Slides Chapter 1-7 Dickhoff-Van Neck

- Preliminary material covered in slides of Chs. 1-5 assumed more or less familiar
- Green's function formulation of single-particle problem in Ch.6 slides useful preparation for general formulation
- Single-particle propagator in many-fermion system introduced in Ch.7 slides

Symmetric and antisymmetric states

When is quantum physics expected?

Consider the energy levels for a particle of mass m
enclosed in a box with volume $V = L^3$

$$\varepsilon_{n_x,n_y,n_z} = \frac{h^2}{8mL^2}(n_x^2 + n_y^2 + n_z^2)$$ positive integers

Total number of states below energy E

$$\Omega(E) = \frac{\pi}{6}\left(\frac{8mL^2E}{h^2}\right)^{3/2} = \frac{\pi}{6}\left(\frac{8mE}{h^2}\right)^{3/2} V$$

"Quantumness" --> indistinguishability not important when

$$1 \gg Q \equiv \frac{N}{\Omega} = \frac{6}{\pi}\rho\left(\frac{h^2}{12mk_BT}\right)^{3/2}$$

Use $E = \frac{3}{2}k_BT$

Q

System	T (K)	Density (m^{-3})	Mass (u)	Q
He (l)	4.2	1.9×10^{28}	4.0	1.1
He (g)	4.2	2.5×10^{27}	4.0	1.4×10^{-1}
He (g)	273	2.7×10^{25}	4.0	2.9×10^{-6}
Ne (l)	27.1	3.6×10^{28}	20.2	1.1×10^{-2}
Ne (g)	273	2.7×10^{25}	20.2	2.5×10^{-7}
e^- Na metal	273	2.5×10^{28}	5.5×10^{-4}	1.7×10^{3}
e^- Al metal	273	1.8×10^{29}	5.5×10^{-4}	1.2×10^{4}
e^- white dwarfs	10^{7}	10^{36}	5.5×10^{-4}	8.5×10^{3}
p,n nuclear matter	10^{10}	1.7×10^{44}	1.0	6.5×10^{2}
n neutron star	10^{8}	4.0×10^{44}	1.0	1.5×10^{6}
^{87}Rb condensate	10^{-7}	10^{19}	87	1.5

Bosons and Fermions

- Use experimental observations to conclude about consequences of identical particles
- Two possibilities
  - antisymmetric states ⇒ **fermions** half-integer spin
    - Pauli from properties of electrons in atoms
  - symmetric states ⇒ **bosons** integer spin
    - Considerations related to electromagnetic radiation (photons)
- Can also consider quantization of "field" equations
  - e.g. quantize "free" Maxwell equations (see standard textbooks)

Wolfgang Pauli (1900-1958)

- The Nobel Prize in Physics 1945 was awarded to Wolfgang Pauli "for the discovery of the Exclusion Principle, also called the Pauli Principle".

- paper Zeitschr. f. Phys. 31, 765 (1925)

Review single-particle states

- Notation $|\ldots\rangle$
- … list of quantum numbers associated with a CSCO
- Normalization $\langle\alpha|\beta\rangle = \delta_{\alpha,\beta}$
- Continuous quantum numbers
  - Example $\langle \boldsymbol{r}, m_s | \boldsymbol{r}', m_s' \rangle = \delta(\boldsymbol{r} - \boldsymbol{r}')\delta_{m_s, m_s'}$
- Completeness $\sum_\alpha |\alpha\rangle\langle\alpha| = 1$

Consequences for two-particle states

- CVS for two particles: product space
- Notation $|\alpha_1\alpha_2) = |\alpha_1\rangle\,|\alpha_2\rangle$ ←
- Orthogonality $(\alpha_1\alpha_2|\alpha_1'\alpha_2') = \delta_{\alpha_1,\alpha_1'}\delta_{\alpha_2,\alpha_2'}$
- Completeness $\sum_{\alpha_1\alpha_2} |\alpha_1\alpha_2)(\alpha_1\alpha_2| = 1$

Exchange degeneracy

- Consider $\alpha_1 \neq \alpha_2$
- Then $|\alpha_2\alpha_1) \neq |\alpha_1\alpha_2)$
- All states $|\alpha_1\alpha_2)$

$$|\alpha_2\alpha_1)$$

$$c_1|\alpha_1\alpha_2) + c_2|\alpha_2\alpha_1)$$

yield α_1 for one particle and α_2 for the other upon measurement

- Yet, unclear which state describes this system and therefore inconsistent with quantum postulates
- Consider permutation operator

$$P_{12}|\alpha_1\alpha_2) = |\alpha_2\alpha_1)$$

with $P_{12} = P_{21} \text{ and } P_{12}^2 = 1$

- Hamiltonian for two particles is symmetric for 1 ⇔ 2

Development

- Typical Hamiltonian $H = \frac{\boldsymbol{p}_1^2}{2m} + \frac{\boldsymbol{p}_2^2}{2m} + V(|\boldsymbol{r}_1 - \boldsymbol{r}_2|)$
- Consider operator acting on particle 1 and corresponding eigenvalue $A_1|\alpha_1\alpha_2) = a_1|\alpha_1\alpha_2)$
- Similarly, the same operator acting on particle 2 yields
$$A_2|\alpha_1\alpha_2) = a_2|\alpha_1\alpha_2)$$
- Note $P_{12}A_1|\alpha_1\alpha_2) = a_1 P_{12}|\alpha_1\alpha_2) = a_1|\alpha_2\alpha_1) = A_2|\alpha_2\alpha_1)$
- and $P_{12}A_1|\alpha_1\alpha_2) = P_{12}A_1P_{12}^{-1}P_{12}|\alpha_1\alpha_2) = P_{12}A_1P_{12}^{-1}|\alpha_2\alpha_1)$
- Holds for any state; therefore $P_{12}A_1P_{12}^{-1} = A_2$
- It follows that $P_{12}HP_{12}^{-1} = H$ or $[P_{12}, H] = 0$

Symmetric and antisymmetric two-particle states

- So $$[P_{12}, H] = 0$$
- Common eigenkets either
$$|\alpha_1\alpha_2\rangle_+ = \frac{1}{\sqrt{2}}\{|\alpha_1\alpha_2) + |\alpha_2\alpha_1)\}$$
or
$$|\alpha_1\alpha_2\rangle_- = \frac{1}{\sqrt{2}}\{|\alpha_1\alpha_2) - |\alpha_2\alpha_1)\}$$
- Eigenstates of the Hamiltonian either symmetric ⇒ bosons

  or antisymmetric ⇒fermions
- Two-boson state $$|\alpha_1\alpha_2\rangle_S = \left[\frac{1}{2n_\alpha!n_{\alpha'}!\ldots}\right]^{1/2}\{|\alpha_1\alpha_2) + |\alpha_2\alpha_1)\}$$

$$\alpha_1 = \alpha_2 = \alpha \Rightarrow |n_\alpha = 2\rangle = |\alpha\alpha\rangle_S = |\alpha\rangle\,|\alpha\rangle$$

$$\alpha_1 \neq \alpha_2 \Rightarrow |\alpha_1\alpha_2\rangle_S = \frac{1}{\sqrt{2}}\{|\alpha_1\alpha_2) + |\alpha_2\alpha_1)\}$$

Fermions

- Antisymmetry: $|\alpha_2\alpha_1\rangle = -|\alpha_1\alpha_2\rangle$
- Both kets represent the same physical state: count only once in completeness relation ⇒ "order" quantum numbers

$$|1\rangle , |2\rangle , |3\rangle , ...$$

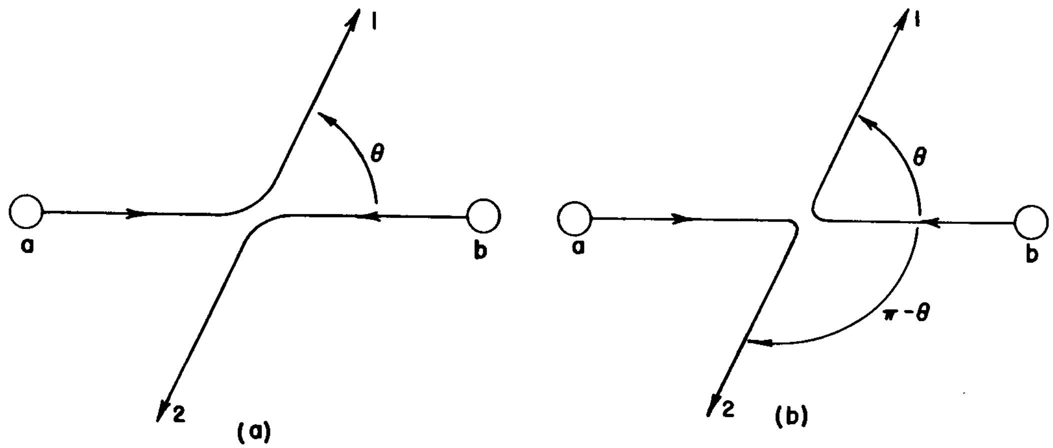
- Ordered: $$\sum_{i<j} |ij\rangle\langle ij| = 1$$
- Not ordered: $$\frac{1}{2!}\sum_{ij} |ij\rangle\langle ij| = 1$$

Bosons ordered: $$\sum_{i\leq j} |ij\rangle\langle ij| = 1$$

not ordered: $$\sum_{ij} \frac{n_1!n_2!...}{2!} |ij\rangle\langle ij| = 1$$

Scattering of identical particles

Particles that can be "distinguished"



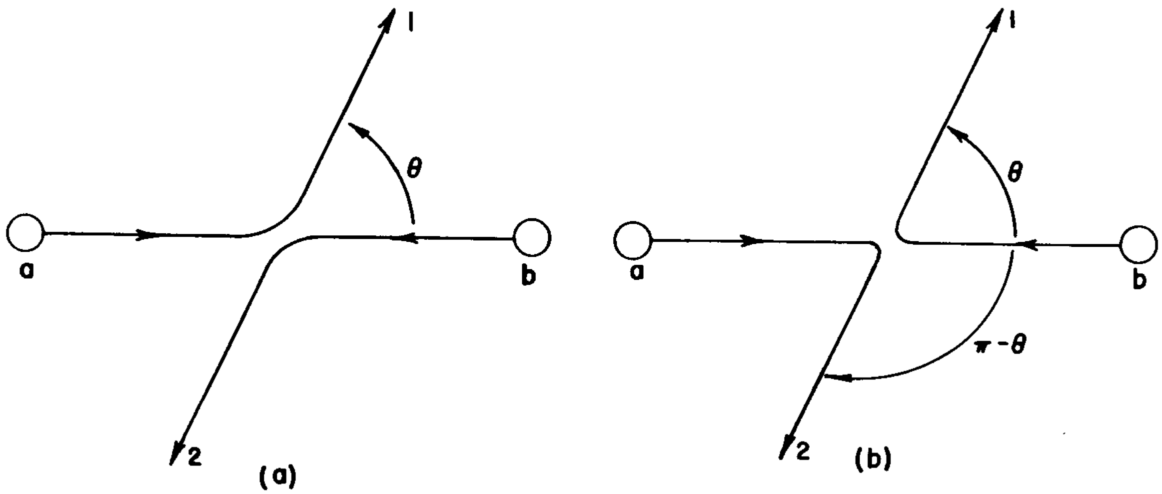
particle a in D1 (a) $$\frac{d\sigma}{d\Omega}(a\ in\ D_1, b\ in\ D_2) = |f(\theta)|^2$$

particle a in D2 (b) $$\frac{d\sigma}{d\Omega}(a\ in\ D_2, b\ in\ D_1) = |f(\pi-\theta)|^2$$

any particle in D1 $$\frac{d\sigma}{d\Omega}(particle\ in\ D_1) = |f(\theta)|^2 + |f(\pi-\theta)|^2$$

Identical bosons

- Cannot distinguish (a) and (b)



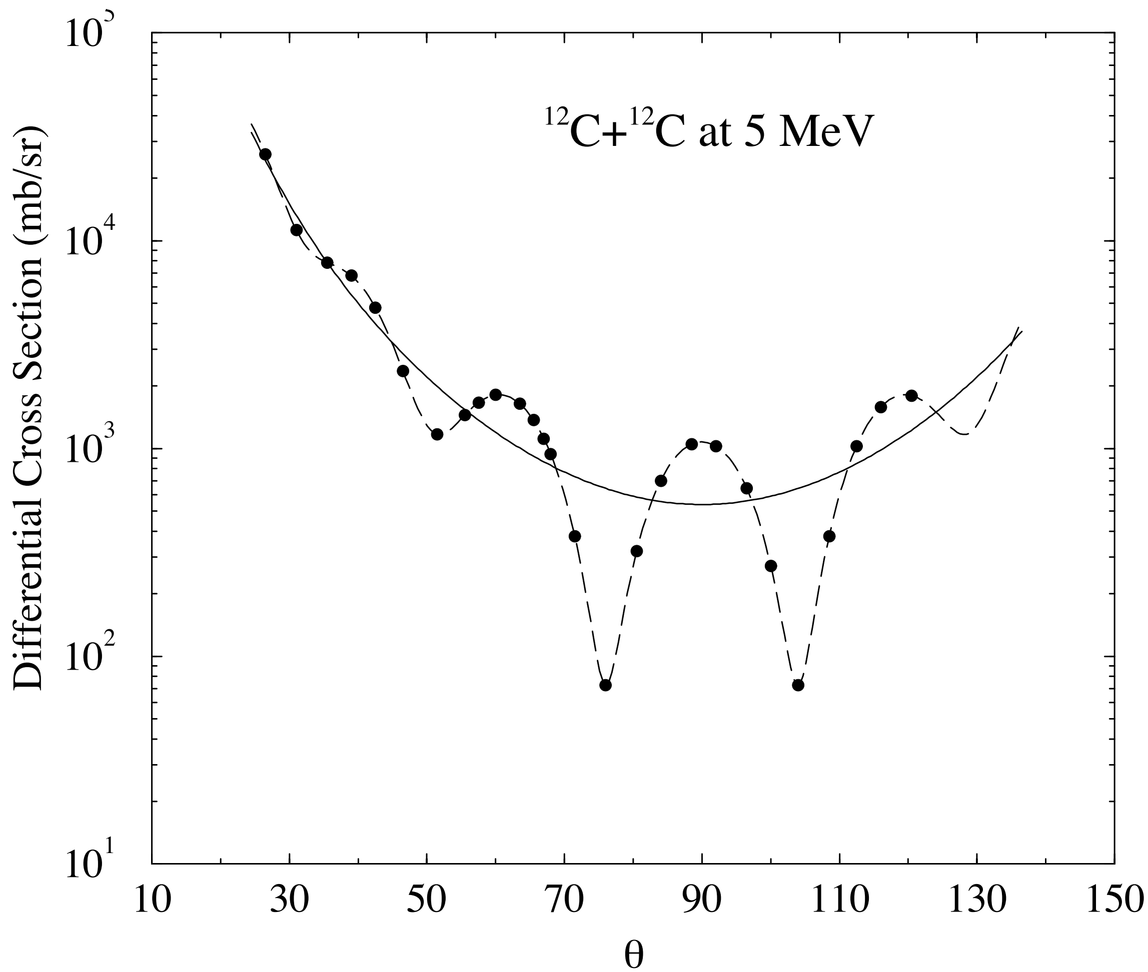
- Rule for bosons: add amplitudes then square!

$$\frac{d\sigma}{d\Omega}(bosons) = \left|f(\theta) + f(\pi - \theta)\right|^2$$

- Interference
- 90 degrees: factor of 2 compared to "classical" cross section

$^{12}C + ^{12}C$

Low-energy boson-boson scattering

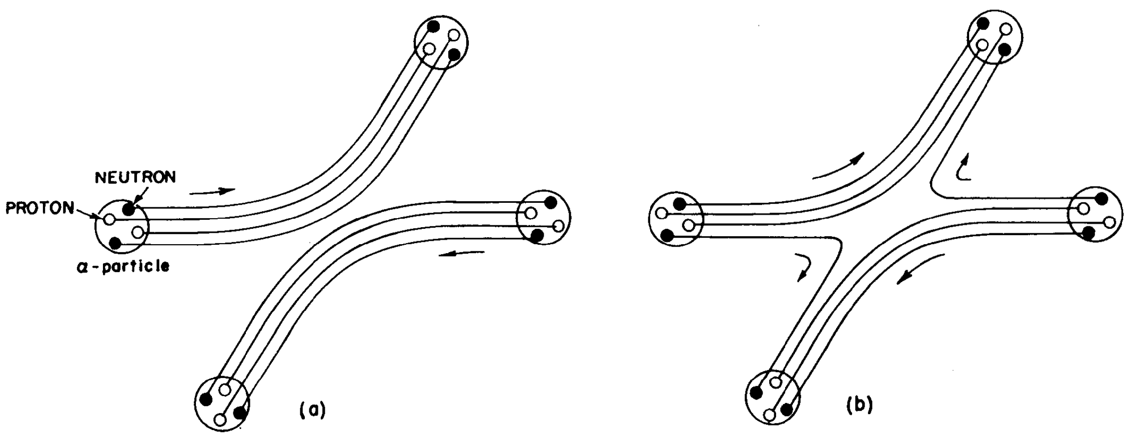


Phys. Rev. **123**, 878 (1961)

^{12}C a boson?

- 6 protons and 6 neutrons
- total angular momentum integer (made of 12 spin-$\frac{1}{2}$ particles)
- ground state 0^+
- first excited state above 4 MeV

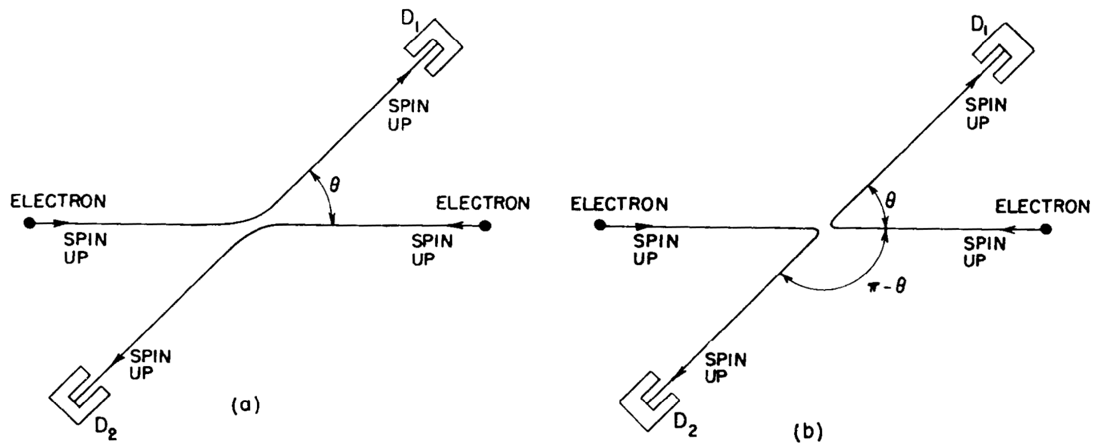
- ^{4}He atom: 2p + 2n + 2e $\Rightarrow$**boson**
- ^{3}He atom: 2p + 1n + 2e $\Rightarrow$**fermion**
- but



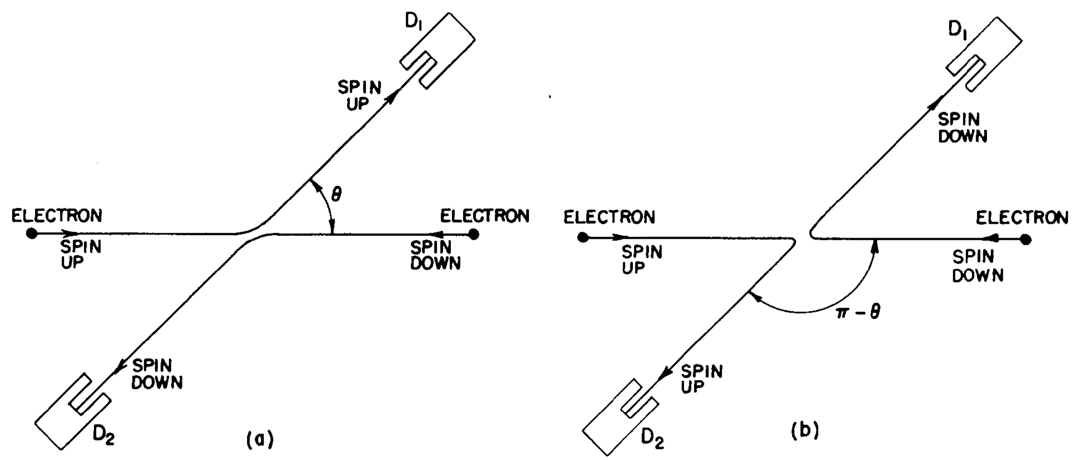
Fermion-fermion scattering

- Identical fermions: electrons with spin up

$$\frac{d\sigma}{d\Omega}(fermions) = \left|f(\theta) - f(\pi - \theta)\right|^2$$



- What about



N-particle states (fermions)

- Product states $|\alpha_1\alpha_2 ... \alpha_N) = |\alpha_1\rangle\,|\alpha_2\rangle\,...\,|\alpha_N\rangle$
- Normalization

$$\begin{aligned}(\alpha_1\alpha_2...\alpha_N|\alpha_1'\alpha_2'...\alpha_N') &= \langle\alpha_1|\alpha_1'\rangle\langle\alpha_2|\alpha_2'\rangle...\langle\alpha_N|\alpha_N'\rangle \\ &= \delta_{\alpha_1,\alpha_1'}\delta_{\alpha_2,\alpha_2'}...\delta_{\alpha_N,\alpha_N'}\end{aligned}$$

- Completeness $\sum_{\alpha_1\alpha_2...\alpha_N} |\alpha_1\alpha_2...\alpha_N)(\alpha_1\alpha_2...\alpha_N| = 1$
- Identical particles: symmetric or antisymmetric states
- Fermions: use antisymmetrizer $\mathcal{A} = \frac{1}{N!}\sum_p (-1)^p P$
- Permutation operator: product of two-particle permutations
- # of two-particle permutations odd/even ⇒ **sign**

Example for 3 particles

- Check odd/even permutation

$$
\begin{aligned}
|\alpha_1\alpha_2\alpha_3\rangle &= \frac{1}{\sqrt{6}}\{|\alpha_1\alpha_2\alpha_3) - |\alpha_2\alpha_1\alpha_3) + |\alpha_2\alpha_3\alpha_1) \\
&- |\alpha_3\alpha_2\alpha_1) + |\alpha_3\alpha_1\alpha_2) - |\alpha_1\alpha_3\alpha_2)\}.
\end{aligned}
$$

- Note normalization (6 states)
- Also note antisymmetry $|\alpha_1\alpha_2\alpha_3\rangle = -|\alpha_2\alpha_1\alpha_3\rangle$
- No two fermions can occupy the same state!!
- Example for three bosons (symmetric state) [Check!]

$$
\begin{aligned}
|\alpha_1\alpha_1\alpha_2\rangle &= \frac{1}{\sqrt{3!2!}}\{|\alpha_1\alpha_1\alpha_2) + |\alpha_1\alpha_1\alpha_2) + |\alpha_1\alpha_2\alpha_1) \\
&+ |\alpha_2\alpha_1\alpha_1) + |\alpha_2\alpha_1\alpha_1) + |\alpha_1\alpha_2\alpha_1)\} \\
&= \frac{1}{\sqrt{3}}\{|\alpha_1\alpha_1\alpha_2) + |\alpha_1\alpha_2\alpha_1) + |\alpha_2\alpha_1\alpha_1)\}.
\end{aligned}
$$

N fermions

- Completeness with ordered single-particle (sp) quantum numbers

$$\sum_{\alpha_1\alpha_2...\alpha_N}^{ordered} |\alpha_1\alpha_2...\alpha_N\rangle\langle\alpha_1\alpha_2...\alpha_N| = 1$$

- Not ordered $\frac{1}{N!}\sum_{\alpha_1\alpha_2...\alpha_N} |\alpha_1\alpha_2...\alpha_N\rangle\langle\alpha_1\alpha_2...\alpha_N| = 1$

- Normalization with ordered single-particle (sp) quantum numbers

$$\begin{aligned}\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha'_N\rangle &= \langle\alpha_1|\alpha'_1\rangle\langle\alpha_2|\alpha'_2\rangle...\langle\alpha_N|\alpha'_N\rangle \\ &= \delta_{\alpha_1,\alpha'_1}\delta_{\alpha_2,\alpha'_2}...\delta_{\alpha_N,\alpha'_N}\end{aligned}$$

- Not ordered ⇒ determinant

$$\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha'_N\rangle = \begin{vmatrix} \langle\alpha_1|\alpha'_1\rangle & \langle\alpha_1|\alpha'_2\rangle & \dots & \langle\alpha_1|\alpha'_N\rangle \\ \langle\alpha_2|\alpha'_1\rangle & \langle\alpha_2|\alpha'_2\rangle & \dots & \langle\alpha_2|\alpha'_N\rangle \\ \vdots & \vdots & \ddots & \vdots \\ \langle\alpha_N|\alpha'_1\rangle & \langle\alpha_N|\alpha'_2\rangle & \dots & \langle\alpha_N|\alpha'_N\rangle \end{vmatrix}.$$

Normalized N-particle wave function

- Called a Slater determinant

$$\psi_{\alpha_1\alpha_2\ldots\alpha_N}(x_1x_2\ldots x_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \langle x_1|\alpha_1\rangle & \ldots & \langle x_N|\alpha_1\rangle \\ \langle x_1|\alpha_2\rangle & \ldots & \langle x_N|\alpha_2\rangle \\ \vdots & \ddots & \vdots \\ \langle x_1|\alpha_N\rangle & \ldots & \langle x_N|\alpha_N\rangle \end{vmatrix}.$$

- Hard to work with Slater determinants
- Use occupation number representation or second quantization

Second quantization

- Motivation:
  - Slater determinants tedious to work with
  - Relevant operators change only the quantum numbers of one or two particles (and in exceptional cases three)
- Consider states that are labeled by the # of particles occupying sp states ⇒ occupation number representation
- Allow states in CVS with different # of particles ⇒ Fock space
- Includes new state: the vacuum $|0\rangle$
  - all sp states $\{|\alpha\rangle\}$
  - all antisymmetric two-particle (tp) states $\{|\alpha_1\alpha_2\rangle\}$
  - ..
  - all antisymmetric N-particle states $\{|\alpha_1\alpha_2...\alpha_N\rangle\}$
  - up to infinite number of particles .....

Alternative writing

- Vacuum state $$|0\rangle = \underset{\alpha_1\alpha_2 ...}{|0\ 0 ...}\ \underset{\alpha_\infty}{0\rangle}$$
- Sp state $$|\alpha_i\rangle = |0\ 0\ ...0\ \underset{\alpha_i}{1}\ 0...0\rangle$$
- Tp state $$|\alpha_i\alpha_j\rangle = |0\ 0\ ...0\ \underset{\alpha_i}{1}\ 0...0\ \underset{\alpha_j}{1}\ 0...0\rangle$$
- etc.
- Use ordered states $$\sum_{N=0}^{\infty} \sum_{\alpha_1\alpha_2..\alpha_N}^{ordered} |\alpha_1\alpha_2...\alpha_N\rangle\langle\alpha_1\alpha_2...\alpha_N| = 1$$
- Introduce new operator in Fock space $a^\dagger_\alpha$

Particle addition (creation) operator

- Definition $a_\alpha^\dagger \left|\alpha_1\alpha_2...\alpha_N\right\rangle \equiv \left|\alpha\alpha_1\alpha_2...\alpha_N\right\rangle$
- Takes an antisymmetric N-particle state and turns it into an antisymmetric N+1-particle state with α occupied!!!!
- Note:
  - $\alpha = \alpha_i$ ⇒ not a state
  - $\alpha \neq \alpha_i$ ⇒ i=1,…,N new state (may require ordering)
- Acts on any state
- Including

$$a_\alpha^\dagger \left|0\right\rangle = \left|\alpha\right\rangle$$

$$a_\alpha^\dagger \left|\beta\right\rangle = \left|\alpha\beta\right\rangle$$

- and
- etc.
- What about the adjoint operator a_α ?

