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- Before putting together our BCS results, let's go back and fill in a few pieces in our derivations.

- Start with $\boxed{\langle BCS|\hat{N}|BCS\rangle = \sum_{k\alpha} \langle BCS|a^\dagger_{k\alpha} a_{k\alpha}|BCS\rangle}$

- Recall that $\boxed{|BCS\rangle = \prod_{k_1}(u_{k_1} + v_{k_1} a^\dagger_{k_1\uparrow} a^\dagger_{-k_1\downarrow})|0\rangle}$

and on the other side $\boxed{\langle BCS| = \langle 0|\prod_{k_2}(u_{k_2} + v_{k_2} a_{-k_2\downarrow} a_{k_2\uparrow})}$

- For any particular value of k and α, the operator $a^\dagger_{k\alpha} a_{k\alpha}$ will commute with all terms except for the ones with $k_1 = k$ and $k_2 = k$.
  - The others will combine to give $\boxed{u_{k_1}^2 + v_{k_1}^2 = 1}$.
  - So we are left only with

$$\boxed{\langle BCS|\hat{N}|BCS\rangle = 2\sum_k \langle 0|(u_k + v_k a_{-k\downarrow} a_{k\uparrow}) a^\dagger_{k\uparrow} a_{k\uparrow} (u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow})|0\rangle}$$

- The terms with u_k don't contribute, since either $a_{k\alpha}|0\rangle = 0$ or $\langle 0|a^\dagger_{k\alpha} = 0$ kills them.
- The 2 comes from picking k and $\downarrow$ as another possibility

$$\Rightarrow \langle BCS|\hat{N}|BCS\rangle = 2\sum_k v_k^2 \langle 0|a_{-k\downarrow} a_{k\uparrow} a^\dagger_{k\uparrow} a_{k\uparrow} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}|0\rangle$$

$$= 2\sum_k v_k^2$$ by moving a's to the right. (or just saying $\hat{n}_{k\uparrow} = a^\dagger_{k\uparrow} a_{k\uparrow}$ just counts the one occupied $k\uparrow$ state)

$$\Rightarrow \boxed{N = \langle BCS|\hat{N}|BCS\rangle = 2\sum_k v_k^2} \quad \text{or} \quad \boxed{\sum_k v_k^2 = \frac{N}{2}}$$

Similarly,

$$\boxed{\langle BCS|K_0|BCS\rangle = \sum_{k\alpha}(\epsilon_k^0 - \mu) a^\dagger_{k\alpha} a_{k\alpha} = 2\sum_k (\epsilon_k^0 - \mu) v_k^2}$$

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- The matrix element of $\sum_{kpq}\sum_{\alpha_1\alpha_2} a^\dagger_{k+q,\alpha_1} a^\dagger_{p-q,\alpha_2} a_{p\alpha_2} a_{k\alpha_1}$ is more involved. In principle we can use the same approach of matching k,p,q's up and then evaluating the resulting matrix element by the anticommutation relations.

- In practice, there is a better way $\Rightarrow$ define new combinations of $a_{k\uparrow}$ and $a^\dagger_{-k\downarrow}$ (and so on) that correspond to destruction operators for $|BCS\rangle$, the way that $a_{k\alpha}|0\rangle = 0$ or $a_{k\alpha}|F\rangle = 0$ for $k > k_F$.

- In particular, define a canonical transformation:

$$\boxed{\alpha_k = u_k a_{k\uparrow} - v_k a^\dagger_{-k\downarrow}} \qquad \boxed{\beta_{-k} = u_k a_{-k\downarrow} + v_k a_{k\uparrow}}$$

This is canonical if the anticommutation relations still hold:

$$\boxed{\{\alpha_k, \alpha^\dagger_{k'}\} = \{\beta_k, \beta^\dagger_{k'}\} = \delta_{kk'}}, \quad \text{all other } \{\,,\,\}\text{'s} = 0$$

Using $\{a_{k\alpha}, a^\dagger_{k'\alpha'}\} = \delta_{kk'}\delta_{\alpha\alpha'}$, it is simple to see that this is true if $u_k^2 + v_k^2 = 1$, which we have already required.

- This is called a Bogolyubov transformation.
  - Note that it doesn't conserve particle number since it mixes creation and destruction operators.

- We can invert the transformation to obtain

$$\boxed{a_{k\uparrow} = u_k \alpha_k + v_k \beta^\dagger_{-k}} \qquad \boxed{a_{-k\downarrow} = u_k \beta_{-k} - v_k \alpha^\dagger_k}$$

and rewrite $\mathcal{K}$ in terms of the new operators.

