

February 19, 1980

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Situation: You have a perturbation  $H = H_0 + H'$  of a self-adjoint operator on  $\mathcal{H}$ . One has a second quantization of  $H_0$  which is a Fock space  $\mathcal{F}$  ~~which~~ which is roughly the exterior algebra of  $\mathcal{H}$ , equipped with the extension of  $H_0$  as a derivation, and equipped with a ground state  $|E\rangle$  which is element corresponding to the negative eigenspace of  $H_0$ . Thus  $|E\rangle$  is the state with all negative energy levels filled. If the perturbation is sufficiently ~~weak~~ weak, then the negative eigenspace for  $H$  should project nicely on that for  $H_0$ , so Fock space should contain a ground state  $|E\rangle$  for  $H$  such that  $\langle E|E\rangle \neq 0$ . I want to understand two numbers:

$$\Delta E = \langle E|H'|E\rangle \quad \text{assuming } \|E\|=1 \text{ and } H_0|E\rangle=0$$

$$|\langle E|E\rangle|^2$$

The formulas for these are messy in the case of discrete spectrum and maybe become simpler for continuous spectrum.

Example: Take  $H_0 = \frac{p^2}{2}$  on  $\mathcal{H} = L^2(\mathbb{R})$  and take  $H = \frac{p^2}{2} + V(x)$ . Now fix a  $\mu = \varepsilon_F$  = Fermi-energy. Then we get a splitting

$$\mathcal{H} = \mathcal{H}^- \oplus \mathcal{H}^+$$

where  $\mathcal{H}^-$  is spanned by  $e^{ikx}$  with  $\frac{k^2}{2} < \varepsilon_F$  or  $|k| < k_F$  where  $\frac{1}{2}k_F^2 = \varepsilon_F$ . (Normally one works in a box  $[-L/2, L/2]$  of volume  $L$  with periodic boundary conditions. Then  $k \in \frac{2\pi}{L}\mathbb{Z}$  and the number  $N$  of  $k$  with  $|k| < k_F$  is

$$N \sim 2k_F / \left(\frac{2\pi}{L}\right)$$

or

$$\boxed{N/L = k_F/\pi}$$

so

$k_F$  is essentially the particle density.)

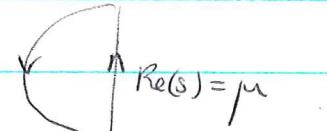
Let's compute the ground energy shift. We do this by figuring out the formulas in the discrete case and then extending them formally. We consider  $H_1 = H_0 + \lambda V$  and let  $E_\lambda = \langle \Psi_\lambda | H_1 | \Psi_\lambda \rangle$  be the ground energy. One has

$$\frac{dE_\lambda}{d\lambda} = \langle \Psi_\lambda | V | \Psi_\lambda \rangle = \text{tr}(P_\lambda^- V)$$

where  $P_\lambda^-$  is the projection onto the eigenspaces for  $H_1$  belonging to eigenvalues  $\leq \mu$ . Now

$$P_\lambda^- = \frac{1}{2\pi i} \int_{\mu-i\infty}^{\mu+i\infty} \frac{ds}{s - H_\lambda}$$

or better the contour is



Thus

$$\frac{dE_\lambda}{d\lambda} = \frac{1}{2\pi i} \int_C \text{tr}\left(\frac{1}{s - H_\lambda} V\right) ds$$

$\underbrace{\hspace{10em}}$

$$\boxed{\frac{1}{s - H_0} V + \frac{1}{s - H_0} \lambda V \frac{1}{s - H_0} V + \dots}$$

and so integrating from  $\lambda=0$  to  $\lambda=1$  gives

$$\Delta E = \frac{1}{2\pi i} \int_C \text{tr}\left(\frac{1}{s - H_0} V + \frac{1}{2} \left(\frac{1}{s - H_0} V\right)^2 + \dots\right) ds$$

$\underbrace{\hspace{10em}}$

$$\boxed{-\log\left(1 - \frac{1}{s - H_0} V\right)}$$

or

$$\boxed{+\Delta E = \frac{1}{2\pi i} \int_C -\log \det\left(1 - \frac{1}{s - H_0} V\right) ds}$$

$\boxed{\hspace{10em}}$

$\uparrow \text{Re}(s) = \mu$

In the case  $H_0 = \frac{p^2}{2} = -\frac{1}{2} \frac{d^2}{dx^2}$ , recall that for  $\text{Im } k > 0$  we have

$$\det(1 - \frac{1}{k^2 + D^2} 2V) = A(k)$$

where  $A(k)$  is determined by the scattering for the equation  $(k^2 + D^2 - 2V)\psi = 0$ :

$$e^{-ikx} \longleftrightarrow A(k)e^{ikx} + B(k)e^{ikx}.$$

So let's substitute  $s = k^2/2$  and we get

$$\Delta E = \frac{1}{2\pi i} \int -\log(A(k)) k dk$$



and the contour should enclose the bound states at  $k = ik_g$ . Suppose there are no bound states.

Then we have

$$\Delta E = \frac{1}{2\pi i} \int_{-k_F}^{k_F} \log\left(\frac{A(k)}{A(-k)}\right) k dk$$

and  $\frac{A(k)}{A(-k)}$  is essentially the determinant of the scattering matrix.

Recall the basic asymptotic behavior of

$$\det(1 - \frac{1}{k^2 + D^2} g) = A(k)$$

One has

$$\log A(k) = - \left[ \text{tr}\left(\frac{1}{k^2 + D^2} g\right) + \frac{1}{2} \text{tr}\left(\frac{1}{k^2 + D^2} g\right)^2 + \dots \right]$$

$$= - \iint \frac{e^{2ik|x-x'|}}{2ik} g(x) dx + \frac{1}{2} \int \frac{e^{2ik|x-x'|}}{(2ik)^2} g(x)g(x') dx dx' + \dots$$

so

$$\log A(k) \sim -\frac{1}{2ik} \int_{-\infty}^{\infty} g(x) dx + O\left(\frac{1}{k^3}\right) \quad \text{as } k \rightarrow \pm\infty.$$

(see p. 543). Consequently provided  $\int g(x) dx = 0$  one sees  $\Delta E$  remains finite as  $k_F \rightarrow \infty$ .

February 20, 1980

We are considering a gas of independent fermions, which we think of ~~as~~ as electrons in a metal, and then we introduce an impurity and try to see what happens. We describe a single fermion by  $H_0 = \frac{P^2}{2}$  on  $L^2(\mathbb{R})$ , and to get the gas we have to give a chemical potential or Fermi energy  $\epsilon_F$ . The impurity is represented by a perturbation  $H = H_0 + U(x)$ . As the impurity potential is turned on :  $H_2 = H_0 + \lambda U$  the density of the gas changes, the total charge, energy changes, and we want to compute these quantities.

The way to visualize things is to start off in a box so as to have discrete spectra, but this really shouldn't be necessary. Let's work on the line in a box  $-L/2 \leq x \leq L/2$  with  $H_0 = -\Delta = -\frac{d^2}{dx^2}$ .