Particle removal (destruction) operator

- Action of adjoint operator?

$$a_\alpha |\alpha_1\alpha_2...\alpha_N\rangle = \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2..\alpha'_M}^{ordered} |\alpha'_1\alpha'_2..\alpha'_M\rangle \langle\alpha'_1\alpha'_2..\alpha'_M| a_\alpha |\alpha_1\alpha_2..\alpha_N\rangle$$

$$= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2..\alpha'_M}^{ordered} |\alpha'_1\alpha'_2..\alpha'_M\rangle \langle\alpha_1\alpha_2..\alpha_N| a_\alpha^\dagger |\alpha'_1\alpha'_2..\alpha'_M\rangle^*$$

$$= \sum_{M=0}^{\infty} \sum_{\alpha'_1\alpha'_2..\alpha'_M}^{ordered} |\alpha'_1\alpha'_2..\alpha'_M\rangle \langle\alpha_1\alpha_2..\alpha_N|\alpha\alpha'_1\alpha'_2..\alpha'_M\rangle^*$$

- Consider once α placed in the correct location ⇒ $(-1)^{i-1}$

$$\langle\alpha_1\alpha_2...\alpha_N|\alpha'_1\alpha'_2...\alpha\alpha'_i...\alpha'_M\rangle = \delta_{\alpha_1,\alpha'_1}\delta_{\alpha_2,\alpha'_2}...\delta_{\alpha_i,\alpha}\delta_{\alpha_{i+1},\alpha'_i}...\delta_{\alpha_N,\alpha'_{N-1}}$$

- So $\quad a_\alpha |\alpha_1\alpha_2...\alpha_N\rangle = (-1)^{i-1} |\alpha_1\alpha_2...\alpha_{i-1}\alpha_{i+1}...\alpha_N\rangle \quad$ if $\alpha = \alpha_i$
- or $\quad a_\alpha |\alpha_1\alpha_2...\alpha_N\rangle = 0 \quad$ if $\alpha \neq \alpha_i, i = 1, ..., N$
- Example: $a_\alpha |0\rangle = 0$ Note: again antisymmetric state!

Fermion anticommutation relations

$$\{a_\alpha, a_\beta^\dagger\} = a_\alpha a_\beta^\dagger + a_\beta^\dagger a_\alpha = \delta_{\alpha,\beta}$$

$$\{a_\alpha, a_\beta\} = \{a_\alpha^\dagger, a_\beta^\dagger\} = 0$$

- "Easy" to demonstrate
- Rewrite antisymmetric state

$$\begin{aligned} |\alpha_1\alpha_2\alpha_3...\alpha_N\rangle &= a_{\alpha_1}^\dagger |\alpha_2\alpha_3...\alpha_N\rangle = a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger |\alpha_3...\alpha_N\rangle = ... \\ &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger |0\rangle = \prod_i a_{\alpha_i}^\dagger |0\rangle \end{aligned}$$

- Ensures Pauli principle

$$\begin{aligned} |\alpha_1\alpha_2...\alpha_N\rangle &= a_{\alpha_1}^\dagger a_{\alpha_2}^\dagger ... a_{\alpha_N}^\dagger |0\rangle = -a_{\alpha_2}^\dagger a_{\alpha_1}^\dagger ... a_{\alpha_N}^\dagger |0\rangle \\ &= -|\alpha_2\alpha_1...\alpha_N\rangle \end{aligned}$$

- Occupation numbers

$$|n_{\alpha_1} = 1, n_{\alpha_2} = 0, n_{\alpha_3} = 1, 0, ..., 0, ...\rangle = |\alpha_1\alpha_3\rangle$$

One-body operators in Fock space

- Examples?

- 1 particle in sp space $F = \sum_\alpha \sum_\beta |\alpha\rangle \langle\alpha| F |\beta\rangle \langle\beta|$

- Operator completely determined by all $\langle\alpha| F |\beta\rangle$ matrix elements

- N-particle space $F_N = F(1) + F(2) + ... + F(N) = \sum_{i=1}^{N} F(i)$
- Action of $F(i)$ on a product state

$$F(i)|\alpha_1\alpha_2\alpha_3...\alpha_N) = |\alpha_1\rangle |\alpha_2\rangle ... |\alpha_{i-1}\rangle \left\{\sum_{\beta_i} |\beta_i\rangle \langle\beta_i| F |\alpha_i\rangle\right\} |\alpha_{i+1}\rangle ... |\alpha_N\rangle$$

$$= \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle |\alpha_1...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N)$$

One-body operators (continued)

- Matrix element $\langle \beta_i | F | \alpha_i \rangle$ same for any particle (dummy variables)
- Then

$$F_N|\alpha_1\alpha_2\alpha_3...\alpha_N) = F(1)|\alpha_1\rangle|\alpha_2\rangle...|\alpha_N\rangle + ... + |\alpha_1\rangle|\alpha_2\rangle...F(N)|\alpha_N\rangle$$

$$= \sum_{\beta_1}\langle\beta_1|F|\alpha_1\rangle|\beta_1\alpha_2...\alpha_N) + ... + \sum_{\beta_N}\langle\beta_N|F|\alpha_N\rangle|\alpha_1\alpha_2...\beta_N)$$

$$= \sum_{i=1}^{N}\sum_{\beta_i}\langle\beta_i|F|\alpha_i\rangle|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N)$$

- Since F_N is symmetric it commutes with the antisymmetrizer $\mathcal{A}$
- Thus

$$F_N|\alpha_1\alpha_2\alpha_3...\alpha_N\rangle = \sum_{i=1}^{N}\sum_{\beta_i}\langle\beta_i|F|\alpha_i\rangle|\alpha_1\alpha_2...\alpha_{i-1}\beta_i\alpha_{i+1}...\alpha_N\rangle$$

Fock-space one-body operator

- Consider Fock-space operator $\hat{F} = \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, a^\dagger_\alpha a_\beta$
- Note the "^" notation
- This operator accomplishes the same as F_N for any N!
- Use

$$
\begin{aligned}
[\hat{F}, a^\dagger_{\alpha_i}] &= \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, [a^\dagger_\alpha a_\beta, a^\dagger_{\alpha_i}] = \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, (a^\dagger_\alpha a_\beta a^\dagger_{\alpha_i} - a^\dagger_{\alpha_i} a^\dagger_\alpha a_\beta) \\
&= \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, a^\dagger_\alpha (a_\beta a^\dagger_{\alpha_i} + a^\dagger_{\alpha_i} a_\beta) = \sum_{\alpha\beta} \langle\alpha| F |\beta\rangle \, a^\dagger_\alpha \delta_{\beta,\alpha_i} \\
&= \sum_{\alpha} \langle\alpha| F |\alpha_i\rangle \, a^\dagger_\alpha = \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle \, a^\dagger_{\beta_i}
\end{aligned}
$$

- and apply

$$
\begin{aligned}
\hat{F} \, |\alpha_1 \alpha_2 \alpha_3 ... \alpha_N\rangle &= \hat{F} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} \, |0\rangle \\
&= [\hat{F}, a^\dagger_{\alpha_1}] a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} \, |0\rangle + a^\dagger_{\alpha_1} \hat{F} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} \, |0\rangle \\
&= [\hat{F}, a^\dagger_{\alpha_1}] a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N} \, |0\rangle + a^\dagger_{\alpha_1} [\hat{F}, a^\dagger_{\alpha_2}] ... a^\dagger_{\alpha_N} \, |0\rangle + ... + a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... [\hat{F}, a^\dagger_{\alpha_N}] \, |0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle \, a^\dagger_{\alpha_1} ... a^\dagger_{\alpha_{i-1}} a^\dagger_{\beta_i} a^\dagger_{\alpha_{i+1}} ... a^\dagger_{\alpha_N} \, |0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i} \langle\beta_i| F |\alpha_i\rangle \, |\alpha_1 ... \alpha_{i-1} \beta_i \alpha_{i+1} ... \alpha_N\rangle
\end{aligned}
$$

✓

Examples

- Density operator for N particles $\rho_N(\boldsymbol{r}) = \sum_{i=1}^{N} \delta(\boldsymbol{r} - \boldsymbol{r}_i)$
- Second-quantized form: choose $\{|\boldsymbol{r}, m_s\rangle\}$ basis
- In Fock space

$$\begin{aligned}\hat{\rho}(\boldsymbol{r}) &= \sum_{m_s, m_{s'}} \int d^3r_1 \int d^3r_1' \; \langle \boldsymbol{r}_1 m_s | \, \delta(\boldsymbol{r} - \boldsymbol{r}_{op}) \, | \boldsymbol{r}_1' m_{s'} \rangle \, a^\dagger_{\boldsymbol{r}_1 m_s} a_{\boldsymbol{r}_1' m_{s'}} \\ &= \sum_{m_s} a^\dagger_{\boldsymbol{r} m_s} a_{\boldsymbol{r} m_s}\end{aligned}$$

- Kinetic energy

$$\begin{aligned}\hat{T} &= \sum_{\alpha\beta} \langle \alpha | \, T \, | \beta \rangle \, a^\dagger_\alpha a_\beta \\ &= \sum_{\boldsymbol{p}_1 m_1 \boldsymbol{p}_2 m_2} \langle \boldsymbol{p}_1 m_1 | \, \frac{\boldsymbol{p}_{op}^2}{2m} \, | \boldsymbol{p}_2 m_2 \rangle \, a^\dagger_{\boldsymbol{p}_1 m_1} a_{\boldsymbol{p}_2 m_2} \\ &= \sum_{\boldsymbol{p}_1 m_1} \frac{\boldsymbol{p}_1^2}{2m} a^\dagger_{\boldsymbol{p}_1 m_1} a_{\boldsymbol{p}_1 m_1}\end{aligned}$$

More examples

- Consider $\hat{N} = \sum_\alpha a^\dagger_\alpha a_\alpha$

- Determine $\left[\hat{N}, a^\dagger_{\alpha_i}\right]$

$$\begin{aligned} \left[\hat{N}, a^\dagger_{\alpha_i}\right] &= \sum_\alpha \left[a^\dagger_\alpha a_\alpha, a^\dagger_{\alpha_i}\right] \\ &= a^\dagger_{\alpha_i} \end{aligned}$$

- Therefore $\hat{N}\,|\alpha_1 ... \alpha_N\rangle = N\,|\alpha_1 ... \alpha_N\rangle$

Change of basis $\quad a^\dagger_\alpha\,|0\rangle = |\alpha\rangle = \sum_\lambda |\lambda\rangle\,\langle\lambda|\alpha\rangle = \sum_\lambda a^\dagger_\lambda\,|0\rangle\,\langle\lambda|\alpha\rangle$

Can be done for any state in Fock space ⇒ $\quad a^\dagger_\alpha = \sum_\lambda \langle\lambda|\alpha\rangle a^\dagger_\lambda$

Also $\quad a_\alpha = \sum_\lambda \langle\alpha|\lambda\rangle a_\lambda$

Two-body operators in Fock space

- Similar strategy $$V = \sum_{\alpha\beta}\sum_{\gamma\delta} |\alpha\beta)(\alpha\beta|V|\gamma\delta)(\gamma\delta|$$
- N-particles

$$V_N = \begin{cases} V(1,2)+ & V(1,3)+ & V(1,4)+ & \ldots + & V(1,N)+ \\ & V(2,3)+ & V(2,4)+ & \ldots + & V(2,N)+ \\ & & V(3,4)+ & \ldots + & V(3,N)+ \\ & & & \ddots & \vdots \\ & & & & V(N-1,N) \end{cases}$$

$$= \sum_{i<j=1}^{N} V(i,j) = \frac{1}{2}\sum_{i\neq j}^{N} V(i,j)$$

- Consider

$$V(i,j)|\alpha_1..\alpha_i..\alpha_j..\alpha_N) = \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j)|\alpha_1..\alpha_{i-1}\beta_i\alpha_{i+1}..\alpha_{j-1}\beta_j\alpha_{j+1}..\alpha_N)$$

- Matrix elements do not depend on the selected pair
- $(\beta_i\beta_j|V|\alpha_i\alpha_j)$ identical for any pair as long as quantum numbers are the same, so

$$V_N|\alpha_1\alpha_2\alpha_3...\alpha_N) = \sum_{i<j=1}^{N}\sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j)|\alpha_1...\beta_i...\beta_j...\alpha_N)$$

More on two-body operators

- Note: V_N symmetric and therefore commutes with antisymmetrizer
- As a consequence

$$V_N \left|\alpha_1\alpha_2\alpha_3 \ldots \alpha_N\right\rangle = \sum_{i<j=1}^{N} \sum_{\beta_i\beta_j} (\beta_i\beta_j|V|\alpha_i\alpha_j) \left|\alpha_1 \ldots \beta_i \ldots \beta_j \ldots \alpha_N\right\rangle$$

- Fock-space operator

$$\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma$$

- accomplishes the same result for any particle number!
- Note ordering

Two-body operator

- Use

$$
\begin{aligned}
[\hat{V}, a^\dagger_{\alpha_i}] &= \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)a^\dagger_\alpha a^\dagger_\beta [a_\delta a_\gamma, a^\dagger_{\alpha_i}] \\
&= \ldots\ldots a^\dagger_\alpha a^\dagger_\beta (a_\delta a_\gamma a^\dagger_{\alpha_i} - a^\dagger_{\alpha_i} a_\delta a_\gamma) \\
&= \ldots\ldots a^\dagger_\alpha a^\dagger_\beta (a_\delta(\delta_{\gamma,\alpha_i} - a^\dagger_{\alpha_i} a_\gamma) - a^\dagger_{\alpha_i} a_\delta a_\gamma) \\
&= \ldots\ldots a^\dagger_\alpha a^\dagger_\beta (a_\delta \delta_{\gamma,\alpha_i} - \delta_{\delta,\alpha_i} a_\gamma) \\
&= \frac{1}{2}\sum_{\alpha\beta\delta}(\alpha\beta|V|\alpha_i\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta - \frac{1}{2}\sum_{\alpha\beta\gamma}(\alpha\beta|V|\gamma\alpha_i)a^\dagger_\alpha a^\dagger_\beta a_\gamma \\
&= \sum_{\alpha\beta\delta}(\alpha\beta|V|\alpha_i\delta)a^\dagger_\alpha a^\dagger_\beta a_\delta = \sum_{\beta_i\beta_j\alpha_{i'}}(\beta_i\beta_j|V|\alpha_i\alpha_{i'})a^\dagger_{\beta_i} a^\dagger_{\beta_j} a_{\alpha_{i'}}
\end{aligned}
$$

- Note $(\alpha\beta|V|\gamma\delta) = (\beta\alpha|V|\delta\gamma)$ since $V(i,j) = V(j,i)$

Two-body operators

- Use to show
$$
\begin{aligned}
\hat{V}\,|\alpha_1\alpha_2\alpha_3...\alpha_N\rangle &= \hat{V} a^\dagger_{\alpha_1} a^\dagger_{\alpha_2} ... a^\dagger_{\alpha_N}\,|0\rangle \\
&= \sum_{i=1}^{N} a^\dagger_{\alpha_1} ... [\hat{V}, a^\dagger_{\alpha_i}] ... a^\dagger_{\alpha_N}\,|0\rangle \\
&= \sum_{i=1}^{N} \sum_{\beta_i \beta_{i'} \alpha_{i'}} (\beta_i \beta_{i'}|V|\alpha_i \alpha_{i'}) a^\dagger_{\alpha_1} ... a^\dagger_{\beta_i} a^\dagger_{\beta_{i'}} a_{\alpha_{i'}} a^\dagger_{\alpha_{i+1}} ... a^\dagger_{\alpha_N}\,|0\rangle \\
&= \sum_{i=1}^{N} \sum_{j>i}^{N} \sum_{\beta_i \beta_j} (\beta_i \beta_j|V|\alpha_i \alpha_j) a^\dagger_{\alpha_1} ... a^\dagger_{\beta_i} ... a^\dagger_{\beta_j} ... a^\dagger_{\alpha_N}\,|0\rangle
\end{aligned}
$$
✔

- Employ
$$
\sum_{\beta_j \alpha_{i'}} f(\beta_j, \alpha_{i'}) [a^\dagger_{\beta_j} a_{\alpha_{i'}}, a^\dagger_{\alpha_j}] = \sum_{\beta_j} f(\beta_j, \alpha_j) a^\dagger_{\beta_j}
$$

- Often used
$$
\hat{V} = \frac{1}{4} \sum_{\alpha\beta\gamma\delta} \langle\alpha\beta|\, V \,|\gamma\delta\rangle\, a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma
$$

- with
$$
\langle\alpha\beta|\, V \,|\gamma\delta\rangle \equiv (\alpha\beta|V|\gamma\delta) - (\alpha\beta|V|\delta\gamma) = \langle\alpha\beta|\, \hat{V} \,|\gamma\delta\rangle
$$

- Check!

Hamiltonian

- Most common operator
$$\hat{H} = \hat{T} + \hat{V} = \sum_{\alpha\beta} \langle\alpha|\, T\, |\beta\rangle\, a^\dagger_\alpha a_\beta + \frac{1}{2}\sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$$
- Notation often used $\psi^\dagger_{m_s}(\boldsymbol{r}) \equiv a^\dagger_{\boldsymbol{r}m_s}$
- Use
$$\begin{aligned}\langle \boldsymbol{r}m_s|\, T\, |\boldsymbol{r}'m_s'\rangle &= \langle \boldsymbol{r}m_s|\, \frac{\boldsymbol{p}^2}{2m}\, |\boldsymbol{r}'m_s'\rangle \\ &= \frac{-i\hbar}{2m}\nabla\cdot\langle\, \boldsymbol{r}m_s|\, \boldsymbol{p}\, |\boldsymbol{r}'m_s'\rangle \\ &= \frac{-\hbar^2}{2m}\nabla^2\langle \boldsymbol{r}m_s|\boldsymbol{r}'m_s'\rangle \\ &= \frac{-\hbar^2}{2m}\nabla^2\delta(\boldsymbol{r}-\boldsymbol{r}')\delta_{m_s,m_s'}\end{aligned}$$
- and
$$\begin{aligned}(\boldsymbol{r}_1 m_{s_1}\ \boldsymbol{r}_2 m_{s_2}|V(\boldsymbol{r},\boldsymbol{r}')|\boldsymbol{r}_3 m_{s_3}\ \boldsymbol{r}_4 m_{s_4}) &= \delta(\boldsymbol{r}_1-\boldsymbol{r}_3)\delta(\boldsymbol{r}_2-\boldsymbol{r}_4) \\ &\times\ \delta_{m_{s_1},m_{s_3}}\delta_{m_{s_2},m_{s_4}}V(|\boldsymbol{r}_3-\boldsymbol{r}_4|)\end{aligned}$$
- In this basis
$$\begin{aligned}\hat{H} &= \sum_{m_s}\int d^3r\ \psi^\dagger_{m_s}(\boldsymbol{r})\{\frac{-\hbar^2}{2m}\nabla^2\}\psi_{m_s}(\boldsymbol{r}) \\ &+ \frac{1}{2}\sum_{m_s m_s'}\int d^3r\ \int d^3r'\ \psi^\dagger_{m_s}(\boldsymbol{r})\psi^\dagger_{m_s'}(\boldsymbol{r}')V(|\boldsymbol{r}-\boldsymbol{r}'|)\psi_{m_s'}(\boldsymbol{r}')\psi_{m_s}(\boldsymbol{r})\end{aligned}$$
- appears as "second quantization"

IPM for fermions in finite systems

- IPM = independent particle model
- Only consider Pauli principle
- Localized fermions (for now)
- Examples
- Hamiltonian many-body problem: $\hat{H} = \hat{T} + \hat{V} = \hat{H}_0 + \hat{H}_1$
- with $\hat{H}_0 = \hat{T} + \hat{U}$
- and $\hat{H}_1 = \hat{V} - \hat{U}$
- Suitably chosen auxiliary one-body potential U
- Many-body problem can be solved for $\hat{H}_0$!!
- Also works with fixed external potential U_{ext}

$$\hat{H} = \hat{T} + \hat{U}_{ext} + \hat{V} = \hat{H}_0 + \hat{H}_1$$

Role of U

- Can be chosen to minimize effect of two-body interaction
- Ground state of total Hamiltonian may break a symmetry
  - Spontaneous magnetization
- Can speed up convergence of perturbation expansion in $\hat{H}_1$
- Spherical symmetry: sp problem straightforward but may have to be done numerically
- Assume solved: e.g. 3D-harmonic oscillator in nuclear physics

$$H_0 \left|\lambda\right\rangle = (T+U) \left|\lambda\right\rangle = \varepsilon_\lambda \left|\lambda\right\rangle$$

- For nuclei $\left|\lambda\right\rangle = \left|n(\ell\tfrac{1}{2})jm_j\right\rangle$
- For atoms (include Coulomb attraction to nucleus)

$$\left|\lambda\right\rangle = \left|n\ell m_\ell \tfrac{1}{2} m_s\right\rangle$$

Use second quantization

- Consider in the $\{|\lambda\rangle\}$ basis (discrete sums for simplicity)

$$\begin{aligned}\hat{H}_0 &= \sum_{\lambda\lambda'} \langle\lambda|\,(T+U)\,|\lambda'\rangle\, a^\dagger_\lambda a_{\lambda'} \\ &= \sum_{\lambda\lambda'} \varepsilon_{\lambda'}\ \delta_{\lambda,\lambda'}\ a^\dagger_\lambda a_{\lambda'} = \sum_\lambda \varepsilon_\lambda a^\dagger_\lambda a_\lambda\end{aligned}$$

- All many-body eigenstates of $\hat{H}_0$ are of the form

$$|\Phi^N_n\rangle = |\lambda_1\lambda_2...\lambda_N\rangle = a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} ... a^\dagger_{\lambda_N}\,|0\rangle$$

- with eigenvalue

$$E^N_n = \sum_{i=1}^N \varepsilon_{\lambda_i}$$

Explicitly

- Employ $$\left[\hat{H}_0, a^\dagger_{\lambda_i}\right] = \varepsilon_{\lambda_i} a^\dagger_{\lambda_i}$$

- and therefore

$$\hat{H}_0 \left|\lambda_1 \lambda_2 \lambda_3 ... \lambda_N\right\rangle = \hat{H}_0 a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} ... a^\dagger_{\lambda_N} \left|0\right\rangle$$

$$\begin{aligned}
&= [\hat{H}_0, a^\dagger_{\lambda_1}] a^\dagger_{\lambda_2} ... a^\dagger_{\lambda_N} \left|0\right\rangle + a^\dagger_{\lambda_1} \hat{H}_0 a^\dagger_{\lambda_2} ... a^\dagger_{\lambda_N} \left|0\right\rangle \\
&= [\hat{H}_0, a^\dagger_{\lambda_1}] a^\dagger_{\lambda_2} ... a^\dagger_{\lambda_N} \left|0\right\rangle + a^\dagger_{\lambda_1} [\hat{H}_0, a^\dagger_{\lambda_2}] ... a^\dagger_{\lambda_N} \left|0\right\rangle + ... + a^\dagger_{\lambda_1} a^\dagger_{\lambda_2} ... [\hat{H}_0, a^\dagger_{\lambda_N}] \left|0\right\rangle \\
&= \left\{ \sum_{i=1}^{N} \varepsilon_{\lambda_i} \right\} \left|\lambda_1 \lambda_2 \lambda_3 ... \lambda_N\right\rangle
\end{aligned}$$

- Corresponding many-body problem solved!
- Ground state $$\left|\Phi_0^N\right\rangle = \prod_{\lambda_i \le F} a^\dagger_{\lambda_i} \left|0\right\rangle$$
- Fermi sea ⇒ F

