Notes on Siemens Ch. 6

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Interactions Beyond the Mean Field

- The mean field approximation gives us basic features of nuclei. But now we're going to move beyond the mean field approximation.
- The first thing we are going to do is look at the pairing term to the binding energy (equation 4.3.2).

$$B_p = \frac{\left[(-1)^N + (-1)^Z\right]\delta}{A^{1/2}} \tag{1}$$

- This gives even-even nuclei a tighter binding energy. Also it turns out that the ground state of even-even nuclei have zero angular momentum.
- To explain these things we are going to go beyond the independent-particle motion (mean field).

Interactions Beyond the Mean Field

- Add a perturbation to the mean field Hamiltonian (H_R is called the residual interaction)

$$H = H_{MF} + H_R \tag{2}$$

    - The eigenstates of H_{MF} are Slater determinants.
- One solution to this is to diagonalize H_R in the H_{MF} basis, but this requires large calculations.
- We are going to use other methods in this chapter. We will split (crudely) into long-range and short-range parts, and look at short-range parts here.

The δ-Force

- Look at degenerate states of H_{MF} because H_R with have a decisive influence.
- Start with H_{MF} in a full j state and two identical nucleons in the next j state.

$$\psi_{JM}^{nlj}(1,2) = \sum_{m_1 m_2} \langle j m_1 j m_2 | JM \rangle \mathcal{A} \left[\Phi_{nljm_1}(1) \Phi_{nljm_2}(2) \right] \tag{3}$$

$$\Phi_{nljm_1} = \frac{1}{r} u_{nlj}(r) \sum_{m,s} \left\langle l m \frac{1}{2} s \middle| j m_1 \right\rangle Y_l^m(\theta, \phi) \chi_s \tag{4}$$

- The shortest range for H_R is a δ-force.

$$H_R = V_0 \delta(\mathbf{r}_1 - \mathbf{r}_2) \tag{5}$$

The δ-Force

- This Hamiltonian gives an energy

$$E_R = V_0 \int \psi^*_{JM} \delta(\mathbf{r}_1 - \mathbf{r}_2) \psi_{JM} d^3\mathbf{r}_1 d^3\mathbf{r}_2 \tag{6}$$

$$= \frac{V_0 \left[1 + (-1)^J\right] (2j+1)^2}{32\pi(2J+1)} \left| \left\langle j, \frac{1}{2}, j, -\frac{1}{2} \middle| J, 0 \right\rangle \right|^2 \int\limits_0^\infty r^{-2} u^4_{nlj(r)dr} \tag{7}$$

- Note here that E_R vanishes for odd values of J. This means that two identical Fermi particles in the same j-shell can only be in even angular-momentum states.
- For an attractive force $(V_0 < 0)$ the lowest energy has $J = 0$ and the first excited state is $J = 2$.

The δ-Force

- For all $j > \frac{3}{2}$ the difference in energies of these two states is

$$|(E_2 - E_0)/E_0| \approx \frac{3}{4} \tag{8}$$

  which is large as seen in figure 6.2 of the book.
- The two nucleons have their largest spatial overlap in this state $(J = 0)$.
- Thus an attractive δ-interaction decreases the energy.

The Degenerate Pairing Model

- A main feature of the δ-force that is maintained in the pairing force is that it only has non-zero matrix elements between time-reversed states. Also, they non-zero elements are all identital

$$\left\langle jm_1\overline{jm_1}\right| V \left|jm_2\overline{jm_2}\right\rangle \equiv -G \tag{9}$$

- Let's use the basis states $j + \frac{1}{2} \equiv \Omega$. Now the Schrödinger equation becomes

$$-G\begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & & & 1 \\ \vdots & \ddots & \vdots & \\ 1 & & \cdots & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_\Omega \end{pmatrix} = E\begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_\Omega \end{pmatrix} \tag{10}$$

$$-G(x_1 + \cdots + x_\Omega) = Ex_1 = Ex_2 = \cdots = Ex_\Omega \tag{11}$$

The Degenerate Pairing Model

$$-G(x_1 + \cdots + x_\Omega) = Ex_1 = Ex_2 = \cdots = Ex_\Omega \tag{12}$$

- This has solutions

$$E = -G\Omega, \qquad \vec{x} = \frac{1}{\sqrt{\Omega}}(1, 1, \cdots, 1) \tag{13}$$

and

$$E = 0, \qquad x_1 + x_2 + \cdots + x_\Omega = 0. \tag{14}$$

- Equation 13 refers to the $J = 0$ state and the degerarate $J > 0$ states have energy of equation 14.