Basic eigenfunctions are

$$u_k(x) = \frac{1}{\sqrt{L}} e^{ikx} \quad k \in \frac{2\pi}{L} \mathbb{Z}$$

and  $H u_k = k^2 u_k$ . Extend  $H_0$  to a derivation of the exterior algebra of  $\mathcal{H} = L^2([-L/2, L/2])$  and let  $N$  be the number of particles belonging to the Fermi energy  $\epsilon_F = k_F^2$ . Thus

$$N = \text{card}\{k \mid k < k_F\}$$

$$N \cdot \frac{2\pi}{L} \sim 2k_F \quad \text{or} \quad \frac{N}{L} \sim \frac{1}{\pi} k_F$$

where this last relation becomes exact as ~~when~~  $N, L \rightarrow \infty$ . So now we have this  $N$ -particle ground state which

is the filled Fermi sea. Let's compute the particle density at a given point  $x$ . What does this mean? Answer: It is  $\langle \underline{\Phi} | \psi^*(x) \psi(x) | \underline{\Phi} \rangle$  where  $\psi(x)$  is the interior product on the exterior algebra associated to the linear functional  $\psi(f) = f(x)$  on  $H$ . So if the constants  $c_k$  are such that

$$\psi(x) = \sum_k c_k a_k$$

we have  $c_k = \psi(x) u_k = u_k(x) = \frac{1}{\sqrt{L}} e^{-ikx}$ , so

$$\psi(x) = \sum \frac{1}{\sqrt{L}} e^{-ikx} a_k$$

Hence

$$\begin{aligned} \langle \underline{\Phi} | \psi(x)^* \psi(x) | \underline{\Phi} \rangle &= \sum_{k, k'} \frac{1}{L} e^{-ik'x + ikx} \underbrace{\langle \underline{\Phi} | a_k^* a_{k'} | \underline{\Phi} \rangle}_{\begin{cases} 0 & \text{unless } k' = k < k_F \\ 1 & \text{otherwise} \end{cases}} \\ &= \frac{N}{L} \end{aligned}$$

which checks.

Let's carry out the analogous construction for the perturbed operator  $H = H_0 + U$ . Again work in a box so the spectrum is discrete. Let  $u_\alpha(x)$  be an orthonormal basis of eigenfunctions  $H u_\alpha = \varepsilon_\alpha u_\alpha$ . Then

$$\psi(x) = \sum c_\alpha a_\alpha \quad c_\alpha = \psi(x) u_\alpha = u_\alpha(x)$$

$$\psi(x) = \sum u_\alpha(x) a_\alpha$$

so the particle density in the ground state  $\underline{\Phi}$  corresponding to the Fermi energy  $\varepsilon_F$  is

$$\begin{aligned} \langle \underline{\Phi} | \psi(x)^* \psi(x) | \underline{\Phi} \rangle &= \sum_{\alpha, \alpha'} \overline{u_{\alpha'}(x)} u_\alpha(x) \underbrace{\langle \underline{\Phi} | a_{\alpha'}^* a_\alpha | \underline{\Phi} \rangle}_{\begin{cases} 0 & \text{unless } \alpha = \alpha' \\ 1 & \text{and } \varepsilon_\alpha < \varepsilon_F \\ 0 & \text{otherwise} \end{cases}} \\ &= \sum_{\varepsilon_\alpha < \varepsilon_F} \overline{u_\alpha(x)} u_\alpha(x) \end{aligned}$$

This is the diagonal of the kernel for orthogonal projection  $P^-$  on the eigenspaces of  $H$  for energies  $< \varepsilon_F$ .

$$P^- = \frac{1}{2\pi i} \int \frac{1}{s - H} ds$$

$$\text{Re}(s) = \varepsilon_F$$

Recall that

$$G(t, t') = \begin{cases} e^{-H(t-t')} P^+ & t > t' \\ e^{-H(t-t')} (-P^-) & t < t' \end{cases}$$

$$\psi(xt) = \sum u_\alpha(x) e^{-\varepsilon_\alpha t} a_\alpha$$

$$\psi^*(x't') = \sum \overline{u_\alpha(x')} e^{\varepsilon_\alpha t'} a_\alpha^*$$

$$G(xt, x't') = \langle \Xi | \psi(xt) \psi^*(x't') | \Xi \rangle \quad t > t'$$

$$= \sum u_\alpha(x) e^{-\varepsilon_\alpha t} \overline{u_{\alpha'}(x')} e^{\varepsilon_{\alpha'} t'} \langle \Xi | a_\alpha a_{\alpha'}^* | \Xi \rangle$$

$$G(xt, x't') = \begin{cases} \sum_{\varepsilon_\alpha > \varepsilon_F} u_\alpha(x) \overline{u_{\alpha'}(x')} e^{-\varepsilon_\alpha (t-t')} & t > t' \\ - \sum_{\varepsilon_\alpha < \varepsilon_F} u_\alpha(x) \overline{u_{\alpha'}(x')} e^{-\varepsilon_\alpha (t-t')} & t < t' \end{cases}$$

The particle density is

$$\langle \Xi | \psi^*(x) \psi(x) | \Xi \rangle = \lim_{t \rightarrow 0^-} -G(xt, x0)$$

February 22, 1980

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Consider  $H = -\Delta + V$  on  $\mathcal{H} = L^2(\mathbb{R})$  where  $V \in C_0^\infty$ .

Fix a Fermi energy  $\varepsilon_F$ . Then we get a splitting  $\mathcal{H} = \mathcal{H}^- \oplus \mathcal{H}^+$ , where  $H < \varepsilon_F$  on  $\mathcal{H}^-$  and  $H > \varepsilon_F$  on  $\mathcal{H}^+$ . We then form the <sup>fermion</sup> Fock space of  $\mathcal{H}$  ~~with~~ with ground state  $\mathbb{E}$  representing the Fermi sea with all the states in  $\mathcal{H}^-$  filled:

$$\mathcal{F} = \Lambda^{\mathcal{H}^-} \otimes \Lambda^{\mathcal{H}^+}$$

We have a Green's function

$$G(xt, x't') = \langle \mathbb{E} | T[\psi(xt) \psi^*(x't')] | \mathbb{E} \rangle$$

which we worked out yesterday in the case where  $\mathbb{R}$  is replaced by a box, or where  $V$  grows fast enough so that the spectrum is discrete. Recall this: Let  $u_\alpha$  be an orthonormal basis of eigenfunctions for  $H$ ,  $H u_\alpha = \varepsilon_\alpha u_\alpha$ . Then

$\psi(x) = \text{"interior mult. by } f \mapsto f(x) \text{ on } \Lambda \mathcal{H}"$

$$= \sum u_\alpha(x) a_\alpha$$

so  $\psi(xt) = \sum u_\alpha(x) a_\alpha(t)$

$$a_\alpha(t) = e^{Ht} a_\alpha e^{-Ht} = e^{-\varepsilon_\alpha t} a_\alpha$$

$$\psi(xt) = \sum u_\alpha(x) e^{-\varepsilon_\alpha t} a_\alpha$$

$$\psi^*(x't') = \sum \overline{u_\alpha(x)} e^{\varepsilon_\alpha t'} a_\alpha^*$$

$t > t'$   $G(xt, x't') = \sum u_\alpha(x) \overline{u_{\alpha t}(x')} e^{-\varepsilon_\alpha t + \varepsilon_{\alpha t} t'} \langle \mathbb{E} | a_\alpha a_\alpha^* | \mathbb{E} \rangle$

$t < t'$

$$\langle \mathbb{E} | -a_\alpha^*, a_\alpha | \mathbb{E} \rangle$$

So

$$G(xt, x't') = \sum_{\substack{\varepsilon_x > \varepsilon_F \\ \alpha}} u_\alpha(x) \overline{u_\alpha(x')} e^{-\varepsilon_\alpha(t-t')} \quad t > t'$$

$$- \sum_{\substack{\varepsilon_x < \varepsilon_F \\ \alpha}} u_\alpha(x) \overline{u_\alpha(x')} e^{-\varepsilon_\alpha(t-t')} \quad t < t'$$

In the finite temperature case one has

$$\langle a_\alpha a_{\alpha'}^* \rangle = \delta_{\alpha\alpha'} \frac{1}{1 + e^{-\beta\varepsilon_\alpha}}$$

$$\langle a_{\alpha'}^* a_\alpha \rangle = \delta_{\alpha\alpha'} \frac{e^{-\beta\varepsilon_\alpha}}{1 + e^{-\beta\varepsilon_\alpha}}$$

The reason is that

$$\langle a_\alpha a_{\alpha'}^* \rangle = \frac{\text{tr}(e^{-\beta H} a_\alpha a_{\alpha'}^*)}{\text{tr}(e^{-\beta H})}$$

and because  $H$  is diagonal, the exterior algebra can be written as a tensor product of the  $\alpha, \alpha'$  part and the rest of  $H$ . Thus the finite temperature Green's function is

$$G(xt, x't') = \sum_{\alpha} u_\alpha(x) \overline{u_\alpha(x')} e^{-\varepsilon_\alpha(t-t')} \begin{cases} \frac{1}{1 + e^{-\beta\varepsilon_\alpha}} & t > t' \\ \frac{-e^{-\beta\varepsilon_\alpha}}{1 + e^{-\beta\varepsilon_\alpha}} & t < t' \end{cases}$$

The problem now is to understand what happens to these formulas as the box  gets infinite and the spectrum is continuous

Note: The above formulas for finite temperature case should have  $H$  replaced by  $H - i\varepsilon_F$ . In the sequel let's assume this has been done, so that  $\varepsilon_F = 0$ .

Formulas for the finite temperature Green's function

$$1) \quad G(t, t') = e^{-H(t-t')} \begin{cases} \frac{1}{1+e^{-\beta H}} & t > t' \\ \frac{-e^{-\beta H}}{1+e^{-\beta H}} & t < t' \end{cases}$$

Note that  $0 \leq t, t' \leq \beta$  and that

$$G(\beta, t') = e^{-H(\beta-t')} \frac{1}{1+e^{-\beta H}} = -G(0, t')$$

so that  $G$  is the inverse of  $\frac{d}{dt} + H$  on  $[0, \beta]$  with anti-periodic boundary conditions. Hence we can compute it by Fourier series and get

$$2) \quad G(t, t') = \sum_{k \in \frac{2\pi}{\beta}(\frac{1}{2} + \mathbb{Z})} \frac{1}{\beta} \frac{e^{-ik(t-t')}}{ik + H}$$

Next let us use contour integration to evaluate the above sum. The summation takes place over those  $z = ik$  with  $k \in \frac{2\pi}{\beta}(\frac{1}{2} + \mathbb{Z})$ , i.e. where  $e^{\beta z} + 1 = 0$ . At such a zero, one has  $\frac{d}{dz}(e^{\beta z} + 1) = \beta e^{\beta z} = -\beta$ . Hence by residues:

$$3) \quad G(t, t') = \frac{-1}{2\pi i} \int \frac{e^{z(t-t')}}{(z + H)(e^{\beta z} + 1)} dz$$

The contour is a thin rectangle enclosing the zeroes of  $e^{\beta z} + 1$ , thin enough so as to avoid the spectrum of  $H$  which we think of as being separated by  $\epsilon_F = 0$ . Another formula is

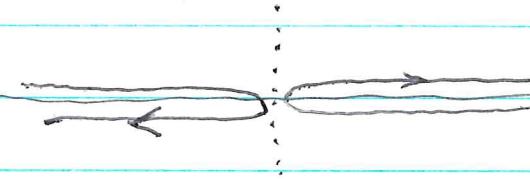
$$3') \quad G(t, t') = \frac{-1}{2\pi i} \int \frac{e^{z(t-t')}}{z+H} \left( \frac{1}{e^{\beta z} + 1} - 1 \right) dz$$

$\frac{-e^{\beta z}}{1+e^{\beta z}}$

If  $t-t' > 0$ , then  $\boxed{\text{the function decays as } \operatorname{Re}(z) \rightarrow \pm\infty}$  at least when  $t \in (0, \beta)$  one has  $0 < t-t' < \beta$  and so

$$\frac{e^{z(t-t')}}{e^{z\beta} + 1}$$

decays as either  $\operatorname{Re}(z) \rightarrow +\infty$  or  $-\infty$ . Hence the contour <sup>in 3)</sup> can be deformed to



which gives

$$G(t, t') = \frac{e^{-H(t-t')}}{1 + e^{-\beta H}} \quad t > t'$$

On the other hand if  $t-t' < 0$ , then  $\boxed{-\beta < t-t' < 0}$

so

$$\frac{e^{z(t-t')}}{1 + e^{\beta z}} \frac{(-e^{\beta z})}{(-e^{\beta z})}$$

decays as either  $\operatorname{Re}(z) \rightarrow +\infty$  or  $\operatorname{Re}(z) \rightarrow -\infty$  so the contour in (3') can be deformed in the same  $\boxed{\text{way}}$  to yield

$$G(t, t') = - \frac{e^{-H(t-t')}}{1 + e^{-\beta H}} \frac{e^{-\beta H}}{1 + e^{-\beta H}} \quad t < t'$$

which checks the formula  $\boxed{1}$ .

February 23, 1980

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Yesterday we worked out the Green's function at non-zero temperature for a system of independent fermions governed by a 1-particle Hamiltonian  $H$  and with a given Fermi energy. We found (for  $\varepsilon_F = 0$ )

$$G(t, t') = e^{-H(t-t')} \begin{cases} \frac{1}{1+e^{-\beta H}} & t > t' \\ \frac{-e^{-\beta H}}{1+e^{-\beta H}} & t < t' \end{cases}$$

It follows that the density matrix is

$$-G(0^-, 0) = \frac{e^{-\beta H}}{1+e^{-\beta H}} = \frac{1}{e^{\beta H} + 1}.$$

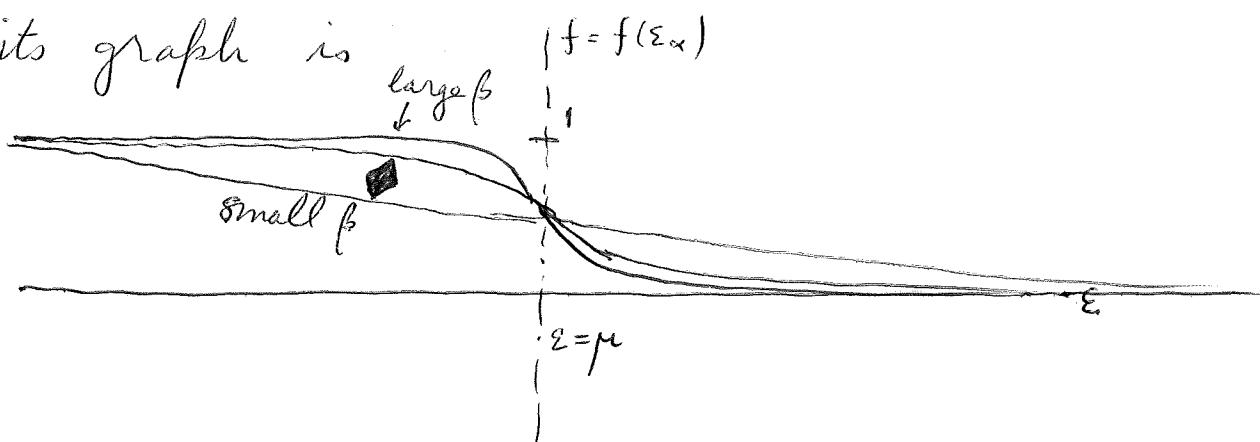
Thus the density of particles at a point  $x$

$$\langle \psi^*(x) \psi(x) \rangle = -G(x0^-, x0) = \sum_{\alpha} |u_{\alpha}(x)|^2 \frac{1}{e^{\beta \varepsilon_{\alpha}} + 1}$$

if  $u_{\alpha}$  is an orthonormal basis of eigenfunctions. The last function is the Fermi function; in general is would be

$$f_{\alpha} = \langle a_{\alpha}^* a_{\alpha} \rangle = \frac{1}{e^{\beta(\varepsilon_{\alpha}-\mu)} + 1}$$

and its graph is



The above extends to the case where  $H$  has

continuous spectrum:

$$\langle x | \frac{1}{e^{\beta H} + 1} | x \rangle = \int \frac{1}{e^{\beta E_k} + 1} dE_k(x, x)$$

The next project will be to take  $H = -\Delta + V$  with  $V \in C_0^\infty$  and see if we <sup>can</sup> compute the particle density well enough so as to understand Friedel oscillations.

We need to review eigenfunctions for  $H$ . Notation:  $\psi(x, k) \stackrel{(phi(x, k))}{=} \text{is the solution of } (H - k^2)\psi = 0 \text{ or}$

$$1) \quad (k^2 + \Delta)\psi = V\psi$$

such that

$$\begin{aligned} \psi(x, k) &\sim e^{ikx} & \text{as } x \rightarrow +\infty \\ \phi(x, k) &\sim e^{-ikx} & \text{as } x \rightarrow -\infty \end{aligned}$$

where we think of  $k$  as being in the UHP. The scattering is given by

$$e^{-ikx} \longleftrightarrow A(k)e^{-ikx} + B(k)e^{ikx}$$

$$\text{or } \phi(x, k) = A(k)\psi(x, -k) + B(k)\psi(x, k)$$

and the Green's function is

$$G_k(x, x') = \frac{\phi(x_1, k) \psi(x_2, k)}{A(k) 2ik}$$

Let's go over physics notation:  $\psi_k^+(x)$  denotes the solution of the Schrödinger equation 1) which differs from  $e^{ikx}$  by an outgoing wave. Recall how this

goes: Consider a solution of  $i\partial_t \psi = H\psi$  of

the form

$$\psi(x, t) = \int e^{ikx - ik^2 t / 2m} f(k) dk \quad x \text{ large}$$

where  $f$  has support close to  $k_0$ . Then for large  $(x, t)$ ,  $\psi(x, t)$  is negligible unless the exponent is stationary near  $k=k_0$ . But

$$\frac{d}{dk} \left( kx - \frac{k^2 t}{2m} \right) = x - \frac{k}{m} t = 0$$

means ~~that~~ that  $\psi$  represents a wave packet travelling with velocity  $k/m$ , hence momentum  $k$ . Thus  $e^{ikx}$  represents a wave travelling in the direction  $k$ . It follows that for  $k > 0$

$$\psi_k^+ : \tilde{R}(k)e^{-ikx} + e^{ikx} \longleftrightarrow T(k)e^{ikx}$$

and for  $k < 0$

~~$\psi_k^+ :$~~

$$T(k)e^{ikx} \longleftrightarrow e^{ikx} + R(k)e^{-ikx}$$

Unfortunately if we give  $k$  a small positive imaginary part:  $k+i\eta$ , then

$$e^{i(k+i\eta)x} = e^{-\eta x + ikx}$$

decays as  $x \rightarrow +\infty$  which is not what you expect.

?

The problem is that  $\psi_k^+$  is defined via Leppmann-Schwinger

$$\psi_k^+ = \varphi_k + \frac{1}{k^2 + i\varepsilon + \Delta} V \psi_k^+$$

so that one wants to push  $k$  so that  $k^2 \in \text{UHP}$ . Thus we want  $k \mapsto k + i\eta$ , where  $(k + i\eta)^2 = k^2 - \eta^2 + 2ik\eta \in \text{UHP}$  so we want  $k\eta > 0$ . The same formula will work in 3dms.

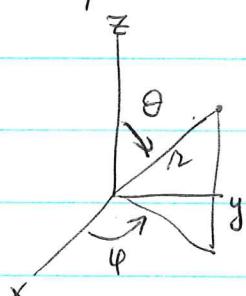
Note that

$$e^{i(k+i\eta)x} = e^{ikx} e^{-\eta x}$$

decays in the direction  $y$  which since  $k \cdot y > 0$  means this function decays in the  $k$ -direction. Thus we look at complex  $\vec{k}$  with  $\text{Im}(k^2) > 0$  and define  $\psi_k^+$  to be the eigenfunction for  $H$  with eigenvalue  $k^2$  which differs from  $e^{ikx}$  by an  $L^2$  function.

So the moral is that the physics way of thinking about the scattering <sup>on  $\mathbb{R}^3$</sup>  differs from the way I am familiar with. Hence one should perhaps work with a symmetrical situation.

Let's try to do the scattering in 3 dimensions with a spherically symmetric potential  $V(r)$ .  Recall the formulas



$$\Delta = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2}{\partial \phi^2}$$

$$(1 + r^2 - 2r \cos \theta)^{-1/2} = \sum_{l=0}^{\infty} r^l P_l(\cos \theta)$$

$$\left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \sin \theta \frac{\partial}{\partial \theta} + l(l+1) \right] P_l(\cos \theta) = 0$$

$$\int_{-1}^1 P_l(x) P_{l'}(x) dx = \frac{2}{2l+1} \delta_{ll'}$$

$$P_l(x) = \frac{(2l-1)!!}{l!} x^l + O(x^{l+1})$$

$$e^{ikr \cos \theta} = \sum_{l=0}^{\infty} (2l+1) i^l j_l(kr) P_l(\cos \theta)$$

$$j_l(r) \sim \frac{\sin(r - l\pi/2)}{r} \quad \text{as } r \rightarrow \infty$$

$$j_l(r) \sim \frac{1}{(2l+1)!!} r^l \quad \text{as } r \rightarrow 0$$

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Given a free eigenfunction  $e^{ik \cdot x}$  the perturbed eigenfunction asymptotic to it as  $t \rightarrow \infty$  in some sense is obtained by solving the Lippmann-Schwinger equation:

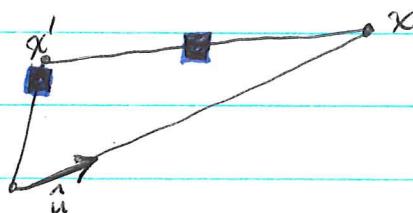
$$\psi_{\underline{k}}^+(x) = e^{ik \cdot x} + \frac{1}{k^2 + i0^+ - H_0} V \psi_{\underline{k}}^+ \quad \text{where}$$

$$\langle x | \frac{1}{k^2 + i0^+ + \Delta} | x' \rangle = \frac{e^{ikr}}{-4\pi r} \quad h = |x-x'| \quad \text{and } k > 0.$$

Thus

$$\psi_{\underline{k}}^+(x) = e^{ik \cdot x} + \int \frac{e^{ik|x-x'|}}{-4\pi|x-x'|} V(x') \psi_{\underline{k}}^+(x') d^3x'$$

Let's look at this for  $x = r\hat{u}$ ,  $\hat{u}$  a fixed unit vector and  $r \rightarrow \infty$ .



$$\begin{aligned} |x-x'| &= \sqrt{r^2 + |x'|^2 - 2r\hat{u} \cdot x'} \\ &= r \left( 1 - \frac{\hat{u} \cdot x'}{r} \right) + O\left(\frac{1}{r}\right) \\ &= r - \hat{u} \cdot x' + O\left(\frac{1}{r}\right) \end{aligned}$$

$$\psi_{\underline{k}}^+(x) - e^{ik \cdot x} = \int \frac{e^{ikr}}{r} \frac{e^{-ik\hat{u} \cdot x'}}{-4\pi} \left( 1 + O\left(\frac{1}{r}\right) \right) V(x') \psi_{\underline{k}}^+(x') dx'$$

Thus we see that provided we let ~~x~~  $x \rightarrow \infty$  radially:  $x = r\hat{u}$  with  $r \rightarrow \infty$ , we have

$$\psi_{\underline{k}}^+(x) = e^{ik \cdot x} + \frac{e^{ikr}}{r} f(k\hat{u}, \underline{k}) + O\left(\frac{1}{r^2}\right)$$

$$f(k', \underline{k}) = -\frac{1}{4\pi} \int e^{-ik' \cdot x} V(x) \psi_{\underline{k}}^+(x) dx$$

Consider the situation where  $V = V(r)$ . Then

we use partial wave expansions:

$$e^{ikz} = \sum_{\ell} i^{\ell} (2\ell+1) \underbrace{j_{\ell}(kr)}_{\sim \frac{\sin(kr - \frac{1}{2}\ell\pi)}{kr}} P_{\ell}(\cos\theta) = \frac{e^{ikr} - e^{-ikr}}{2ikr}$$

Let  $\psi_k^+(x) = \psi_k^-(x) = \boxed{\phantom{000}} e^{ikz} + \text{scattered wave, i.e. } \underline{k} = (0, 0, k) \text{ and } k > 0 \text{ always. Partial waves.}$

$$\psi_k^+(r, \theta) = \sum_{\ell} \boxed{\phantom{000}} R_{\ell}(r, k) P_{\ell}(\cos\theta)$$

where  $R_{\ell}(r, k)$  satisfies

$$\left\{ -\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} + \frac{\ell(\ell+1)}{r^2} + V(r) - k^2 \right\} R_{\ell} = 0$$

$$R_{\ell} \sim \text{const. } r^{\ell} \quad \text{as } r \rightarrow 0.$$

For large  $r$  one has

$$R_{\ell} \sim \text{const. } \frac{\sin(kr - \frac{1}{2}\ell\pi + \delta_{\ell}(k))}{r}$$

where  $\delta_{\ell}(k)$  is the so-called phase shift. Since  $\psi_k^+ - e^{ikz} \boxed{\phantom{000}} \sim A \frac{e^{ikr}}{r}$ , we expect in

$$R_{\ell} \sim \text{const. } \frac{e^{ikr} i^{\ell} e^{i\delta_{\ell}} - e^{-ikr} - i^{\ell} e^{-i\delta_{\ell}}}{r}$$

that the constant makes the  $\frac{e^{-ikr}}{r}$  term agree with that for  $e^{ikz}$ . Thus

$$R_{\ell}(r, k) \sim_{(2\ell+1)} \frac{e^{2i\delta_{\ell}(k)}}{2ikr} e^{ikr} - (-1)^{\ell} e^{-ikr}$$

and so we get

$$\psi_k^+(r, \theta) - e^{ikz} \sim A(k, \theta) \frac{e^{ikr}}{r} \quad \text{as } r \rightarrow \infty$$

where

$$A(k, \theta) = \sum_l (2l+1) \frac{S_l(k)-1}{2ik} P_l(\cos \theta)$$

scattering amplitude

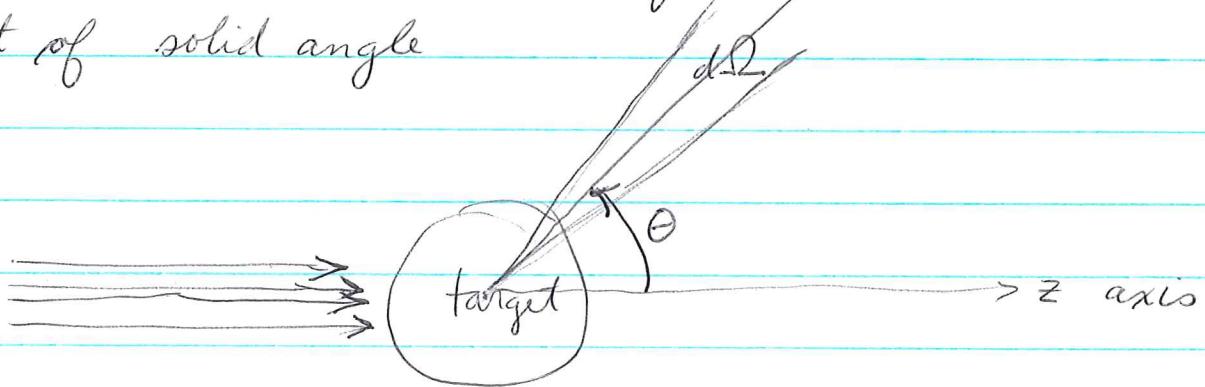
$$S_l(k) = e^{2i\delta_l(k)}$$

The differential cross-section is the quantity

~~(differential cross-section)~~

$$\frac{d\sigma}{d\Omega} = |A(k, \theta)|^2$$

and it has the following interpretation. One thinks of  $e^{ikz}$  as representing a beam of particles with momentum  $k$ ,  $V(r)$  is the potential of many sufficiently separated identical atoms which form the target. ~~and it contributes to the interaction of other beams~~  $d\Omega$  is an element of solid angle



and  $d\sigma$  measures the fraction of the beam scattered into  $d\Omega$ . The total scattering cross-section is

$$\sigma = \int A(k, \theta)^2 \frac{d\Omega}{2\pi \sin \theta d\theta} = \sum_l \left| \frac{S_l(k)-1}{2ik} \right|^2 (2l+1)^2 \frac{2\pi \cdot 2}{2l+1}$$

$$\sigma = \frac{4\pi}{k^2} \sum_l (2l+1) \sin^2 \delta_l(k)$$

$$\text{Im } A(k, \theta) = \sum_l (2l+1) \frac{1 - \cos 2\delta_l(k)}{2k} P_l(\cos \theta)$$

$$\boxed{\text{Im } A(k, \theta) = \frac{1}{k} \sum_l (2l+1) \sin^2 \delta_l(k) \cdot P_l(\cos \theta)}$$

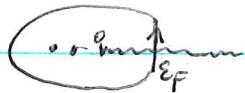
Since  $P_l(1) = 1$  we get the optical thm.

$$\boxed{\sigma = \frac{4\pi}{k} \text{Im } A(k, 0)}$$

$A(k, 0)$  = forward scattering amp.