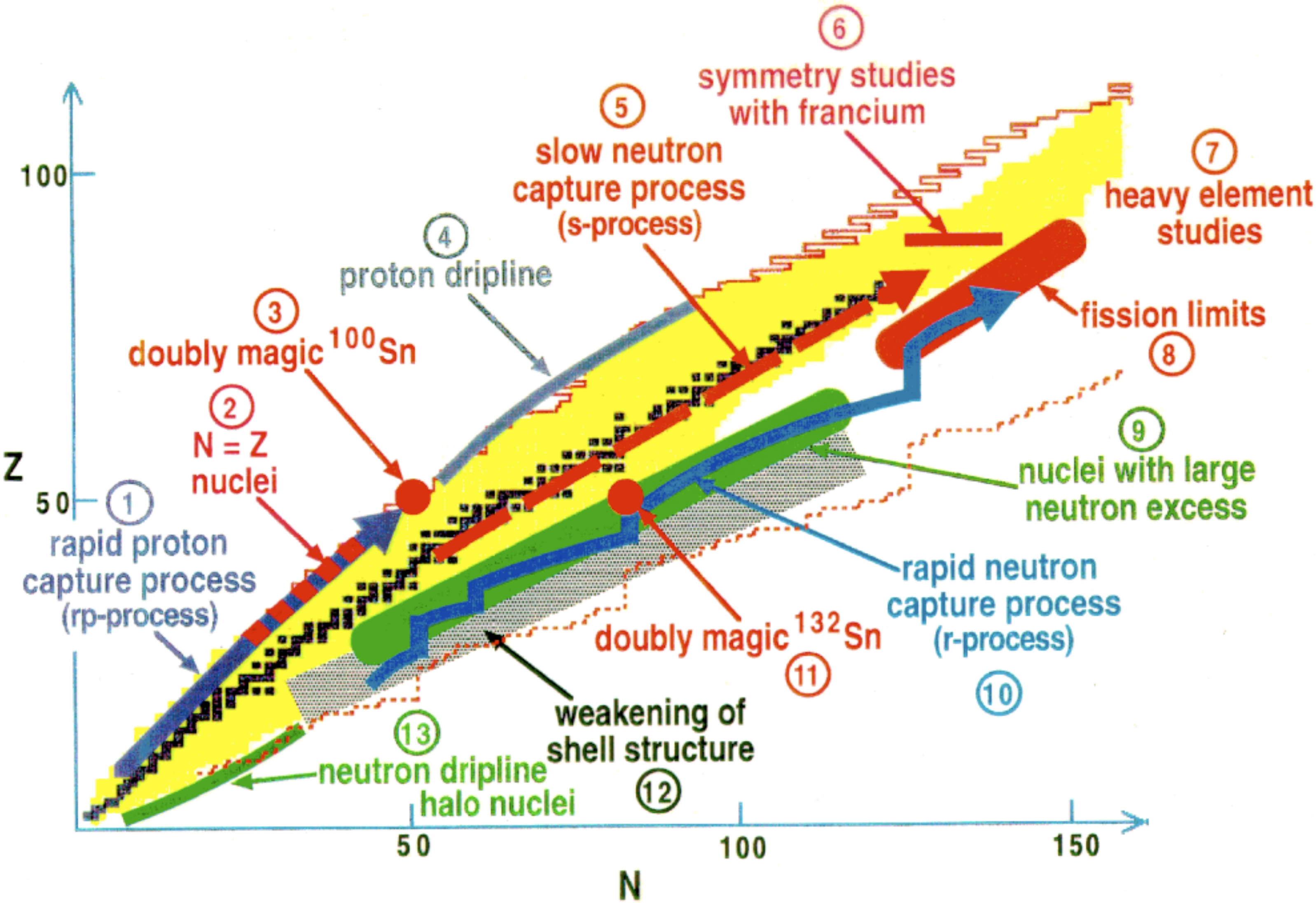
Nucleons in nuclei

- Atoms: shell closures at 2,10,18,36,54,86
- Similar features observed in nuclei
- Notation:
  - # of neutrons N
  - # of protons Z
  - # of nucleons $A = N + Z$
- Equivalent of ionization energy: separation energy
  - for protons $S_p(N,Z) = B(N,Z) - B(N,Z-1)$
  - for neutrons $S_n(N,Z) = B(N,Z) - B(N-1,Z)$
  - binding energy

$$M(N,Z) = \frac{E(N,Z)}{c^2} = N\ m_n\ +\ Z\ m_p\ -\ \frac{B(N,Z)}{c^2}$$

Chart of nuclides

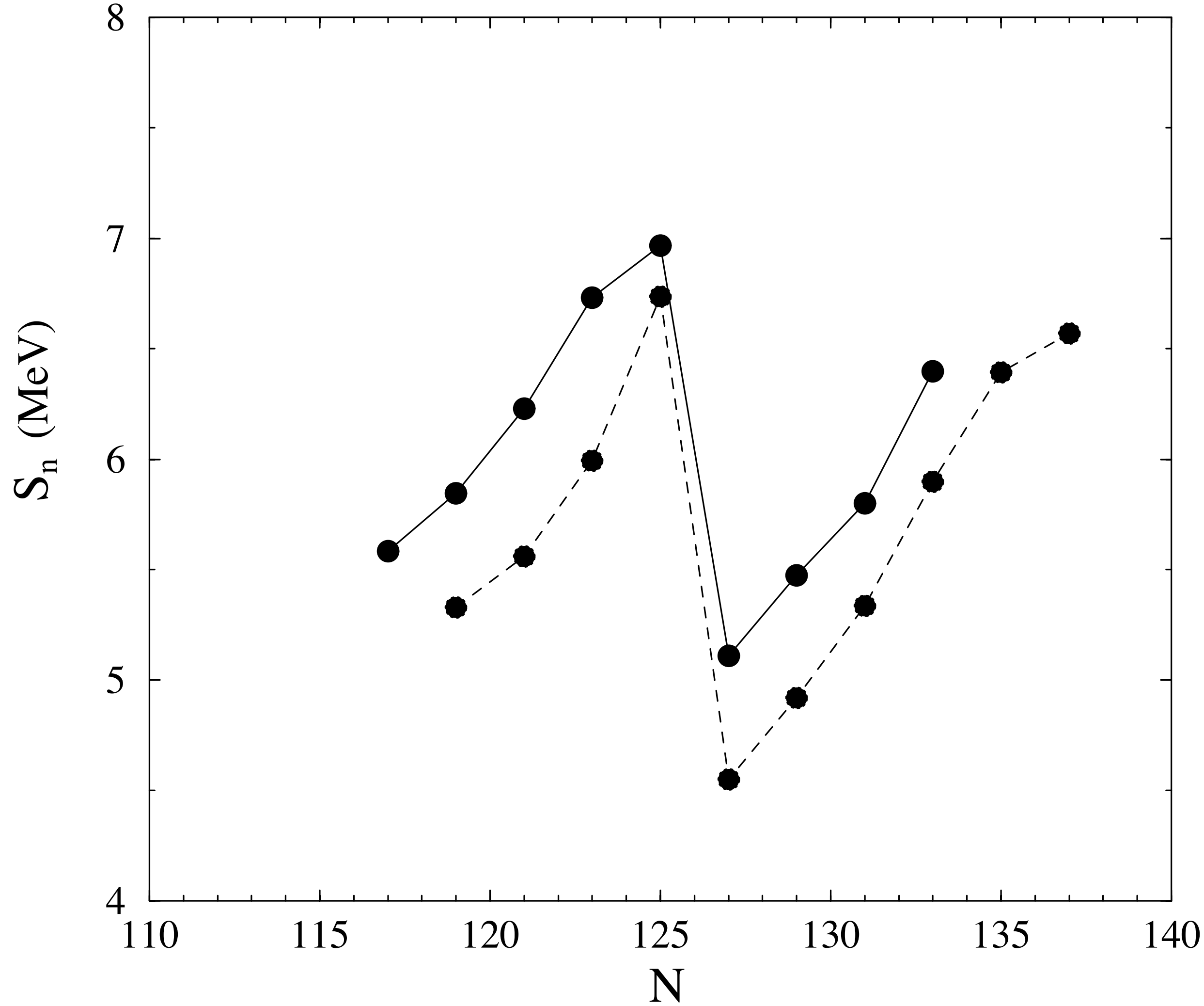
- Lots of nuclei and lots to be discovered



- Links to astrophysics

Shell closure at N=126

- Odd-even effect: plot only even Z

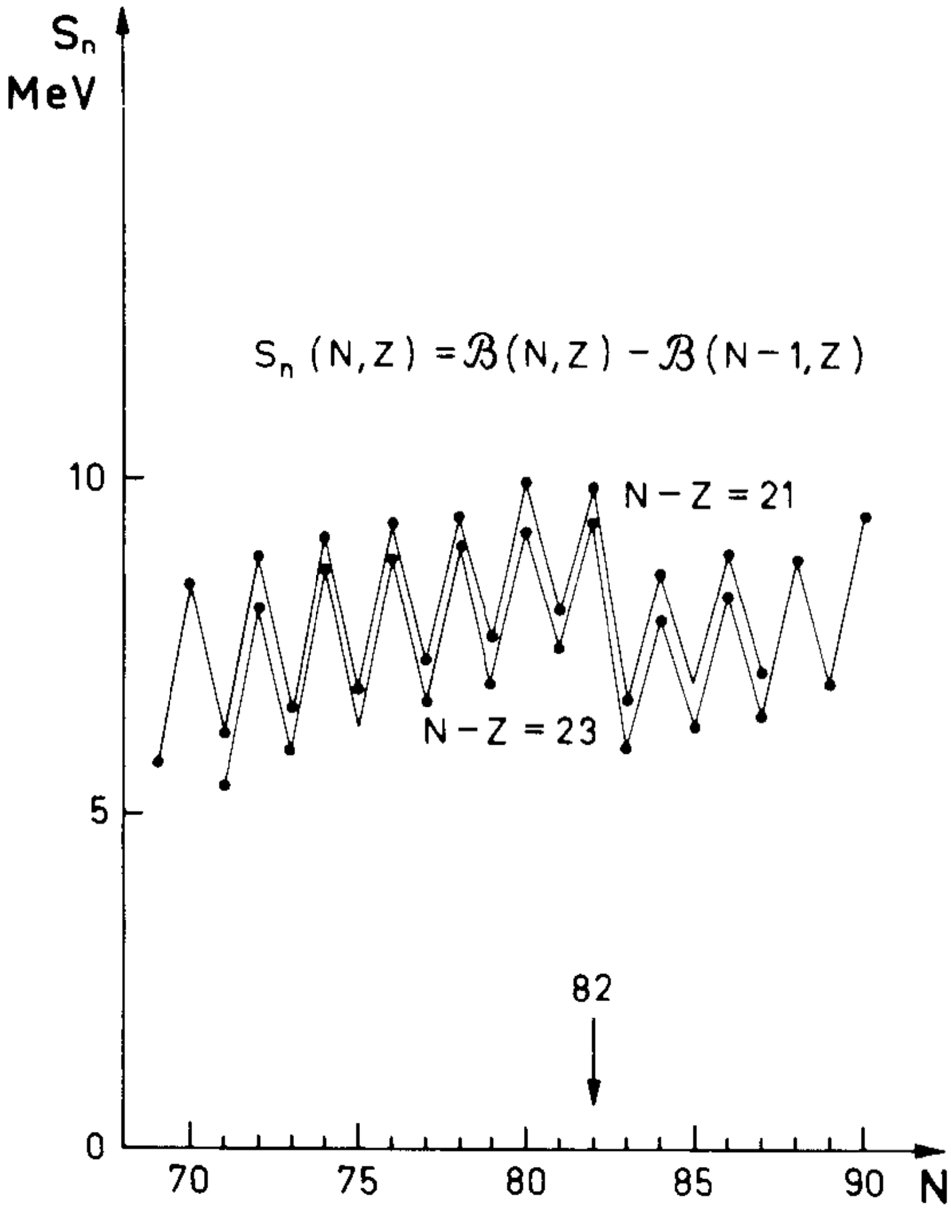


Solid: N-Z=41
Dashed: N-Z=43

- Also at other values N and Z

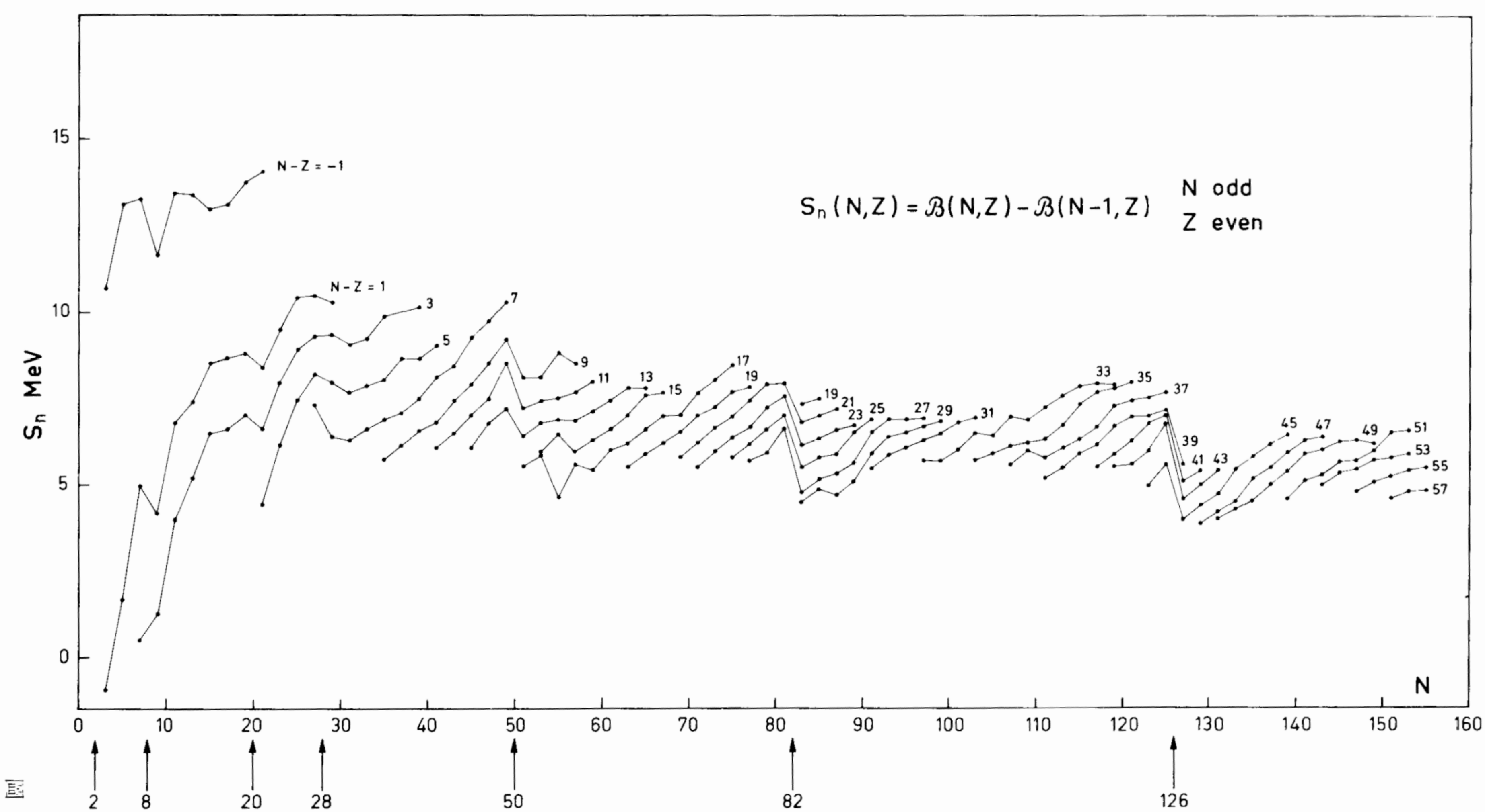
Illustration of odd-even effect

- from Bohr & Mottelson Vol.1 (BM1)



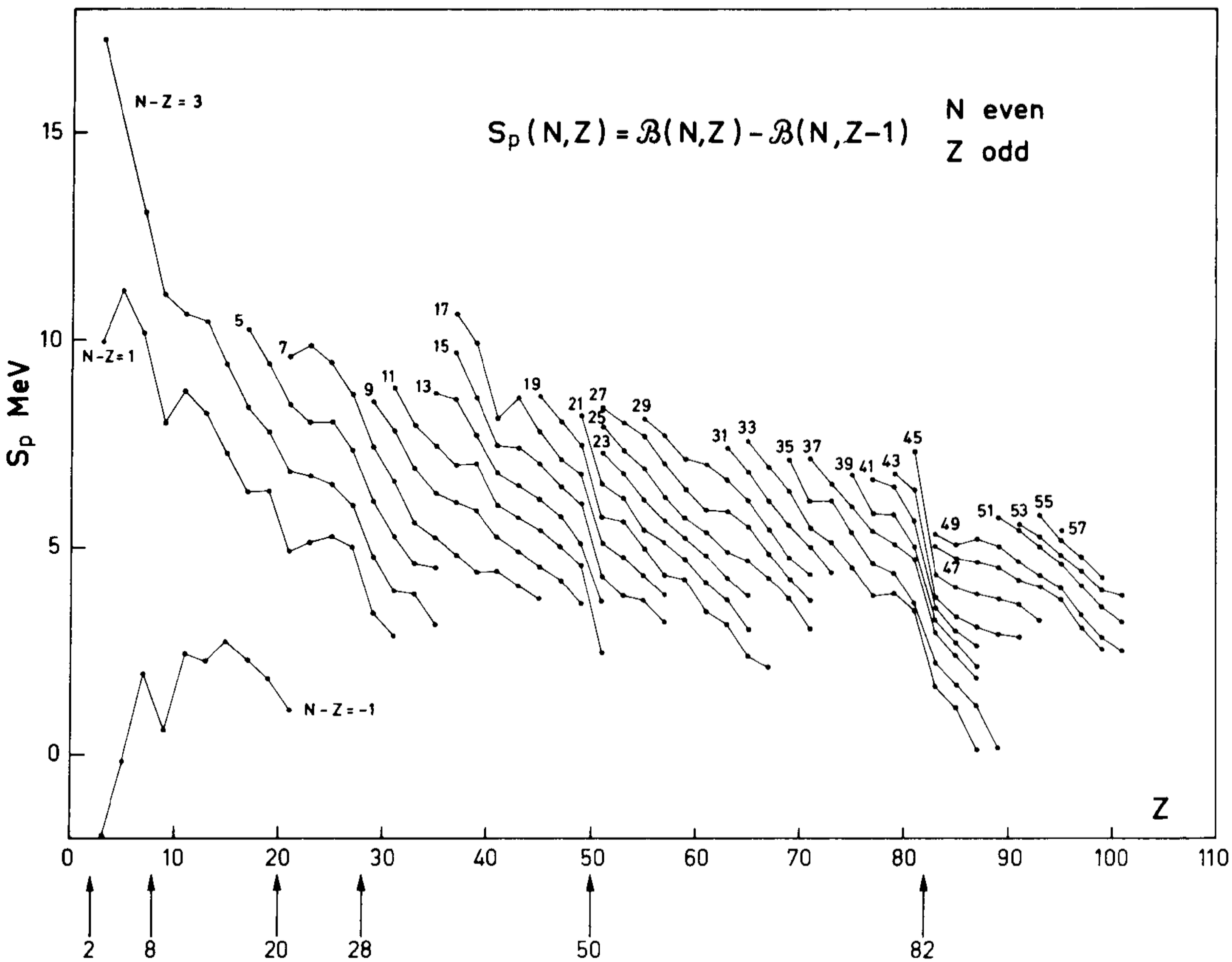
Neutrons

- BM1 figure



Protons

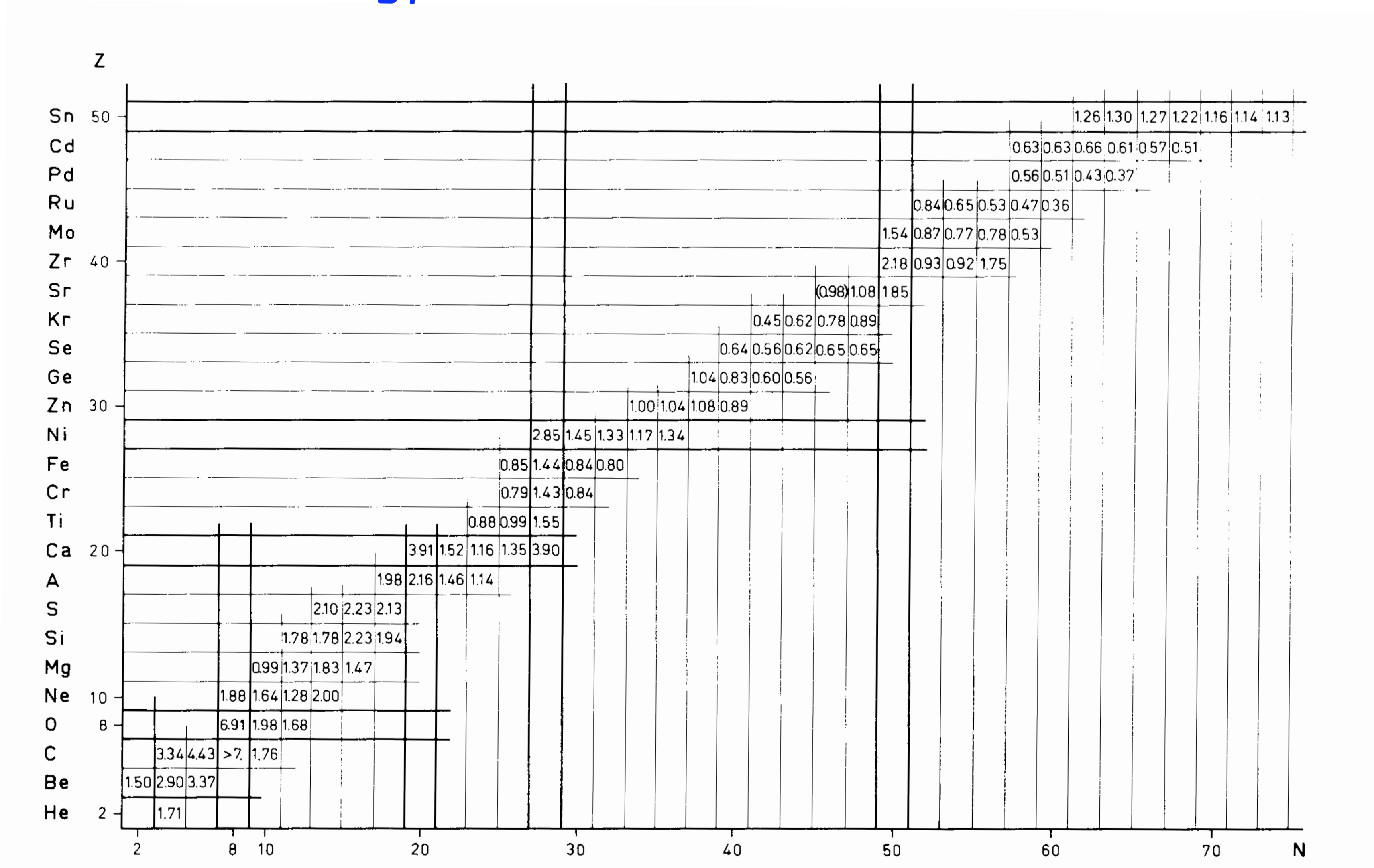
- BM1 figure



QMPT 540

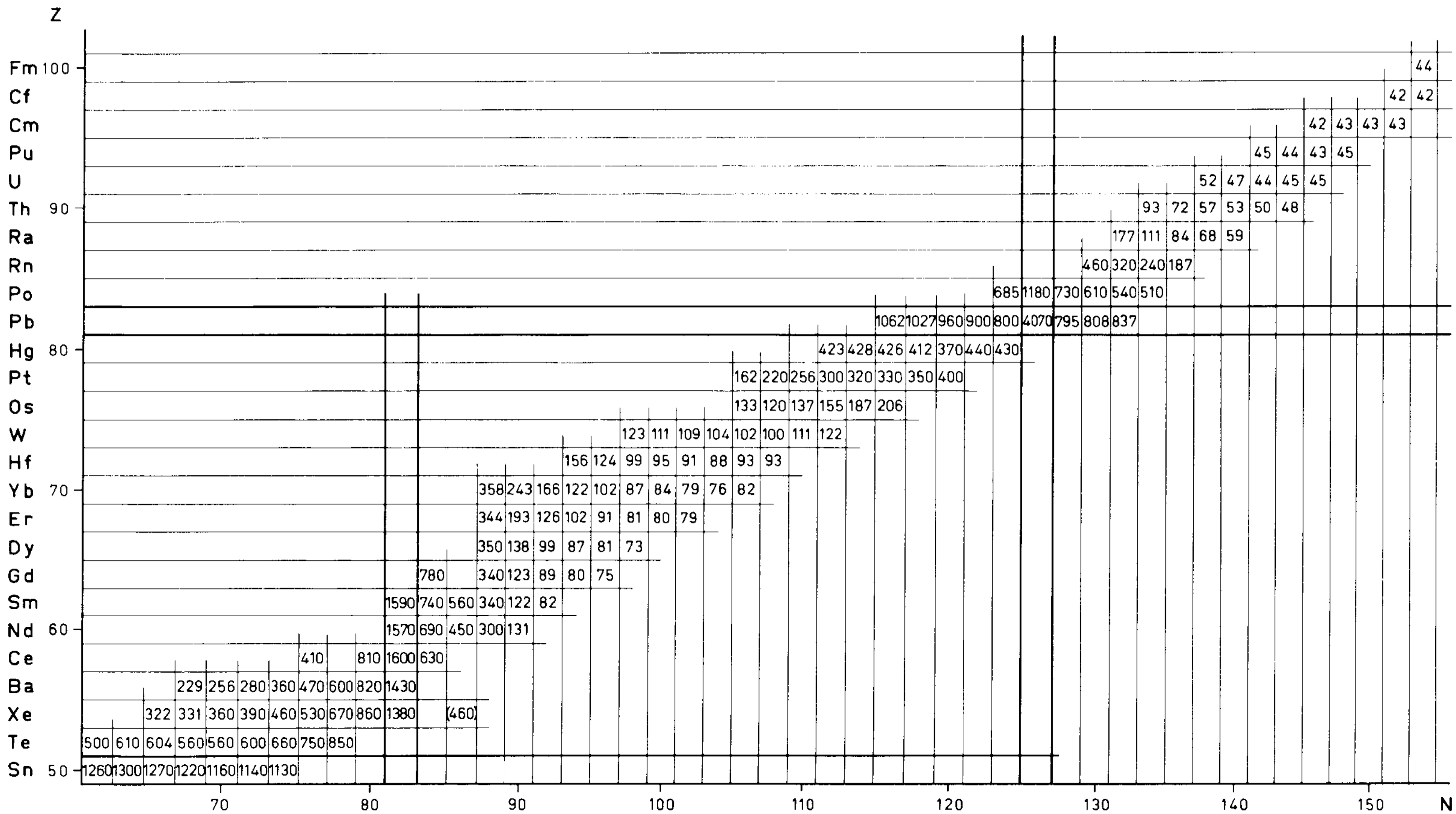
Systematics excitation energies in even-even nuclei

- Ground states 0^+
- First excited state almost always 2^+
- Excitation energy in MeV



Heavy nuclei

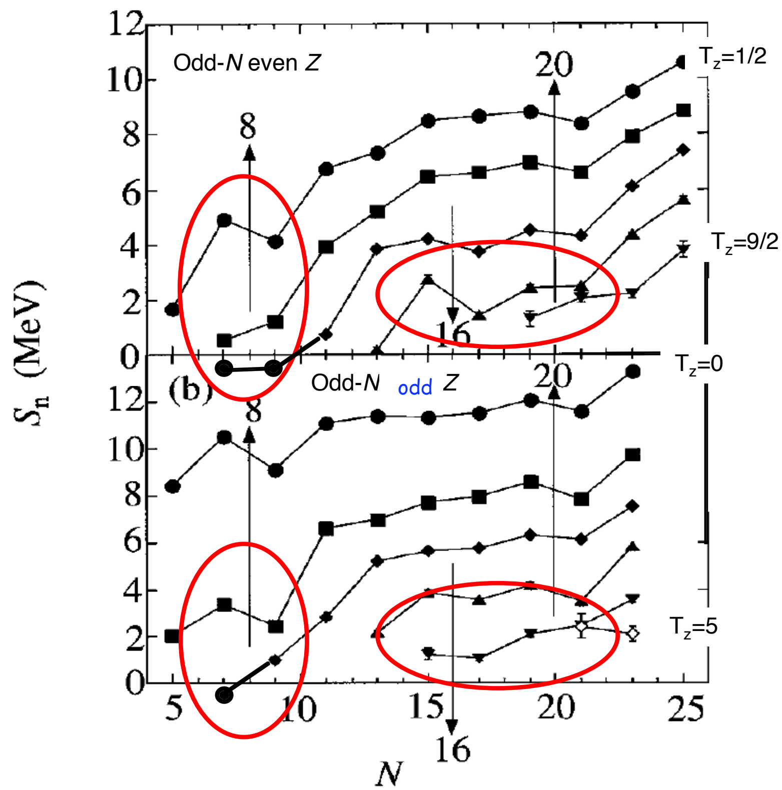
- Magic numbers for nuclei near stability:
  - Z=2, 8, 20, 28, 50, 82
  - N=2, 8, 20, 28, 50, 82, 126



Nuclear shell structure

- Ground-state spins and parity of odd nuclei provide further evidence of "magic numbers"
- Character of magic numbers may change far from stability (hot)

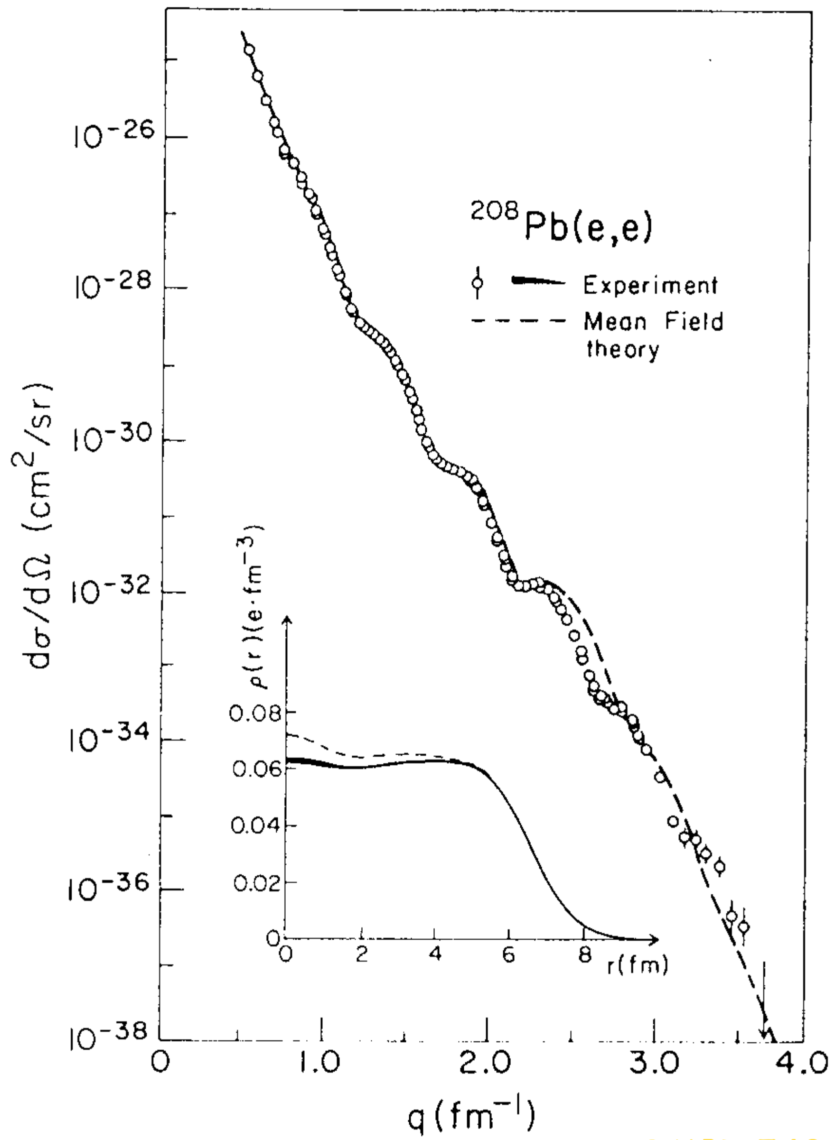
A. Ozawa *et al.*, Phys. Rev. Lett. 84, 5493 (2000)



