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The S-Eqn in First and Second Quantization

- see F+W, sect. 1

- The time-dependent Schrodinger equation is

$$i\hbar \frac{\partial}{\partial t} \Psi(x_1, \ldots, x_N, t) = H \Psi(x_1, \ldots, x_N, t)$$

where $x_k \equiv \{\vec{x}_k, s_{z_k}, \ldots\}$ specifies fully the k^{th} particle.
With an appropriate set of boundary conditions and

$$H = \sum_{k=1}^{N} T(x_k) + \frac{1}{2} \sum_{k \neq l=1}^{N} V(x_k, x_l)$$

we have our problem to solve.

- We start by expanding Ψ in a complete set of time-independent, single-particle wavefunctions that incorporate the boundary conditions.
  - eg. large, uniform system, expand in plane waves in a large box with periodic boundary conditions
  - in harmonic trap, expand in harmonic oscillator wf's
  - in atoms, expand in complete set of Coulomb wf's

- Let $\psi_{E_k}(x_k)$ be the single particle wavefunction, where E_k is a complete set of single-particle quantum numbers
  - spinless bosons in a box: $E_k \to \vec{p}$
  - " " in central field: $E_k \to E, J, m$
  - fermions in a box: $E_k \to \vec{p}, s_z$

- Imagine that this infinite set E_k is ordered:
  $(1, 2, 3, \ldots, r, s, t, \ldots, \infty)$

- ASSUME THE $\psi_{E_k}(x_k)$ ARE ORTHONORMAL.

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Consider 1 particle first, with $U(x_1)$ instead of $V(x_1, x_2)$

$$\Psi(x_1,t) = \sum_{E_1'} C(E_1',t)\psi_{E_1'}(x_1)$$

- eg. expanding in harmonic oscillator w.f.'s, so E_1' runs over $n=0, l=0$, $n=1, l=0$, $n=2, l=0$, $n=0, l=1$, and so on.

- Let's find an equation for the C's from the S-eqn. Plug in:

$$i\hbar \sum_{E_1'} \left[\frac{\partial}{\partial t} C(E_1',t)\right]\psi_{E_1'}(x_1) = \sum_{E_1'} C(E_1',t)\, H\psi_{E_1'}(x_1)$$

- Use orthonormality of ψ_{E_k} to project out $C(E_1,t)$ out of all the E_1' terms. Do this by multiplying by $\psi^*_{E_1}(x_1)$ and integrating over x_1 (which may mean a sum over spin) ← (so that spinor is correct)

$$\int dx_1\, \psi^*_{E_1}(x_1)\psi_{E_1'}(x_1) = \delta_{E_1 E_1'} = \begin{cases} 0 \text{ if } E_1 \neq E_1' \\ 1 \text{ if } E_1 = E_1' \end{cases}$$

$$\Rightarrow i\hbar \frac{\partial}{\partial t} C(E_1,t) = \sum_{E_1'} \int dx_1\, \psi^*_{E_1}(x_1)\left[\underbrace{-\frac{\hbar^2}{2m}\nabla_1^2}_{T(x_1)} + U(x_1)\right]\psi_{E_1}(x_1) \cdot C(E_1',t)$$

Hamiltonian matrix element ⇒ number

- We get an equation for each E_1 ⇒ infinite set of coupled differential equations for the C's.

- If we want a stationary state, then time dependence of all C's is proportional to $e^{-iEt/\hbar}$, so we get a matrix eigenvalue problem
  - in practice, truncate basis to get finite matrix to diagonalize

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Now suppose we have two (identical) particles, with $V(x_k, x_l)$ again.

- Expand $\boxed{\Psi(x_1, x_2, t) = \sum_{E_1', E_2'} C(E_1', E_2', t)\, \psi_{E_1'}(x_1)\, \psi_{E_2'}(x_2)}$

$\Rightarrow$ complete basis for $\mathcal{H}$.

- Plug into S-eqn again, multiply by $\psi^*_{E_1}(x_1)\psi^*_{E_2}(x_2)$ and integrate over x_1 and x_2.

$$\boxed{\begin{aligned} i\hbar \frac{\partial}{\partial t} C(E_1, E_2, t) = \sum_{E_1', E_2'} \int dx_1 dx_2\, \psi^*_{E_1}(x_1)\psi^*_{E_2}(x_2) \Big[T(x_1) + T(x_2) \\ + \tfrac{1}{2}V(x_1, x_2) + \tfrac{1}{2}V(x_2, x_1) \Big] \\ \psi_{E_1'}(x_1)\psi_{E_2'}(x_2) \\ \times C(E_1', E_2', t) \end{aligned}}$$

$\Rightarrow$ Kinetic energy T involves only one E_k at a time, while V involves two E_k's (since two-body operator).

- If a coordinate x_k is not "mentioned" by T or V in a given term, then orthonormality just sets $E_k' = E_k$

$$\Rightarrow \boxed{\begin{aligned} i\hbar \frac{\partial}{\partial t} C(E_1, E_2, t) = \int dx_1\, \psi^*_{E_1}(x_1) T(x_1) \psi_{E_1'}(x_1)\, C(E_1', E_2, t) \\ + \int dx_2\, \psi^*_{E_2}(x_2) T(x_2) \psi_{E_2'}(x_2)\, C(E_1, E_2', t) \\ + \tfrac{1}{2}\Big[\int dx_1 dx_2\, \psi^*_{E_1}(x_1)\psi^*_{E_2}(x_2) V(x_1, x_2) \psi_{E_1'}(x_1)\psi_{E_2'}(x_2) \Big] \\ \times C(E_1', E_2', t) \\ + (1 \leftrightarrow 2) \end{aligned}}$$

- So, again, we have an infinite set of coupled differential equations. Stationary states $\Rightarrow$ just a bigger matrix problem.