Let's now return to the problem of computing the particle density in the fermi gas given by a Fermi energy  $\varepsilon_F = k_F^2$  and the 1-particle Hamiltonian  $H = -\Delta + V$ . We want the diagonal of the kernel for the projection  $P^-$  on states of energy  $< \varepsilon_F$ .

$$P^- = \frac{1}{2\pi i} \int \frac{ds}{s - H}$$



In the case of three dims with  $V = V(r)$ , this will be a sum over  $l$ , and the spectrum of angular momentum  $l$  will be  $(2l+1)$ -fold degenerate. So we should first look at the radial case

$$\left( -\frac{d^2}{dx^2} + V(x) \right) \psi = k^2 \psi \quad \text{on } [0, \infty)$$

with some boundary condition at  $x=0$ . Then the resolvent is

$$G_k(x, x') = \langle x \left| \frac{1}{k^2 + \Delta - V} \right| x' \rangle = \frac{\phi(x_s, k) \psi(x_s, k)}{W(\phi, \psi)}$$

and we have

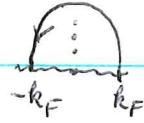
$$\phi(x, k) \sim A(k) e^{-ikx} + A(-k) e^{ikx} \quad x \gg 0$$

$$\phi(x, k) = A(k) \psi(x, -k) + A(-k) \psi(x, k)$$

$$\text{so } W(\phi, \psi) = A(k) 2ik$$

Then

$$\langle x | P^- | x' \rangle = \frac{1}{2\pi i} \int_{-k_F}^{k_F} G_k(x, x') 2k dk$$



$$= \sum_{\text{bdd states}} u_\alpha(x) \overline{u_\alpha(x')} + \frac{i}{2\pi} \int_{-k_F}^{k_F} G_k(x, x') 2k dk$$

If  $k_F = \infty$ , we get the completeness relation. The last term can be written

$$\frac{i}{2\pi} \int_0^{k_F} \left\{ \frac{\phi(x_<, k) \psi(x_>, k)}{2ikA(k)} + \frac{\psi(x_>, -k)}{2ikA(-k)} \right\} 2k dk = \frac{1}{2\pi} \int_0^{k_F} \phi(x_<, k) \psi(x_>, k) \frac{dk}{|A(k)|^2}$$

Thus

$$\langle x | P^- | x' \rangle = \sum_{\text{bdd states}} u_\alpha(x) \overline{u_\alpha(x')} + \frac{1}{2\pi} \int_0^{k_F} \phi(x, k) \psi(x', k) \frac{dk}{|A(k)|^2}$$

For  $x$  outside the support of  $\psi$  we have

$$\begin{aligned} \phi(x, k) &= A(k) e^{-ikx} + A(-k) e^{ikx} = |A(k)| (e^{-ikx+i\delta_0} + e^{ikx-i\delta_0}) \\ &= 2|A(k)| \sin(kx + \delta_0(k)) \end{aligned}$$

where  $\delta_0(k)$  is essentially the argument of  $A(k)$ . Hence

$$\int_0^{k_F} \frac{\phi(x, k)^2 dk}{|A(k)|^2} = 4 \int_0^{k_F} \sin^2(kx + \delta_0(k)) dk$$

Now compare with  $V=0$ , where  $\phi(x, k) = \sin(kx) = \frac{e^{ikx} - e^{-ikx}}{2i}$  so that  $A(k) = \frac{i}{2}$  and  $|A(k)|^2 = \frac{1}{4}$ , and so the density is

$$4 \int_0^{k_F} \sin^2(kx) dk.$$

Difference oscillates.

February 27, 1980

Consider  $\mathbb{C}^n = \mathbb{C}^P \oplus \mathbb{C}^{n-P}$  and let  $e_w = e_1 \wedge \dots \wedge e_p$  denotes the element of  $\Lambda^p(\mathbb{C}^n)$  associated to the subspace  $W = \mathbb{C}^P$ . Given  $A \in GL_n(\mathbb{C})$  we can write it in block form

$$A = \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} \quad \text{with } \alpha \text{ a } p \times p \text{ matrix}$$

and we have  $\langle e_w | \tilde{A} | e_w \rangle = \det(\alpha)$ , where  $\tilde{A}$  denotes the <sup>functional</sup> extension of  $A$  to the exterior algebra. Now

$$\|\tilde{A}e_w\|^2 = \langle e_w | \tilde{A}^* \tilde{A} | e_w \rangle$$

If  $\tilde{A}^* = \tilde{A}^*$ , then since  $\|A^* A\| = \begin{pmatrix} \alpha^* & \beta^* \\ \gamma^* & \delta^* \end{pmatrix} \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix} = \begin{pmatrix} \alpha^* \alpha + \gamma^* \gamma & \cdot \\ \cdot & \cdot \end{pmatrix}$  we get

$$\|\tilde{A}e_w\|^2 = \det(\alpha^* \alpha + \gamma^* \gamma).$$

To verify  $\tilde{A}^* = \tilde{A}^*$  take decomposable vectors,

$$\begin{aligned} \langle v_1 \wedge \dots \wedge v_p | \tilde{A}(w_1 \wedge \dots \wedge w_p) \rangle &= \boxed{\text{det}(v_i | Aw_j)} \langle v_1 \wedge \dots \wedge v_p | Aw_1 \wedge \dots \wedge Aw_p \rangle \\ &= \det \langle v_i | Aw_j \rangle = \det \langle A^* v_i | w_j \rangle = \langle \tilde{A}^*(v_1 \wedge \dots \wedge v_p) | w_1 \wedge \dots \wedge w_p \rangle \end{aligned}$$

March 2, 1980

Review Fredholm formulas for  $(I-\lambda K)^{-1} = \frac{\text{adj}(I-\lambda K)}{\det(I-\lambda K)}$   
 Put  $\det(I-\lambda K) = \sum \lambda^n D_n$ ,  $\text{adj}(I-\lambda K) = \sum \lambda^n A_n$ . Then

$$(I-\lambda K) \sum \lambda^n A_n = \sum \lambda^n D_n$$

$$\boxed{A_n - KA_{n-1} = D_n}$$

Also  $\frac{d}{d\lambda} \det(I-\lambda K) = -\text{tr}(K \text{adj}(I-\lambda K))$  or

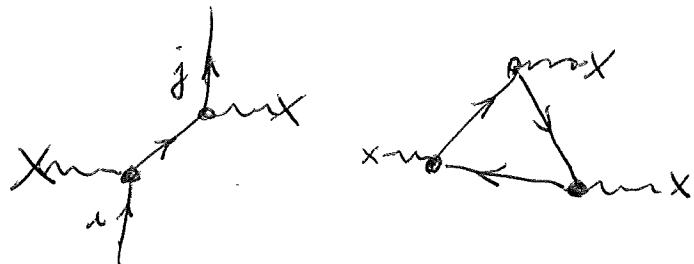
$$\boxed{n D_n = -\text{tr}(KA_{n-1})}$$

There's a diagrammatic version of these recursion formulas using

$$\frac{\int e^{-\psi^*(I-\lambda K)\psi} \psi_i \psi_j^*}{\int e^{-\psi^*\psi}} = \frac{\int e^{-\psi^*(I-\lambda K)\psi} \psi_i \psi_j^*}{\int e^{-\psi^*(I-\lambda K)K}} \cdot \frac{\int e^{-\psi^*(I-\lambda K)\psi}}{\int e^{-\psi^*\psi}}$$

$$= (I-\lambda K)_{ij}^{-1} \cdot \det(I-\lambda K) = [\text{adj}(I-\lambda K)]_{ij}$$

Expanding in powers of the interaction  $\lambda K$  gives  $[\text{adj}(I-\lambda K)]_{ij}$  as a sum over diagrams with directed edges labelled by a variable  $i$  and vertices of the form  $\begin{smallmatrix} j \\ \nearrow \\ i \\ \searrow \\ k \end{smallmatrix} \lambda K_{ji}$ . Thus  $(A_n)_{ij}$  is the sum over  $n$ -vertex diagrams with entering arrows labelled by  $j$  and exiting arrow labelled by  $i$ . A typical one is



$D_n$  is similar without external lines. The formula

$$A_n = D_n + K A_{n-1}$$

results from ~~█~~ dividing the diagrams according to whether the interaction occurs on the  $j-i$  path. The formula

$$h D_n = - \text{tr}(K A_{n-1})$$

results from breaking a contribution to  $D_n$  at any of its  $n$ -vertices; the minus sign is due to the fact we have cut a fermion loop.