- N=20 may disappear and N=16 may appear

Empirical potential

- Analogy to atoms suggests finding a sp potential ⇒ shells + IPM
- Difference(s) with atoms?
- Properties of empirical potential
  - overall?
  - size?
  - shape?
- Consider nuclear charge density



Frois & Papanicolas, Ann. Rev. Nucl. Part. Sci. **37**, 133 (1987)

Nuclear density distribution

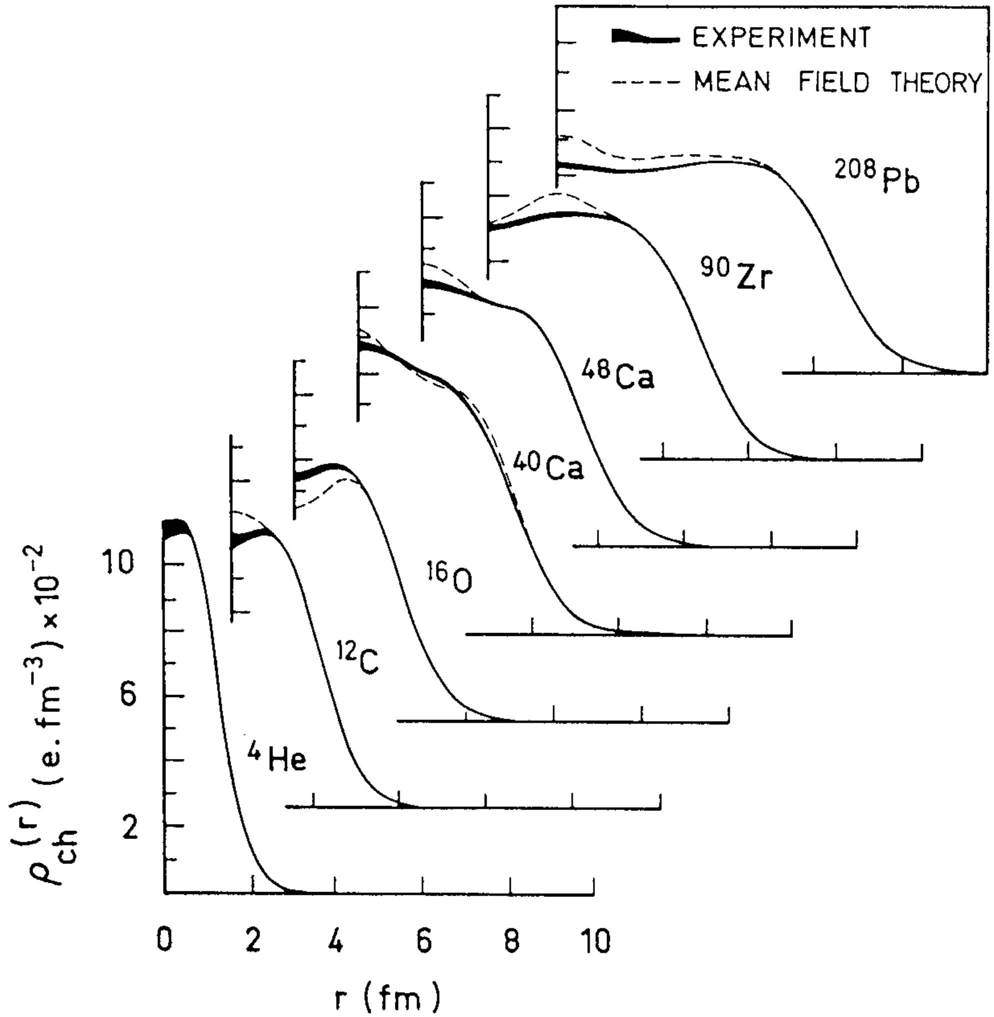
- Central density (A/Z* charge density) about the same for nuclei heavier than ^{16}O, corresponding to 0.16 nucleons/fm^3
- Important quantity
- Shape roughly represented by
-

$$\rho_{ch}(r) = \frac{\rho_0}{1 + \exp\left(\frac{r-c}{z}\right)}$$

$$c \approx 1.07 A^{\frac{1}{3}} \mathrm{fm}$$

$$z \approx 0.55 \mathrm{fm}$$

- Potential similar shape



Empirical potential

- Bohr Mottelson Vol.1

$$U = V f(r) + V_{\ell s} \left(\frac{\boldsymbol{\ell} \cdot \boldsymbol{s}}{\hbar^2} \right) r_0^2 \frac{1}{r} \frac{d}{dr} f(r)$$

- Central part roughly follows shape of density

$$f(r) = \left[1 + \exp\left(\frac{r - R}{a} \right) \right]^{-1}$$

- Woods-Saxon form
- Depth $V = \left[-51 \pm 33 \left(\frac{N - Z}{A} \right) \right] \text{ MeV}$

  + neutrons

  - protons

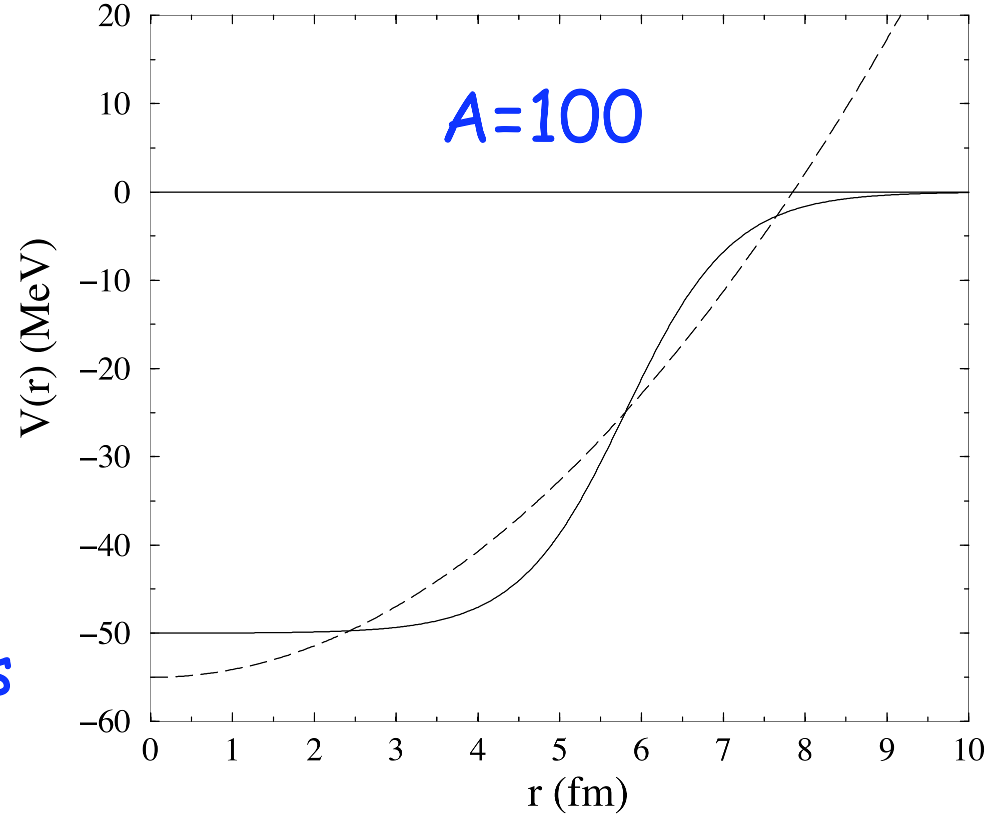
- radius $R = r_0 \, A^{1/3}$ with $r_0 = 1.27 \text{ fm}$
- diffuseness $a = 0.67 \text{ fm}$

Analytically solvable alternative

- Woods-Saxon (WS) generates finite number of bound states
- IPM: fill lowest levels ⇒ nuclear shells ⇒ magic numbers
- reasonably approximated by 3D harmonic oscillator

$$U_{HO}(r) = \frac{1}{2}m\omega^2 r^2 - V_0$$

$$H_0 = \frac{\boldsymbol{p}^2}{2m} + U_{HO}(r)$$



- Eigenstates in spherical basis

$$H_{HO}\,|n\ell m_\ell m_s\rangle = \left(\hbar\omega(2n + \ell + \tfrac{3}{2}) - V_0\right)|n\ell m_\ell m_s\rangle$$

Harmonic oscillator

- Filling of oscillator shells
- # of quanta $N = 2n + \ell$

N	n	ℓ	# of particles	"magic #"	parity
0	0	0	2	2	+
1	0	1	6	8	-
2	1	0	2		+
2	0	2	10	20	+
3	1	1	6		-
3	0	3	14	40	-
4	2	0	2		+
4	1	2	10		+
4	0	4	18	70	+

Need for another type of sp potential

- 1949 Mayer and Jensen suggest the need of a spin-orbit term
- Requires a coupled basis

$$|n(\ell s)jm_j\rangle = \sum_{m_\ell m_s} |n\ell m_\ell m_s\rangle\,(\ell\ m_\ell\ s\ m_s|\ j\ m_j)$$

- Use $\boldsymbol{\ell}\cdot\boldsymbol{s} = \frac{1}{2}(\boldsymbol{j}^2 - \boldsymbol{\ell}^2 - \boldsymbol{s}^2)$ to show that these are eigenstates

$$\frac{\boldsymbol{\ell}\cdot\boldsymbol{s}}{\hbar^2}\,|n(\ell s)jm_j\rangle = \tfrac{1}{2}\left(j(j+1) - \ell(\ell+1) - \tfrac{1}{2}(\tfrac{1}{2}+1)\right)|n(\ell s)jm_j\rangle$$

- For $j = \ell + \frac{1}{2}$ eigenvalue $\frac{1}{2}\ell$
- while for $j = \ell - \frac{1}{2}$ $-\frac{1}{2}(\ell + 1)$
- so SO splits these levels! and more so with larger ℓ

Inclusion of SO potential and magic numbers

- Sign of SO?

$$V_{\ell s}\left(\frac{\boldsymbol{\ell}\cdot\boldsymbol{s}}{\hbar^2}\right) r_0^2 \frac{1}{r}\frac{d}{dr} f(r)$$

$$V_{\ell s} = -0.44V$$

- Consequence for

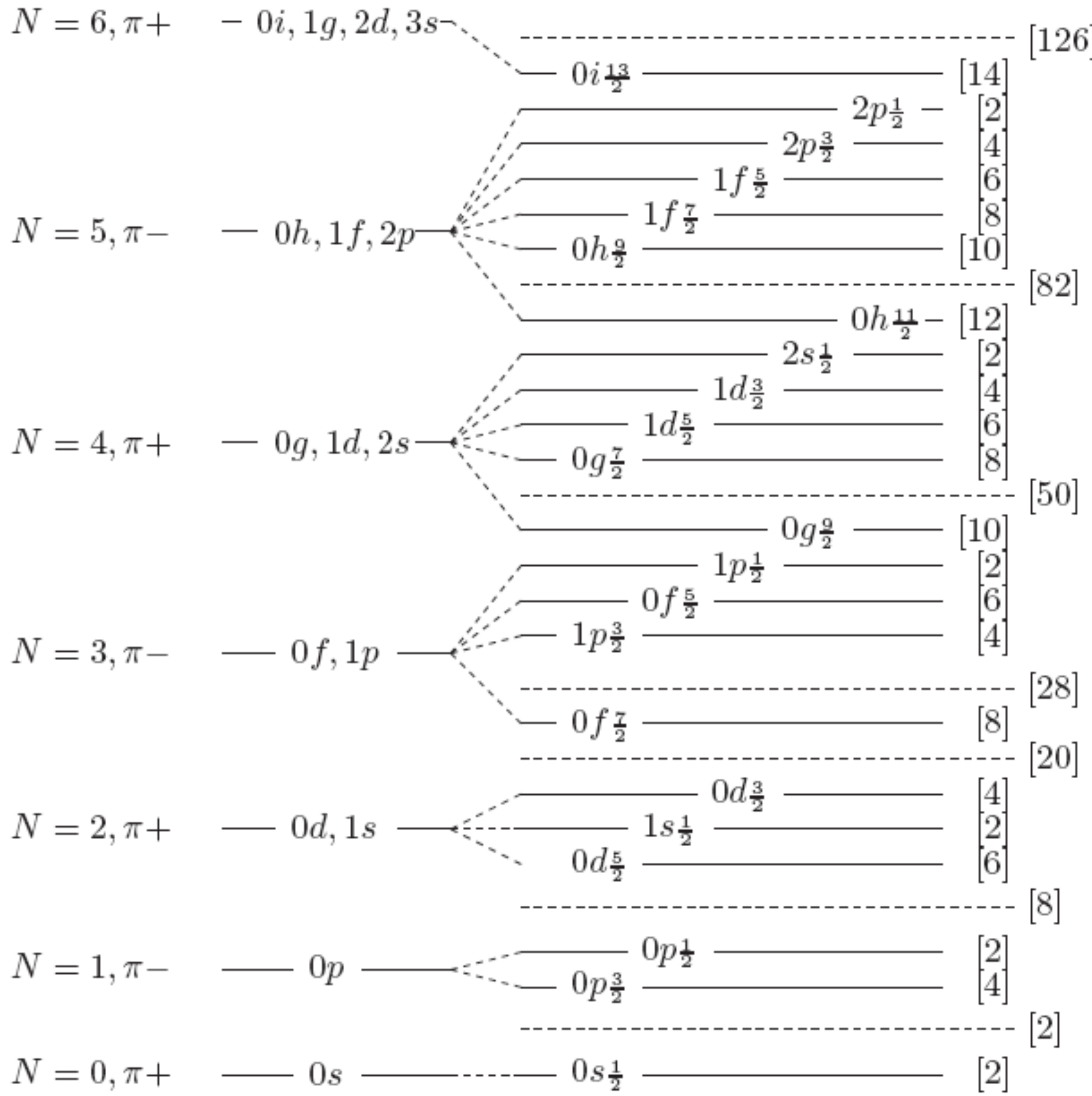
$$0f\,\tfrac{7}{2}$$

$$0g\,\tfrac{9}{2}$$

$$0h\,\tfrac{11}{2}$$

$$0i\,\tfrac{13}{2}$$

- Noticeably shifted
- Correct magic numbers!



^{208}Pb for example

- Empirical potential & sp energies

$$\hat{H}_0 \; a_\alpha^\dagger \left| {}^{208}\mathrm{Pb}_{g.s.} \right\rangle = \left[\varepsilon_\alpha + E({}^{208}\mathrm{Pb}_{g.s.}) \right] \; a_\alpha^\dagger \left| {}^{208}\mathrm{Pb}_{g.s.} \right\rangle$$

- *A*+1: "sp energies" $E_n^{A+1} - E_0^A$ directly from experiment
- *A*-1:

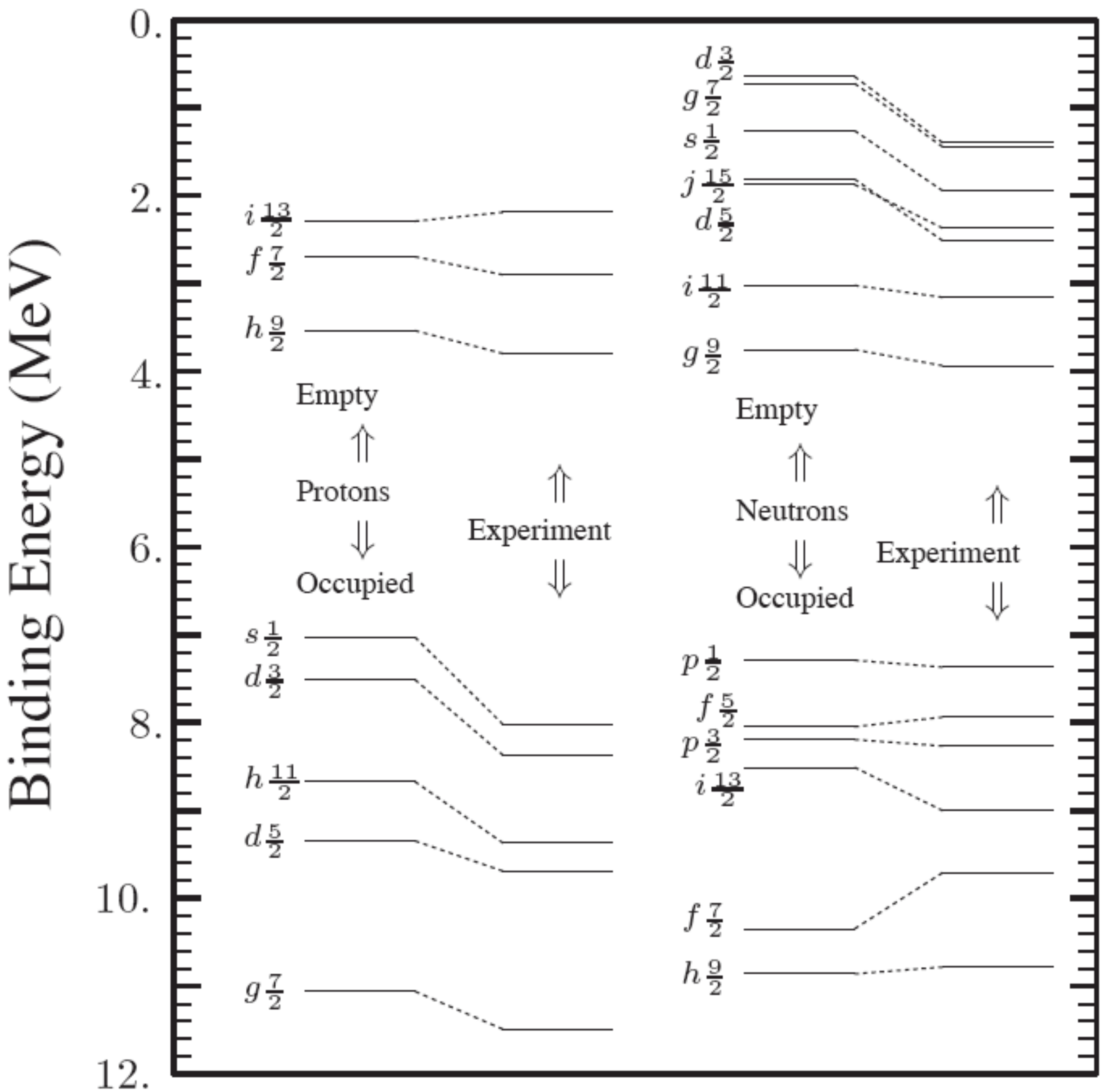
$$\hat{H}_0 \; a_\alpha \left| {}^{208}\mathrm{Pb}_{g.s.} \right\rangle = \left[E({}^{208}\mathrm{Pb}_{g.s.}) - \varepsilon_\alpha \right] \; a_\alpha \left| {}^{208}\mathrm{Pb}_{g.s.} \right\rangle$$

- also directly from $E_0^A - E_n^{A-1}$

- Shell filling for nuclei near stability follows empirical potential

Comparison with experiment

- Now how to explain this potential …



Nucleon-nucleon interaction

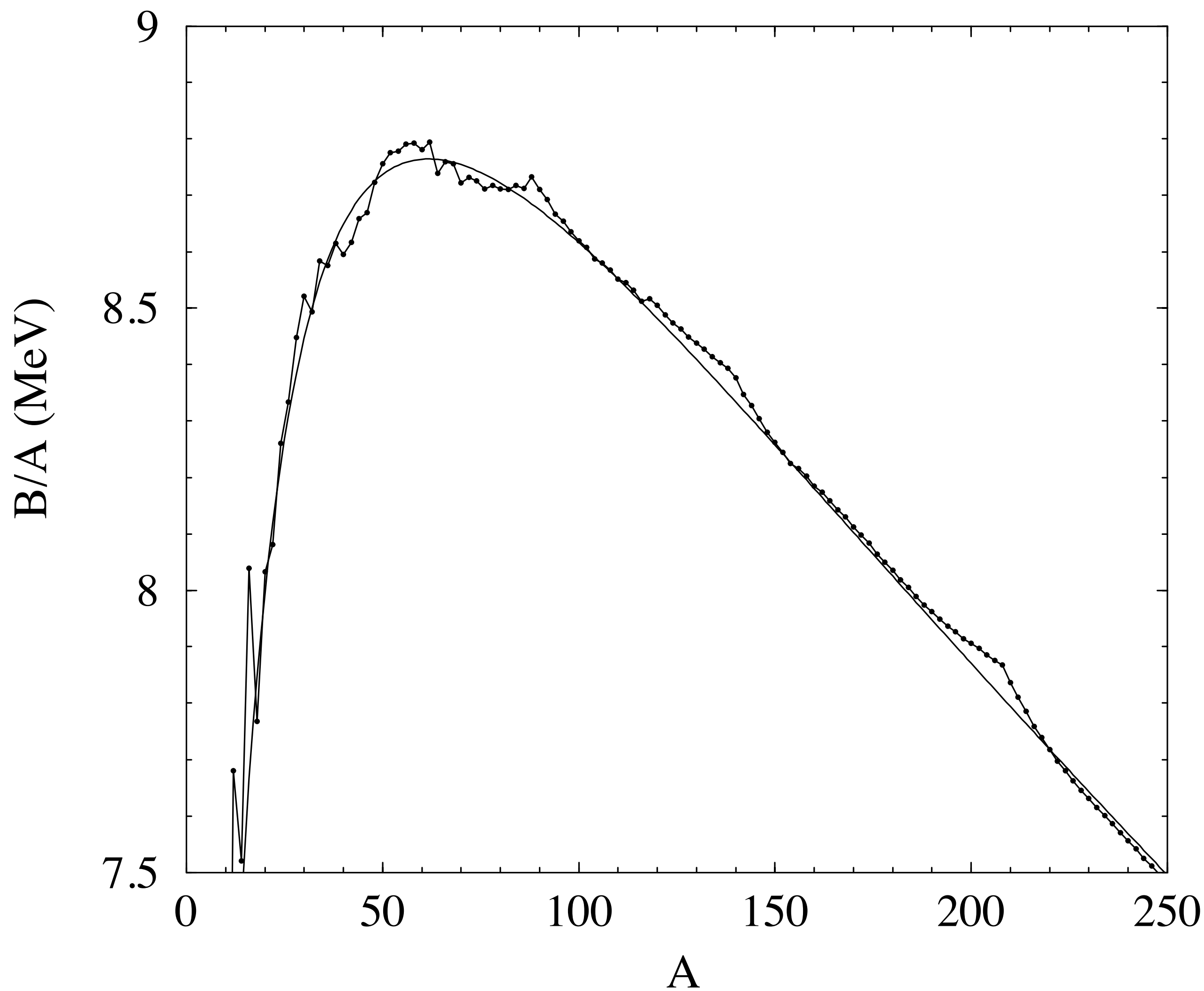
- Shell structure in nuclei and lots more to be explained on the basis of how nucleons interact with each other in free space

- QCD
- Lattice calculations
- Effective field theory
- Exchange of lowest bosonic states
- Phenomenology

- Realistic NN interactions: describe NN scattering data up to pion production threshold plus deuteron properties
- Note: extra energy scale from confinement of nucleons

Nuclear Matter

- Nuclear masses near stability $M(N,Z) = \frac{E(N,Z)}{c^2} = N\ m_n\ +\ Z\ m_p\ -\ \frac{B(N,Z)}{c^2}$
- Data
- Each A most stable N,Z pair



- Where fission?
- Where fusion?