The Degenerate Pairing Model

- Now assume we have n particles in the j-shell ($n \leq 2\Omega$), and p pairs of particles, i.e. $J = 0$ states.
- Using equation 13 and the fact that Ω is the number of possible pairs we get
$$E(n,p) = -Gp\left(\Omega - n + p + 1\right) \tag{15}$$
- Introduce *seniority*, $S = n - 2p$, the number of unpaired nucleons.

$$E(n,S) = -\frac{G}{4}(n-S)(2\Omega - n - S + 2) \tag{16}$$
$$E(n,0) = -\frac{1}{4}Gn(2\Omega - n + 2),\ \text{lowest} \tag{17}$$
$$E(2,0) = -G\Omega,\ \text{what we got before} \tag{18}$$
$$E(2\Omega,0) = -Gn/2,\ \text{what you expect from mean field} \tag{19}$$

The Degenerate Pairing Model

- The pairing force creates as many pairs of particles as possible.
- Even-even have zero spin.
- Odd numbers of nuclei, spin is determined by unpaired nucleon.
- Comparing odd-mass and even-mass nuclei we get,

$$E(2p+1,p) - E(2p,p) = Gp \tag{20}$$

  which seems to agree with experiment.
- For even-even nuclei, the lowest excited state is that of one broken pair, which has symmetric energy

$$E(2p,p-1) - E(2p,p) = G\Omega \tag{21}$$

- For us to use degenerate perturbation theory we assume that the perturbed energy shifts should be small compared to the energy spacing. Since the shifts are $G\Omega$ this is not the case (G is small but he says $G\Omega$ is much larger). So we have to do something else.
- We generalize our residual interaction and write it with creation and destruction operators.

$$H_R = -G \sum_{i,k}{}' a_{\bar{k}}^{\dagger} a_{k}^{\dagger} a_i a_{\bar{i}} \tag{22}$$

Where the primed sum means a truncated sum around the fermi energy $|\varepsilon_k - \mu| \leq S$.

- Since now we can't assume $H_R \ll H_{MF}$ we have to do some fancy footwork.

$$H = H_0 + \delta H \tag{23}$$

$$H_0 = \sum_k \varepsilon_k \left(a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}} \right) - \Delta \sum_k{}' \left(a_{\bar{k}}^\dagger a_k^\dagger + a_k a_{\bar{k}} \right) \tag{24}$$

$$\delta H = -G \sum_{i,k}{}' a_{\bar{k}}^\dagger a_k^\dagger a_i a_{\bar{i}} + \Delta \sum_k{}' \left(a_{\bar{k}}^\dagger a_k^\dagger + a_k a_{\bar{k}} \right) \tag{25}$$

- We want eigenfunctions of both H and N, but without δH we can't have that.

$$N = \sum_k (a_k^\dagger a_k + a_{\bar{k}}^\dagger a_{\bar{k}}) \tag{26}$$

- Thus we don't have conservation of particles and at most we can have a given average number particles. We account for this by modifying out Hamiltonian.

- We then use the Lagrange multiplier μ (we will have a constraint on the expectation value of N) to write

$$H' = H - \mu N = H_0' + \delta H, \qquad H_0' = H_0 - \mu N \tag{27}$$

- Minimizing the expectation value of H_0 ($\delta \langle H_0' \rangle$) gives us

$$\mu = \frac{\delta \langle H_0 \rangle}{\delta \langle N \rangle} \tag{28}$$

- This is the amound of energy that is needed to remove one nucleon, i.e. the chemical potential.

- We can diagonalize H_0' exactly, we only have to do so for the interval $|\varepsilon_k - \mu| \leq S$.
- Inside the interval we introduce new creation and annihilation operators.

$$\alpha_k = \mathrm{u}_k a_k + \mathrm{v}_k a_{\bar{k}}^\dagger \qquad \alpha_{\bar{k}} = \mathrm{u}_k a_{\bar{k}} - \mathrm{v}_k a_k^\dagger \tag{29}$$

- This is called the Bogolyubov transformation and the variables u_k and v_k are used to minimize $\langle H_0' \rangle$ with the normalization requirement

$$\mathrm{u}_k^2 + \mathrm{v}_k^2 = 1, \tag{30}$$

which ensures the same (anti)commutation relations between the α's as thos of the a's.