Suppose  $K = |v\rangle\langle\bar{v}|$  is of rank 1. Then

$$\begin{aligned} \frac{1}{1-\lambda K} &= 1 + \lambda K + \lambda^2 K^2 + \dots \\ &= 1 + \lambda |v\rangle\langle\bar{v}| + \lambda^2 |v\rangle\langle\bar{v}| |v\rangle\langle\bar{v}| + \dots \\ &= 1 + \frac{\lambda |v\rangle\langle\bar{v}|}{1 - \lambda \langle\bar{v}|v\rangle} \\ &= \frac{1 + \lambda [ |v\rangle\langle\bar{v}| - \langle\bar{v}|v\rangle ]}{1 - \lambda \langle\bar{v}|v\rangle} \end{aligned}$$


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Alternative version which leads to the denominator  $\sum_{n>0} \tilde{D}_n \lambda^n = \det(1-\lambda K) e^{\lambda \text{tr } K}$ , where one has "pulled the poison tooth". ~~█~~ The numerator will be

$$\sum_{n>0} \tilde{N}_n \lambda^n = \underbrace{[(1-\lambda K)^{-1} - 1]}_{\text{diagrams}} \underbrace{\det(1-\lambda K) e^{\lambda \text{tr } K}}_{\substack{\text{vacuum diagrams} \\ \text{where } \text{O } \text{ are} \\ \text{deleted.}}} \quad \text{where } \text{O } \text{ has} \\ \text{been deleted}$$

Recursion formulas are

$$\begin{cases} n\tilde{D}_n = -\text{tr}(K\tilde{N}_{n-1}) \\ \tilde{N}_n = K(\tilde{N}_{n-1} + \tilde{D}_{n-1}) \end{cases}$$

Diagrams contributing to  $\tilde{N}_n$  involve incoming and outgoing external lines, together with  $n$  vertices of interaction, <sup>at least</sup> one of which occurs on the path connecting the external lines.

$$\tilde{N}_0 = 0 \quad \tilde{N}_1 = K \quad \tilde{N}_2 = K^2$$

$$\tilde{D}_0 = 1 \quad \tilde{D}_1 = 0 \quad \tilde{D}_2 = -\frac{1}{2} \text{tr}(K^2)$$


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March 3, 1980

Weinberg's analysis of a  $N$ -body system (in Brandeis Summer Institute in Theor. Physics 1964 Vol. II - Lectures on particles and field theory).

We work with  $N$ -distinguishable particles, so the Hilbert space is  $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_N$  and  $H = H_0 + V$  where

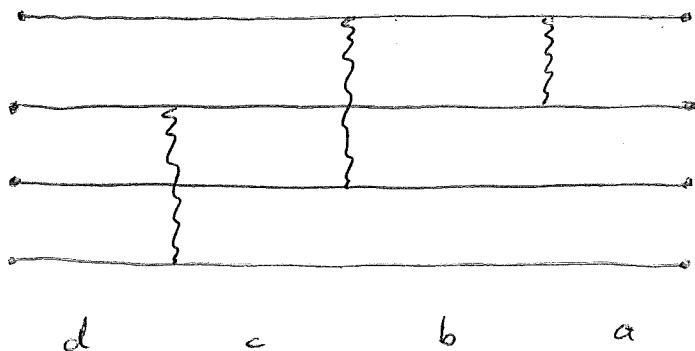
$$H_0 |p_1, \dots, p_N\rangle = \sum \frac{p_i^2}{2m_i} |p_1, \dots, p_N\rangle$$

$$V = \sum_{i < j} V_{ij}$$

The problem is to understand matrix elements of

$$\begin{aligned} G(w) &= [w - H]^{-1} = G_0(w) + G_0(w)VG_0(w) + \dots \\ &= G_0(w) + G_0(w) \sum_{i < j} V_{ij} G_0(w) + G_0(w) \sum_{i < j} V_{ij} G_0(w) \sum_{k < l} V_{kl} \dots \\ &\quad + \dots \end{aligned}$$

We draw diagrams as follows:



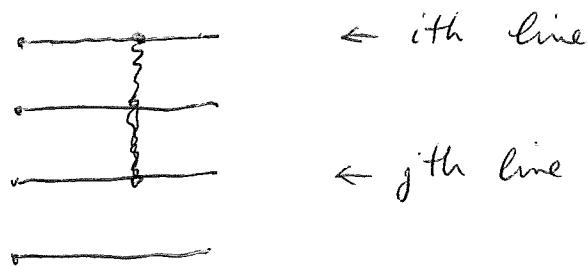
a represents the initial state, d the final state; a vertical wavy line between  $i$ th and  $j$ th line represents  $V_{ij}$ . The above diagram represents the contribution to  $\langle d | G(w) | a \rangle$  coming from the term  $G_0(w)V_{24}G_0(w)V_{13}G_0(w)V_{12}G_0(w)$ , that is

$$\langle d | G | a \rangle = \langle d | G_0 V_{24} G_0 V_{13} G_0 V_{12} G_0 | a \rangle$$

$$= \int dc \int db \frac{\langle d | V_{24} | c \rangle \langle c | V_{13} | b \rangle \langle b | V_{12} | a \rangle}{(w - E_d)(w - E_c)(w - E_b)(w - E_a)}$$

Put  $K = G_0 V$  so that  $G = [I - K]^{-1} G_0$ .

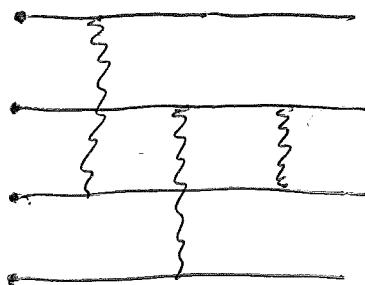
One has  $K = \sum_{ij} G_0 V_{ij}$  where  $G_0 V_{ij}$  is represented by the diagram



The dots missing on the right mean that  $G_0$  doesn't appear. The equation  $G = G^0 + KG$  has the obvious diagram interpretation of looking at the left-most interaction

$$\begin{aligned}
 \text{Diagram with a circle labeled } G \text{ connected to three lines} &= \text{Diagram with a circle labeled } G \text{ connected to two lines} + \text{Diagram with a circle labeled } G \text{ connected to one line} \\
 &\quad + \text{other } K_{ij} \text{ terms} \\
 &= \text{Diagram with a circle labeled } G \text{ connected to two lines} + \text{Diagram with a circle labeled } K \text{ connected to one line}
 \end{aligned}$$