Nuclear Matter

- Smooth curve

$$B = b_{vol} A - b_{surf} A^{2/3} - \frac{1}{2} b_{sym} \frac{(N-Z)^2}{A} - \frac{3}{5} \frac{Z^2 e^2}{R_c}$$

- volume $b_{vol} = 15.56 \text{ MeV}$
- surface $b_{surf} = 17.23 \text{ MeV}$
- symmetry $b_{sym} = 46.57 \text{ MeV}$
- Coulomb $R_c = 1.24 A^{1/3} \text{ fm}$

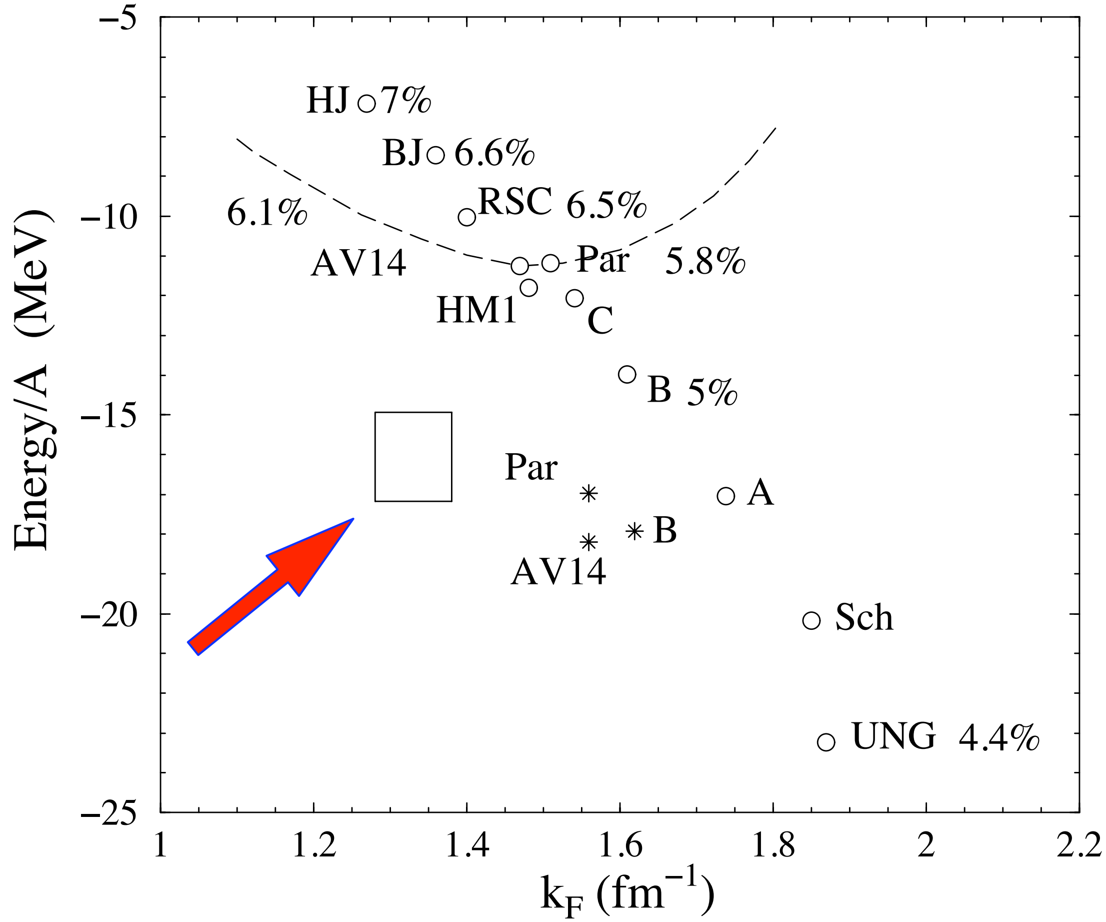
Great interest in limit: N=Z; no Coulomb; A ⇒∞

Two most important numbers in Nuclear Physics

$$\frac{B}{A} \approx 16 \text{ MeV} \qquad \rho_0 \approx 0.16 \text{ fm}^3$$

Saturation problem of nuclear matter

Given V_{NN} ⇒ explain correct minimum of E/A in nuclear matter as a function of density inside empirical box



Describe the infinite system of neutrons

⇒ properties of neutron stars

Isospin

- Shell closures for N and Z the same!!
- Also $m_n c^2 \approx m_p c^2$ 939.56 MeV vs. 938.27 MeV
- So strong interaction Hamiltonian (QCD) invariant for p ⇔ n
- But weak and electromagnetic interactions are not
- Strong interaction dominates ⇒ consequences
- Notation (for now) $p_\alpha^\dagger$ adds proton $n_\alpha^\dagger$ adds neutron
- Anticommutation relations $\{p_\alpha^\dagger, p_\beta\} = \delta_{\alpha,\beta}$ $\{n_\alpha^\dagger, n_\beta\} = \delta_{\alpha,\beta}$

Isospin

- Z proton & N neutron state

$$|\alpha_1\alpha_2...\alpha_Z;\beta_1\beta_2...\beta_N\rangle = p^\dagger_{\alpha_1}p^\dagger_{\alpha_2}...p^\dagger_{\alpha_Z}n^\dagger_{\beta_1}n^\dagger_{\beta_2}...n^\dagger_{\beta_N}\,|0\rangle$$

- Exchange all p with n $\hat{T}^+ = \sum_\alpha p^\dagger_\alpha n_\alpha$
- and vice versa $\hat{T}^- = \sum_\alpha n^\dagger_\alpha p_\alpha$
- Expect $[\hat{H}_S, \hat{T}^\pm] = 0$
- Consider

$$\begin{aligned}\hat{T}_3 &= \frac{1}{2}[\hat{T}^+,\hat{T}^-] = \frac{1}{2}\sum_{\alpha\beta}(p^\dagger_\alpha n_\alpha n^\dagger_\beta p_\beta - n^\dagger_\beta p_\beta p^\dagger_\alpha n_\alpha)\\ &= \frac{1}{2}\sum_{\alpha\beta}(p^\dagger_\alpha p_\beta \delta_{\alpha,\beta} - n^\dagger_\beta n_\alpha \delta_{\alpha,\beta}) = \frac{1}{2}\sum_\alpha (p^\dagger_\alpha p_\alpha - n^\dagger_\alpha n_\alpha)\end{aligned}$$

- will also commute with H_S

Isospin

- Check $[\hat{T}_3, \hat{T}^{\pm}] = \pm\hat{T}^{\pm}$
- Then operators

$$\hat{T}_1 = \tfrac{1}{2}\left(\hat{T}^+ + \hat{T}^-\right)$$
$$\hat{T}_2 = \tfrac{1}{2i}\left(\hat{T}^+ - \hat{T}^-\right)$$
$$\hat{T}_3$$

obey the same algebra as J_x, J_y, J_z

so spectrum identical and $\hat{H}_S, \hat{\boldsymbol{T}}^2, \hat{T}_3$ simultaneously diagonal !

proton $\left|\boldsymbol{r} m_s\right\rangle_p = \left|\boldsymbol{r} m_s m_t = \tfrac{1}{2}\right\rangle$

neutron $\left|\boldsymbol{r} m_s\right\rangle_n = \left|\boldsymbol{r} m_s m_t = -\tfrac{1}{2}\right\rangle$

For this doublet $\boldsymbol{T}^2 \left|\boldsymbol{r} m_s m_t\right\rangle = \tfrac{1}{2}(\tfrac{1}{2}+1)\left|\boldsymbol{r} m_s m_t\right\rangle$

and $T_3 \left|\boldsymbol{r} m_s m_t\right\rangle = m_t \left|\boldsymbol{r} m_s m_t\right\rangle$

States with total isospin constructed as for angular momentum

Closed-shells and angular momentum

- Atoms: consider one closed shell (argument the same for more)

$$|n\ell m_\ell = \ell m_s = \tfrac{1}{2}, n\ell m_\ell = \ell m_s = -\tfrac{1}{2}, \ldots n\ell m_\ell = -\ell m_s = \tfrac{1}{2}, n\ell m_\ell = -\ell m_s = -\tfrac{1}{2}\rangle$$

- Expect?
- Example: He

$$\begin{aligned} \left|(1s)^2\right\rangle &= \frac{1}{\sqrt{2}}\left\{|1s\uparrow 1s\downarrow\rangle - |1s\downarrow 1s\uparrow\rangle\right\} \\ &= \left|(1s)^2; L=0 S=0\right\rangle \end{aligned}$$

- Consider nuclear closed shell

$$|\Phi_0\rangle = |n(\ell\tfrac{1}{2})jm_j = j, n(\ell\tfrac{1}{2})jm_j = j-1, \ldots, n(\ell\tfrac{1}{2})m_j = -j\rangle$$

Angular momentum and second quantization

- z-component of total angular momentum

$$\hat{J}_z = \sum_{n\ell jm} \sum_{n'\ell' j'm'} \langle n\ell jm | \, j_z \, | n'\ell' j'm' \rangle \, a^\dagger_{n\ell jm} a_{n'\ell' j'm'}$$

$$= \sum_{n\ell jm} \hbar m \; a^\dagger_{n\ell jm} a_{n\ell jm}$$

- Action on single closed shell

$$\hat{J}_z \, | n\ell j; m = -j, -j+1, ..., j \rangle = \sum_m \hbar m \; a^\dagger_{n\ell jm} a_{n\ell jm} \, | n\ell j; m = -j, -j+1, ..., = j \rangle$$

$$= \left\{ \sum_{m=-j}^{j} \hbar m \right\} | n\ell j; m = -j, -j+1, ..., j \rangle$$

$$= 0 \times | n\ell j; m = -j, -j+1, ..., j \rangle$$

- Also $\hat{J}_\pm \, | n\ell j; m = -j, -j+1, ..., j \rangle = 0$
- So total angular momentum $J = 0$
- Closed shell atoms $L = 0$

$S = 0$

Two-particle states and interactions

- Pauli principle has important effect on possible states
- Free particles ⇒ plane waves
- Eigenstates of $T = \frac{\boldsymbol{p}^2}{2m}$ notation (isospin)
- Use box normalization (should be familiar)
- Nucleons $|\boldsymbol{p}\ s=\frac{1}{2}\ m_s\ t=\frac{1}{2}\ m_t\rangle \equiv |\boldsymbol{p} m_s m_t\rangle$
- Electrons, ^{3}He atoms $|\boldsymbol{p}\ s=\frac{1}{2}\ m_s\rangle \equiv |\boldsymbol{p} m_s\rangle$
- Bosons with zero spin (^{4}He atoms) $|\boldsymbol{p}\rangle$

- Use successive basis transformations for two-nucleon states to survey angular momentum restrictions
- Total spin & isospin; CM and relative momentum; orbital angular momentum relative motion; total angular momentum

Antisymmetric two-nucleon states

- Start with

$$|\boldsymbol{p}_1 m_{s_1} m_{t_1}; \boldsymbol{p}_2 m_{s_2} m_{t_2}\rangle = \frac{1}{\sqrt{2}} \left\{ |\boldsymbol{p}_1 m_{s_1} m_{t_1}\rangle |\boldsymbol{p}_2 m_{s_2} m_{t_2}\rangle - |\boldsymbol{p}_2 m_{s_2} m_{t_2}\rangle |\boldsymbol{p}_1 m_{s_1} m_{t_1}\rangle \right\}$$

$$= \frac{1}{\sqrt{2}} \sum_{SM_S} \sum_{TM_T} \{ (\tfrac{1}{2}\ m_{s_1}\ \tfrac{1}{2}\ m_{s_2}\ |S\ M_S) (\tfrac{1}{2}\ m_{t_1}\ \tfrac{1}{2}\ m_{t_2}\ |T\ M_T) |\boldsymbol{p}_1\ \boldsymbol{p}_2\ S\ M_S\ T\ M_T)$$

$$- (\tfrac{1}{2}\ m_{s_2}\ \tfrac{1}{2}\ m_{s_1}\ |S\ M_S) (\tfrac{1}{2}\ m_{t_2}\ \tfrac{1}{2}\ m_{t_1}\ |T\ M_T) |\boldsymbol{p}_2\ \boldsymbol{p}_1\ S\ M_S\ T\ M_T) \}$$

- then

$$\boldsymbol{P} = \boldsymbol{p}_1 + \boldsymbol{p}_2$$
$$\boldsymbol{p} = \tfrac{1}{2} (\boldsymbol{p}_1 - \boldsymbol{p}_2)$$

- and use

$$|\boldsymbol{p}\rangle = \sum_{LM_L} |pLM_L\rangle \langle LM_L|\hat{\boldsymbol{p}}\rangle = \sum_{LM_L} |pLM_L\rangle Y^*_{LM_L}(\hat{\boldsymbol{p}})$$

$$|-\boldsymbol{p}\rangle = \sum_{LM_L} |pLM_L\rangle \langle LM_L|\widehat{-\boldsymbol{p}}\rangle = \sum_{LM_L} |pLM_L\rangle (-1)^L Y^*_{LM_L}(\hat{\boldsymbol{p}})$$

$$Y^*_{LM_L}(\widehat{-\boldsymbol{p}}) = Y^*_{LM_L}(\pi - \theta_p, \phi_p + \pi) = (-1)^L Y^*_{LM_L}(\hat{\boldsymbol{p}})$$

- as well as

$$(\tfrac{1}{2}\ m_{s_2}\ \tfrac{1}{2}\ m_{s_1}\ |S\ M_S) = (-1)^{\frac{1}{2}+\frac{1}{2}-S}\ (\tfrac{1}{2}\ m_{s_1}\ \tfrac{1}{2}\ m_{s_2}\ |S\ M_S)$$

$$(\tfrac{1}{2}\ m_{t_2}\ \tfrac{1}{2}\ m_{t_1}\ |T\ M_T) = (-1)^{\frac{1}{2}+\frac{1}{2}-T}\ (\tfrac{1}{2}\ m_{t_1}\ \tfrac{1}{2}\ m_{t_2}\ |T\ M_T)$$

Antisymmetry constraints for two nucleons

- Summarize

$$|\boldsymbol{p}_1 m_{s_1} m_{t_1}; \boldsymbol{p}_2 m_{s_2} m_{t_2}\rangle =$$

$$\frac{1}{\sqrt{2}} \sum_{SM_S TM_T LM_L} \left(\tfrac{1}{2}\ m_{s_1}\ \tfrac{1}{2}\ m_{s_2}\ |S\ M_S\right)\left(\tfrac{1}{2}\ m_{t_1}\ \tfrac{1}{2}\ m_{t_2}\ |T\ M_T\right) Y^*_{LM_L}(\hat{\boldsymbol{p}})$$

$$\times \left[1-(-1)^{L+S+T}\right] |\boldsymbol{P}\ p\ LM_L SM_S\ TM_T)$$

$$= \frac{1}{\sqrt{2}} \sum_{SM_S TM_T LM_L JM_J} \left(\tfrac{1}{2}\ m_{s_1}\ \tfrac{1}{2}\ m_{s_2}\ |S\ M_S\right)\left(\tfrac{1}{2}\ m_{t_1}\ \tfrac{1}{2}\ m_{t_2}\ |T\ M_T\right) Y^*_{LM_L}(\hat{\boldsymbol{p}})$$

$$\times\ (L\ M_L\ S\ M_S\ |J\ M_J) \left[1-(-1)^{L+S+T}\right] |\boldsymbol{P}\ p\ (LS)JM_J\ TM_T)$$

- $L+S+T$ must be odd!
  - Notation

T=0	T=1
${}^3S_1 - {}^3D_1$	${}^1S_0$
${}^1P_1$	${}^3P_0$
${}^3D_2$	${}^3P_1$
$\dots$	${}^3P_2 - {}^3F_2$
	${}^1D_2$

Two electrons and two spinless bosons

- Remove isospin

$$|\boldsymbol{p}_1 m_{s_1}; \boldsymbol{p}_2 m_{s_2}\rangle = \frac{1}{\sqrt{2}} \sum_{S M_S L M_L} (\tfrac{1}{2}\ m_{s_1}\ \tfrac{1}{2}\ m_{s_2}\ | S\ M_S)\, Y^*_{L M_L}(\hat{\boldsymbol{p}}) \times \left[1 + (-1)^{L+S}\right] |\boldsymbol{P}\ p\ L M_L S M_S\ )$$

- $L + S$ even!

- Two spinless bosons

$$|\boldsymbol{p}_1; \boldsymbol{p}_2\rangle = \frac{1}{\sqrt{2}} \sum_{L M_L} Y^*_{L M_L}(\hat{\boldsymbol{p}}) \left[1 + (-1)^{L}\right] |\boldsymbol{P}\ p\ L M_L\ )$$

- L even!

Nuclei

- Different shells only Clebsch-Gordan constraint
- Uncoupled states in the same shell $|\Phi_{jm,jm'}\rangle = a^\dagger_{jm} a^\dagger_{jm'} |\Phi_0\rangle$
- Coupling

$$
\begin{aligned}
|\Phi_{jj,JM}\rangle &= \sum_{mm'} (j\ m\ j\ m'\ |J\ M)\, |\Phi_{jm,jm'}\rangle = \sum_{mm'} (j\ m'\ j\ m\ |J\ M)\, |\Phi_{jm',jm}\rangle \\
&= \sum_{mm'} (-1)^{2j-J} (j\ m\ j\ m'\ |J\ M)\, (-1)\, |\Phi_{jm,jm'}\rangle \\
&= (-1)^J \sum_{mm'} (j\ m\ j\ m'\ |J\ M)\, |\Phi_{jm,jm'}\rangle \\
&= (-1)^J\ |\Phi_{jj,JM}\rangle
\end{aligned}
$$

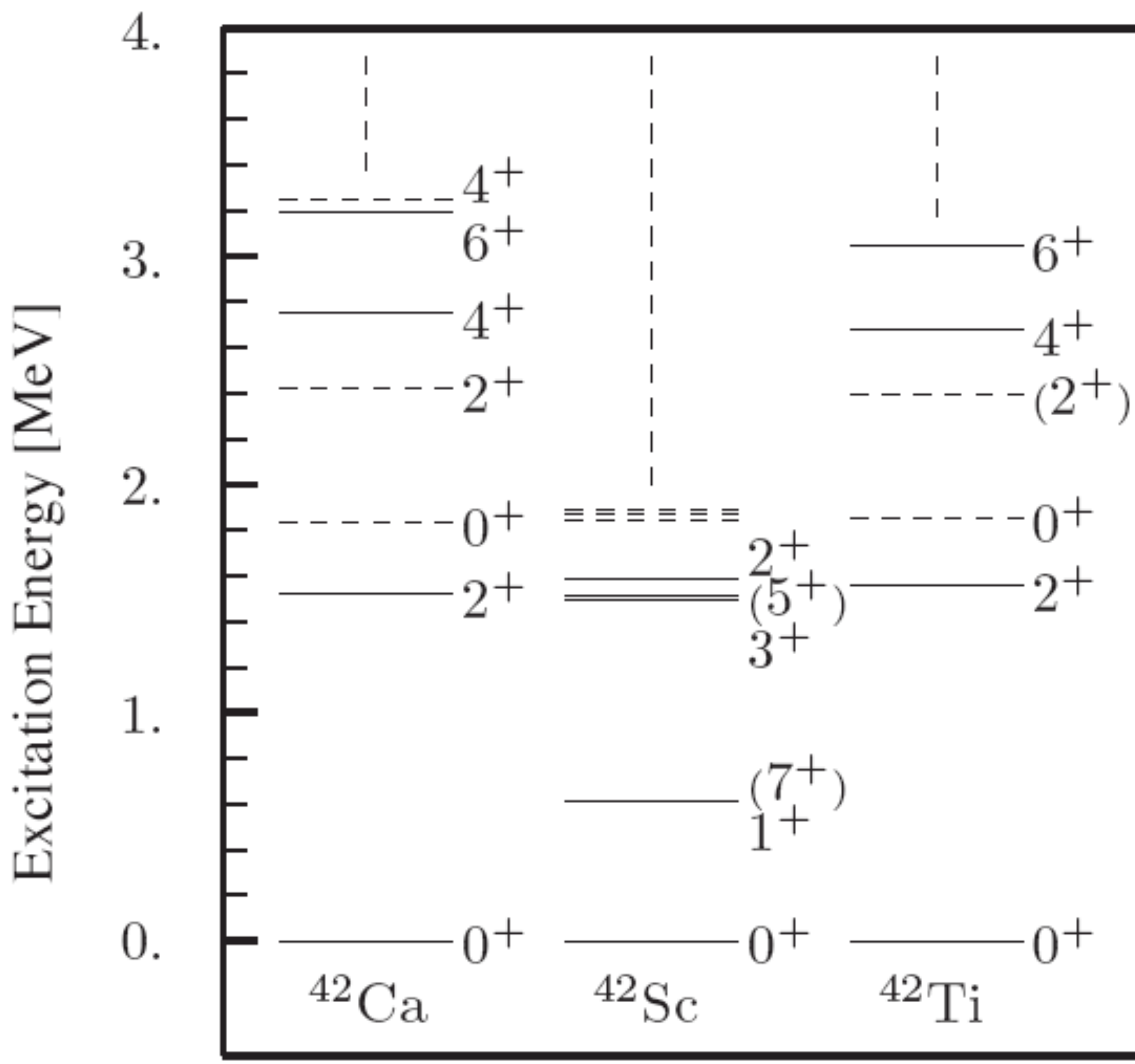
- Only even total angular momentum
- With isospin

$$
\begin{aligned}
|\Phi_{jj,JM,TM_T}\rangle &= \sum_{mm'm_tm'_t} (j\ m\ j\ m'\ |J\ M)\, (\tfrac{1}{2}\ m_t\ \tfrac{1}{2}\ m'_t\ |T\ M_T)\, |\Phi_{jmm_t,jm'm'_t}\rangle \\
&= (-1)^{J+T+1}\, |\Phi_{jj,JM,TM_T}\rangle
\end{aligned}
$$

- J+T odd!

^{40}Ca + two nucleons

- Spectrum



Two-body interactions and matrix elements

- To determine $\hat{V} = \frac{1}{2} \sum_{\alpha\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a^\dagger_\alpha a^\dagger_\beta a_\delta a_\gamma$
- we need a basis and calculate $(\alpha\beta|V|\gamma\delta)$ for given interaction
- Simplest type: spin-independent & local (also for spinless bosons)

$$
\begin{aligned}
(\boldsymbol{r}_1 \boldsymbol{r}_2|V|\boldsymbol{r}_3 \boldsymbol{r}_4) &= (\boldsymbol{R}\boldsymbol{r}|V|\boldsymbol{R}'\boldsymbol{r}') \\
&= \delta(\boldsymbol{R}-\boldsymbol{R}') \langle \boldsymbol{r}| V |\boldsymbol{r}'\rangle = \delta(\boldsymbol{R}-\boldsymbol{R}')\delta(\boldsymbol{r}-\boldsymbol{r}')V(r)
\end{aligned}
$$

- with

$$
\begin{aligned}
\boldsymbol{R} &= \tfrac{1}{2}(\boldsymbol{r}_1 + \boldsymbol{r}_2) \\
\boldsymbol{r} &= \boldsymbol{r}_1 - \boldsymbol{r}_2
\end{aligned}
$$

- Therefore

$$
\hat{V} = \frac{1}{2} \sum_{mm'} \int d^3R \int d^3r \; V(r) a^\dagger_{\boldsymbol{R}+\boldsymbol{r}/2 m} a^\dagger_{\boldsymbol{R}-\boldsymbol{r}/2 m'} a_{\boldsymbol{R}-\boldsymbol{r}/2 m'} a_{\boldsymbol{R}+\boldsymbol{r}/2 m}
$$

Nucleon-nucleon interaction

- Yukawa 1935
- short-range interaction requires exchange of massive particle

$$V_Y(r) = V_0 \frac{e^{-\mu r}}{\mu r}$$

- mass of particle $\mu \hbar c = mc^2$
- mesons are the bosonic excitations of the QCD vacuum
- many quantum numbers
- So one encounters also spin and isospin dependence

$$V_{spin} = V_\sigma(r) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$$

$$V_{isospin} = V_\tau(r) \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

$$V_{s-i} = V_{\sigma\tau}(r) \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2$$

Spin and isospin matrix elements

- Pauli spin matrices $\boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$
- represent $\frac{4}{\hbar^2} \boldsymbol{s}_1 \cdot \boldsymbol{s}_2$
- Use $\boldsymbol{S} = \boldsymbol{s}_1 + \boldsymbol{s}_2$
- Then $\boldsymbol{s}_1 \cdot \boldsymbol{s}_2 = \frac{1}{2} \left(\boldsymbol{S}^2 - \boldsymbol{s}_1^2 - \boldsymbol{s}_2^2 \right)$
- So coupled states are required

$$\langle S' M_S' | \, \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \, | S M_S \rangle = \left(2S \left(S+1 \right) - 3 \right) \delta_{S,S'} \delta_{M_S, M_S'}$$

- Same for isospin

$$\langle T' M_T' | \, \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \, | T M_T \rangle = \left(2T \left(T+1 \right) - 3 \right) \delta_{T,T'} \delta_{M_T, M_T'}$$

Realistic NN interaction

- Required for NN scattering

$$
\begin{array}{rrrr}
1 & \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 & \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 & \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
S_{12} & S_{12} \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 & \boldsymbol{L} \cdot \boldsymbol{S} & \boldsymbol{L} \cdot \boldsymbol{S} \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
\boldsymbol{L}^2 & \boldsymbol{L}^2 \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 & \boldsymbol{L}^2 \; \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 & \boldsymbol{L}^2 \; \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2 \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 \\
(\boldsymbol{L} \cdot \boldsymbol{S})^2 & (\boldsymbol{L} \cdot \boldsymbol{S})^2 \; \boldsymbol{\tau}_1 \cdot \boldsymbol{\tau}_2 & &
\end{array}
$$

- plus radial dependence
- Tensor force $\quad S_{12}(\hat{\boldsymbol{r}}) = 3\,(\boldsymbol{\sigma}_1 \cdot \hat{\boldsymbol{r}})\,(\boldsymbol{\sigma}_2 \cdot \hat{\boldsymbol{r}}) - \boldsymbol{\sigma}_1 \cdot \boldsymbol{\sigma}_2$
- Short-range interaction suggests use of angular momentum basis
- Angular momentum algebra
- Spherical tensor algebra
- Often calculations are done in momentum space

Momentum space

- Transform to total and relative momentum basis

$$(\boldsymbol{p}_1\boldsymbol{p}_2|V|\boldsymbol{p}_3\boldsymbol{p}_4) = (\boldsymbol{P}\boldsymbol{p}|V|\boldsymbol{P}'\boldsymbol{p}') = \delta_{\boldsymbol{P},\boldsymbol{P}'}\langle\boldsymbol{p}|V|\boldsymbol{p}'\rangle$$

- or wave vectors

$$\langle\boldsymbol{k}|V|\boldsymbol{k}'\rangle = \frac{1}{V}\int d^3r\ \exp\{i(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}\}V(r)$$

- Use

$$\exp\{i\boldsymbol{q}\cdot\boldsymbol{r}\} = 4\pi\sum_{\ell m} i^{\ell}Y^*_{\ell m}(\hat{\boldsymbol{r}})Y_{\ell m}(\hat{\boldsymbol{q}})\mathrm{j}_{\ell}(qr)$$

- to find

$$\langle\boldsymbol{k}|V|\boldsymbol{k}'\rangle = \frac{4\pi}{V}\int dr\ r^2\ \mathrm{j}_0(qr)V(r) \quad \text{with} \quad q = |\boldsymbol{k}-\boldsymbol{k}'|$$

- Yukawa $\langle\boldsymbol{k}|V_{\mathrm{Y}}|\boldsymbol{k}'\rangle = \frac{4\pi}{V}\frac{V_0}{\mu}\frac{1}{\mu^2+(\boldsymbol{k}'-\boldsymbol{k})^2}$

- Helps for Coulomb $\langle\boldsymbol{k}|V_C|\boldsymbol{k}'\rangle = \frac{4\pi}{V}\frac{q_1q_2e^2}{(\boldsymbol{k}'-\boldsymbol{k})^2}$ when $\boldsymbol{k}\neq\boldsymbol{k}'$

Partial wave basis

- Requires matrix elements of the form

$$\langle kLM_L|\, V\, |k'L'M_L'\rangle = \int d\hat{\boldsymbol{k}}\ \langle LM_L|\hat{\boldsymbol{k}}\rangle \int d\hat{\boldsymbol{k}}'\ \langle\hat{\boldsymbol{k}}'|L'M_L'\rangle\, \langle\boldsymbol{k}|\, V(r)\, |\boldsymbol{k}'\rangle$$

- For Yukawa write

$$\langle\boldsymbol{k}|\, V_Y(r)\, |\boldsymbol{k}'\rangle = \frac{4\pi}{V}\frac{V_0}{\mu}\frac{1}{2kk'}\frac{1}{\frac{\mu^2+k^2+k'^2}{2kk'} - \cos\theta_{kk'}}$$

- and use

$$\frac{1}{\frac{\mu^2+k^2+k'^2}{2kk'} - \cos\theta_{kk'}} = \sum_{\ell=0}^{\infty}(2\ell+1)\ Q_\ell\left(\frac{\mu^2+k^2+k'^2}{2kk'}\right)P_\ell(\cos\theta_{kk'})$$

$$= \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{\ell} 4\pi\ Q_\ell\left(\frac{\mu^2+k^2+k'^2}{2kk'}\right)Y^*_{\ell m}(\hat{\boldsymbol{k}})Y_{\ell m}(\hat{\boldsymbol{k}}')$$

- with Legendre functions

$$\begin{aligned} Q_0(z) &= \frac{1}{2}\ln\left(\frac{z+1}{z-1}\right) \\ Q_1(z) &= \frac{z}{2}\ln\left(\frac{z+1}{z-1}\right) - 1 \\ Q_2(z) &= \frac{3z^2-1}{4}\ln\left(\frac{z+1}{z-1}\right) - \frac{3}{2}z \end{aligned}$$

- yields

$$\langle kLM_L|\, V\, |k'L'M_L'\rangle = \delta_{L,L'}\ \delta_{M_L,M_L'}\frac{(4\pi)^2V_0}{V\mu 2kk'}\ Q_L\left(\frac{\mu^2+k^2+k'^2}{2kk'}\right)$$