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Now N-body: same thing:

$$\Psi(x_1,\dots,x_N,t) = \sum_{E_1',\dots,E_N'} C(E_1'\cdots E_N',t)\,\psi_{E_1'}(x_1)\cdots\psi_{E_N'}(x_N)$$

- Multiplying by $\psi^+_{E_1}(x_1)\cdots\psi^+_{E_N}(x_N)$ and integrating, orthonormality eliminates all but one integration in each term in the sum of kinetic energy terms and all but 2 integrations in the potential energy sum.

("single particle")

- We say that only one s.p. wavefunction is "changed" in the first case and only 2 in the second case:

$$i\hbar\frac{\partial}{\partial t}C(E_1,\dots,E_N,t) = \sum_{k=1}^{N}\sum_{W}\int dx_k\,\psi^+_{E_k}(x_k)\,T(x_k)\,\psi_W(x_k)\,C(E_1,\dots E_{k-1},W E_{k+1}\dots E_N,t)$$

$$+\frac{1}{2}\sum_{k\neq l=1}^{N}\sum_{W}\sum_{W'}\iint dx_k\,dx_l\,\psi^+_{E_k}(x_k)\psi^+_{E_l}(x_l)\,V(x_k,x_l)\,\psi_W(x_k)\psi_{W'}(x_l)\times C(E_1\cdots E_{k-1},W E_{k+1}\cdots E_{l-1},W' E_{l+1}\cdots E_N,t)$$

- So this "works", but you can see the practical difficulties if we have 100 or 10^{23} particles!
  - Big waste of effort, since only 1 or 2 change

- What about the fact that the particles are identical?
  - it means that lots of the C's must be the same:

$$\Psi(\cdots x_i\cdots x_j\cdots,t) = \pm\Psi(\cdots x_j\cdots x_i\cdots,t)$$

for bosons/fermions.

This implies

$$C(\cdots E_i\cdots E_j\cdots,t) = \pm C(\cdots E_j\cdots E_i\cdots t)$$

So with two particles, $C(E_1,E_2) = +C(E_2,E_1)$ for bosons

$C(E_1,E_2) = -C(E_1,E_2)$ for fermions ($=0$ if $E_1=E_2$)

Pauli!

So lots of redundancy.

↑ means basis states are Slater determinants

- so "real" basis for bosons is $\psi_1(x_1)\psi_2(x_2)$, $\psi_1(x_1)\psi_2(x_2)+\psi_2(x_1)\psi_1(x_2)$, ...
for fermions $\psi_1(x_1)\psi_2(x_2)-\psi_2(x_1)\psi_1(x_2)$, ...
$\Rightarrow$ slater determinants

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We can regroup the equations and sums by just counting how many times E_1 appears, E_2 appears, and so on.
- Since identical, doesn't matter if particle 1 or particle 2 or whatever
$\Rightarrow$ Keep track of "occupation number" n_k of E_k.

- In gory detail one can show how one can rewrite the results in terms of occupation number basis states. We refer the reader to F+W and just jump to the answer without proof.

Introduce time-independent abstract state vectors:

$$|n_1 n_2 \cdots n_\infty\rangle$$

where n_1 particles in single-particle eigenstate 1, n_2 in eigenstate 2 and so on.

- Make it complete and orthonormal

$$\langle n_1' n_2' \cdots n_\infty' | n_1 n_2 \cdots n_\infty\rangle = \delta_{n_1 n_1'} \cdots \delta_{n_\infty n_\infty'}$$

$$\sum_{n_1, n_2, \cdots n_\infty} |n_1 n_2 \cdots n_\infty\rangle\langle n_1 n_2 \cdots n_\infty| = 1$$

- for bosons n_k goes from 0 to ∞ in the complete space
- for fermions n_k is either 0 or 1

- In fact, $|n_1 n_2 \cdots n_\infty\rangle = |n_1\rangle|n_2\rangle \cdots |n_\infty\rangle$
since (as seen below) the eigenstates can be simultaneous eigenstates of each of the number operators for individual modes.
  - For each mode n_i, think about harmonic oscillator.

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To work with this basis, we recall the raising and lowering operators of the harmonic oscillator, and for bosons introduce $b_k, b_k^\dagger$ that satisfy

$$\boxed{[b_k, b_{k'}^\dagger] = \delta_{kk'} \quad \text{bosons}}$$

$$\boxed{[b_k, b_{k'}] = [b_k^\dagger, b_{k'}^\dagger] = 0}$$

As in HO case, the properties of these operators follow from the commutation relations:

$$\boxed{b_k^\dagger b_k |n_k\rangle = n_k |n_k\rangle} \quad n_k = 0, 1, 2, \ldots \infty \quad \text{"number operator"}$$

$$\boxed{b_k |n_k\rangle = (n_k)^{1/2} |n_k - 1\rangle} \quad \text{"destruction operator"}$$

$$\boxed{b_k^\dagger |n_k\rangle = (n_k + 1)^{1/2} |n_k + 1\rangle} \quad \text{"creation operator"}$$

↙ hermitian ⇒ real eigenvalues

Proofs:

Since $n = \langle n | b^\dagger b | n \rangle = \sum_m \langle n | b^\dagger | m \rangle \langle m | b | n \rangle = \sum_m |\langle m | b | n \rangle|^2 \geq 0$, we can't have a negative eigenvalue of the number operator.

So use b to "count down" from $|n\rangle$: ↙ from commutation relations

$$b^\dagger b (b|n\rangle) = b(b^\dagger b)|n\rangle + [b^\dagger b, b]|n\rangle = (n-1)(b|n\rangle)$$

which must terminate in zero eventually if repeated to avoid going negative. The same argument applying $b^\dagger$ establishes the first and we get the normalization (up to a phase chosen to be 1) by combining the last two equations.

The extension to many modes is immediate since $[b_k^\dagger b_k, b_{k'}^\dagger b_{k'}] = 0$ for $k \neq k'$ ⇒ eigenstates of total system can be simultaneous number operator eigenstates.