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These new operators α_k and β_k annihilate the BCS ground state:

$$\boxed{\alpha_k|BCS\rangle = \beta_k|BCS\rangle = 0}$$

eg. $(u_k a_{k\uparrow} - v_k a^\dagger_{-k\downarrow})\prod_{k_1}(u_{k_1} + v_{k_1} a^\dagger_{k_1\uparrow} a^\dagger_{-k_1\downarrow})|0\rangle$

$$= \prod_{k_1\neq k}(u_{k_1} + v_{k_1} a^\dagger_{k_1\uparrow} a^\dagger_{-k_1\downarrow})(u_k a_{k\uparrow} - v_k a^\dagger_{-k\downarrow})(u_k + v_k a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow})|0\rangle$$

$$= (\quad\text{"}\quad)[u_k^2 \underbrace{a_{k\uparrow}|0\rangle}_{0} + (u_k v_k) a_{k\uparrow} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}|0\rangle - v_k u_k a^\dagger_{-k\downarrow}|0\rangle - v_k^2 a^\dagger_{-k\downarrow} a^\dagger_{k\uparrow} a^\dagger_{-k\downarrow}|0\rangle]$$

$$= (\quad)[u_k v_k a^\dagger_{-k\downarrow}|0\rangle - v_k u_k a^\dagger_{-k\downarrow}|0\rangle] = 0$$

- Rearranging the Hamiltonian in terms of the α's and β's is a bit tedious, we'll leave that to Fetter and Walecka, section 37, who carry it out for a more general potential.

- The end result is

$$\boxed{\hat{K} = U + \hat{H}_1 + \hat{H}_2 + N(\hat{V})}$$

where $\langle BCS|N(\hat{V})|BCS\rangle = 0$ ("normal-ordered") and

$$\boxed{U = 2\sum_k(\epsilon_k^0 - \mu)v_k^2 - \frac{|\lambda|}{L}\sum_{kk'}(v_k v_{k'}^2 + u_k v_k u_{k'} v_{k'})}$$

$$\boxed{\hat{H}_1 = \sum_k(\alpha_k^\dagger\alpha_k + \beta_{-k}^\dagger\beta_{-k})\left\{\left[\epsilon_k^0 - \mu - \frac{|\lambda|}{L}\sum_{k'}v_{k'}^2\right](u_k^2 - v_k^2) + 2\frac{|\lambda|}{L}u_k v_k\sum_{k'}u_{k'}v_{k'}\right\}}$$

$$\boxed{\hat{H}_2 = \sum_k(\alpha_k^\dagger\beta_{-k}^\dagger + \beta_{-k}\alpha_k)\left\{2\left[\epsilon_k^0 - \mu - \frac{|\lambda|}{L}\sum_{k'}v_{k'}^2\right]u_k v_k - \frac{|\lambda|}{L}(u_k^2 - v_k^2)\sum_{k'}u_{k'}v_{k'}\right.}$$

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Applying the results and definitions from the minimization, we find that $\hat{H}_2$ vanishes and

$$\boxed{U = \sum_k (\epsilon_k^0 - \mu)\left(1 - \xi_k/E_k\right) - \frac{|\lambda|\rho}{4} N - \frac{1}{|\lambda|}\Delta^2}$$

$$\boxed{\hat{H}_1 = \sum_k E_k\left(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k\right)}$$

with $\boxed{E_k \equiv \sqrt{\xi_k^2 + \Delta^2}}$

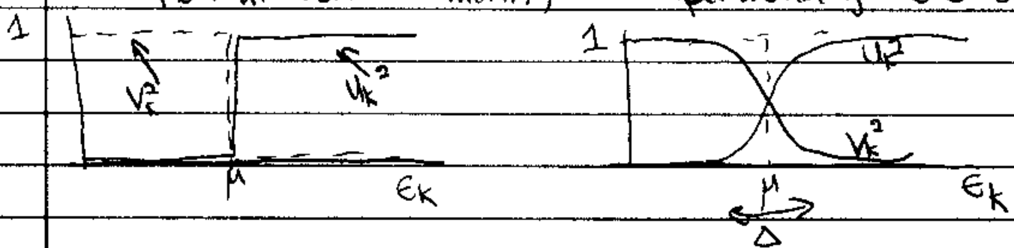
- We see that $\langle BCS | \hat{H}_1 | BCS \rangle = 0$, so U gives the ground state energy. If we neglect $N(\hat{V})$, which is a good approximation in many cases, then each excited quasiparticle requires energy