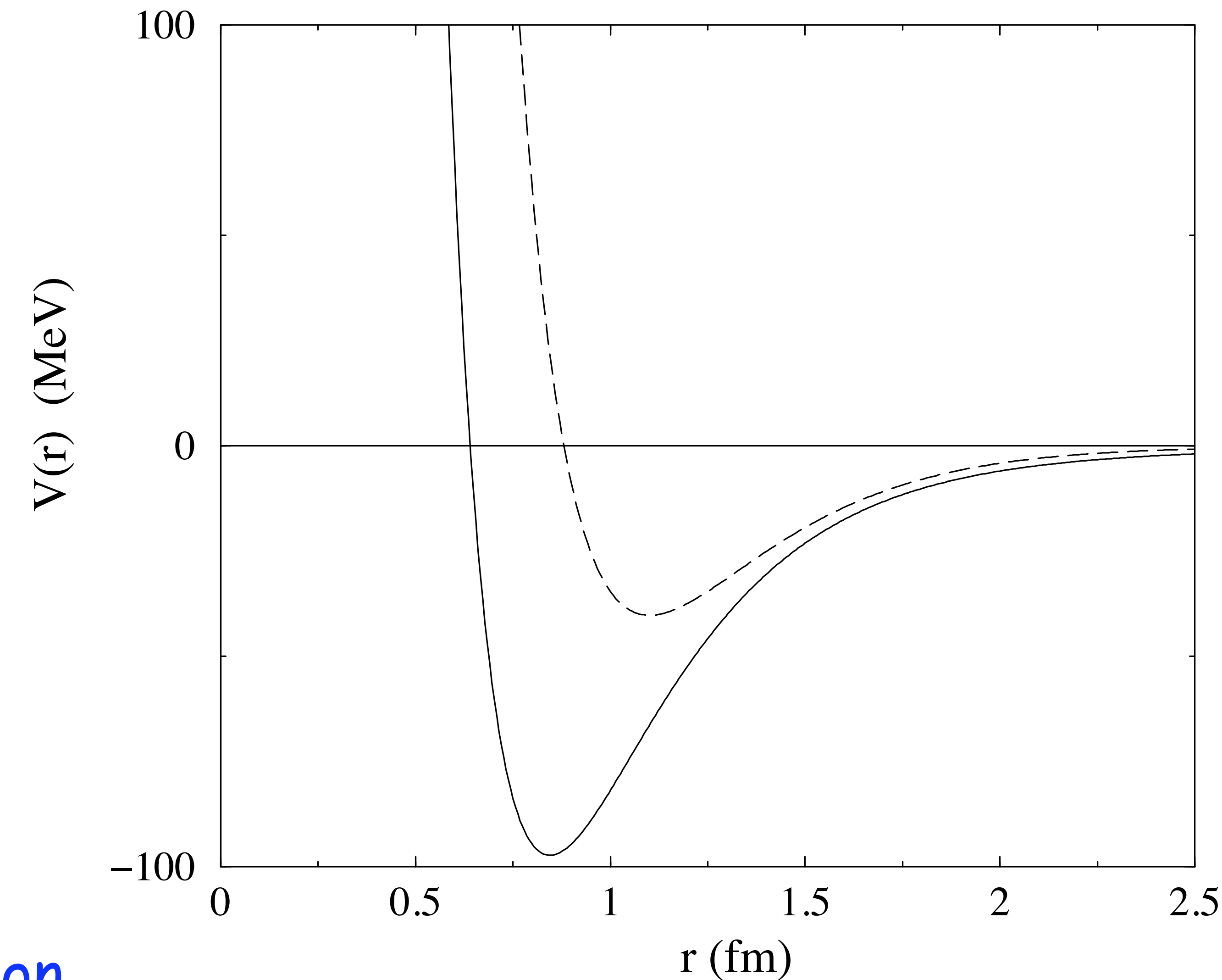
Example

- Reid soft-core interaction (1968)

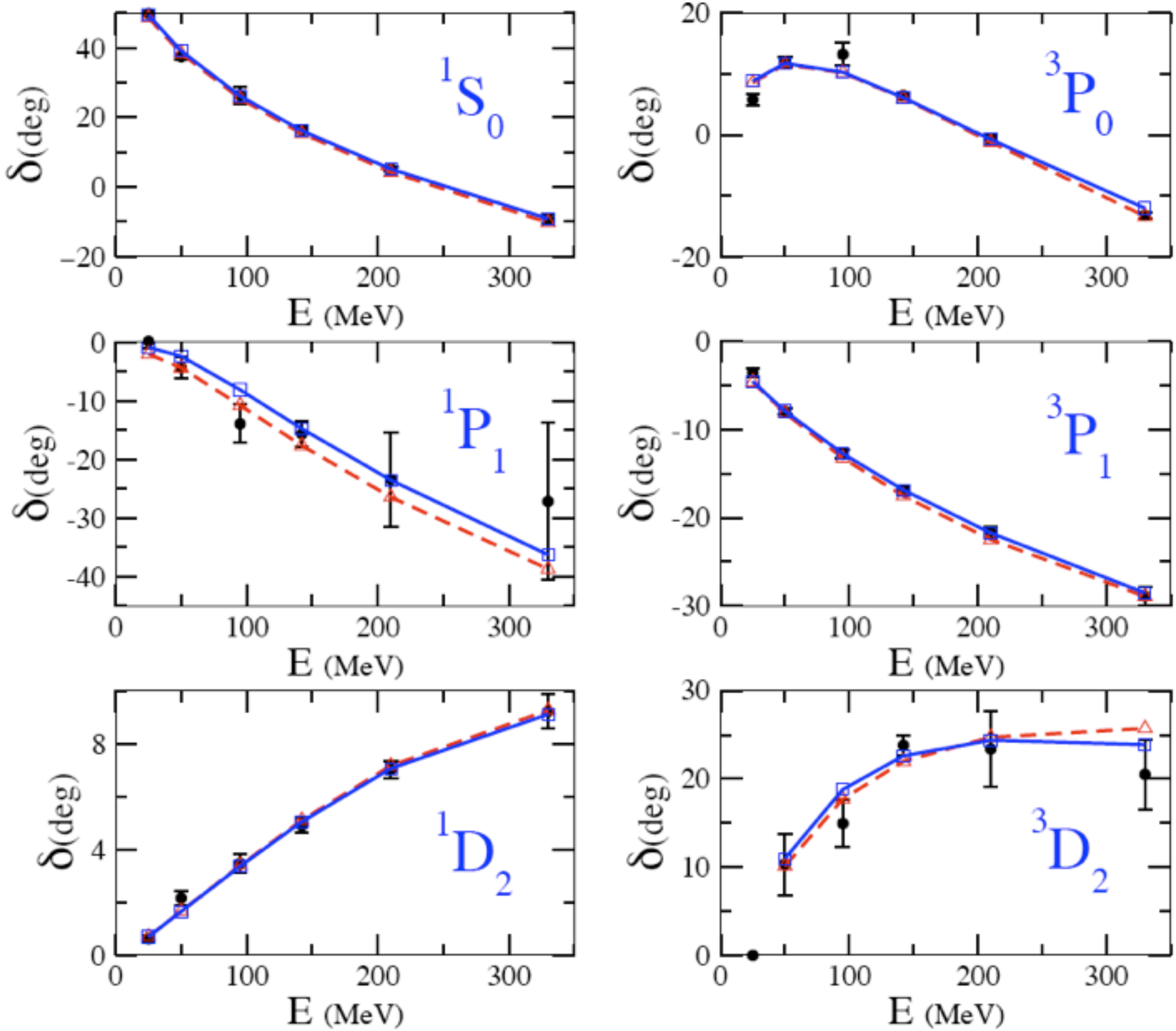
- solid $^1S_0$
- no bound state

- dashed $^3S_1$
- deuteron
- ??

note similarity to
atom-atom interaction



Phase shifts 1968...

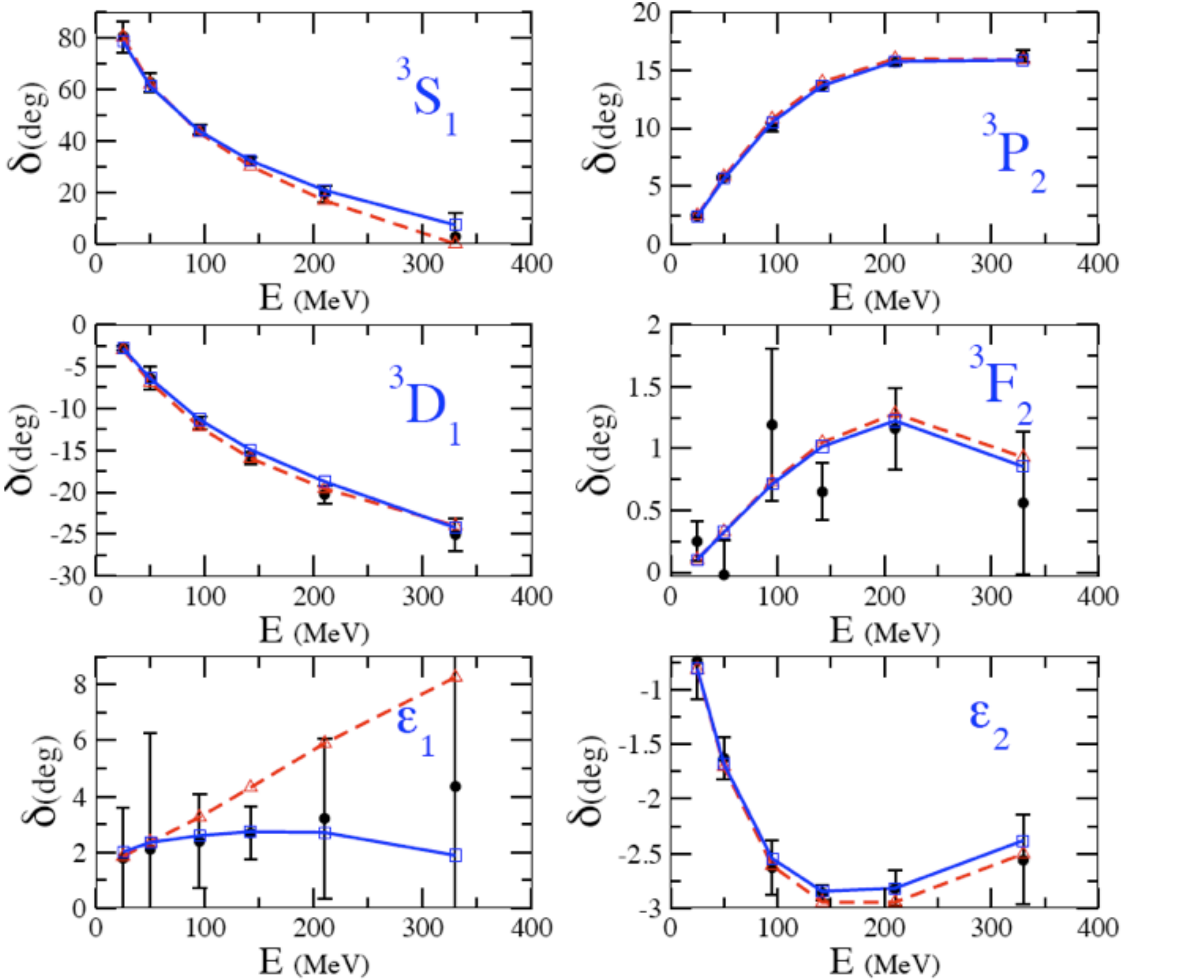


Dynamic

Static

Nucleon correlations

Phase shifts 1968...



Infinite systems & plane-wave states

- Suppress for now discrete quantum numbers (for fermions)
- Momentum eigenstates of kinetic energy

$$\frac{\boldsymbol{p}_{op}^2}{2m}\left|\boldsymbol{p}'\right\rangle = \frac{\boldsymbol{p}'^2}{2m}\left|\boldsymbol{p}'\right\rangle$$

- Associated wave function $\langle \boldsymbol{r}|\boldsymbol{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\boldsymbol{p}\cdot\boldsymbol{r}}$
- Normalization condition $\langle \boldsymbol{p}'|\boldsymbol{p}\rangle = \frac{1}{(2\pi\hbar)^3}\int d\boldsymbol{r}\; e^{\frac{i}{\hbar}(\boldsymbol{p}-\boldsymbol{p}')\cdot\boldsymbol{r}} = \delta(\boldsymbol{p}'-\boldsymbol{p})$
- Often used: wave vectors $\boldsymbol{k} = \frac{\boldsymbol{p}}{\hbar}$
- Wave function $\langle \boldsymbol{r}|\boldsymbol{k}\rangle = \frac{1}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
- and $\langle \boldsymbol{k}'|\boldsymbol{k}\rangle = \delta(\boldsymbol{k}'-\boldsymbol{k})$

Box normalization

- Confinement to cubic box $V = L^3$
- Wave function $\langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{\sqrt{V}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$
- Boundary conditions: only discrete $\langle \boldsymbol{k}' | \boldsymbol{k} \rangle = \delta_{\boldsymbol{k}',\boldsymbol{k}}$
- Means $\langle \boldsymbol{k}' | \boldsymbol{k} \rangle = \int_{box} d\boldsymbol{r}\ \langle \boldsymbol{k}' | \boldsymbol{r} \rangle \langle \boldsymbol{r} | \boldsymbol{k} \rangle = \frac{1}{V} \int_{box} d\boldsymbol{r}\ e^{i(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} = \delta_{\boldsymbol{k}',\boldsymbol{k}}$
- For example: periodic bc
- x-direction $e^{ik_x x} = e^{ik_x(x+L)} = e^{ik_x x} e^{ik_x L}$
- therefore $\cos(k_x L) + i \sin(k_x L) = 1$
- Hence $k_x = n_x \frac{2\pi}{L}$ where $n_x = 0, \pm 1, \pm 2, ...$
- Also for y and z
- Each allowed triplet $\{k_x, k_y, k_z\}$ corresponds to $\{n_x, n_y, n_z\}$
- Ground state: fill the lowest-energy states up to a maximum
- Fermi momentum; wave vector $p_F = \hbar k_F$

Thermodynamic limit

- Determine Fermi wave vector by calculating the expectation value of the number operator in the ground state

$$|\Phi_0\rangle = \prod_{|\boldsymbol{k}|<k_F,\mu} a^\dagger_{\boldsymbol{k}\mu}\,|0\rangle$$

- with μ representing discrete quantum numbers (spin, isospin)
- Thermodynamic limit $N \rightarrow \infty$

$$V \rightarrow \infty$$

- with fixed density $\rho = \dfrac{N}{V}$
- Replace summations by integrations for any function f

$$\sum_{\boldsymbol{k}\mu} f(\boldsymbol{k},\mu) = \sum_{n_x n_y n_z} \sum_{\mu} f(\frac{2\pi \boldsymbol{n}}{L},\mu)$$

$$L \rightarrow \infty \quad \Rightarrow \int d\boldsymbol{n} \sum_{\mu} f(\frac{2\pi \boldsymbol{n}}{L},\mu) = \frac{V}{(2\pi)^3} \int d\boldsymbol{k} \sum_{\mu} f(\boldsymbol{k},\mu)$$

Properties of Fermi gas ground state

- Remember $$N = \langle\Phi_0|\,\hat{N}\,|\Phi_0\rangle = \sum_{\boldsymbol{k}\mu}\langle\Phi_0|\,a^\dagger_{\boldsymbol{k}\mu}a_{\boldsymbol{k}\mu}\,|\Phi_0\rangle = \sum_{\boldsymbol{k}\mu}\theta(k_F-k)$$
$$= \frac{V}{(2\pi)^3}\sum_\mu\int d^3k\;\theta(k_F-k) = \frac{\nu V}{6\pi^2}k_F^3$$
- degeneracy ν so $k_F = \left\{\frac{6\pi^2 N}{\nu V}\right\}^{1/3}$ fixed ρ: k_F smaller if ν larger
- Energy from $$\hat{T} = \sum_{\boldsymbol{k}\mu}\sum_{\boldsymbol{k}'\mu'}\langle\boldsymbol{k}\mu|\,\frac{\hbar^2\boldsymbol{k}^2}{2m}\,|\boldsymbol{k}'\mu'\rangle\,a^\dagger_{\boldsymbol{k}\mu}a_{\boldsymbol{k}'\mu'} = \sum_{\boldsymbol{k}'\mu'}\frac{\hbar^2\boldsymbol{k}'^2}{2m}a^\dagger_{\boldsymbol{k}'\mu'}a_{\boldsymbol{k}'\mu'}$$
- yielding $$\hat{T}\,|\Phi_0\rangle = \left(\sum_{\boldsymbol{k}'\mu'}\frac{\hbar^2\boldsymbol{k}'^2}{2m}a^\dagger_{\boldsymbol{k}'\mu'}a_{\boldsymbol{k}'\mu'}\right)\prod_{|\boldsymbol{k}|<k_F\,\mu}a^\dagger_{\boldsymbol{k}\mu}\,|0\rangle$$
$$\hat{T}\,|\Phi_0\rangle = E_0\,|\Phi_0\rangle = \left(\sum_{|\boldsymbol{k}|<k_F,\mu}\frac{\hbar^2\boldsymbol{k}^2}{2m}\right)|\Phi_0\rangle$$
- and therefore $$E_0 = \sum_{|\boldsymbol{k}|<k_F,\mu}\frac{\hbar^2\boldsymbol{k}^2}{2m} = \frac{V}{(2\pi)^3}\sum_\mu\int d^3k\frac{\hbar^2k^2}{2m}\theta(k_F-k)$$
$$= V\frac{\nu}{(2\pi)^3}\,4\pi\,\frac{\hbar^2}{2m}\,\frac{1}{5}k_F^5$$
- written as $$\frac{E_0}{N} = \frac{V}{N}\,\frac{\nu}{2\pi^2}\,\frac{\hbar^2k_F^5}{10m} = \frac{3}{5}\frac{\hbar^2k_F^2}{2m} = \frac{3}{5}\varepsilon_F = \frac{3}{5}k_BT_F$$

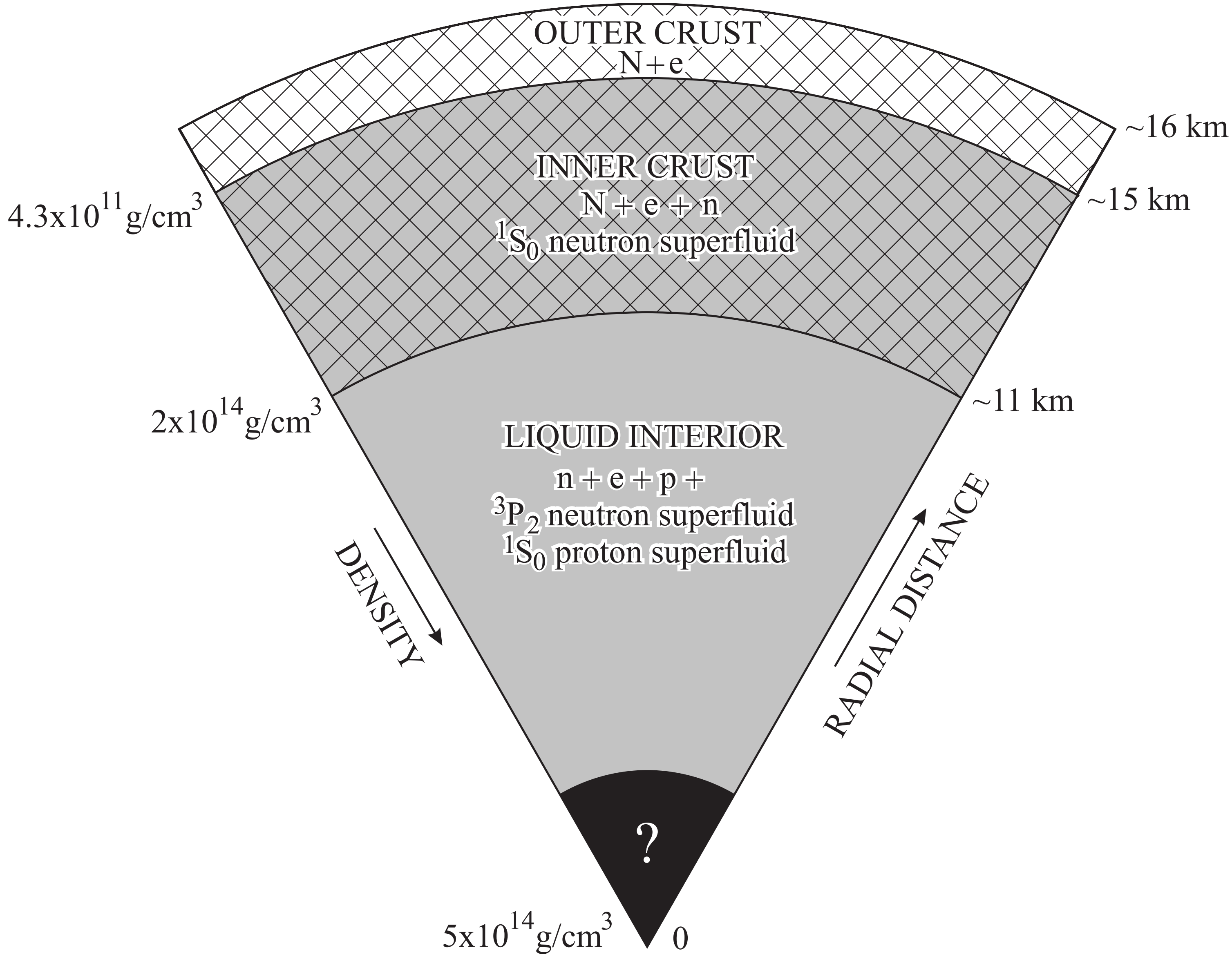
Nuclear matter

- Key quantities
  - Saturation density: 0.16 nucleons per $\text{fm}^3 \Rightarrow$ $k_F = 1.33\ \text{fm}^{-1}$ $\nu = 4$

    interparticle spacing $r_0 \approx 1.14\ \text{fm}$
  - Energy per particle at saturation: ~-16 MeV
- Relation between V_{NN} (including possible V_{NNN}) and these quantities still debated
- Bethe contributed ~10 years of his scientific life to this problem
- No global consensus on precise mechanism of saturation
  - role of pions
  - role of three-body interaction
  - role of relativity if any
  - many phenomenological ways to represent saturation properties

Neutron matter

- Interior of neutron star



What is a propagator or Green's function?

- Time evolution governed by Hamiltonian
- Single particle with a Hamiltonian that doesn't depend on time
- At t_0 initial state $|\alpha, t_0\rangle$
- At $t > t_0$ evolves to $|\alpha, t_0; t\rangle = e^{-\frac{i}{\hbar}H(t-t_0)}|\alpha, t_0\rangle$
- Indeed $i\hbar\frac{\partial}{\partial t}|\alpha, t_0; t\rangle = H|\alpha, t_0; t\rangle$
- Relation between wave function at t and t_0

$$\begin{aligned}\psi(\boldsymbol{r}, t) &= \langle \boldsymbol{r}|\alpha, t_0; t\rangle = \langle \boldsymbol{r}|e^{-\frac{i}{\hbar}H(t-t_0)}|\alpha, t_0\rangle \\ &= \int d\boldsymbol{r}' \; \langle \boldsymbol{r}|e^{-\frac{i}{\hbar}H(t-t_0)}|\boldsymbol{r}'\rangle \langle \boldsymbol{r}'|\alpha, t_0\rangle \\ &\equiv i\hbar\int d\boldsymbol{r}' \; G(\boldsymbol{r}, \boldsymbol{r}'; t-t_0)\psi(\boldsymbol{r}', t_0)\end{aligned}$$

- with propagator or Green's function

Huygens

$$G(\boldsymbol{r}, \boldsymbol{r}'; t-t_0) \equiv -\frac{i}{\hbar}\langle \boldsymbol{r}|e^{-\frac{i}{\hbar}H(t-t_0)}|\boldsymbol{r}'\rangle$$

Alternative expressions

- Rewrite propagator assuming a discrete spectrum with $H\left|n\right\rangle = \varepsilon_n \left|n\right\rangle$

$$
\begin{aligned}
G(\boldsymbol{r},\boldsymbol{r}';t-t_0) &= -\frac{i}{\hbar}\left\langle \boldsymbol{r}\right| e^{-\frac{i}{\hbar}H(t-t_0)}\left|\boldsymbol{r}'\right\rangle = -\frac{i}{\hbar}\left\langle 0\right| a_{\boldsymbol{r}} e^{-\frac{i}{\hbar}H(t-t_0)} a^\dagger_{\boldsymbol{r}'}\left|0\right\rangle \\
&= -\frac{i}{\hbar}\sum_n \left\langle 0\right| a_{\boldsymbol{r}}\left|n\right\rangle \left\langle n\right| a^\dagger_{\boldsymbol{r}'}\left|0\right\rangle e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)} \\
&= -\frac{i}{\hbar}\sum_n u_n(\boldsymbol{r})u_n^*(\boldsymbol{r}')e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}
\end{aligned}
$$

- Note $\left\langle 0\right| a_{\boldsymbol{r}}\left|n\right\rangle = \left\langle \boldsymbol{r}|n\right\rangle = u_n(\boldsymbol{r})$ and $H\left|n\right\rangle = \varepsilon_n\left|n\right\rangle$

Propagator yields information on wave functions and eigenvalues of H

- Use integral representation of step function

$$\theta(t-t_0) = -\int \frac{dE'}{2\pi i}\,\frac{e^{-iE'(t-t_0)/\hbar}}{E'+i\eta} \qquad \text{with} \qquad \frac{d}{dt}\theta(t-t_0) = \delta(t-t_0)$$

- includes causality to facilitate Fourier transform (FT)

FT

- Consider alternatives of FT

$$G(\boldsymbol{r},\boldsymbol{r}';E) = -\frac{i}{\hbar}\int_{-\infty}^{\infty} d(t-t_0)\; e^{\frac{i}{\hbar}E(t-t_0)}\left\{\theta(t-t_0)\sum_n u_n(\boldsymbol{r})u_n^*(\boldsymbol{r}')e^{-\frac{i}{\hbar}\varepsilon_n(t-t_0)}\right\}$$

$$= \sum_n \frac{u_n(\boldsymbol{r})u_n^*(\boldsymbol{r}')}{E-\varepsilon_n+i\eta} = \sum_n \frac{\langle 0|\, a_{\boldsymbol{r}}\,|n\rangle\,\langle n|\, a_{\boldsymbol{r}'}^\dagger\,|0\rangle}{E-\varepsilon_n+i\eta}$$

$$= \langle 0|\, a_{\boldsymbol{r}}\frac{1}{E-H+i\eta}a_{\boldsymbol{r}'}^\dagger\,|0\rangle = \langle \boldsymbol{r}|\,\frac{1}{E-H+i\eta}\,|\boldsymbol{r}'\rangle$$

- Clearly other basis sets can be used

$$G(\alpha,\beta;E) = \langle 0|\, a_\alpha \frac{1}{E-H+i\eta}a_\beta^\dagger\,|0\rangle$$

- Relevant operator $\quad G(E) = \dfrac{1}{E-H+i\eta}$

- facilitates expansion

Expansion of propagator

- Relation between exact propagator and approximate one
- Decompose Hamiltonian $H = H_0 + V$
- With $G^{(0)}(E) = \dfrac{1}{E - H_0 + i\eta}$
- solved according to $H_0 |\alpha\rangle = \varepsilon_\alpha |\alpha\rangle$
- In this basis

$$G^{(0)}(\alpha, \beta; E) = \frac{\delta_{\alpha,\beta}}{E - \varepsilon_\alpha + i\eta}$$

- Use operator identity

$$\frac{1}{A-B} = \frac{1}{A} + \frac{1}{A} B \frac{1}{A-B}$$

- with $A = E - H_0 + i\eta$ and $B = V$

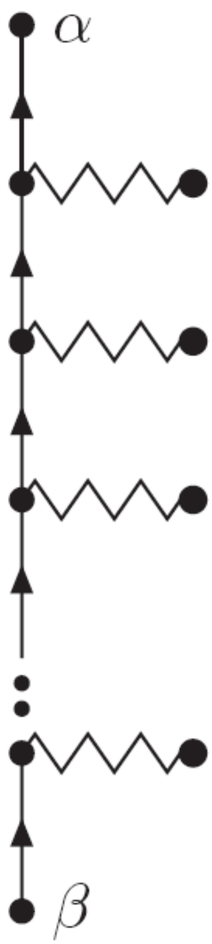
Propagator equation and expansion

- Result $$G = G^{(0)} + G^{(0)}\ V\ G$$
- or $$\langle\alpha|\,\frac{1}{E-H+i\eta}\,|\beta\rangle = \langle\alpha|\,\frac{1}{E-H_0+i\eta}\,|\beta\rangle$$
$$+\sum_{\gamma\delta}\langle\alpha|\,\frac{1}{E-H_0+i\eta}\,|\gamma\rangle\,\langle\gamma|\,V\,|\delta\rangle\,\langle\delta|\,\frac{1}{E-H+i\eta}\,|\beta\rangle$$
- and therefore
$$G(\alpha,\beta;E) = G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\,\langle\gamma|\,V\,|\delta\rangle\,G(\delta,\beta;E)$$
- allows expansion $$G = G^{(0)} + G^{(0)}\ V\ G^{(0)} + G^{(0)}\ V\ G^{(0)}\ V\ G^{(0)} + \ldots$$
$$\begin{aligned} G(\alpha,\beta;E) &= G^{(0)}(\alpha,\beta;E) + \sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\,\langle\gamma|\,V\,|\delta\rangle\,G^{(0)}(\delta,\beta;E) \\ &+ \sum_{\gamma,\delta,\theta,\eta} G^{(0)}(\alpha,\gamma;E)\,\langle\gamma|\,V\,|\theta\rangle\,G^{(0)}(\theta,\eta;E)\,\langle\eta|\,V\,|\delta\rangle\,G^{(0)}(\delta,\beta;E) + \ldots \end{aligned}$$