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Now here's the big claim: We can exactly rewrite the many-body S-equation as

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

with

$$\boxed{\hat{H} = \sum_{ij} b_i^\dagger \langle i|T|j\rangle b_j + \frac{1}{2}\sum_{ijkl} b_i^\dagger b_j^\dagger \langle ij|V|kl\rangle b_l b_k}$$

- The b_i's and $b_i^\dagger$'s take care of the symmetrization for us
- Kinetic term $\Rightarrow$ destroy in state j, create in state i ($\Rightarrow$ "change" j to i as before)
- potential term $\Rightarrow$ 2 states changed by 1.

- Could expand $|\Psi(t)\rangle$ in coefficients $F(n_1, n_2, \ldots, n_\infty, t)|n_1 \ldots n_\infty\rangle$ and show we get the same answer as before. We'll defer that!
  $\Rightarrow$ See Fetter and Walecka, section 7.

- Note that the matrix elements $\langle i|T|j\rangle$ and $\langle ij|V|kl\rangle$ are exactly the same sort we had in the equations for the C's.
  - The b_i's just do the accounting for us now!

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· For fermions we need to use anticommutation relations

$$\{a_r, a_s^\dagger\} = \delta_{rs} \quad \text{fermions}$$

$$\{a_r, a_s\} = [a_r^\dagger, a_s^\dagger] = 0 \qquad \{A,B\} \equiv [A,B]_+ \equiv AB + BA$$

1. $a_s^2 = a_s^{\dagger 2} = 0$ so $a_s^\dagger a_s^\dagger |0\rangle = 0 \Rightarrow$ no two particles in same state

2. $\hat{n}_s = a_s^\dagger a_s$ is the number operator

3. $a^\dagger|0\rangle = |1\rangle \qquad a|1\rangle = |0\rangle$ (overall choice of phase has been made)

$a^\dagger|1\rangle = 0 \qquad a|0\rangle = 0$

4. $|n_1 \cdots n_\infty\rangle = (a_1^\dagger)^{n_1} \cdots (a_\infty^\dagger)^{n_\infty} |0\rangle$ ← just counts how many $a_i^\dagger$'s $a_s^\dagger$ must be commuted with to get to its proper place.

implies signs. Define $S_s = n_1 + n_2 + \cdots + n_{s-1}$

$$a_s|\cdots n_s \cdots\rangle = \begin{cases} 0 & \text{if } n_s = 0 \\ (-1)^{S_s}|\cdots n_s - 1 \cdots\rangle & \text{if } n_s = 1 \end{cases}$$

$$a_s^\dagger|\cdots n_s \cdots\rangle = \begin{cases} (-1)^{S_s}(n_s+1)^{1/2}|\cdots n_s + 1 \cdots\rangle & \text{if } n_s = 0 \\ 0 & \text{if } n_s = 1 \end{cases}$$

$$* \quad a_s^\dagger a_s |\cdots n_s \cdots\rangle = n_s |\cdots n_s \cdots\rangle \qquad n_s = 0, 1$$

5. $i\hbar \frac{\partial}{\partial t}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$

$$\hat{H} = \sum_{rs} a_r^\dagger \langle r|T|s\rangle a_s + \frac{1}{2}\sum_{rstu} a_r^\dagger a_s^\dagger \langle rs|V|tu\rangle a_u a_t$$

note ordering

Alternative example: degenerate electron gas (see F+W) sec. 3

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Example: Dilute Fermi Gas with Short-Range Interaction

- As an prototype system we can consider a set of atoms confined magnetically or optically (the difference is important; see below) where we can consider the trap potential constant (therefore constant energy contribution). Very big trap, so treat as effectively infinite.

$$\Rightarrow \boxed{V(\vec{x}-\vec{x}') = \lambda \delta^3(\vec{x}-\vec{x}')} \qquad \left(\text{recall } \int d^3x' f(\vec{x}')\delta^3(\vec{x}-\vec{x}') = f(\vec{x})\right)$$

so integrals are easy

  - spin-independent (same matrix element between any combination of spin up and spin down)
  - if $\lambda > 0 \Rightarrow$ repulsive, $\lambda < 0 \Rightarrow$ attractive
  - $g \equiv 2S+1$ spin states in general

- Goal: Find ground state energy per particle as a function of density. Also find the pressure and consider stability.
  - Plan: Do perturbation theory about non-interacting system

- To treat a bulk medium, put the system in a large box of side L and take $L \to \infty$ at the end. ← all physical properties
  - Uniform, infinite $\Rightarrow$ translationally invariant so apply periodic boundary conditions on the single-particle wave functions

$\Rightarrow$ plane waves (momentum eigenstates)

$$\boxed{\psi_{\vec{k}\alpha}(\vec{x}) = \frac{1}{\sqrt{\Omega}} e^{i\vec{k}\cdot\vec{x}} \eta_\alpha}$$

where $\Omega \equiv L^3$ is the volume of the box and η_α is the spin function. For spin-1/2 along a given z-axis,

$$\boxed{\eta_\uparrow = \begin{bmatrix} 1 \\ 0 \end{bmatrix}} \text{ and } \boxed{\eta_\downarrow = \begin{bmatrix} 0 \\ 1 \end{bmatrix}} \Rightarrow \boxed{\eta_\alpha^\dagger \eta_\beta = \delta_{\alpha\beta}}$$

$\alpha = 0$ or 1 and $\beta = 0$ or 1

- Periodic boundary conditions imply

$$\boxed{k_i = \frac{2\pi n_i}{L} \quad i = x, y, z \quad n_i = 0, \pm 1, \pm 2}$$

