$

with $\boxed{L^a_p(z) = \frac{\Gamma(a+p+1)}{\Gamma(p+1)}\frac{e^z}{z^a}\frac{d^p}{dz^p}\left(z^{a+p}e^{-z}\right)}$ ⇒ Laguerre polynomials

with $\boxed{q \equiv r/b}$ $\boxed{\hbar\omega = \hbar^2/mb^2}$ and $n = 1, 2, \dots, \infty$.

The normalization is $\boxed{N^2_{n\ell} = \frac{2(n-1)!}{b\left[\Gamma(n+\ell+\frac{1}{2})\right]^3}}$

and $\boxed{\epsilon_{n\ell} = \hbar\omega\left(N+\frac{3}{2}\right) - V_0}$ $\boxed{N = 2(n-1)+\ell = 0, 1, 2, \dots, \infty}$

- Now consider the handout with the energy levels of the square well and the harmonic oscillator, with an intermediate shape approximating the nuclear single-particle potential.
  - This potential will be finite depth

    but, except for levels near the surface, there is not a large effect on the energy from taking the boundaries to infinity (what is the effect on wave functions?)
  - Note the oscillator shells and the degeneracies.
  - n and l are good throughout. Why is higher l lowered most from HO to square well?

4/21/03

- The handouts show experimental evidence that a single-particle picture with energy levels like these is realistic (nucleon knock-out reactions).

- But there is also strong evidence for shell closure effects (cf. the "magic numbers" for atoms in the periodic table of the elements) that occur at 2, 8, 20, 28, 50, 82, 126, ...
  - These do not agree with the energy level figure after the first 3.
  - See other pictures for evidence of single particle structure and splitting of levels
    - (last page) deviation of nuclear masses (or binding energy) from mean value shows largest negative deviations at magic numbers.
    - energy of 2^+ excitation is extra large at magic numbers
    - $(p, 2p)$ knockout $\Rightarrow$ levels in ^{16}O
    - $^{A}Z(d,p)^{A+1}Z$ deuteron stripping
    - (not shown) $(e, e'p)$ proton knock out

show spectrum.

wave function: last quarter from (e,e') experiments $^{206}Pb - ^{205}Tl$

- Mayer and Jensen first suggested attractive single-particle spin-orbit term:

$$\boxed{H' = -\alpha(r)\vec{l}\cdot\vec{s}}$$

Recall that:

$$\boxed{\begin{aligned}\vec{l}\cdot\vec{s}\,|n\,l\,\tfrac{1}{2}\,j\,m_j\rangle &= \tfrac{1}{2}(\vec{j}^2-\vec{l}^2-\vec{s}^2)\,|n\,l\,\tfrac{1}{2}\,m_j\rangle \\ &= \tfrac{1}{2}[j(j+1)-l(l+1)-s(s+1)]\,|n\,l\,\tfrac{1}{2}\,j\,m_j\rangle\end{aligned}}$$

- also, $s = 1/2$ so $\boxed{j = l + 1/2}$ or $\boxed{j = l - 1/2}$ (for $l > 0$, no spin-orbit).

4/21/03

In these configurations,

stretched: $\boxed{j = l + 1/2} \Rightarrow \boxed{\langle \vec{l} \cdot \vec{s} \rangle = l/2}$

jack-knifed: $\boxed{j = l - \frac{1}{2}} \Rightarrow \boxed{\langle \vec{l} \cdot \vec{s} \rangle = -(l+1)/2}$

$\Rightarrow \boxed{\epsilon_{l-\frac{1}{2}} - \epsilon_{l+\frac{1}{2}} = \alpha_{nl} \frac{1}{2}(2l+1)}$ "spin-orbit splitting"

where $\boxed{\alpha_{nl} \equiv \int u_{nl}^2(r)\, \alpha(r)\, dr}$

- $\alpha(r)$ is surface peaked, e.g. $\boxed{\alpha(r) = -0.5\,\text{fm}^2 \frac{1}{r}\frac{dV}{dr}}$

- For fixed l and j, the $2j+1$ degenerate m_j states form a "j-shell"

- Attractive $\vec{l} \cdot \vec{s} \Rightarrow \alpha_{nl} > 0 \Rightarrow$ stretched (higher j) for given l is lower in energy
  - e.g. $1d^{5/2}$ is lower than $1d^{3/2}$, and so on.