$$\boxed{E_k = \left(\Delta_k^2 + \xi_k^2\right)^{1/2} \geq \Delta_k}$$

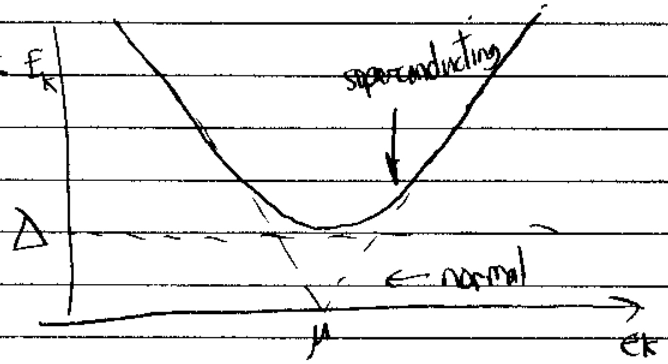
so the excited states are separated from the ground state.

- We find for the u_k's and v_k's

normal solution (with IF?) "superconducting" BCS solution



and the spectrum E_k



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What do pairing and gaps have to do with nuclear physics?

- Look at nuclear spectra for different isotopes of tin or cerium.

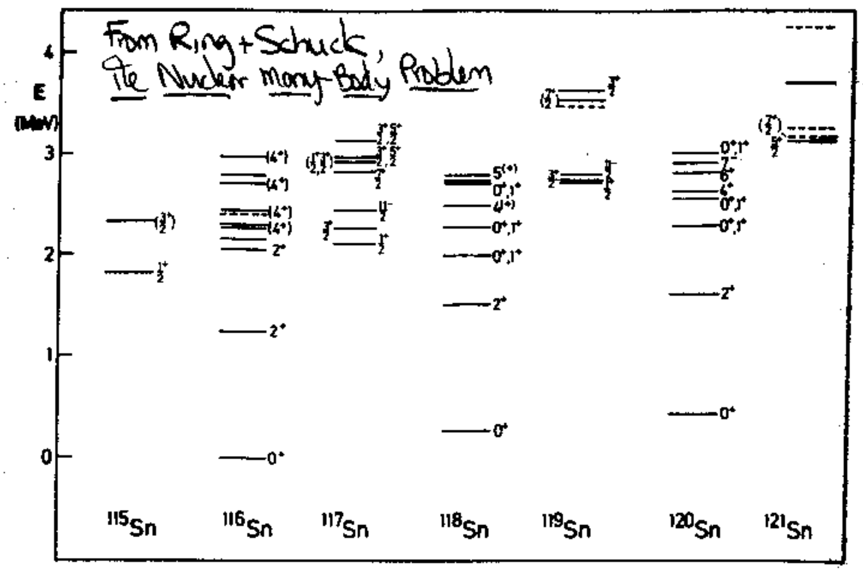
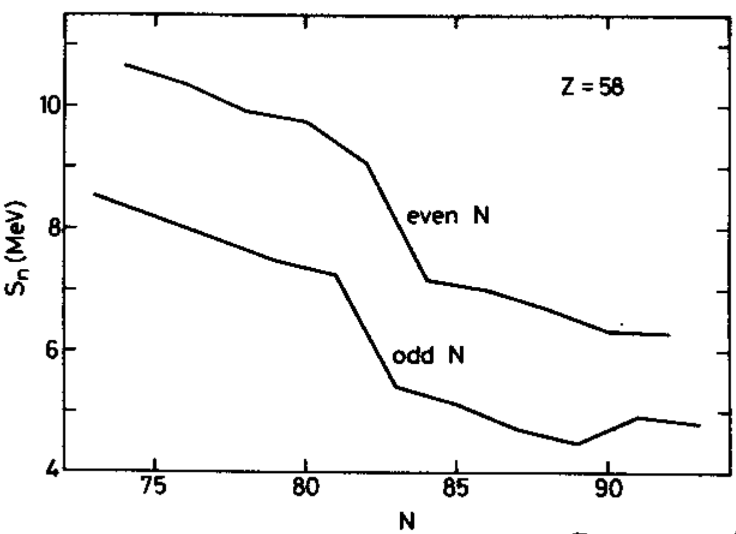


Figure 6.1. Excitation spectra of the $_{50}Sn$ isotopes.