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• Note that $\int \psi^\dagger_{k\alpha}(\vec{x})\,\psi_{k\alpha}(\vec{x})\,d^3x = \frac{1}{\Omega}\int e^{-i(\vec{k}-\vec{k})\cdot\vec{x}}\,\underbrace{\eta^\dagger_\alpha \eta_\alpha}_{=1}\,d^3x$

$= \frac{1}{\Omega}\int d^3x = 1 \Rightarrow$ normalized

• Hamiltonian is (with $\hat{p}_i \to -i\hbar\vec{\nabla}$)

$$H = \sum_{i=1}^{N} \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\lambda \sum_{i\neq j}^{N} \delta^3(\vec{x}_i - \vec{x}_j)$$

[Warning: As we'll note later this is ill-defined without a regularization/renormalization scheme]

Write this in 2nd quantization

$$\langle \vec{k}_1\alpha_1 | \frac{\hat{p}^2}{2m} | \vec{k}_2\alpha_2\rangle = \frac{1}{2m\Omega}\int d^3x\, e^{-i\vec{k}_1\cdot\vec{x}}\,\eta^\dagger_{\alpha_1}(-\hbar^2\nabla^2)\,e^{i\vec{k}_2\cdot\vec{x}}\,\eta_{\alpha_2}$$

$$= \frac{\hbar^2 k_2^2}{2m\Omega}\delta_{\alpha_1\alpha_2}\int d^3x\, e^{i(\vec{k}_2-\vec{k}_1)\cdot\vec{x}} \sim \Omega\delta_{\vec{k}_1,\vec{k}_2}$$

(to see this, integrate in Cartesian coordinates from $-\frac{L}{2} \le x \le \frac{L}{2}$ or $0 \le x_i \le L$)

$$= \frac{\hbar^2 k_2^2}{2m}\delta_{\alpha_1\alpha_2}\delta_{\vec{k}_1\vec{k}_2}$$

kinetic energy $\Rightarrow$ $\hat{T} = \sum_{k\alpha}\frac{\hbar^2 k^2}{2m} a^\dagger_{k\alpha} a_{k\alpha}$ ← same for any V

• add up the kinetic energy of each occupied mode, as checked by the number operator $a^\dagger_{k\alpha}a_{k\alpha}$.
• Simple since diagonal in this basis

• The potential energy is (from wf's)

$$\langle \vec{k}_1\alpha_1\,\vec{k}_2\alpha_2 | V | \vec{k}_3\alpha_3\,\vec{k}_4\alpha_4\rangle = \frac{1}{\Omega^2}\iint d^3x_1 d^3x_2\, e^{-i\vec{k}_1\cdot\vec{x}_1}\eta^\dagger_{\alpha_1}(1)\,e^{-i\vec{k}_2\cdot\vec{x}_2}\eta^\dagger_{\alpha_2}(2)$$

$$\times\lambda\delta^3(\vec{x}_1-\vec{x}_2)\,e^{i\vec{k}_3\cdot\vec{x}_1}\eta_{\alpha_3}(1)\,e^{i\vec{k}_4\cdot\vec{x}_2}\eta_{\alpha_4}(2)$$

1 2

$$= \frac{\lambda}{\Omega^2}\int d^3x_1\, e^{-i(\vec{k}_1+\vec{k}_2-\vec{k}_3-\vec{k}_4)\cdot\vec{x}_1}\,\delta_{\alpha_1\alpha_3}\delta_{\alpha_2\alpha_4}$$

$$= \frac{\lambda}{\Omega}\delta_{\alpha_1\alpha_3}\delta_{\alpha_2\alpha_4}\,\delta_{\vec{k}_1+\vec{k}_2,\,\vec{k}_3+\vec{k}_4}$$

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So now the 2nd quantized Hamiltonian $\hat{H}$ is

$$\hat{H} = \sum_{\vec{k}\alpha} \frac{\hbar^2 k^2}{2m} a^+_{\vec{k}\alpha} a_{\vec{k}\alpha} + \frac{\lambda}{2\Omega} \sum_{\vec{k}_1\vec{k}_2\vec{k}_3\vec{k}_4} \sum\sum\sum a^+_{\vec{k}_1\alpha_1} a^+_{\vec{k}_2\alpha_2} a_{\vec{k}_4\alpha_4} a_{\vec{k}_3\alpha_3} \times \delta_{\alpha_1\alpha_3}\delta_{\alpha_2\alpha_4}\delta_{\vec{k}_1+\vec{k}_2,\vec{k}_3+\vec{k}_4}$$

- The Kronecker delta's let us do two spin summations and one of the momentum summations (momentum conservation)

- We have many possibilities for choosing three independent momenta — until you get some experience you have no way of knowing what choice is best, but you will find in most cases that a particular choice can simplify your life.
  (this $\vec{k},\vec{p}$ in, exchange $\vec{k}_2$, so $\vec{k}+\vec{q}$, $\vec{p}-\vec{q}$ out.)
- Here we'll just follow Fetter+Walecka's (F+W's) lead and change to

$$\vec{k}_1 = \vec{k}+\vec{q} \qquad \vec{k}_3 = \vec{k}$$
$$\vec{k}_2 = \vec{p}-\vec{q} \qquad \vec{k}_4 = \vec{p}$$

so $\vec{q}$ is a momentum transfer.

$$\Rightarrow \hat{H} = \sum_{\vec{k}\alpha} \frac{\hbar^2 k^2}{2m} a^+_{\vec{k}\alpha} a_{\vec{k}\alpha} + \frac{\lambda}{2\Omega} \sum_{\vec{k}\vec{p}\vec{q}} \sum_{\alpha_1\alpha_2} a^+_{\vec{k}+\vec{q}\alpha_1} a^+_{\vec{p}-\vec{q}\alpha_2} a_{\vec{p}\alpha_2} a_{\vec{k}\alpha_1}$$

- In principle the a's and a^+'s should have $\hat{}$'s, since they are operators, but that gets too messy!

- It will be assumed that we have N particles in the volume Ω, so the density is $\rho \equiv N/\Omega$. (F+W: $n \equiv N/V$) We keep ρ fixed in the implied limit $N\to\infty$, $\Omega\to\infty$.

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- We can see what to expect about the relative contributions of the two terms in $\hat{H}$ by introducing dimensionless variables. This is a good way to analyze the expected size of different parts of the energy.

- One length scale comes from the volume per particle, which we use to define the radius r_0 of a sphere equal to that volume:

$$\boxed{\frac{\text{volume}}{\text{particle}} = \frac{\Omega}{N} \equiv \frac{4}{3}\pi r_0^3} \Rightarrow r_0 \text{ is more-or-less the interparticle spacing.}$$

- Another length scale for comparison comes from the interaction strength λ. We'll find out later that

$$\boxed{\lambda = \frac{4\pi\hbar^2 a_s}{m}} \qquad k\cot\delta_0 = -\frac{1}{a_s} + O(k^2)$$

for small k, where δ_0 is the s-wave phase shift.

where a_s is the S-wave "scattering length." (We'll come back to it.)

- So the dimensionless ratio $\tilde{r}_s \equiv \frac{r_0}{a_s}$ (scaled particle separation) characterizes the density of the system:
  - $\tilde{r}_s \to 0 \Rightarrow$ high density ($r_0 \to 0$)
  - $\tilde{r}_s \to \infty \Rightarrow$ low density

- If we rescale the volume and momenta by r_0:

$$\boxed{\Pi = \Omega/r_0^3 \qquad \vec{K} = r_0\vec{k} \qquad \vec{p} = r_0\vec{p} \qquad \vec{q} = r_0\vec{q}}$$

Then we can rewrite $\hat{H}$ as

$$\boxed{\hat{H} = \frac{\hbar^2}{m r_0^2}\left(\sum_{\vec{K}\lambda} \frac{1}{2} K^2 a^\dagger_{\vec{K}\lambda} a_{\vec{K}\lambda} + \frac{a_s}{r_0}\frac{4\pi}{2\Pi} \sum_{\vec{k}\vec{p}\vec{q}} \sum_{\alpha_1\alpha_2} a^\dagger_{\vec{k}+\vec{q},\alpha_1} a^\dagger_{\vec{p}-\vec{q},\alpha_2} a_{\vec{p}\alpha_2} a_{\vec{k}\alpha_1} \right)}$$

$$\frac{1}{\tilde{r}_s} \qquad '' \qquad \frac{1}{\tilde{r}_s}$$

1/8/03 $(\tilde{r}_s \to \infty)$

- So at low density, the potential energy becomes a perturbation to the kinetic energy

$\Rightarrow$ if $a_s \ll r_0$, apply perturbation theory to find the energy

- You might expect that the ground state energy has a power-series expansion in a_s, but we'll find, in fact, that it doesn't (stay tuned!)

- So let us assume from now on that we are in the dilute (low-density) limit

- Separate $\boxed{\hat{H} = \hat{H}_0 + \hat{H}_1}$ where

$\boxed{\hat{H}_0 = \frac{\hbar^2 k^2}{2m} a^\dagger_{\vec{k}\alpha} a_{\vec{k}\alpha}}$ is the unperturbed Hamiltonian, which represents a non interacting Fermi system

$$\boxed{\hat{H}_1 = \frac{\lambda}{2\Omega} \sum_{\vec{k}\vec{p}\vec{q}} \sum_{\alpha_1\alpha_2} a^\dagger_{\vec{k}+\vec{q}\,\alpha_1} a^\dagger_{\vec{p}-\vec{q}\,\alpha_2} a_{\vec{p}\alpha_2} a_{\vec{k}\alpha_1}}$$

is the small perturbation.

- Expand the ground-state energy E as $E^{(0)} + E^{(1)} + \ldots$ where $E^{(0)}$ is the ground-state energy of a free Fermi gas while $E^{(1)}$ is the first-order energy shift

- In carrying out the evaluation of $E^{(0)}$ and $E^{(1)}$ we'll evaluate sums by converting to integrals (in the $L \to \infty$ limit)

$$\int F(k)\,dk \doteq \sum_i F(k_i)\,\Delta k_i = \sum_i F(k_i) \frac{2\pi}{L} \Delta n_i^{\prime\prime 1} = \frac{2\pi}{L} \sum_i F(k_i)$$

$$\Rightarrow \boxed{\sum_{\vec{k}\alpha} f_\alpha(\vec{k}) = \Omega \sum_\alpha \int \frac{d^3k}{(2\pi)^3} f_\alpha(\vec{k})}$$ [dk always comes with 2π's]

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- We denote the ground state of the non-interacting Fermi gas by $|F\rangle$.
  - If spin 1/2, then Pauli exclusion principle allows 2 fermions per momentum state ($\uparrow$ and $\downarrow$)
  - If spin S, then $g = 2S+1$ per momentum state
  - Lowest energy by minimizing kinetic energy $\Rightarrow$ fill lowest momentum states
  - Call the highest filled momentum the Fermi momentum $p_F = \hbar k_F$

- Find k_F in terms of N, Ω, and $\rho = N/\Omega$ by taking the expectation value of the number operator

$\theta(x) = \begin{cases} 1 \text{ if } x > 0 \\ 0 \text{ if } x < 0 \end{cases}$

$$N = \langle F|\hat{N}|F\rangle = \sum_{k\alpha} \langle F|\hat{n}_{k\alpha}|F\rangle = \sum_{k\alpha} \theta(k_F - k)$$

$$= \frac{\Omega}{(2\pi)^3} \sum_{\alpha} \int d^3k\, \theta(k_F - k) = \frac{\Omega}{(2\pi)^3}\, g \times (\text{volume of sphere of radius } k_F)$$

$$= \frac{\Omega}{(2\pi)^3}\, g\, \tfrac{4}{3}\pi k_F^3 = \Omega\left(\frac{g k_F^3}{6\pi^2}\right)$$

$$\Rightarrow \boxed{\rho = \frac{g k_F^3}{6\pi^2}} \quad \text{and} \quad \boxed{k_F = \left(\frac{6\pi^2 \rho}{g}\right)^{1/3} = \left(\frac{18\pi}{4g}\right)^{1/3} \frac{1}{r_0} \xrightarrow{g=2} \frac{1.92}{r_0}}$$

so k_F^{-1} is comparable to the interparticle spacing.

- Also, our small parameter $\frac{a_s}{r_0}$ can be replaced by an alternative small parameter: $k_F a_s$.
  - This is the usual expansion parameter for a dilute Fermi system.

1/8/03

So now evaluate $E^{(0)}$ → expectation value of $\hat{H}_0$ in $|F\rangle$

$$E^{(0)} = \langle F|\hat{H}_0|F\rangle = \frac{\hbar^2}{2m}\sum_{k\alpha} k^2 \langle F|\hat{n}_{k\alpha}|F\rangle$$

$$\hat{n}_{k\alpha}|F\rangle = \begin{cases} 0 & \text{if } |\vec{k}|>k_f \\ |F\rangle & \text{if } |\vec{k}|<k_f \end{cases}$$

$$= \frac{\hbar^2}{2m}\sum_{k\alpha} k^2\,\theta(k_f - |\vec{k}|) \quad \leftarrow$$

$$= \frac{\hbar^2}{2m}\sum_{\alpha}\frac{\Omega}{(2\pi)^3}\int d^3k\, k^2\,\theta(k_f-k)$$

$$\int d^3k\, k^2\,\theta(k_f-k) = 4\pi\int_0^{k_f} k^4\,dk$$

$$= \frac{\hbar^2}{2m}\frac{g\Omega}{2\pi^2}\frac{k_f^5}{5} = \frac{\hbar^2 k_f^2}{2m}\frac{3}{5}\frac{gk_f^3}{6\pi^2}\Omega$$

$$\rho = \frac{N}{\Omega}$$

$$= \frac{3}{5}\frac{\hbar^2 k_f^2}{2m}N$$

$$\Rightarrow \boxed{E^{(0)}/N = \frac{3}{5}\frac{\hbar^2 k_f^2}{2m} = \frac{3}{5}\epsilon_f^0}$$

Fermi energy $\epsilon_f^0 = \frac{\hbar^2 k_f^2}{2m}$ ← energy of last atom at top of Fermi sea

- So in a free Fermi gas, the kinetic energy per particle is $\frac{3}{5}$ the kinetic energy of the last particle.

- The first-order energy shift is

$$\boxed{E^{(1)} = \langle F|\hat{H}_1|F\rangle = \frac{\lambda}{2\Omega}\sum_{\vec{k},\vec{p},\vec{q}}\sum_{\alpha_1\alpha_2}\langle F|a^\dagger_{\vec{k}+\vec{q}\alpha_1}\, a^\dagger_{\vec{p}-\vec{q}\alpha_2}\, a_{\vec{p}\alpha_2}\, a_{\vec{k}\alpha_1}|F\rangle}$$

- Ok, we'll analyze it by hand
  - $a_{\vec{k}\alpha_1}$ and $a_{\vec{p}\alpha_2}$ annihilate particles in $|F\rangle$. If there is no particle to destroy, the result is zero. ⇒ $|\vec{k}|, |\vec{p}| < k_f$ or zero
  - acting to the left, we similarly conclude $|\vec{k}+\vec{q}|, |\vec{p}-\vec{q}| < k_f$
  - The states must match up, or we'll get zero by orthogonality.

$$\Rightarrow \boxed{\vec{k}+\vec{q},\alpha_1 = \vec{k}\alpha_1 \text{ and } \vec{p}-\vec{q},\alpha_2 = \vec{p}\alpha_2}$$

or

$$\boxed{\vec{k}+\vec{q},\alpha_1 = \vec{p}\alpha_2 \text{ and } \vec{p}-\vec{q},\alpha_2 = \vec{k}\alpha_1}$$

} two terms call them "direct" and "exchange"

1/8/03

direct: the first pairing forces $\vec{q}=0$ but doesn't constrain $\vec{k}$ or $\vec{p}$ (except we know they are less than k_F in magnitude) or either spin sum. (So the energy will be proportional to g^2.)

exchange: The second pairing determines $\vec{p}$ in terms of $\vec{k}$ and $\vec{q}$ (you can pick any one of the three momenta), eliminating the $\vec{p}$ sum. Also, we must have $\alpha_1=\alpha_2$, eliminating one spin sum (so this part of the energy will be proportional to g.)

- Work out each one in turn, using $\boxed{\hat{n}_{\vec{k}\alpha}|F\rangle = \theta(k_F-|\vec{k}|)|F\rangle}$ repeatedly,

direct: $\boxed{\langle F|a^\dagger a^\dagger a a|F\rangle \longrightarrow \delta_{\vec{q},0}\langle F|a^\dagger_{\vec{k}\alpha_1}a^\dagger_{\vec{p}\alpha_2}a_{\vec{p}\alpha_2}a_{\vec{k}\alpha_1}|F\rangle}$

- Note that $\{\vec{p}\alpha_2\}\neq\{\vec{k}\alpha_1\}$, since otherwise the product of the a's (or $a^\dagger$'s) would be zero.