Diagrammatic interpretation

- Practical choice $$G^{(0)}(\alpha,\beta;E) = \frac{\delta_{\alpha,\beta}}{E - \varepsilon_\alpha + i\eta}$$

- In k^{th} order



Rule 1 Draw a directed line with k zigzag (horizontal) interaction lines V and $k+1$ directed unperturbed propagators $G^{(0)}$

Rule 2 Label external points (α and β)
Label each V

$$\langle\gamma|\, V\, |\delta\rangle$$

For each full line with arrow write

$$G^{(0)}(\mu,\nu;E)$$

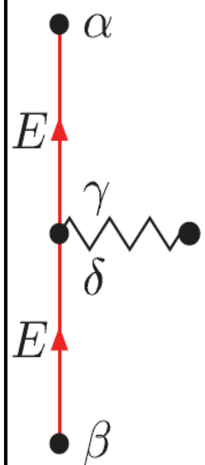
Rule 3 Sum (integrate) over all internal quantum numbers

Examples

- Lowest order

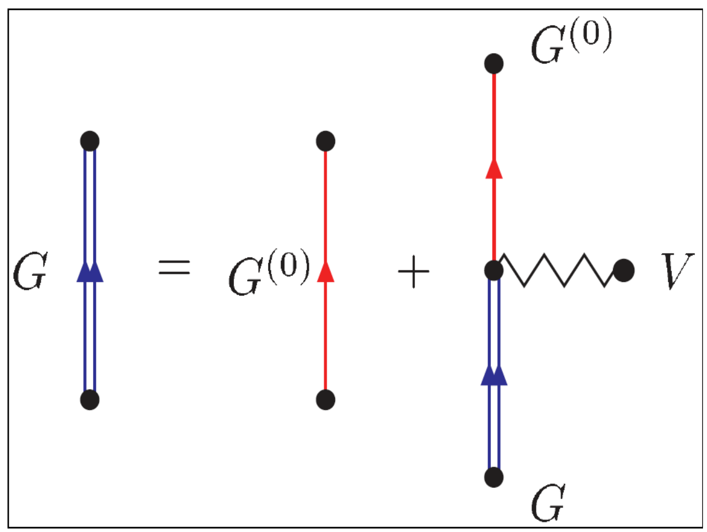
$$G^{(0)}(\alpha,\beta;E)$$

- First order



$$\sum_{\gamma,\delta} G^{(0)}(\alpha,\gamma;E)\,\langle\gamma|\,V\,|\delta\rangle\,G^{(0)}(\delta,\beta;E)$$

- All diagrams summed by



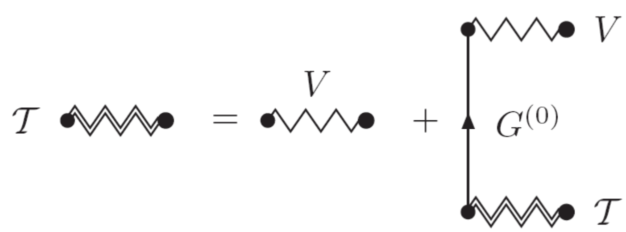
Rearrange series expansion

- Often useful (in operator form)

$$
\begin{aligned}
G &= G^{(0)} + G^{(0)}\ V\ G^{(0)} + G^{(0)}\ V\ G^{(0)}\ V\ G^{(0)} + \ldots \\
&= G^{(0)} + G^{(0)}\ V\ \{G^{(0)} + G^{(0)}\ V\ G^{(0)} + \ldots\} = G^{(0)} + G^{(0)}\ V\ G \\
&= G^{(0)} + \{G^{(0)} + G^{(0)}\ V\ G^{(0)} + \ldots\}\ V\ G^{(0)} = G^{(0)} + G\ V\ G^{(0)} \\
&= G^{(0)}\ + G^{(0)}\{V + V\ G^{(0)}\ V + \ldots\}\ G^{(0)} = G^{(0)} + G^{(0)}\ \mathcal{T}\ G^{(0)}
\end{aligned}
$$

- with

$$
\begin{aligned}
\mathcal{T} &= V + V\ G^{(0)}\ V + V\ G^{(0)}\ V\ G^{(0)}\ V + \ldots \\
&= V + V\ G^{(0)}\ \{V + V\ G^{(0)}\ V + \ldots\} \\
&= V + V\ G^{(0)}\ \mathcal{T} = V + \mathcal{T}\ G^{(0)}\ V = V + V\ G\ V
\end{aligned}
$$

- Illustrated by
- T-matrix equation 

(take matrix elements)

Solution strategy for discrete (bound) states

- Also useful in the many-body problem
- Exact discrete eigenstates $H\left|m\right\rangle = \varepsilon_m \left|m\right\rangle$
- Exact continuum states $H\left|\mu\right\rangle = \varepsilon_\mu \left|\mu\right\rangle$
- Completeness

$$1 = \sum_m \left|m\right\rangle \left\langle m\right| + \int d\mu \ \left|\mu\right\rangle \left\langle \mu\right|$$

- Rewrite $G(\alpha,\beta;E) = \left\langle 0\right| a_\alpha \dfrac{1}{E - H + i\eta} a_\beta^\dagger \left|0\right\rangle$

$$G(\alpha,\beta;E) = \sum_m \frac{\langle\alpha|m\rangle\langle m|\beta\rangle}{E - \varepsilon_m + i\eta} + \int d\mu \ \frac{\langle\alpha|\mu\rangle\langle\mu|\beta\rangle}{E - \varepsilon_\mu + i\eta}$$

- Assume $H_0 = T$ and work with momentum states $\{|\alpha\rangle\} = \{|\boldsymbol{p}\rangle\}$

Limits

- Remember

$$G(\alpha,\beta;E) = \sum_m \frac{\langle\alpha|m\rangle\langle m|\beta\rangle}{E-\varepsilon_m+i\eta} + \int d\mu\ \frac{\langle\alpha|\mu\rangle\langle\mu|\beta\rangle}{E-\varepsilon_\mu+i\eta}$$

- Then perform

$$\lim_{E\rightarrow\varepsilon_n}(E-\varepsilon_n)\{G = G^{(0)} + G^{(0)}\ V\ G\}$$

- Three terms
  - $$\lim_{E\rightarrow\varepsilon_n}(E-\varepsilon_n)\left\{\sum_m \frac{\langle\alpha|m\rangle\langle m|\beta\rangle}{E-\varepsilon_m+i\eta} + \ldots\right\} = \langle\alpha|n\rangle\langle n|\beta\rangle$$
    $$\Rightarrow \langle\boldsymbol{p}|n\rangle\langle n|\boldsymbol{p}'\rangle$$
  - $$\lim_{E\rightarrow\varepsilon_n}(E-\varepsilon_n)\langle\alpha|\frac{1}{E-T+i\eta}|\beta\rangle \Rightarrow \lim_{E\rightarrow\varepsilon_n}(E-\varepsilon_n)\frac{\delta(\boldsymbol{p}-\boldsymbol{p}')}{E-\frac{\boldsymbol{p}^2}{2m}+i\eta} = 0$$
  - $$\lim_{E\rightarrow\varepsilon_n}(E-\varepsilon_n) \times \sum_{\gamma\delta}\langle\alpha|\frac{1}{E-T+i\eta}|\gamma\rangle\langle\gamma|V|\delta\rangle\left\{\sum_m \frac{\langle\delta|m\rangle\langle m|\beta\rangle}{E-\varepsilon_m+i\eta}+\ldots\right\}$$
    $$= \sum_{\gamma\delta}\langle\alpha|\frac{1}{\varepsilon_n-T}|\gamma\rangle\langle\gamma|V|\delta\rangle\langle\delta|n\rangle\langle n|\beta\rangle$$
    $$\Rightarrow \int d\boldsymbol{p}''\frac{1}{\varepsilon_n-\frac{\boldsymbol{p}^2}{2m}}\langle\boldsymbol{p}|V|\boldsymbol{p}''\rangle\langle\boldsymbol{p}''|n\rangle\langle n|\boldsymbol{p}'\rangle$$

Rearrange

- Collect

$$\langle \boldsymbol{p}|n\rangle = \frac{1}{\varepsilon_n - \frac{\boldsymbol{p}^2}{2m}} \int d\boldsymbol{p}'' \, \langle \boldsymbol{p}| V |\boldsymbol{p}''\rangle \, \langle \boldsymbol{p}''|n\rangle$$

- or $$\frac{\boldsymbol{p}^2}{2m}\phi_n(\boldsymbol{p}) + \int d\boldsymbol{p}'' \, \langle \boldsymbol{p}| V |\boldsymbol{p}''\rangle \, \phi_n(\boldsymbol{p}'') = \varepsilon_n \phi_n(\boldsymbol{p})$$

- with $\langle \boldsymbol{p}|n\rangle = \phi_n(\boldsymbol{p})$ momentum space wave function
- Schrödinger equation in momentum space!
- In general basis $\langle \alpha|n\rangle = \sum_{\gamma\delta} \langle \alpha| \frac{1}{\varepsilon_n - H_0} |\gamma\rangle \, \langle \gamma| V |\delta\rangle \, \langle \delta|n\rangle$
- or

$$\sum_{\alpha} \langle \beta| (\varepsilon_n - H_0) |\alpha\rangle \, \langle \alpha|n\rangle = \sum_{\delta} \langle \beta| V |\delta\rangle \, \langle \delta|n\rangle$$

- and therefore $\varepsilon_n \langle \beta|n\rangle = \sum_{\alpha} \{\langle \beta| H_0 |\alpha\rangle + \langle \beta| V |\alpha\rangle\} \, \langle \alpha|n\rangle$

Scattering theory with propagators

- Also useful for description of scattering processes
- Use both forms

$$\begin{aligned} G &= G^{(0)} + G^{(0)}\ V\ G \\ &= G^{(0)} + G^{(0)}\ \mathcal{T}\ G^{(0)} \end{aligned}$$

- Spinless particle, wave vectors, and $H_0 = T$

$$G^{(0)}(\boldsymbol{k}, \boldsymbol{k}'; E) = \delta(\boldsymbol{k} - \boldsymbol{k}') \frac{1}{E - \hbar^2 k^2/2m + i\eta}$$

- Insert

$$\begin{aligned} G(\boldsymbol{k}, \boldsymbol{k}'; E) &= G^{(0)}(\boldsymbol{k}, \boldsymbol{k}'; E) + G^{(0)}(\boldsymbol{k}; E) \int d\boldsymbol{q}\ \langle \boldsymbol{k} | V | \boldsymbol{q} \rangle\ G(\boldsymbol{q}, \boldsymbol{k}'; E) \\ &= G^{(0)}(\boldsymbol{k}, \boldsymbol{k}'; E) + G^{(0)}(\boldsymbol{k}; E)\ \langle \boldsymbol{k} | \mathcal{T}(E) | \boldsymbol{k}' \rangle\ G^{(0)}(\boldsymbol{k}'; E) \end{aligned}$$

- notation

$$G^{(0)}(\boldsymbol{k}, \boldsymbol{k}'; E) = \delta(\boldsymbol{k} - \boldsymbol{k}') G^{(0)}(\boldsymbol{k}; E)$$

But...

- Analysis for short-range potential in coordinate space...
- So FT

$$G(\boldsymbol{r},\boldsymbol{r}';E) = \int \frac{d\boldsymbol{k}}{(2\pi)^{3/2}} \int \frac{d\boldsymbol{k}'}{(2\pi)^{3/2}} e^{i\boldsymbol{k}\cdot\boldsymbol{r}} G(\boldsymbol{k},\boldsymbol{k}';E) e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'}$$

- and

$$\begin{aligned} G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) &= \int \frac{d\boldsymbol{k}}{(2\pi)^{3/2}} \int \frac{d\boldsymbol{k}'}{(2\pi)^{3/2}}\ e^{i\boldsymbol{k}\cdot\boldsymbol{r}} G^{(0)}(\boldsymbol{k},\boldsymbol{k}';E) e^{-i\boldsymbol{k}'\cdot\boldsymbol{r}'} \\ &= \int \frac{d\boldsymbol{k}}{(2\pi)^{3}}\ e^{i\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} G^{(0)}(\boldsymbol{k};E) \end{aligned}$$

- yielding

$$\begin{aligned} G(\boldsymbol{r},\boldsymbol{r}';E) &= G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) + \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2\ G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;E)\ \langle \boldsymbol{r}_1 | V | \boldsymbol{r}_2 \rangle\ G(\boldsymbol{r}_2,\boldsymbol{r}';E) \\ &= G^{(0)}(\boldsymbol{r},\boldsymbol{r}';E) + \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2\ G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;E)\ \langle \boldsymbol{r}_1 | \mathcal{T}(E) | \boldsymbol{r}_2 \rangle\ G^{(0)}(\boldsymbol{r}_2,\boldsymbol{r}';E) \end{aligned}$$

- Could have been done directly too
- Asymptotic analysis

Ingredients

- Define $E \equiv \frac{\hbar^2 k_0^2}{2m}$
- Perform angular integrals, extend integration to $-\infty$ (even integrand), introduce k_0, and factorize denominator

$$\begin{aligned} G^{(0)}(\boldsymbol{r}, \boldsymbol{r}'; E) &= \frac{2m}{\hbar^2} \frac{1}{i|\boldsymbol{r}-\boldsymbol{r}'|} \frac{1}{8\pi^2} \int_{-\infty}^{\infty} dk\ k \frac{e^{ik|\boldsymbol{r}-\boldsymbol{r}'|} - e^{-ik|\boldsymbol{r}-\boldsymbol{r}'|}}{(k_0 - k + i\eta)(k_0 + k + i\eta)} \\ &= \frac{2m}{\hbar^2} \frac{-1}{4\pi|\boldsymbol{r}-\boldsymbol{r}'|} e^{ik_0|\boldsymbol{r}-\boldsymbol{r}'|} \end{aligned}$$

- last equality: contour integration
- Need e.g. limit for $r' \gg r$
- Expand $k_0|\boldsymbol{r}-\boldsymbol{r}'| = k_0 r' \sqrt{1 + \left(\frac{r}{r'}\right)^2 - \frac{2\boldsymbol{r}\cdot\boldsymbol{r}'}{r'^2}} \approx k_0 r' - k_0 \hat{\boldsymbol{r}}' \cdot \boldsymbol{r}$
- In that limit

$$G^{(0)}(\boldsymbol{r}, \boldsymbol{r}'; E) \to -\frac{m}{2\pi\hbar^2} \frac{e^{ik_0 r'}}{r'} e^{-ik_0 \hat{\boldsymbol{r}}' \cdot \boldsymbol{r}}$$

Separability

- Insert for both $r' \gg r$ and $r' \gg r_2$ in equation with $\mathcal{T}$, and assume finite range of potential (doesn't work for Coulomb)
- then propagator is separable $G(\boldsymbol{r},\boldsymbol{r}';E) = -\frac{m}{2\pi\hbar^2}\frac{e^{ik_0 r'}}{r'}\psi_{k_0}(\boldsymbol{r})$
- with (second equality)

$$\begin{aligned}\psi_{k_0}(\boldsymbol{r}) &= e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}} + \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2\, G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;E)\,\langle \boldsymbol{r}_1|V|\boldsymbol{r}_2\rangle\,\psi_{k_0}(\boldsymbol{r}_2) \\ &= e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}} + \int d\boldsymbol{r}_1 \int d\boldsymbol{r}_2\, G^{(0)}(\boldsymbol{r},\boldsymbol{r}_1;E)\,\langle \boldsymbol{r}_1|\mathcal{T}(E)|\boldsymbol{r}_2\rangle\, e^{-ik_0\hat{\boldsymbol{r}}'\cdot\boldsymbol{r}_2}\end{aligned}$$

- Insert again (standard integral equation = first equality)
- Identify positive z-direction $\boldsymbol{k} \equiv -k_0\hat{\boldsymbol{r}}'$
- Use separable form in second equality to identify coefficient multiplying spherical wave as scattering amplitude

$f_{k_0}(\theta,\phi) = -\frac{4m\pi^2}{\hbar^2}\langle \boldsymbol{k}'|\mathcal{T}(E)|\boldsymbol{k}\rangle$ cross section $\frac{d\sigma}{d\Omega} = |f_{k_0}(\theta,\phi)|^2$

Short-range and spherical potential

- Angular momentum basis $|\boldsymbol{k}\rangle = \sum_{\ell m_\ell} |k\ell m_\ell\rangle \langle \ell m_\ell|\hat{\boldsymbol{k}}\rangle = \sum_{\ell m_\ell} |k\ell m_\ell\rangle Y^*_{\ell m_\ell}(\hat{\boldsymbol{k}})$
- Noninteracting propagator

$$\begin{aligned} G^{(0)}(k\ell m_\ell, k'\ell' m_{\ell'}; E) &= \frac{\delta(k-k')}{k^2}\delta_{\ell,\ell'}\delta_{m_\ell,m_{\ell'}}\frac{1}{E-\hbar^2k^2/2m+i\eta} \\ &= \frac{\delta(k-k')}{k^2}\delta_{\ell,\ell'}\delta_{m_\ell,m_{\ell'}}G^{(0)}(k;E) \end{aligned}$$

- Equations for propagator become (assuming spherical symmetry)

$$\begin{aligned} G_\ell(k,k';E) &= \frac{\delta(k-k')}{k^2}G^{(0)}(k;E) + G^{(0)}(k;E)\int_0^\infty dq q^2 \langle k|V^\ell|q\rangle G_\ell(q,k';E) \\ &= \frac{\delta(k-k')}{k^2}G^{(0)}(k;E) + G^{(0)}(k;E)\langle k|\mathcal{T}^\ell(E)|k'\rangle G^{(0)}(k';E) \end{aligned}$$

- For $\mathcal{T}$ -matrix

$$\langle k|\mathcal{T}^\ell(E)|k'\rangle = \langle k|V^\ell|k'\rangle + \int_0^\infty dq\ q^2 \langle k|V^\ell|q\rangle G^{(0)}(q;E)\langle q|\mathcal{T}^\ell(E)|k'\rangle$$

Asymptotic analysis in coordinate space

- Fourier-Bessel transform (FBT)

$$G_\ell(r,r';E) = \frac{2}{\pi}\int_0^\infty dk\ k^2 \int_0^\infty dk'\ k'^2\ \mathrm{j}_\ell(kr)\mathrm{j}_\ell(k'r')G_\ell(k,k';E)$$

- with $\langle k\ell m_\ell | r\ell' m_{\ell'}\rangle = \delta_{\ell,\ell'}\delta_{m_\ell,m_{\ell'}}\sqrt{\frac{2}{\pi}}\mathrm{j}_\ell(kr)$
- Noninteracting propagator (show)

$$\begin{aligned} G_\ell^{(0)}(r,r';E) &= \frac{2}{\pi}\int_0^\infty dk\ k^2\ \mathrm{j}_\ell(kr)\mathrm{j}_\ell(kr')G^{(0)}(k;E) \\ &= -ik_0\frac{2m}{\hbar^2}\mathrm{j}_\ell(k_0 r_<)\mathrm{h}_\ell(k_0 r_>) \end{aligned}$$

- Propagator equations

$$\begin{aligned} G_\ell(r,r';E) &= G_\ell^{(0)}(r,r';E) + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2\ G_\ell^{(0)}(r,r_1;E)\ \langle r_1|V^\ell|r_2\rangle\ G_\ell(r_2,r';E) \\ &= G_\ell^{(0)}(r,r';E) + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2\ G_\ell^{(0)}(r,r_1;E)\ \langle r_1|\mathcal{T}^\ell(E)|r_2\rangle\ G_\ell^{(0)}(r_2,r';E) \end{aligned}$$

- Assume finite range potential
- Substitute noninteracting propagator in second equation

Again separable but without approximation

- Then for $r' > r$ and $r' > r_0$ with $\langle r|V^\ell|r'\rangle = 0$ for r and $r' > r_0$

$$G_\ell(r,r';E) = -ik_0\frac{2m}{\hbar^2}\left\{\mathrm{j}_\ell(k_0r)\mathrm{h}_\ell(k_0r') + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2\; G_\ell^{(0)}(r,r_1;E)\langle r_1|\mathcal{T}^\ell(E)|r_2\rangle \mathrm{j}_\ell(k_0r_2)\mathrm{h}_\ell(k_0r')\right\}$$
$$= -ik_0\frac{2m}{\hbar^2}\psi_{\ell k_0}(r)\mathrm{h}_\ell(k_0r')$$

- where

$$\psi_{\ell k_0}(r) = \mathrm{j}_\ell(k_0r) + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2\; G_\ell^{(0)}(r,r_1;E)\langle r_1|\mathcal{T}^\ell(E)|r_2\rangle \mathrm{j}_\ell(k_0r_2)$$

- A substitution of separable result in first propagator equation yields integral equation

$$\psi_{\ell k_0}(r) = \mathrm{j}_\ell(k_0r) + \int_0^\infty dr_1 r_1^2 \int_0^\infty dr_2 r_2^2\; G_\ell^{(0)}(r,r_1;E)\langle r_1|V^\ell|r_2\rangle \psi_{\ell k_0}(r_2)$$

- Asymptotic analysis as before using properties of Bessel and Hankel functions

Phase shift

- Asymptotic propagator

$$G_\ell(r,r';E) \to -i\left(\frac{m}{\hbar^2}\right)k_0\mathrm{h}_\ell(k_0r')\left\{\mathrm{h}^*_\ell(k_0r)+\mathrm{h}_\ell(k_0r)\left[1-4i\frac{m}{\hbar^2}k_0\right.\right.$$

$$\left.\left.\times\int_0^\infty dr_1r_1^2\int_0^\infty dr_2r_2^2\ \langle r_1|\mathcal{T}^\ell(E)|r_2\rangle \mathrm{j}_\ell(k_0r_1)\mathrm{j}_\ell(k_0r_2)\right]\right\}$$

$$= -i\frac{m}{\hbar^2}k_0\mathrm{h}_\ell(k_0r')\left\{\mathrm{h}^*_\ell(k_0r)+\mathrm{h}_\ell(k_0r)\left[1-2\pi i\left(\frac{mk_0}{\hbar^2}\right)\langle k_0|\mathcal{T}^\ell(E)|k_0\rangle\right]\right\}$$

- Term in square brackets defines phase shift

$$\langle k_0|\mathcal{S}^\ell(E)|k_0\rangle = \left[1-2\pi i\left(\frac{mk_0}{\hbar^2}\right)\langle k_0|\mathcal{T}^\ell(E)|k_0\rangle\right] \equiv e^{2i\delta_\ell}$$

- or

$$\tan\delta_\ell = \frac{\mathrm{Im}\ \langle k_0|\mathcal{T}^\ell(E)|k_0\rangle}{\mathrm{Re}\ \langle k_0|\mathcal{T}^\ell(E)|k_0\rangle}$$

- Asymptotic propagator for $\ell = 0$

$$G_{\ell=0}(r,r';E) \to -\frac{2m}{k_0\hbar^2}\frac{1}{rr'}e^{i(k_0r'+\delta_0)}\sin(k_0r+\delta_0)$$

Scattering amplitude

- Decomposition of scattering amplitude

$$f(\theta,\phi) = \sum_l \frac{2l+1}{k_0}\left\{\frac{-mk_0\pi}{\hbar^2}\right\}\langle k_0|\mathcal{T}^\ell(E)|k_0\rangle P_\ell(\cos\theta)$$
$$= \sum_\ell \frac{2\ell+1}{k_0} e^{i\delta_\ell}\sin\delta_\ell P_\ell(\cos\theta)$$

- → Differential cross section and

- Total cross section $\sigma_{tot} = \frac{4\pi}{k_0^2}\sum_\ell (2\ell+1)\sin^2\delta_\ell$

Pictures in Quantum Mechanics

- Quick review (see Appendix A)

Schrödinger picture (usual) $|\Psi_S(t)\rangle = |\Psi(t)\rangle$

- Schrödinger equation (SE) for many-particle state

$$i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle = \hat{H}\,|\Psi_S(t)\rangle$$

- given $|\Psi_S(t_0)\rangle$ at t_0
- time-independent Hamiltonian

$$|\Psi_S(t)\rangle = \hat{U}_S(t-t_0)\,|\Psi_S(t_0)\rangle$$

- with

$$\hat{U}_S(t-t_0) = \exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\}$$

- time-evolution operator in Schrödinger picture

Heisenberg picture

- Transform time dependence to operators while making state kets "timeless"
- Define $$|\Psi_H(t)\rangle = \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}|\Psi_S(t)\rangle$$
- It follows that $$i\hbar\frac{\partial}{\partial t}|\Psi_H(t)\rangle = -\hat{H}|\Psi_H(t)\rangle + \hat{H}|\Psi_H(t)\rangle = 0$$
- and therefore $$|\Psi_H(t)\rangle \equiv |\Psi_H\rangle$$
- For operators employ $$\hat{O}_S|\Psi_S(t)\rangle = |\Psi'_S(t)\rangle$$
- to obtain $$|\Psi'_H\rangle = \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}|\Psi'_S(t)\rangle$$
$$= \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\hat{O}_S\exp\left\{-\frac{i}{\hbar}\hat{H}t\right\}\exp\left\{\frac{i}{\hbar}\hat{H}t\right\}|\Psi_S(t)\rangle = \hat{O}_H(t)|\Psi_H\rangle$$
- with $$\hat{O}_H(t) = \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\hat{O}_S\exp\left\{-\frac{i}{\hbar}\hat{H}t\right\}$$

Equation of motion for Heisenberg operators

- Use definition

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{O}_H(t) &= \left\{i\hbar\frac{\partial}{\partial t}\exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\right\}\hat{O}_S\exp\left\{-\frac{i}{\hbar}\hat{H}t\right\} \\
&\quad + \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\hat{O}_S\left\{i\hbar\frac{\partial}{\partial t}\exp\left\{-\frac{i}{\hbar}\hat{H}t\right\}\right\} \\
&= -\hat{H}\hat{O}_H(t) + \hat{O}_H(t)\hat{H} = \left[\hat{O}_H(t), \hat{H}\right] \\
&= \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\left[\hat{O}_S, \hat{H}\right]\exp\left\{-\frac{i}{\hbar}\hat{H}t\right\}
\end{aligned}
$$

- showing that if the Schrödinger operator commutes with Hamiltonian, the corresponding Heisenberg operator is constant of motion

Properties

- Note that $$|\Psi_H\rangle = |\Psi_S(t=0)\rangle$$
- and $$\hat{O}_S = \hat{O}_H(t=0)$$
- For energy eigenkets $$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$$
- and $$\begin{aligned} |\Psi_{n_S}(t)\rangle &= e^{-iE_n t/\hbar}\,|\Psi_n\rangle \\ &= e^{-i\hat{H}t/\hbar}\,|\Psi_n\rangle \end{aligned}$$
- So $$|\Psi_n\rangle = |\Psi_{n_H}\rangle$$

Sp propagator in many-body system

- Similar definition as in sp problem
- Also very useful both for discrete and continuum problems
- Fermion definition

$$G(\alpha,\beta;t,t') = -\frac{i}{\hbar}\langle\Psi_0^N|\,\mathcal{T}[a_{\alpha_H}(t)a^\dagger_{\beta_H}(t')]\,|\Psi_0^N\rangle$$

- with normalized Heisenberg ground state

$$\hat{H}\,|\Psi_0^N\rangle = E_0^N\,|\Psi_0^N\rangle$$

- Heisenberg picture operators

$$a_{\alpha_H}(t) = e^{\frac{i}{\hbar}\hat{H}t}a_\alpha e^{-\frac{i}{\hbar}\hat{H}t}$$

$$a^\dagger_{\alpha_H}(t) = e^{\frac{i}{\hbar}\hat{H}t}a^\dagger_\alpha e^{-\frac{i}{\hbar}\hat{H}t}$$

- and time-ordering operation is defined according to (fermions)

$$\mathcal{T}[a_{\alpha_H}(t)a^\dagger_{\beta_H}(t')] \equiv \theta(t-t')a_{\alpha_H}(t)a^\dagger_{\beta_H}(t') - \theta(t'-t)a^\dagger_{\beta_H}(t')a_{\alpha_H}(t)$$

Use definitions

- Write in detail

$$G(\alpha,\beta;t-t') = -\frac{i}{\hbar}\left\{\theta(t-t')e^{\frac{i}{\hbar}E_0^N(t-t')}\langle\Psi_0^N|\,a_\alpha e^{-\frac{i}{\hbar}\hat{H}(t-t')}a_\beta^\dagger\,|\Psi_0^N\rangle\right.$$

$$\left.-\theta(t'-t)e^{\frac{i}{\hbar}E_0^N(t'-t)}\langle\Psi_0^N|\,a_\beta^\dagger e^{-\frac{i}{\hbar}\hat{H}(t'-t)}a_\alpha\,|\Psi_0^N\rangle\right\}$$

$$= -\frac{i}{\hbar}\left\{\theta(t-t')\sum_m e^{\frac{i}{\hbar}(E_0^N-E_m^{N+1})(t-t')}\langle\Psi_0^N|\,a_\alpha\,|\Psi_m^{N+1}\rangle\langle\Psi_m^{N+1}|\,a_\beta^\dagger\,|\Psi_0^N\rangle\right.$$

$$\left.-\theta(t'-t)\sum_n e^{\frac{i}{\hbar}(E_0^N-E_n^{N-1})(t'-t)}\langle\Psi_0^N|\,a_\beta^\dagger\,|\Psi_n^{N-1}\rangle\langle\Psi_n^{N-1}|\,a_\alpha\,|\Psi_0^N\rangle\right\}$$

- introducing appropriate completeness relations with exact eigenstates

$$\hat{H}\,|\Psi_m^{N+1}\rangle = E_m^{N+1}\,|\Psi_m^{N+1}\rangle$$

$$\hat{H}\,|\Psi_n^{N-1}\rangle = E_n^{N-1}\,|\Psi_n^{N-1}\rangle$$

Lehmann representation

- Introduce FT for practical applications

$$G(\alpha,\beta;E) = \int_{-\infty}^{\infty} d(t-t')\; e^{\frac{i}{\hbar}E(t-t')}\; G(\alpha,\beta;t-t')$$

- Use again integral representation of step function

$$\begin{aligned} G(\alpha,\beta;E) &= \sum_m \frac{\langle \Psi_0^N | a_\alpha | \Psi_m^{N+1}\rangle \langle \Psi_m^{N+1} | a_\beta^\dagger | \Psi_0^N\rangle}{E-(E_m^{N+1}-E_0^N)+i\eta} \\ &+ \sum_n \frac{\langle \Psi_0^N | a_\beta^\dagger | \Psi_n^{N-1}\rangle \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N\rangle}{E-(E_0^N-E_n^{N-1})-i\eta} \\ &= \langle \Psi_0^N | a_\alpha \frac{1}{E-(\hat{H}-E_0^N)+i\eta} a_\beta^\dagger | \Psi_0^N\rangle \\ &+ \langle \Psi_0^N | a_\beta^\dagger \frac{1}{E-(E_0^N-\hat{H})-i\eta} a_\alpha | \Psi_0^N\rangle \end{aligned}$$

- Any sp basis can be used
- Still "wave functions" and eigenvalues as in sp problem!!