$$\left\{\alpha_i, \alpha_k\right\} = \left\{\alpha_i^\dagger, \alpha_k^\dagger\right\} = 0, \qquad \left\{\alpha_i, \alpha_k^\dagger\right\} = \delta_{ik} \tag{31}$$

- The transformation for a is then

$$a_k = \mathrm{u}_k \alpha_k - \mathrm{v}_k \alpha_{\bar{k}}^\dagger, \qquad a_{\bar{k}} = \mathrm{u}_k \alpha_{\bar{k}} + \mathrm{v}_k \alpha_k^\dagger. \tag{32}$$

- Plugging this into equations 24 and 27 gives us

$$H_0' = \Omega_{gs} + \sum_k H_k^{(1)} \left(\alpha_k^\dagger \alpha_k + \alpha_{\bar{k}}^\dagger \alpha_{\bar{k}} \right) + {\sum_k}' H_k^{(2)} \left(\alpha_{\bar{k}}^\dagger \alpha_k^\dagger + \alpha_k \alpha_{\bar{k}} \right) \tag{33}$$

$$\Omega_{gs} = 2 {\sum_k}' \left[(\varepsilon_k - \mu) \mathrm{v}_k^2 - \delta \mathrm{u}_k \mathrm{v}_k \right] \tag{34}$$

$$H_k^{(1)} = (\varepsilon_k - \mu)(\mathrm{u}_k^2 - \mathrm{v}_k^2) + 2\mathrm{u}_k \mathrm{v}_k \Delta \tag{35}$$

$$H_k^{(2)} = 2(\varepsilon_k - \mu)\mathrm{u}_k \mathrm{v}_k - (\mathrm{u}_k^2 - \mathrm{v}_k^2)\Delta \tag{36}$$

- Where for $\varepsilon_k - \mu > S, \mathrm{u}_k = 1, \mathrm{v}_k = 0$ and for $\varepsilon_k - \mu < -S, \mathrm{u}_k = 0, \mathrm{v}_k = 1$.

- To diagonalize H_0' we require that $H_k^{(2)}$ be zero in the interval.

$$2(\varepsilon_k - \mu)\mathrm{u}_k\mathrm{v}_k = (\mathrm{u}_k^2 - \mathrm{v}_k^2)\Delta \tag{37}$$

- This has the following solutions.

$$\mathrm{v}_k^2 = \frac{1}{2}\left(1 - \frac{\varepsilon_k - \mu}{\epsilon_k}\right) \leq 1 \tag{38}$$

$$\mathrm{u}_k^2 = \frac{1}{2}\left(1 + \frac{\varepsilon_k - \mu}{\epsilon_k}\right) \leq 1 \tag{39}$$

$$\epsilon_k = \sqrt{(\varepsilon_k - \mu)^2 + \Delta^2} \tag{40}$$

- With this we get

$$H_0' = \Omega_{gs} + \sum_k \epsilon_k \left(\alpha_k^\dagger \alpha_k + \alpha_{\bar{k}}^\dagger \alpha_{\bar{k}}\right) \tag{41}$$

- The BCS wave function is given by

$$\alpha_k |gs\rangle = \alpha_{\bar{k}} |gs\rangle = 0 \tag{42}$$

$$a_k |vac\rangle = a_{\bar{k}} |vac\rangle = 0 \tag{43}$$

$$|gs\rangle = \prod_k \left(\mathrm{u}_k + \mathrm{v}_k a^\dagger_{\bar{k}} a^\dagger_k \right) |vac\rangle . \tag{44}$$

- Again, since we don't have a fixed number of particles we can get the average number of particles, and the fluctuation in the number.

$$N_0 = \langle gs| N |gs\rangle = 2\sum_k \mathrm{v}_k^2 = \sum_k \left(1 - \frac{\varepsilon_k - \mu}{\epsilon_k} \right) \tag{45}$$

$$\sigma^2 = \langle gs| N^2 |gs\rangle - (\langle gs| N |gs\rangle)^2 = 4\sum_k \mathrm{u}_k^2 \mathrm{v}_k^2 = \Delta^2 {\sum_k}' \frac{1}{\epsilon_k^2} \tag{46}$$

- The energy gain compared to the normal energy is

$$\Delta E = \langle gs| H_0' + \mu N |gs\rangle - 2 \sum_{\varepsilon_k < \mu} \varepsilon_k \tag{47}$$

$$= 2 \sum_k \varepsilon_k \mathrm{v}_k^2 - \Delta^2 \sum_k{}' \frac{1}{\epsilon_k} - 2 \sum_{\varepsilon_k < \mu} \varepsilon_k \tag{48}$$

- Looking at the BCS wave function we see that v_k^2 is the probability of one pair being in the original ε_k. This goes from 1 below μ to 0 above μ.
- The system is now described by quasi-particles, of energy ϵ_k, which are created by the $\alpha_k^\dagger$ and $\alpha_{\bar{k}}^\dagger$ operators. These quasi-particles are linear combinations of "old" holes and "old" particles.

- We can determine Δ by minimizing $\langle gs| H - \mu N |gs\rangle$ with respect to Δ.
- Doing this yields the condition

$$0 = \Delta \left(1 - \frac{1}{2} G \sum{}' \frac{1}{\epsilon_k}\right), \tag{49}$$

which has the solution $\Delta = 0$, corresponding to the original Hartree-Fock solution with no pairing. For $\Delta \neq 0$ we get the condition

$$\frac{2}{G} = \sum{}' \frac{1}{\epsilon_k}. \tag{50}$$

- This must be greater than

$$\sum \frac{1}{|\varepsilon_k - \mu|} = \frac{2}{G_c}. \tag{51}$$

- Thus to have non trivial solutions we must have $G \geq G_c$.

- If we assume Δ to be large compared to the single-particle energy spacings near the Fermi energy we can then take the level density, g, to be continuous. I we also assume that $S \gg \Delta$, and that $g(\varepsilon)$ is constant around μ, we get

$$\frac{2}{G} = {\sum}' \frac{1}{\epsilon_k} = \int\limits_{\mu-S}^{\mu+S} \frac{\frac{1}{2}g(\varepsilon)d\varepsilon}{\sqrt{(\varepsilon-\mu)^2+\Delta^2}} \approx \int\limits_{0}^{S} \frac{d\varepsilon}{\sqrt{\varepsilon^2+\Delta^2}} \tag{52}$$

$$= g(\mu)\ln\left(\frac{S}{\Delta}+\sqrt{1+\left(\frac{S}{\Delta}\right)^2}\right) \approx g(\mu)\ln\left(\frac{2S}{\Delta}\right), \tag{53}$$

which gives us

$$\Delta = 2Se^{-2/Gg(\mu)} \tag{54}$$

The Uniform Model

- It will turn out that Δ is the physically relevant quantity, so in experiments it is reasonable to fix Δ and $g(\mu)$ to relate S and G.
- The energy gain and the fluctuation of particle number can be estimated in similar ways to get

$$\Delta E \approx -\frac{1}{4} g(\mu) \Delta^2 \tag{55}$$

$$\sigma^2 \approx \frac{\pi}{2} g(\mu) \Delta. \tag{56}$$

Relation to Experimental Information

- Let's now relate the Hamiltonian, $H_0' = \Omega_{gs} + \sum_k \epsilon_k \left(\alpha_k^\dagger \alpha_k + \alpha_{\bar{k}}^\dagger \alpha_{\bar{k}} \right)$ to experiment. The lowest excited state for even-even nuclei is the lowest possible two-quasiparticle excitation

$$2\epsilon_k = 2\sqrt{(\varepsilon - \mu)^2 + \Delta^2} \geq 2\Delta. \tag{57}$$

  This corresponds to the breaking of one pair.
- If you take an odd nucleus as an even-even core plus an extra quasiparticle, then you can use this for odd systems as well. For this the ground state energy is $\Omega_{gs} + \epsilon_{k_0}$, giving the lowest excited state an energy of $\epsilon_k - \epsilon_{k_0}$.
- This means that the binding energy for an odd mass nucleus is about $\epsilon_{k_0} \approx \Delta$ larger than for even-even nuclei. This is experimentally known from the liquid-drop model and is roughly

$$\Delta = \frac{2\delta}{\sqrt{A}} = \frac{12\mathrm{MeV}}{\sqrt{A}} \tag{58}$$

- Figure 6.4 shows results for Δ values that match experiment pretty well, which is evidence that the strong force has two-body interactions similar to the pairing force.
- The author then goes on to give some numerical estimates of $g(\mu)$, S, G, and σ.