$\Rightarrow$ we can move $a_{\vec{k}\alpha_1}$ two place to the left without picking up extra terms from the anticommutators:

$$a^\dagger_{\vec{p}\alpha_2}a_{\vec{p}\alpha_2}a_{\vec{k}\alpha_1} = -a^\dagger_{\vec{p}\alpha_2}a_{\vec{k}\alpha_1}a_{\vec{p}\alpha_2} = +a_{\vec{k}\alpha_1}a^\dagger_{\vec{p}\alpha_2}a_{\vec{p}\alpha_2}$$

$$\Rightarrow \boxed{\langle F|a^\dagger a^\dagger a a|F\rangle \longrightarrow \delta_{\vec{q},0}\langle F|\hat{n}_{\vec{k}\alpha_1}\hat{n}_{\vec{p}\alpha_2}|F\rangle = \theta(k_F-|\vec{k}|)\,\theta(k_F-|\vec{p}|)\,\delta_{\vec{q},0}}$$

$$\Rightarrow E^{(1)}_{direct} = \frac{\lambda}{2\Omega}\sum_{\alpha_1\alpha_2}\sum_{\vec{k}\vec{p}\vec{q}}\delta_{\vec{q},0}\,\theta(k_F-|\vec{k}|)\,\theta(k_F-|\vec{p}|)$$

$$= \frac{\lambda}{2\Omega}|g^2|\left(\frac{\Omega}{(2\pi)^3}\int d^3p\,\theta(k_F-|\vec{p}|)\right)\left(\frac{\Omega}{(2\pi)^3}\int d^3k\,\theta(k_F-|\vec{k}|)\right)$$

$$= \frac{\lambda}{2\Omega}N^2 \quad \text{using the previous result for } N.$$

The energy per particle (which is well defined in the thermodynamic limit)

B $\boxed{E^{(1)}_{direct}/N = \frac{\lambda N}{2\Omega} = \frac{\lambda}{2}\rho}$ and the energy density $\mathcal{E}$ (energy/volume)

13 $\boxed{\mathcal{E}^{(1)}_{direct} = \frac{\lambda}{2\Omega^2}N^2 = \frac{\lambda}{2}\rho^2}$

18/03

The other term is similar but messier:

exchange: $\langle F|a^\dagger a^\dagger a a|F\rangle \to \delta_{\vec{k}+\vec{q},\vec{p}}\,\delta_{\alpha_1,\alpha_2}\langle F|a^\dagger_{\vec{k}+\vec{q}\alpha_1}\, a^\dagger_{\vec{k}\alpha_1}\, a_{\vec{k}+\vec{q}\alpha_1}\, a_{\vec{p}\alpha_1}|F\rangle$

only one interchange $\Rightarrow$ $= -\delta_{\vec{k}+\vec{q},\vec{p}}\,\delta_{\alpha_1,\alpha_2}\langle F|\hat{n}_{\vec{k}+\vec{q}\lambda_1}\,\hat{n}_{\vec{k}\lambda_1}|F\rangle$

$= -\delta_{\vec{k}+\vec{q},\vec{p}}\,\delta_{\alpha_1,\alpha_2}\,\theta(k_f-|\vec{k}+\vec{q}|)\,\theta(k_f-k)$

$$\Rightarrow E^{(1)}_{\text{exchange}} = \frac{\lambda}{2\Omega}\sum_{\vec{q}\alpha_1\alpha_2}\sum_{\vec{k}\vec{p}}(-\delta_{\vec{k}+\vec{q},\vec{p}})\,\delta_{\alpha_1,\alpha_2}\,\theta(k_f-|\vec{k}+\vec{q}|)\,\theta(k_f-k)$$

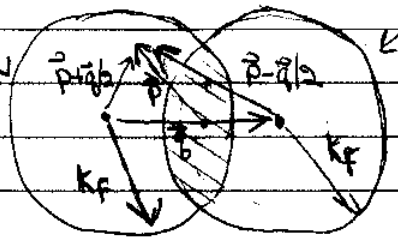
$$= -\frac{\lambda}{2\Omega}\,g\,\frac{\Omega^2}{(2\pi)^6}\int d^3k\, d^3q\;\theta(k_f-|\vec{k}+\vec{q}|)\,\theta(k_f-k)$$

It is convenient (and useful!) to make the integration more symmetric by defining $\vec{P}=\vec{k}+\frac{1}{2}\vec{q}$ and integrating over $\vec{P}$ and $\vec{q}$.

$$\Rightarrow \boxed{E^{(1)}_{\text{exchange}} = -\frac{g\lambda}{2}\frac{\Omega^2}{(2\pi)^6}\int d^3q\int d^3P\;\theta(k_f-|\vec{P}+\tfrac{1}{2}\vec{q}|)\,\theta(k_f-|\vec{P}-\tfrac{1}{2}\vec{q}|)}$$

over $\vec{P}$

We can represent the integration region diagrammatically as (2-d slice)



- The diagram is for fixed $\vec{q}$, which is the separation of the two spheres.
- $\vec{P}$ is measured from the center and is integrated over.
- The two sphere surfaces are the boundaries of the θ-functions.
- The shaded region is the "volume" (in P space) we want. $\Rightarrow q<2k_f$

we want $\frac{1}{2}\times$ this volume

$\cos\theta_{\max} = \frac{q}{2k_f} \equiv x$

$$\Rightarrow \int d^3P\;\theta(k_f-|\vec{P}+\tfrac{1}{2}\vec{q}|)\,\theta(k_f-|\vec{P}-\tfrac{1}{2}\vec{q}|) = 2\,\theta(2k_f-q)\,2\pi\int_x^1 dx\int_{k_f x/\chi}^{k_f} r^2\,dr$$

$$= \frac{4\pi}{3}k_f^3\,\theta(1-x)\int_x^1 dx\left(1-\frac{x^3}{\chi^3}\right) = \frac{4\pi}{3}k_f^3\,\theta(1-x)\left[1-\frac{3}{2}x+\frac{1}{2}x^3\right]$$

$$\Rightarrow \boxed{E^{(1)}_{\text{exchange}} = -\frac{g\lambda}{2}\frac{\Omega}{(2\pi)^6}\,\frac{4\pi k_f^3}{3}(2k_f)^3\int_0^1 dx\,x^2\underbrace{(1-\tfrac{3}{2}x+\tfrac{1}{2}x^3)}_{\frac{1}{2}(2-x)^2(1+x)}\cdot 4\pi = -\frac{1}{2}\frac{1}{g}\left(\frac{gk_f^3}{6\pi^2}\right)\left(\frac{gk_f^3}{6\pi^2}\right)\Omega = -\frac{1}{g}\frac{1}{2}g^2\Omega}$$