It's clear what is meant by a connected graph. An irreducible graph is one of the form



such that if the ~~█~~ right-most interaction is dropped then it becomes disconnected. Any connected graph has a unique irreducible leading (from the left) part, so we have the equation

$$C = I \cdot G$$

$$\text{Diagram with a circle labeled } C \text{ connected to three lines} = \text{Diagram with a circle labeled } I \text{ connected to two lines} \cdot \text{Diagram with a circle labeled } G \text{ connected to one line}$$

An irreducible graph splits into 2 components when the right-most interaction is dropped:

$$I = \frac{1}{2!} \sum_{\substack{\text{partitions} \\ \{1, \dots, N\} = S_1 \cup S_2}} C_{S_1} * C_{S_2} \underbrace{V_{S_1, S_2}}_{\substack{\text{Sum of all interactions} \\ \text{between particles of subsystem } S_1 \\ \text{and particles of subsystem } S_2}}$$

can be omitted  
if ordering of  $S_1, S_2$   
is not counted

Finally any contribution to  $G$  can be built up from its connected components:

$$G = \prod_{m=1}^{\infty} \sum_{\substack{\text{partitions} \\ \{1, \dots, N\} = S_1 \cup \dots \cup S_m}} C_{S_1} * \dots * C_{S_m}$$

can be omitted if ordering of  $S_1, \dots, S_m$  is not counted.

Convolution is defined by

$$f(w) * g(w) = \frac{1}{2\pi i} \oint_{\text{contour enclosed singularities of } f} f(z) g(w-z) dz$$

and has the effect that

$$\frac{1}{w-a} * \frac{1}{w-b} = \frac{1}{w-a-b}.$$

March 5, 1980

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Return to a many electron system and try to understand dielectric response, Kubo formula, polarization propagator, etc. An electron gas with  $N$ -particles is described classically by the Hamiltonian

$$H = \sum_{i=1}^N \frac{p_i^2}{2m} + \sum_{i < j} V(r_i - r_j) \quad V(r) = \frac{e^2}{r}$$

The ~~particle~~ density is

$$\rho(r) = \sum_{i=1}^N \delta(r - r_i)$$

Now

$$\iint dx dx' \rho(x) V(x-x') \rho(x') = \sum_{i,j} V(r_i - r_j)$$

except that this has problems when  $r_i = r_j$ .

Consider next the quantum situation. If we regard the particles as distinguishable, the Hilbert space is  $\mathcal{H}_1 \otimes \dots \otimes \mathcal{H}_N$ , ~~whose elements are wave functions~~ whose elements are wave functions  $\psi(r_1, \dots, r_N)$ . Electrons are fermions, so wave functions are skew-symmetric. The particle density  $\rho(r)$  becomes an operator; more generally any <sup>symmetric</sup> function of  $r_1, \dots, r_n$  gives a multiplication operator on skew-symmetric wave functions. Since  $\rho(r)$  is a sum of the one-particle functions  $r_i \mapsto \delta(r - r_i)$ , its effect on  $\mathbb{A}^N \mathcal{H}_1$  is that of a derivation. ~~whose~~ Let  $u_\alpha$  be an orthonormal basis for  $\mathcal{H}_1$ . Then on  $\mathcal{H}$ , one has

$$\langle u_\beta | \rho(r) | u_\alpha \rangle = \overline{u_\beta(r)} u_\alpha(r)$$

and so on the Fock space

$$\rho(r) = \sum_{\beta, \alpha} a_\beta^* \overline{u_\beta(r)} u_\alpha(r) a_\alpha = \psi(r)^* \psi(r)$$

where  $\psi(r) = \sum u_\alpha(r) a_\alpha$  is the interior multiplication  $f \mapsto f(r)$ .

Assuming  $V(0) = 0$  the potential energy can be written

$$\begin{aligned}
 & \frac{1}{2} \int \int dr dr' \rho(r) V(r-r') \rho(r') \\
 &= \frac{1}{2} \int \int dr dr' \psi(r)^* \psi(r) V(r-r') \psi(r')^* \psi(r') \\
 &= \frac{1}{2} \int \int dr dr' \psi(r)^* \psi(r')^* V(r-r') \psi(r') \psi(r) \\
 &\quad + \frac{1}{2} \int \int dr dr' \psi(r)^* V(r-r') \underbrace{\{\psi(r), \psi(r')^*\}}_{\delta(r-r')} \psi(r')
 \end{aligned}$$

] correct potential energy in general

The 2nd term is  $V(0) \frac{1}{2} \int dr \psi(r)^* \psi(r) = \frac{V(0)}{2} N$ . Thus one sees that the potential energy is essentially

$$\frac{1}{2} \int \int dr dr' \rho(r) V(r-r') \rho(r') + \text{constant}$$

Thomas-Fermi model for an atom. One has a nucleus with charge  $Z_e$ . The first model (due to Pauli) is treat all the electrons as independent particles subject only to the exclusion principle. Then one puts in  $Z$  electrons filling one shell at a time. The Thomas-Fermi and Hartree-Fock models attempt to understand the effects of the Coulomb repulsion between electrons by introducing an average potential due to the other electrons. Let  $\varphi(r)$  denote the average or effective potential; by spherical symmetry it depends only on  $r = |r|$ .

With Thomas-Fermi one treats the electrons as a fermi gas with density  $\rho(r)$  (here  $r = |r|$ ). Once  $\varphi(r)$  is given one can solve Schrödinger's equation to get an orthonormal

basis of eigenfunctions  $u_\alpha(r)$  and then one gets the density

$$\rho(r) = \sum_{\epsilon_\alpha < \epsilon_F} |u_\alpha(r)|^2$$

by giving a Fermi energy. But there is a way to get at this density semi-classically: Recall:

$$\text{number of eigenvalues of } \frac{p^2}{2m} + \varphi(r) < \epsilon_F \stackrel{\text{semi-classical}}{\sim} 2 \int \frac{d^3k d^3r}{(2\pi)^3} = 2 \int \frac{d^3p d^3r}{(2\pi\hbar)^3}$$

$$\frac{\hbar^2 k^2}{2m} + \varphi(r) < \epsilon_F \quad \frac{p^2}{2m} + \varphi(r) < \epsilon_F$$

Thus the number of states belonging to a volume  $d^3p d^3r$  in phase space is  $2 \frac{d^3p d^3r}{(2\pi\hbar)^3}$ . So in a small volume  $dr$  the number of electrons, namely  $\rho(r) dr$ , should have their momenta distributed in such a way as to fill up all the possible states with position  $r$  and energy  $< \epsilon_F$ . Thus

$$\rho(r) = 2 \frac{\text{volume of } \frac{p^2}{2m} + \varphi(r) < \epsilon_F}{(2\pi\hbar)^3} = 2 \frac{1}{(2\pi\hbar)^3} \frac{4}{3} \pi (2m(\epsilon_F - \varphi(r)))^{3/2}$$

Finally  $\varphi(r)$  is determined from  $\rho(r)$  by Poisson's equation

$$\Delta \varphi = 4\pi e \rho \quad -e = \text{charge of electron}$$

together with the boundary condition that

$$\varphi(r) \sim -\frac{Ze^2}{r} \quad \text{as } r \rightarrow 0$$

In connection with the "Weyl" formula  $\circledast$ , recall Victor checked it for the harmonic oscillator. One needs:

$$\text{Vol unit ball in } \mathbb{R}^{2n} = \frac{\pi^n}{n!}$$

Is this related to the  $\pi^{-s/2} \Gamma(s/2)$  in the ful. eqn. for  $\zeta$ ?