$\Rightarrow$ check out the 2nd spectrum.

- Notice the depression of high l stretched states is sufficient to create new shell closures
  $\Rightarrow$ nuclear magic numbers!

- Verify in the figure the observations above:
  - splitting as function of l

- In QED, spin-orbit force is a <u>relativistic</u> effect
  - electromagnetic version is much too small in nuclear case
  - motivation for "relativistic mean-field models"
    $\Rightarrow$ nucleons move in large, self-consistent scalar and vector fields
  - non-relativistic precision calculations require 3-body forces to get spin-orbit

4/21/03

- How do we get the independent particle potential?
  - The nucleon-nucleon potential obtained from fitting N-N phase shift data (more later!) does not lead to a mean-field potential directly (e.g. in Hartree-Fock as in our simple expansion).

- Instead we introduce an "effective interaction", which, in the presence of other nucleons gives the same result (in a limited domain) as a full calculation with the "bare" interaction.

- The Skyrme interaction was proposed back in 1956 by Skyrme but was not applied to nuclei until the early seventies. It remains one of the most common approaches to properties of medium to heavy nuclei. [See "New Skyrme interaction for normal and exotic nuclei", B.A. Brown, Phys. Rev. C <u>58</u> (1998) 220.]

- It has a form very much like our effective field theory expansion:

$$\boxed{V = \sum_{i<j} V(i,j) + \sum_{i<j<k} V(i,j,k)}$$

with

$$\boxed{\begin{aligned} V(1,2) = {} & t_0(1+x_0 P^\sigma)\,\delta(\vec{r}_1-\vec{r}_2) \\ & + \tfrac{1}{2}t_1\left[\delta(\vec{r}_1-\vec{r}_2)\vec{k}'^2 + \vec{k}^2\,\delta(\vec{r}_1-\vec{r}_2)\right] \\ & + t_2\,\vec{k}'\,\delta(\vec{r}_1-\vec{r}_2)\,\vec{k} + iW_0(\vec{\sigma}^{(1)}+\vec{\sigma}^{(2)})\cdot\vec{k}'\times\delta(\vec{r}_1-\vec{r}_2)\,\vec{k} \end{aligned}}$$

$$\boxed{P^\sigma \equiv \tfrac{1}{2}(1+\vec{\sigma}^{(1)}\cdot\vec{\sigma}^{(2)})}$$

with $\boxed{\vec{k} = \dfrac{\vec{p}}{\hbar} = \dfrac{1}{2i}(\vec{\nabla}_1-\vec{\nabla}_2)}$

spin-orbit force

4/21/03

The three-body interaction is:

$$\boxed{V(1,2,3) = t_3\,\delta(\vec{r}_1-\vec{r}_2)\,\delta(\vec{r}_2-\vec{r}_3)}$$

Aside: If a potential V depends only on $\vec{r}=\vec{r}_1-\vec{r}_2$, then in momentum space

$$\boxed{\langle\vec{p}|V|\vec{p}\,'\rangle = \frac{1}{(2\pi\hbar)^3}\int e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}\,V(\vec{r})\,e^{\frac{i}{\hbar}\vec{p}\,'\cdot\vec{r}}\,d^3r}$$

and a momentum expansion

$$\boxed{(2\pi\hbar)^3\langle\vec{p}|V|\vec{p}\,'\rangle = V_0 + V_1(\vec{p}\,'^2+\vec{p}^{\,2}) + V_2\,\vec{p}\cdot\vec{p}\,'}$$

acts to the left   acts to the right

$$\Rightarrow \boxed{V(\vec{r}) = V_0\,\delta(\vec{r}) + V_1\left(\hat{p}^2\,\delta(\vec{r}) + \delta(\vec{r})\,\hat{p}^2\right) + V_2\,\hat{p}\,\delta(\vec{r})\,\hat{p}}$$