1/8/03

Putting the direct and exchange together:

$$\frac{E^{(1)}}{N} = \frac{\lambda}{2}\rho\left(1-\frac{1}{g}\right) = \frac{4\pi\hbar^2 a_s}{2m}\frac{g k_F^3}{6\pi^2}\left(1-\frac{1}{g}\right) = \frac{\hbar^2 k_F^2}{2m}\left((g-1)\frac{2k_F a}{3\pi}\right)$$

The last form provides a direct comparison with $E^{(0)}$:

$$\frac{E}{N} = \frac{E^{(0)}}{N} + \frac{E^{(1)}}{N} + \ldots = \frac{\hbar^2 k_F^2}{2m}\left[\frac{g}{5} + (g-1)\frac{2k_F a_s}{3\pi} + \ldots\right]$$

- Why does the correction vanish for $g=1$? What if we kept only one spin state?

- So for $k_F a_s \ll 1$, we have a meaningful expansion
  $\Rightarrow$ dilute Fermi gas.
- It's actually trickier than this if $a_s<0$ (attractive), since there is a lower energy ground state than this. (more later!)
- This is well defined for a repulsive $a_s>0$ (and small).

How do we find the higher-order terms?

- How do we find the pressure? $\Rightarrow P = -\left(\frac{\partial E}{\partial V}\right)_N = \rho^2 \frac{\partial (E/N)}{\partial \rho}$
  How do you expect the correction term $E^{(1)}$ to go

- Quick preview of Feynman diagrams

direct: $\vec{k}$ $\vec{q}=0$ $\vec{p}$ — "Hartree"

exchange: $\vec{k}$ $\vec{q}$ $\vec{p}=\vec{k}+\vec{q}$ — "Fock"

- $\cdots \Rightarrow$ λ
- conserve momentum at $\bullet$'s
- spin sums by following solid (fermion) lines $\Rightarrow g^2$ vs. g

These come from closely a scattering diagram in two ways.

$\vec{p}$ $\vec{q}$ $\vec{k}+\vec{q}$ $\vec{k}$

1/8/03

Often we want to switch to the $\vec{x}$ basis. We can do this by forming the "field operators" $\hat{\psi}(\vec{x})$ and $\hat{\psi}^\dagger(\vec{x})$:

$$\hat{\psi}(\vec{x}) \equiv \sum_k \psi_k(\vec{x})\, c_k \qquad c_k = a_k \text{ or } b_k$$

$$\hat{\psi}^\dagger(\vec{x}) \equiv \sum_k \psi_k^\dagger(\vec{x})\, c_k^\dagger$$

where $k = \{\vec{k}, s_z\}$ or $\{E, L, J, m\}$ or ... for spin 1/2 fermions

- In that case, $\psi_k(\vec{x}) = \begin{bmatrix} \psi_k(\vec{x})_1 \\ \psi_k(\vec{x})_2 \end{bmatrix} \equiv \psi_k(\vec{x})_\alpha$

- Using $c_k, c_k^\dagger$ relations,

$$\left[\hat{\psi}_\alpha(\vec{x}), \hat{\psi}_\beta^\dagger(\vec{x}')\right]_\pm = \sum_k \psi_k(\vec{x})_\alpha \psi_k(\vec{x}')^*_\beta = \delta_{\alpha\beta}\,\delta(\vec{x}-\vec{x}')$$

$$\left[\hat{\psi}_\alpha(\vec{x}), \hat{\psi}_\beta(\vec{x}')\right]_\pm = \left[\hat{\psi}^\dagger_\alpha(\vec{x}), \hat{\psi}^\dagger_\beta(\vec{x}')\right]_\pm = 0$$

- Operators

$$\hat{H} = \int d^3x\, \hat{\psi}^\dagger(\vec{x})\, T(\vec{x})\, \hat{\psi}(\vec{x}) + \frac{1}{2}\iint d^3x\, d^3x'\, \hat{\psi}^\dagger(\vec{x})\hat{\psi}^\dagger(\vec{x}')\, V(\vec{x},\vec{x}')\, \hat{\psi}(\vec{x}')\hat{\psi}(\vec{x})$$

$\Rightarrow$ "second quantization": looks like expectation values wrt operators!

- The integration over $\vec{x}, \vec{x}'$ generate the matrix elements

If $J = \sum_{i=1}^{N} J(\vec{x}_i)$ is a first-quantized operator $\Rightarrow$

$$\hat{J} = \sum_{rs} \langle r|J|s\rangle\, c_r^\dagger c_s = \int d^3x \sum_{rs} \psi_r(\vec{x})^\dagger J(\vec{x})\, \psi_s(\vec{x})\, c_r^\dagger c_s = \int d^3x\, \hat{\psi}^\dagger(\vec{x})\, J(\vec{x})\, \hat{\psi}(\vec{x})$$

- number density $\rho(\vec{x}) = \sum_{i=1}^{N} \delta(\vec{x}-\vec{x}_i) \Rightarrow$

$$\hat{n}(\vec{x}) = \sum_{rs} \psi_r(\vec{x})^\dagger \psi_s(\vec{x})\, c_r^\dagger c_s = \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})$$

and total number $\hat{N} = \int d^3x\, \hat{n}(\vec{x}) = \sum_r c_r^\dagger c_r = \sum_r \hat{n}_r = \int d^3x\, \hat{\psi}^\dagger(\vec{x})\hat{\psi}(\vec{x})$