From Siemens + Jensen

Figure 6.1 The neutron separation energy, eq. (4.1.8) as function of neutron number for the cerium isotopes (Z=58). The lines connect points of the same neutron-number parity. The even-neutron nuclei clearly bind the neutrons more strongly than the odd-neutron nuclei. The steep decrease is due to the shell closure at N=82. [*Data from A. H. Wapstra and G. Audi, Nucl. Phys.* **A432** *(1985) 55*]

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- The starting point for thinking about nuclei is a "mean-field" picture, in which each nucleon moves in an average potential due to the other nucleons. The ground states has the lowest orbitals filled.
  - In such a picture, we expect to find excited states in which (roughly) one nucleon is in a higher single-particle orbital, with an excitation energy starting at the difference in single-particle eigenvalues (e.g. picture a harmonic oscillator or square well potential).
  - The first figure on the previous page shows that we have such an excitation spectrum for nuclei with even-odd (proton-neutron) nucleon numbers but a much bigger "gap" in the spectrum for even-even nuclei.

- Also evident in the second figure is the systematic difference between the binding energies of nuclei with odd and even numbers of neutrons and protons.
  - The binding energy of nuclei are summarized quite well by the Bethe-von Weiszacker liquid-drop mass formula, which can be written (see Siemens + Jensen) as (other constants work, too)

$$\boxed{\begin{aligned} B_{LD}(N,Z) = (15.6\,\text{MeV})\left[1-1.5\left(\frac{N-Z}{A}\right)^2\right] - (17.2\,\text{MeV})A^{2/3}\left[1-\emptyset\left(\frac{N-Z}{A}\right)^2\right] \\ -0.70\,\text{MeV}\,\frac{Z^2}{A^{1/3}} + (6\,\text{MeV})\left[(-1)^N+(-1)^Z\right]/A^{1/2} \end{aligned}}$$

where $\boxed{N \equiv \#\text{ of neutrons}}$, $\boxed{Z = \#\text{ of protons}}$, and $\boxed{A \equiv N+Z}$.

- The last term is called the "pairing term", and is not explained by an independent-particle, mean-field picture.

- Other evidence (see Ring + Schuck for details) comes from level densities, moments of inertia of deformed nuclei, the trend of deformations with nuclear mass number, and the presence of low-lying 2^+ states in even nuclei near closed shells (which appear to be vibrational)

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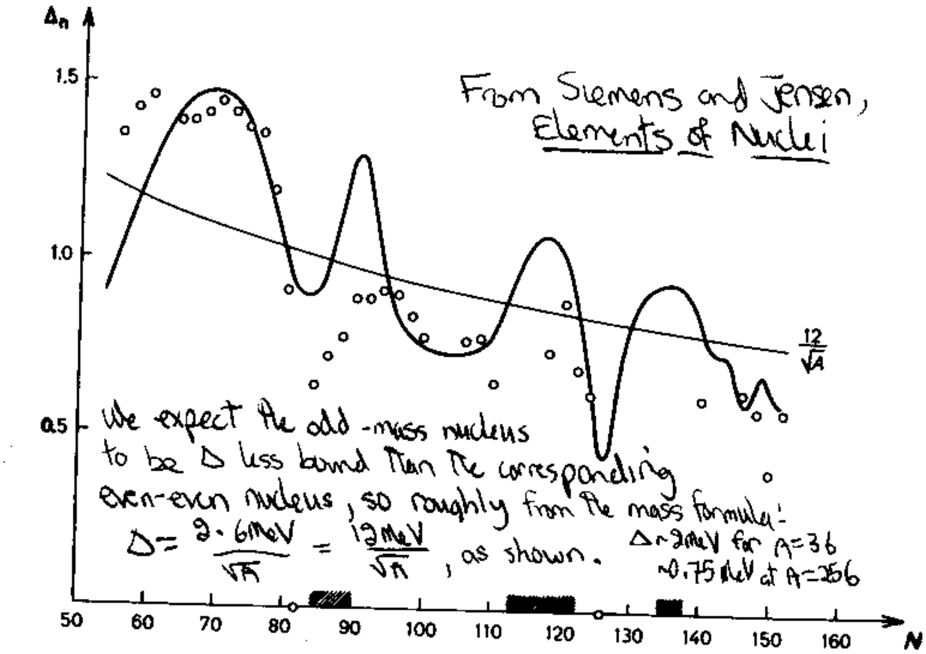
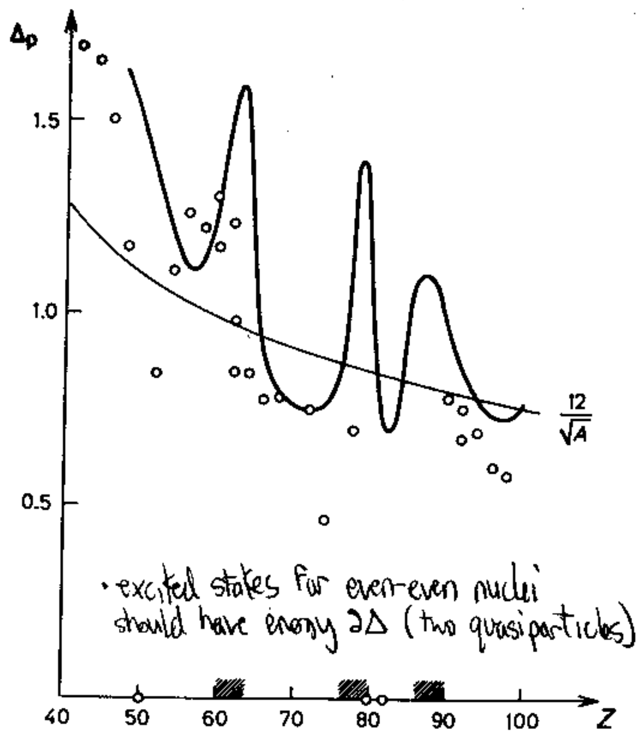
From Siemens and Jensen, Elements of Nuclei