- The non-spin part of the Skyrme interaction in 2nd quantized form is just what we consider for a dilute Fermi gas in effective field theory (EFT). The Lagrangian is:

$$\boxed{\begin{aligned}\mathcal{L}_{EFT} &= \psi^\dagger\left(i\frac{\partial}{\partial t}+\frac{\nabla^2}{2m}\right)\psi - \frac{C_0}{2}(\psi^\dagger\psi)^2 + \frac{C_2}{16}\left[(\psi\psi)^\dagger(\psi\overleftrightarrow{\nabla}^2\psi) + h.c.\right] \\ &\quad + \frac{C_2'}{8}(\psi\overleftrightarrow{\nabla}\psi)^\dagger\cdot(\psi\overleftrightarrow{\nabla}\psi) - \frac{D_0}{6}(\psi^\dagger\psi)^3\end{aligned}}$$

- There are 5 constants in the Skyrme potential given. For Skyrme III they are:

$t_0 = -1128.75$ MeV-fm^3 $t_1 = 395.0$ MeV fm^5

$t_2 = -95.0$ MeV fm^5 $t_3 = 14000.0$ MeV fm^6

$W_0 = 120$ MeV fm^5 $x_0 = 0.45$

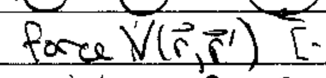
- B.A. Brown adds x_1, x_2, x_3 [take $t_i \to t_i(1+x_iP_\sigma)$ for t_1, t_2, t_3, and $W_0(1+x_WP_\sigma)$] and allows "3-body" term to be a fractional power (see below).

4/21/03

The basic results are nuclear binding energies, charge and neutron radii and densities, and single-particle levels across the periodic table (see handout).

$\Rightarrow$ does remarkably well for relatively few parameters.

How are the calculations done?

- Often called "Skyrme-Hartree-Fock," which gives it away.
- Hartree-Fock corresponds to  in the energy with a non-contact force $V(\vec{r},\vec{r}\,')$ [---]

In a nucleus, we can find equations for the best variational Slater determinant made from $\varphi_k(\vec{r})$ (where k labels the states $\Rightarrow$ quantum numbers) to obtain:

$$\boxed{-\frac{\hbar^2}{2m}\nabla^2\varphi_k(\vec{r}) + \sum_{j=1}^{A}\int d^3r'\, V(\vec{r},\vec{r}\,')\,\varphi_j^*(\vec{r}\,')\left\{\varphi_j(\vec{r}\,')\varphi_k(\vec{r}) - \varphi_j(\vec{r})\varphi_k(\vec{r}\,')\right\} = \epsilon_k\varphi_k(\vec{r})}$$

for each k.

If we define the Hartree or direct potential $\Gamma_H(\vec{r})$:

$$\boxed{\Gamma_H(\vec{r}) = \int d^3r'\, V(\vec{r},\vec{r}\,')\sum_{j=1}^{A}|\varphi_j(\vec{r}\,')|^2 = \int d^3r'\, V(\vec{r},\vec{r}\,')\,\rho(\vec{r}\,')}$$

and the Fock or exchange potential $\Gamma_{ex}(\vec{r},\vec{r}\,')$: density matrix

$$\boxed{\Gamma_{ex}(\vec{r},\vec{r}\,') = -V(\vec{r},\vec{r}\,')\sum_{j=1}^{A}\varphi_j^*(\vec{r}\,')\varphi_j(\vec{r}) \equiv -V(\vec{r},\vec{r}\,')\,\rho(\vec{r},\vec{r}\,')}$$

Then $\varphi_k(\vec{r})$ is the solution of the non-local, integro-differential S-equation:

$$\boxed{\left[-\frac{\hbar^2}{2m}\nabla^2 + \Gamma_H(\vec{r})\right]\varphi_k(\vec{r}) + \int d^3r'\, \Gamma_{ex}(\vec{r},\vec{r}\,')\,\varphi_k(\vec{r}\,') = \epsilon_k\varphi_k(\vec{r})}$$

which must be solved self-consistently. Nonlocality from antisymmetrization.

4/21/03

The solution is <u>drastically</u> simpler with the Skyrme interaction.

The energy is $\boxed{E_0 = \langle \Phi | T + V^{(2)} + V^{(3)} | \Phi \rangle}$
where $|\Phi\rangle$ is the Slater determinant of $\varphi_i(\vec{r}, s, t)$.

If we restrict ourselves to N=Z, no Coulomb, and time-reversal invariant nuclei, then

$$\boxed{\begin{aligned} E_0 &= \sum_{i=1}^{A} \langle i | \frac{p^2}{2m} | i \rangle + \frac{1}{2}\sum_{ij=1}^{A} \langle ij | V^{(2)} | ij \rangle + \frac{1}{6}\sum_{ijk=1}^{A} \langle ijk | V^{(3)} | ijk \rangle \\ &\equiv \int H(\vec{r})\, d^3r \qquad \text{energy functional} \end{aligned}}$$

with

$$\boxed{\begin{aligned} H(\vec{r}) = &\frac{\hbar^2}{2m}\tau(\vec{r}) + \frac{3}{8}t_0\rho^2 + \frac{1}{16}t_3\rho^3 + \frac{1}{16}(3t_1 + 5t_2)\rho\tau \\ &+ \frac{1}{64}(9t_1 - 5t_2)(\nabla\rho)^2 - \frac{3}{4}W_0\,\rho\,\vec{\nabla}\cdot\vec{J} + \frac{1}{32}(t_1 - t_2)\vec{J}^2 \end{aligned}}$$

where

$$\boxed{\rho(\vec{r}) = \sum_{i,s,t}^{\text{occupied}} |\varphi_i(\vec{r}, s, t)|^2} \qquad \text{density}$$

$$\boxed{\tau(\vec{r}) = \sum_{i,s,t}^{\text{occ.}} |\vec{\nabla}\varphi_i(\vec{r}, s, t)|^2} \qquad \text{Kinetic energy density}$$

$$\boxed{\vec{J}(\vec{r}) = (-i)\sum_{i,t,s,s'} \varphi_i^*(\vec{r}, s, t)\left[\vec{\nabla}\varphi_i(\vec{r}, s', t) \times \sigma_{ss'}\right]} \qquad \text{spin-orbit density}$$

In nuclear matter, $\boxed{\varphi_{\vec{k}st} = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}_i\cdot\vec{r}} \chi_s^{1/2}\chi_t^{1/2}}$ and $\boxed{\sum_{i=1}^{A} \to \int^{k_F} d^3k}$

$\Rightarrow \boxed{\rho = \frac{2}{3\pi^2}k_f^3}$ $\boxed{\tau = \frac{2}{3\pi^2}\frac{3}{5}k_f^5 = \frac{3}{5}\rho k_f^2 = \frac{3}{5}\left(\frac{3\pi^2}{2}\right)^{2/3}\rho^{5/3}}$ $\boxed{\vec{\nabla}\rho = \vec{\nabla}\cdot\vec{J} = 0}$

$$\Rightarrow \boxed{\frac{E_0}{A} = \frac{H}{\rho} = \frac{3}{5}\frac{\hbar^2}{2m}k_f^2 + \frac{3}{8}t_0\rho + \frac{1}{16}t_3\rho^2 + \frac{3}{80}(3t_1 + 5t_2)\rho k_f^2}$$