Spectral functions

- Physics of knock-out experiments to be discussed shortly can be interpreted nicely using spectral functions
- For the removal of particles, we have the hole spectral function

$$\begin{aligned} S_h(\alpha;E) &= \frac{1}{\pi}\,\mathrm{Im}\,G(\alpha,\alpha;E) \qquad\qquad E \le \varepsilon_F^- \\ &= \sum_n \left| \langle \Psi_n^{N-1} | \, a_\alpha \, | \Psi_0^N \rangle \right|^2 \delta(E-(E_0^N - E_n^{N-1})) \end{aligned}$$

- with $\varepsilon_F^- = E_0^N - E_0^{N-1}$
- A similar addition probability density is available for adding particles (particle spectral function)

$$\begin{aligned} S_p(\alpha;E) &= -\frac{1}{\pi}\,\mathrm{Im}\,G(\alpha,\alpha;E) \qquad\qquad E \ge \varepsilon_F^+ \\ &= \sum_m \left| \langle \Psi_m^{N+1} | \, a_\alpha^\dagger \, | \Psi_0^N \rangle \right|^2 \delta(E-(E_m^{N+1} - E_0^N)) \end{aligned}$$

$$\varepsilon_F^+ = E_0^{N+1} - E_0^N$$

$$\frac{1}{E \pm i\eta} = \mathcal{P}\frac{1}{E} \mp i\pi\delta(E)$$

Occupation and depletion

- Occupation number

$$n(\alpha) = \langle \Psi_0^N | a_\alpha^\dagger a_\alpha | \Psi_0^N \rangle = \sum_n \left| \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N \rangle \right|^2$$

$$= \int_{-\infty}^{\varepsilon_F^-} dE \sum_n \left| \langle \Psi_n^{N-1} | a_\alpha | \Psi_0^N \rangle \right|^2 \delta(E - (E_0^N - E_n^{N-1}))$$

$$= \int_{-\infty}^{\varepsilon_F^-} dE \; S_h(\alpha; E)$$

- Depletion

$$d(\alpha) = \langle \Psi_0^N | a_\alpha a_\alpha^\dagger | \Psi_0^N \rangle = \sum_m \left| \langle \Psi_m^{N+1} | a_\alpha^\dagger | \Psi_0^N \rangle \right|^2$$

$$= \int_{\varepsilon_F^+}^{\infty} dE \sum_m \left| \langle \Psi_m^{N+1} | a_\alpha^\dagger | \Psi_0^N \rangle \right|^2 \delta(E - (E_m^{N+1} - E_0^N))$$

$$= \int_{\varepsilon_F^+}^{\infty} dE \; S_p(\alpha; E)$$

- Obvious sum rule

$$n(\alpha) + d(\alpha) = \langle \Psi_0^N | a_\alpha^\dagger a_\alpha | \Psi_0^N \rangle + \langle \Psi_0^N | a_\alpha a_\alpha^\dagger | \Psi_0^N \rangle = \langle \Psi_0^N | \Psi_0^N \rangle = 1$$

Expectation values of operators in ground state

- Consider one-body operator

$$\langle\Psi_0^N|\,\hat{O}\,|\Psi_0^N\rangle = \sum_{\alpha,\beta}\langle\alpha|\,O\,|\beta\rangle\,\langle\Psi_0^N|\,a_\alpha^\dagger a_\beta\,|\Psi_0^N\rangle = \sum_{\alpha,\beta}\langle\alpha|\,O\,|\beta\rangle\,n_{\alpha\beta}$$

- One-body density matrix element $\quad n_{\alpha\beta} \equiv \langle\Psi_0^N|\,a_\alpha^\dagger a_\beta\,|\Psi_0^N\rangle$
- can be obtained from sp propagator

$$\begin{aligned}
n_{\beta\alpha} &= \int \frac{dE}{2\pi i}\, e^{iE\eta}\, G(\alpha,\beta;E) \\
&= \int \frac{dE}{2\pi i} e^{iE\eta} \sum_m \frac{\langle\Psi_0^A|\,a_\alpha\,|\Psi_m^{A+1}\rangle\,\langle\Psi_m^{A+1}|\,a_\beta^\dagger\,|\Psi_0^A\rangle}{E-(E_m^{A+1}-E_0^A)+i\eta} \\
&+ \int \frac{dE}{2\pi i}\, e^{iE\eta} \sum_n \frac{\langle\Psi_0^N|\,a_\beta^\dagger\,|\Psi_n^{N-1}\rangle\,\langle\Psi_n^{N-1}|\,a_\alpha\,|\Psi_0^N\rangle}{E-(E_0^N-E_n^{N-1})-i\eta} \\
&= \sum_n \langle\Psi_0^N|\,a_\beta^\dagger\,|\Psi_n^{N-1}\rangle\,\langle\Psi_n^{N-1}|\,a_\alpha\,|\Psi_0^N\rangle = \langle\Psi_0^N|\,a_\beta^\dagger a_\alpha\,|\Psi_0^N\rangle
\end{aligned}$$

- or $\quad n_{\beta\alpha} = \frac{1}{\pi}\int_{-\infty}^{\varepsilon_F^-} dE\;\, \mathrm{Im}\, G(\alpha,\beta;E) = \langle\Psi_0^N|\,a_\beta^\dagger a_\alpha\,|\Psi_0^N\rangle$

Magic?!: energy sum rule

- Consider
$$I_\alpha = \frac{1}{\pi}\int_{-\infty}^{\varepsilon_F^-} dE\ E\ \ \mathrm{Im}\ G(\alpha,\alpha;E) = \int_{-\infty}^{\varepsilon_F^-} dE\ E\ S_h(\alpha;E)$$
$$= \sum_m (E_0^N - E_m^{N-1}) \langle \Psi_0^N | a_\alpha^\dagger | \Psi_m^{N-1} \rangle \langle \Psi_m^{N-1} | a_\alpha | \Psi_0^N \rangle$$
$$= \langle \Psi_0^N | a_\alpha^\dagger a_\alpha \hat{H} | \Psi_0^N \rangle - \sum_m \langle \Psi_0^N | a_\alpha^\dagger E_m^{N-1} | \Psi_m^{N-1} \rangle \langle \Psi_m^{N-1} | a_\alpha | \Psi_0^N \rangle$$
$$= \langle \Psi_0^N | a_\alpha^\dagger a_\alpha \hat{H} | \Psi_0^N \rangle - \langle \Psi_0^N | a_\alpha^\dagger \hat{H} a_\alpha | \Psi_0^N \rangle = \langle \Psi_0^N | a_\alpha^\dagger [a_\alpha, \hat{H}] | \Psi_0^N \rangle$$
- Earlier results yield $[a_\alpha, \hat{H}] = \sum_\beta \langle \alpha | T | \beta \rangle a_\beta + \sum_{\beta\gamma\delta} (\alpha\beta|V|\gamma\delta) a_\beta^\dagger a_\delta a_\gamma$
- Insert $I_\alpha = \sum_\beta \langle \alpha | T | \beta \rangle \langle \Psi_0^N | a_\alpha^\dagger a_\beta | \Psi_0^N \rangle + \sum_{\beta\gamma\delta} (\alpha\beta|V|\gamma\delta)\ \langle \Psi_0^N | a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma | \Psi_0^N \rangle$
- Sum over α
$$\sum_\alpha I_\alpha = \langle \Psi_0^N | \hat{T} | \Psi_0^N \rangle + 2 \langle \Psi_0^N | \hat{V} | \Psi_0^N \rangle$$

Galitski-Migdal energy sum rule (Koltun)

- Combine with half the expectation value of the kinetic energy

$$
\begin{aligned}
E_0^N &= \langle \Psi_0^N | \, \hat{H} \, | \Psi_0^N \rangle \\
&= \frac{1}{2\pi} \int_{-\infty}^{\varepsilon_F^-} dE \, \sum_{\alpha,\beta} \{ \langle \alpha | \, T \, | \beta \rangle + \; E \, \delta_{\alpha,\beta} \} \; \mathrm{Im} \; G(\beta, \alpha; E) \\
&= \frac{1}{2} \left(\sum_{\alpha,\beta} \langle \alpha | \, T \, | \beta \rangle \, n_{\alpha\beta} + \sum_{\alpha} \int_{-\infty}^{\varepsilon_F^-} dE \; E \; S_h(\alpha; E) \right)
\end{aligned}
$$

- complete result only when there are no three- or higher-body interactions
- sp propagator (hole part) yields energy of the ground state
- later: particle part yields elastic scattering cross section

Interaction picture

- Split Hamiltonian $\hat{H} = \hat{H}_0 + \hat{H}_1$
- with $\hat{H}_0$ problem solved (and corresponding time evolution)
- Define $$|\Psi_I(t)\rangle = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}|\Psi_S(t)\rangle$$
- as the interaction picture state ket
- Corresponding equation of motion

$$\begin{aligned} i\hbar\frac{\partial}{\partial t}|\Psi_I(t)\rangle &= -\hat{H}_0|\Psi_I(t)\rangle + \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\} i\hbar\frac{\partial}{\partial t}|\Psi_S(t)\rangle \\ &= -\hat{H}_0|\Psi_I(t)\rangle + \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\left(\hat{H}_0 + \hat{H}_1\right)|\Psi_S(t)\rangle \\ &= \hat{H}_1(t)\,|\Psi_I(t)\rangle \end{aligned}$$

- where $\hat{H}_1(t) = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{H}_1 \exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\}$
- In general $\hat{H}_0$ and $\hat{H}_1$ do not commute!

Operators in the interaction picture

- Consider in Schrödinger picture

$$\hat{O}_S \left|\Psi_S(t)\right\rangle = \left|\Psi'_S(t)\right\rangle$$

- Go to interaction picture

$$\begin{aligned} \left|\Psi'_I(t)\right\rangle &= \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\left|\Psi'_S(t)\right\rangle = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{O}_S\left|\Psi_S(t)\right\rangle \\ &= \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{O}_S \exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\}\exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\left|\Psi_S(t)\right\rangle \\ &= \hat{O}_I(t)\left|\Psi_I(t)\right\rangle \end{aligned}$$

- with

$$\boxed{\hat{O}_I(t) = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{O}_S \exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\}}$$

- is the corresponding operator in the interaction picture

Equation of motion in the interaction picture

- Consider

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\hat{O}_I(t) &= \left\{ i\hbar\frac{\partial}{\partial t}\exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\right\}\hat{O}_S \exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\} \\
&+ \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{O}_S\left\{ i\hbar\frac{\partial}{\partial t}\exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\}\right\} \\
&= -\hat{H}_0\hat{O}_I(t) + \hat{O}_I(t)\hat{H}_0 \\
&= \left[\hat{O}_I(t), \hat{H}_0\right]
\end{aligned}
$$

- Example
  - in its own basis $\hat{H}_0 = \sum_\lambda \varepsilon_\lambda a^\dagger_\lambda a_\lambda$
  - so

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}a_{\lambda_I}(t) &= \left[a_{\lambda_I}(t), \hat{H}_0\right] \\
&= \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\left[a_\lambda, \hat{H}_0\right]\exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\} \\
&= \varepsilon_\lambda a_{\lambda_I}(t)
\end{aligned}
$$

  - and therefore $a_{\lambda_I}(t) = e^{-i\varepsilon_\lambda t/\hbar}a_\lambda$ and $a^\dagger_{\lambda_I}(t) = e^{i\varepsilon_\lambda t/\hbar}a^\dagger_\lambda$

Components of Hamiltonian

- Immediately $$\hat{V}_I(t) = \frac{1}{2}\sum_{\alpha\beta\gamma\delta}(\alpha\beta|V|\gamma\delta)\, a^\dagger_{\alpha_I}(t)a^\dagger_{\beta_I}(t)a_{\delta_I}(t)a_{\gamma_I}(t)$$
- and $$\hat{U}_I(t) = \sum_{\alpha\beta}(\alpha|U|\beta)\, a^\dagger_{\alpha_I}(t)a_{\beta_I}(t)$$
- These operators have simple time dependence
- Critical operator: time-evolution in interaction picture

Interaction picture time-evolution operator

- Define $|\Psi_I(t)\rangle = \hat{\mathcal{U}}(t,t_0)\,|\Psi_I(t_0)\rangle$
- Note subscript "I" suppressed on evolution operator
- Obviously $\hat{\mathcal{U}}(t_0,t_0) = 1$
- Explicit construction

$$\begin{aligned}
|\Psi_I(t)\rangle &= \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}|\Psi_S(t)\rangle \\
&= \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\}|\Psi_S(t_0)\rangle \\
&= \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}_0 t_0\right\}|\Psi_I(t_0)\rangle
\end{aligned}$$

- and therefore

$$\hat{\mathcal{U}}(t,t_0) = \exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}(t-t_0)\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}_0 t_0\right\}$$

Some properties of evolution operator

- Using previous result $\hat{\mathcal{U}}^\dagger(t,t_0)\hat{\mathcal{U}}(t,t_0) = \hat{\mathcal{U}}(t,t_0)\hat{\mathcal{U}}^\dagger(t,t_0) = 1$
- Therefore unitary $\hat{\mathcal{U}}^\dagger(t,t_0) = \hat{\mathcal{U}}^{-1}(t,t_0)$
- Note $\hat{\mathcal{U}}(t_1,t_2)\hat{\mathcal{U}}(t_2,t_3) = \hat{\mathcal{U}}(t_1,t_3)$
- and $\hat{\mathcal{U}}(t,t_0)\hat{\mathcal{U}}(t_0,t) = 1$
- therefore $\hat{\mathcal{U}}(t_0,t) = \hat{\mathcal{U}}^\dagger(t,t_0)$
- For future applications combine SE in interaction picture with definition of evolution operator

$$i\hbar\frac{\partial}{\partial t}\left|\Psi_I(t)\right\rangle = \hat{H}_1(t)\left|\Psi_I(t)\right\rangle \quad \text{so} \quad i\hbar\frac{\partial}{\partial t}\hat{\mathcal{U}}(t,t_0) = \hat{H}_1(t)\hat{\mathcal{U}}(t,t_0)$$

- use boundary condition to integrate

$$\hat{\mathcal{U}}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ \hat{H}_1(t')\hat{\mathcal{U}}(t',t_0)$$

Iterate

- Use

$$\hat{\mathcal{U}}(t,t_0) = 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ \hat{H}_1(t')\hat{\mathcal{U}}(t',t_0)$$

- to generate expansion

$$\begin{aligned}
\hat{\mathcal{U}}(t,t_0) &= 1 - \frac{i}{\hbar}\int_{t_0}^{t} dt'\ \hat{H}_1(t')\left\{1 - \frac{i}{\hbar}\int_{t_0}^{t'} dt''\ \hat{H}_1(t'')\hat{\mathcal{U}}(t'',t_0)\right\} \\
&= 1 + \left(\frac{-i}{\hbar}\right)\int_{t_0}^{t} dt'\ \hat{H}_1(t') \\
&\qquad + \left(\frac{-i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\ \hat{H}_1(t')\hat{H}_1(t'') + \ldots \\
&= \sum_{n=0}^{\infty}\left(\frac{-i}{\hbar}\right)^n \int_{t_0}^{t} dt_1 \int_{t_0}^{t_1} dt_2 \ldots \int_{t_0}^{t_{n-1}} dt_n\ \hat{H}_1(t_1)\hat{H}_1(t_2)\ldots\hat{H}_1(t_n)
\end{aligned}$$

Example: second order

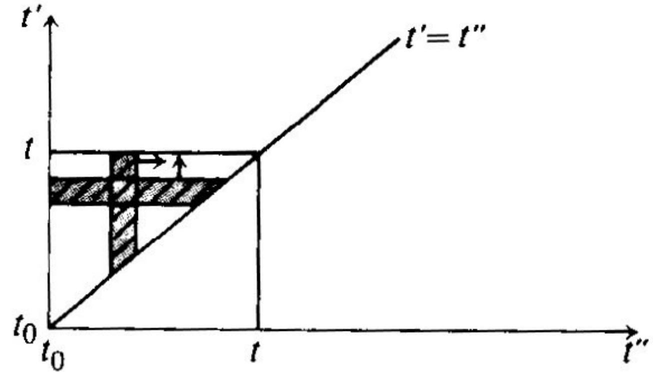
$$\hat{\mathcal{U}}_2(t,t_0) = \left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\ \hat{H}_1(t')\hat{H}_1(t'')$$

$$= \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \left\{ \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\ \hat{H}_1(t')\hat{H}_1(t'') + \int_{t_0}^{t} dt'' \int_{t''}^{t} dt'\ \hat{H}_1(t')\hat{H}_1(t'') \right\}$$

$$= \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \left\{ \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\ \hat{H}_1(t')\hat{H}_1(t'') + \int_{t_0}^{t} dt' \int_{t'}^{t} dt''\ \hat{H}_1(t'')\hat{H}_1(t') \right\}$$

$$= \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \left\{ \int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\ \left[\theta(t'-t'')\hat{H}_1(t')\hat{H}_1(t'') + \theta(t''-t')\hat{H}_1(t'')\hat{H}_1(t')\right] \right\}$$

$$= \frac{1}{2}\left(-\frac{i}{\hbar}\right)^2 \int_{t_0}^{t} dt' \int_{t_0}^{t} dt''\ \mathcal{T}\left[\hat{H}_1(t')\hat{H}_1(t'')\right]$$



- introducing time-ordering
- Extend to all orders

$$\longrightarrow \quad \hat{\mathcal{U}}(t,t_0) = \sum_{n=0}^{\infty} \left(\frac{-i}{\hbar}\right)^n \frac{1}{n!} \int_{t_0}^{t} dt_1 \int_{t_0}^{t} dt_2 \ldots \int_{t_0}^{t} dt_n\ \mathcal{T}\left[\hat{H}_1(t_1)\hat{H}_1(t_2)\ldots\hat{H}_1(t_n)\right]$$

- important for future applications

Links with interaction picture

- Use Schrödinger picture

$$\hat{O}_H(t) = \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\hat{O}_S \exp\left\{-\frac{i}{\hbar}\hat{H}t\right\}$$

$$= \exp\left\{\frac{i}{\hbar}\hat{H}t\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}_0 t\right\}\hat{O}_I(t)\exp\left\{\frac{i}{\hbar}\hat{H}_0 t\right\}\exp\left\{-\frac{i}{\hbar}\hat{H}t\right\}$$

$$= \hat{\mathcal{U}}(0,t)\hat{O}_I(t)\hat{\mathcal{U}}(t,0)$$

- Note that $|\Psi_H\rangle = |\Psi_S(t=0)\rangle = |\Psi_I(t=0)\rangle$
- and $\hat{O}_S = \hat{O}_H(t=0) = \hat{O}_I(t=0)$
- For energy eigenkets

$$|\Psi_{n_S}(t)\rangle = e^{-iE_n t/\hbar}|\Psi_n\rangle = e^{-i\hat{H}t/\hbar}|\Psi_n\rangle$$

- so $|\Psi_n\rangle = |\Psi_{n_H}\rangle$
- Also $|\Psi_H\rangle = |\Psi_I(0)\rangle = \hat{\mathcal{U}}(0,t_0)\,|\Psi_I(t_0)\rangle$

Noninteracting propagator

- Propagator for $\hat{H}_0$ involves interaction picture

$$G^{(0)}(\alpha,\beta;t-t') = -\frac{i}{\hbar}\langle\Phi_0^N|\,\mathcal{T}[a_{\alpha_I}(t)a^\dagger_{\beta_I}(t')]\,|\Phi_0^N\rangle$$

- with corresponding ground state

$$\hat{H}_0\,|\Phi_0^N\rangle = E_{\Phi_0^N}\,|\Phi_0^N\rangle$$

$$E_{\Phi_0^N} = \sum_{\alpha<F}\varepsilon_\alpha$$

- as for IPM so closed-shell atom or nucleus for example
- Operators $\quad a_{\alpha_I}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}a_\alpha e^{-\frac{i}{\hbar}\hat{H}_0 t} = e^{-i\varepsilon_\alpha t/\hbar}a_\alpha$

$$a^\dagger_{\alpha_I}(t) = e^{\frac{i}{\hbar}\hat{H}_0 t}a^\dagger_\alpha e^{-\frac{i}{\hbar}\hat{H}_0 t} = e^{i\varepsilon_\alpha t/\hbar}a^\dagger_\alpha$$

- assuming $\hat{H}_0$ is diagonal in this basis

Evaluate noninteracting sp propagator

- Insert

$$G^{(0)}(\alpha,\beta;t-t') = G_+^{(0)}(\alpha,\beta;t-t') + G_-^{(0)}(\alpha,\beta;t-t')$$

$$= -\frac{i}{\hbar}\delta_{\alpha\beta}\{\theta(t-t')\theta(\alpha-F)e^{-\frac{i}{\hbar}\varepsilon_\alpha(t-t')} - \theta(t'-t)\theta(F-\alpha)e^{\frac{i}{\hbar}\varepsilon_\alpha(t'-t)}\}$$

- propagation of a particle or a hole on top of noninteracting ground state

- directly:

$$\hat{H}_0\; a_\alpha^\dagger\,|\Phi_0^N\rangle = (E_{\Phi_0^N} + \varepsilon_\alpha)\; a_\alpha^\dagger\,|\Phi_0^N\rangle \qquad \alpha > F$$

$$\hat{H}_0\; a_\alpha\,|\Phi_0^N\rangle = (E_{\Phi_0^N} - \varepsilon_\alpha)\; a_\alpha\,|\Phi_0^N\rangle \qquad \alpha < F$$

- FT

$$G^{(0)}(\alpha,\beta;E) = \delta_{\alpha,\beta}\left\{\frac{\theta(\alpha-F)}{E-\varepsilon_\alpha+i\eta} + \frac{\theta(F-\alpha)}{E-\varepsilon_\alpha-i\eta}\right\}$$

Noninteracting spectral functions

- Imaginary parts yield all the strength at one location

$$\begin{aligned} S_h^{(0)}(\alpha;E) &= \frac{1}{\pi}\text{Im } G^{(0)}(\alpha,\alpha;E) & E < \varepsilon_F^{(0)^-} \\ &= \delta(E-\varepsilon_\alpha)\ \theta(F-\alpha) \\ S_p^{(0)}(\alpha;E) &= -\frac{1}{\pi}\text{Im } G^{(0)}(\alpha,\alpha;E) & E > \varepsilon_F^{(0)^+} \\ &= \delta(E-\varepsilon_\alpha)\ \theta(\alpha-F) \end{aligned}$$

- in this basis: either completely full or empty

$$n^{(0)}(\alpha) = \int_{-\infty}^{\varepsilon_F^{(0)^-}} dE\ \delta(E-\varepsilon_\alpha)\ \theta(F-\alpha) = \theta(F-\alpha)$$

- other basis $G^{(0)}(\boldsymbol{r}m_s, \boldsymbol{r}'m_s';E) = \langle\Phi_0^N|\, a_{\boldsymbol{r}m_s} \frac{1}{E-(\hat{H}_0 - E_{\Phi_0^N})+i\eta} a^\dagger_{\boldsymbol{r}'m_s'}\,|\Phi_0^N\rangle$

$$+ \langle\Phi_0^N|\, a^\dagger_{\boldsymbol{r}'m_s'} \frac{1}{E-(E_{\Phi_0^N}-\hat{H}_0)-i\eta} a_{\boldsymbol{r}m_s}\,|\Phi_0^N\rangle$$

$$= \sum_\alpha \left\{ \frac{\langle \boldsymbol{r}m_s|\alpha\rangle\langle\alpha|\boldsymbol{r}'m_s'\rangle\theta(\alpha-F)}{E-\varepsilon_\alpha+i\eta} + \frac{\langle \boldsymbol{r}m_s|\alpha\rangle\langle\alpha|\boldsymbol{r}'m_s'\rangle\theta(F-\alpha)}{E-\varepsilon_\alpha-i\eta} \right\}$$