We expect the odd-mass nucleus to be Δ less bound than the corresponding even-even nucleus, so roughly from the mass formula:

$\Delta = \frac{2 \cdot 6\,\text{MeV}}{\sqrt{A}} = \frac{12\,\text{MeV}}{\sqrt{A}}$, as shown. $\Delta \sim 2\,\text{MeV}$ for $A=36$, $\sim 0.75\,\text{MeV}$ at $A=256$

Figure 6.4a Neutron pairing gaps as a function of the neutron number N. The points are calculations with a realistic single particle model [*from T. Dossing and A. S. Jensen, Nucl. Phys.* A222 *(1974) 493*]. The oscillating solid curve is a smooth extraction of the experimental gaps. [*P. E. Nemirovsky and Y. V. Adamchuk, Nucl. Phys.* 39 *(1962) 551.*] At the shaded regions the deformations change unusually fast.



• excited states for even-even nuclei should have energy 2Δ (two quasiparticles).

Figure 6.4b The same as fig. 6.4.a for protons.

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Aside: Exact Solution to 1-D Attractive δ-Function

- The exact solution of the spin-1/2 Fermi gas with δ-function attraction has the same Hamiltonian as the continuum limit of the Hubbard model.
  - The exact solution of the Hubbard model was originally found by Lieb and Wu (Phys. Rev. Lett. 20 1445 (1968)) using Bethe-ansatz techniques. (See also C.N. Yang, PRL 19 1312 (1967).)
  - The continuum model can be solved by the same techniques

- Here we quote the equations as formulated in
  M. Casas et al, Phys. Rev. A44 (1991) 4915
  who call them the "Gaudin equations" after M. Gaudin, Phys. Lett. 24A (1967) 55.

- We write them in the dimensionless variables we've used before:

$$\boxed{\tilde{\rho} \equiv \rho/m\lambda} \quad \text{and} \quad \boxed{\tilde{\mathcal{E}}(\tilde{\rho}) \equiv (E/N)/(B_2/2) = 8(E/N)/(m\lambda^2)}$$

in which case the equations to solve are:

$$\boxed{F(x) = 2 - \frac{K}{\pi}\int_{-1}^{1} dy \, \frac{F(y)}{1+K^2(x-y)^2}}$$

$$\boxed{\tilde{\rho} = \frac{K}{\pi}\int_{-1}^{1} dy \, F(y)}$$

where K is a non-negative parameter to be eliminated. When we have $F(x)$ and K, then

$$\boxed{\tilde{\mathcal{E}}(\tilde{\rho}) = -1 + \frac{4}{\pi}\frac{K}{\tilde{\rho}}\int_{-1}^{1} dy \, y^2 F(y)}$$

gives the energy and $\boxed{\tilde{\mu} \equiv \frac{\mu}{m\lambda^2} = \left(\tilde{\mathcal{E}} + \tilde{\rho}\frac{d\tilde{\mathcal{E}}}{d\tilde{\rho}}\right)/8}$ follows from a numerical derivative.