4/21/03

Consider the functional $E_0[\rho]$. It is difficult to vary w.r.t. ρ, since not explicit. So vary φ_k instead with constraint of normalization using Lagrange multipliers ϵ_k:

$$\boxed{\frac{\delta}{\delta\varphi_k}\left[E_0[\rho] - \sum_k \epsilon_k \int d^3r\, |\varphi_k(\vec{r})|^2\right) = 0}$$

$$\Rightarrow \boxed{\delta E = \int d^3r \left[\frac{\hbar^2}{2m^*(r)}\delta\tau(\vec{r}) + U(\vec{r})\,\delta\rho(\vec{r}) + \vec{W}(\vec{r})\cdot\delta\vec{J}(\vec{r})\right]}$$

with effective mass:

$$\boxed{m^*(\vec{r}) = \frac{m}{1 + \frac{2m}{\hbar^2}\frac{1}{16}(3t_1 + 5t_2)\rho(\vec{r})}}$$

$$\boxed{U(\vec{r}) = \frac{3}{4}t_0\rho + \frac{3}{16}t_3\rho^2 + \frac{1}{16}(3t_1 + 5t_2)\tau + \frac{1}{32}(5t_2 - 9t_1)\nabla^2\rho - \frac{3}{4}W_0\vec{\nabla}\cdot\vec{J}}$$

$$\boxed{\vec{W}(\vec{r}) = \frac{3}{4}W_0\vec{\nabla}\rho}$$

- insert variations $\delta\tau, \delta\rho, \delta\vec{J}$ w.r.t. φ_k:

$$\boxed{\delta E = 2\sum_{i=1}^{A}\int d^3r\,\delta\varphi_i^*\left\{-\vec{\nabla}\frac{\hbar^2}{2m^*}\vec{\nabla} + U + \vec{W}\cdot\frac{1}{i}(\vec{\nabla}\times\vec{\sigma})\right\}\varphi_i}$$

$$\Rightarrow \boxed{\left\{-\vec{\nabla}\frac{\hbar^2}{2m^*(r)}\vec{\nabla} + U(\vec{r}) + \vec{W}\cdot\frac{1}{i}(\vec{\nabla}\times\vec{\sigma})\right\}\varphi_i(\vec{r}) = \epsilon_i\varphi_i(\vec{r})}$$

spherical symmetry $\Rightarrow \boxed{\frac{3}{2}W_0\left(\frac{1}{r}\frac{d\rho}{dr}\right)\vec{l}\cdot\vec{s}}$

- solve iteratively until self-consistent.

4/21/03

Skyrme III results (1975) (see handout for B.A. Brown 1998 results)

	^{16}O		^{40}Ca		^{48}Ca		^{90}Zr		^{208}Pb	
	expt	SIII	expt	SIII	expt	SIII	expt	SIII	expt	SIII
E/A (MeV)	-7.98	-7.96	-8.55	-8.54	-8.67	-8.71	-8.71	-8.71	-7.87	-7.87
r_{ch} (fm)	2.73	2.69	3.49	3.48	3.48	3.53	4.23	4.32	5.50	5.57

- radii undershoot then overshoot
- modern Skyrme: more parameters and $\rho^3 \to \rho^{2+\alpha}$ with $\alpha = \frac{1}{3}, \frac{1}{2}, \ldots$

How do we add pairing?

Instead of $\boxed{\rho(\vec{r}) = \sum_{i,s,t} |\varphi_i(\vec{r},s,t)|^2 \longrightarrow \sum_{i,s,t}^{\infty} v_i^2 |\varphi_i(\vec{r},s,t)|^2}$

+ pairing energy

with

$$\boxed{v_i^2 = \frac{1}{2}\left(1 - \frac{\epsilon_i - \mu}{\sqrt{(\epsilon_i-\mu)^2+\Delta^2}}\right)}$$

and determine μ by $\boxed{\int d^3r\, \rho(\vec{r}) = A}$

- In principle, solve gap equation with some pairing force to self-consistently find Δ.
  - In practice, often take fixed gap Δ from experiment and solve for pairing force.

- For deformed nuclei, we have coupled r, θ, φ dependence
  - one way to solve: expand in anisotropic harmonic oscillator