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I have written a C-code, called gaudin_test.c, to solve these equations for $\tilde{\epsilon}(\tilde{\rho})$ and $\tilde{\mu}(\tilde{\rho})$.

- note that you only need to specify the dimensionless combination $\tilde{\rho}$ and then everything else follows without additional constants.

- Some notes on how the code works:
  - Given a value of K, the integral equation for F(x) is solved in one of two ways:
    - i) by matrix inversion
    - ii) by iteration
  - both methods are fast and give accurate answers (I looked for agreement to 6 significant figures)
  - In both cases, the integral is evaluated with Gauss-Legendre gaussian quadrature

- Iteration method. This is very straight-forward.
  1. Start by setting $F_i^{old} \equiv F(x_i) = 2$ for all $i = 1$ to N where N is the number of gauss points and x_i and w_i are the corresponding nodes and weights.
  2. Find F_i^{temp} by evaluating the right side of the integral equation using F_j^{old}:

     for $i=1,N$: $$\boxed{F_i^{temp} = 2 - \frac{K}{\pi}\sum_{j=1}^{N} \frac{F_j^{old}\, w_j}{1+K^2\cdot(x_i-x_j)^2}}$$
  3. Form F_i^{new} by "damping" the iteration:

     $$\boxed{F_i^{new} = \eta * F_i^{old} + (1-\eta) * F_i^{temp}}$$ with $0 \le \eta < 1$

     I found $\eta = .4$ to work well in this case.
  4. Set $F_i^{old} = F_i^{new}$ and return to step 3. Calculate $|F_i^{old} - F_i^{new}|$ before setting them equal. When the maximum of this difference is less than a desired tolerance, we stop the iterations.

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- Inversion method. Basically we formulate the integral equation as the matrix equation:

$$\boxed{\underline{A}\,\underline{F} = \underline{B}} \quad \text{or} \quad \boxed{A_{ij} F_j = B_i}$$

which can be solved for F_j by standard packages (I used a gsl linear system routine that uses an LU decomposition).
  - The vector $\underline{B}$ is simple: $B_i = 2$ for $i = 1$ to N.
  - The matrix $\underline{\bar{A}}$ is filled with elements of the integral and also diagonal elements from the left side:

$$\boxed{A_{ij} = \delta_{ij} + \frac{K}{\pi} \frac{w_j}{1 + K^2 (x_i - x_j)^2}}$$

- The array $A_{ij} \to A[i][j]$ and the vector $B_i \to B[i]$ are passed to an appropriate routine and we get our answer F_i for $i = 1$ to N.

- Note that in both cases, F_i is exactly what we want to let us evaluate $\tilde{\varepsilon}(\tilde{\rho})$.

- Ok, so now we have routines to find F_i given K. How do we find K? There are many options for using the second equation, which include solving for K and substituting in the integral equation and use the iteration method.
  - I used a different way, which worked well (so I didn't explore any other methods). [I had a table of results to check against.]
  - The basic idea is to form the function $\boxed{g(K) = \tilde{\rho}_{given} - \frac{K}{\pi} \int_{-1}^{1} dy\, F(y)}$ and find its zero using a root-finding routine.
  - The routine I used employs the Brent algorithm and starts with upper and lower bounds for K; I used $0.00001 < K < 200$.
  - The function $g(K)$ is passed to the routine, where the integral on the right side is evaluated by solving for F_i using the current value of K.

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- Once we have F_i with a self-consistent value of K, we evaluate $\tilde{\mathcal{E}}(\tilde{\rho})$ directly using the third equation.

- To find $\tilde{\mu}(\tilde{\rho})$ I simply took a numerical derivative as

$$\boxed{\frac{d\tilde{\mathcal{E}}(\tilde{\rho})}{d\tilde{\rho}} \doteq \frac{\tilde{\mathcal{E}}(\tilde{\rho}+\delta)-\tilde{\mathcal{E}}(\tilde{\rho}-\delta)}{2\delta}}$$

  - I used $\delta = 0.0005$ but have not studied the errors in order to optimize the calculation.
    - (Too small a δ will result in the answer dominated by round-off error.)

- In the code, I also calculate first and 2^{nd} order perturbation theory results for $\tilde{\varepsilon}(\tilde{\rho})$, and output all of the results to a file in a form suitable for plotting with gnuplot. Here is a plot: