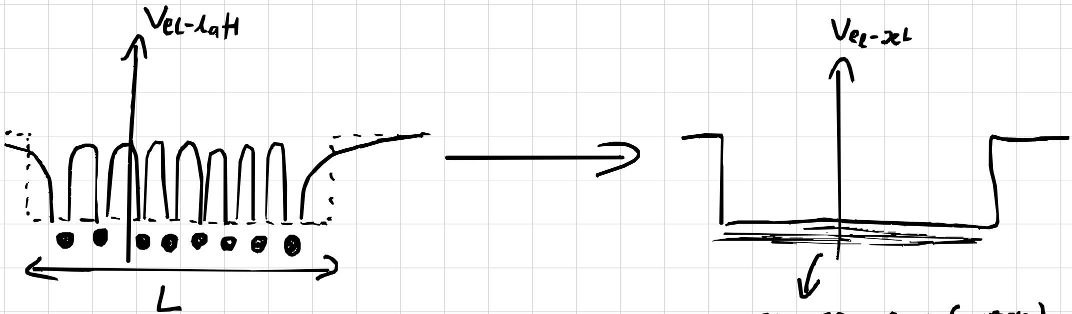
THE JELLIUM MODEL



SMEARED OUT (UNIFORM) CHARGE DENSITY OF IONS

$$H = H_{el} + H_{ion} + H_{el\text{-}ion}$$

$$H_{ion} = \frac{1}{2}\tilde{e}^2 \int d\vec{r} \int d\vec{r}\,' \frac{n(\vec{r})n(\vec{r}\,')}{|\vec{r}-\vec{r}\,'|} e^{-\kappa|\vec{r}-\vec{r}\,'|}$$

(KINETIC ENERGY OF IONS NEGLECTED)

$$H_{el\text{-}ion} = -\tilde{e}^2 \sum_{i=1}^{N} \int d\vec{r} \frac{n(\vec{r})}{|\vec{r}-\vec{r}_i|} e^{-\kappa|\vec{r}-\vec{r}_i|}$$

$$H_{el} = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \frac{1}{2}\tilde{e}^2 \sum_{i\neq j} \frac{1}{|\vec{r}_i-\vec{r}_j|} e^{-\kappa|\vec{r}_i-\vec{r}_j|}$$

- FOR NOW WRITTEN CLASSICALLY
- IN A WHILE WE PUT $n(\vec{r}) = \frac{N}{V} = \text{const}$ ↳ jellium
- $\kappa \to 0^+$ recovers Coulomb.

- $$H_{ion} \overset{\text{jellium}}{=} \frac{1}{2}\tilde{e}^2 \left(\frac{N}{V}\right)^2 \int d\vec{r} \int d\vec{r}\,' \frac{e^{-\kappa|\vec{r}-\vec{r}\,'|}}{|\vec{r}-\vec{r}\,'|} = \left\{\vec{x} = \vec{r}-\vec{r}\,'\right\} = \frac{1}{2}\tilde{e}^2 \left(\frac{N}{V}\right)^2 V \int d\vec{x} \frac{e^{-\kappa x}}{x} =$$
$$= \frac{1}{2}\tilde{e}^2 \frac{N^2}{V} 4\pi \int_0^\infty dx\, x e^{-\kappa x} = \frac{1}{2}\tilde{e}^2 \frac{N^2}{V} \frac{4\pi}{\kappa^2}$$

$$\frac{H_{ion}}{N} = \frac{1}{2}\tilde{e}^2 \frac{N}{V}\frac{4\pi}{\kappa^2} \xrightarrow{\kappa\to 0} \infty \;!$$

REASON — LONG RANGE OF INTERACTIONS. EVERYTHING IS FINITE AS LONG AS $\kappa > 0$.

- $$H_{el\text{-}ion} \overset{\text{jellium}}{=} -\tilde{e}^2 \sum_{i=1}^{N} \frac{N}{V} \underbrace{\int d\vec{r} \frac{e^{-\kappa|\vec{r}-\vec{r}_i|}}{|\vec{r}-\vec{r}_i|}}_{=\frac{4\pi}{\kappa^2}} = -\tilde{e}^2 \frac{N^2}{V}\frac{4\pi}{\kappa^2}$$

$$\frac{H_{el\text{-}ion}}{N} = -\tilde{e}^2 \frac{N}{V}\frac{4\pi}{\kappa^2} \xrightarrow{\kappa\to 0} -\infty$$

$$(*)\quad \frac{H_{el\text{-}ion}}{N} + \frac{H_{ion}}{N} = -\frac{1}{2}\frac{N}{V}\tilde{e}^2\frac{4\pi}{\kappa^2} \to -\infty$$

WE ARE HERE INTERESTED IN THE PHYSICS OF ELECTRONS. THE POSITIVE CHARGE BACKGROUND IS NECESSARY FOR CANCELLING THE DIVERGENT CONTRIBUTIONS. THE ELECTRONIC PART OF THE HAMILTONIAN WE TREAT QUANTUM-MECHANICALLY.

$$H_{el} = \underbrace{\sum_{\bar{k}\sigma} \frac{\hbar^2 \bar{k}^2}{2m} a^\dagger_{\bar{k}\sigma} a_{\bar{k}\sigma}}_{H_0} + \underbrace{\frac{1}{2V} \sum_{\sigma_1\sigma_2} \sum_{\bar{k}_1\bar{k}_2\bar{q}} V_{\bar{q}}\, a^\dagger_{\bar{k}_1+\bar{q},\sigma_1} a^\dagger_{\bar{k}_2-\bar{q}\,\sigma_2} a_{\bar{k}_2\sigma_2} a_{\bar{k}_1\sigma_1}}_{V_{el\text{-}el}}$$

$$V_{\bar{q}} = \frac{4\pi\tilde{e}^2}{\bar{q}^2 + k^2}$$

ISOLATE THE TERM WITH $\bar{q}=0$ IN THE INTERACTION TERM:

THIS GIVES: $\underbrace{\frac{1}{2V} \frac{4\pi\tilde{e}^2}{k^2}}_{V^0_{el\text{-}el}} \sum_{\sigma_1\sigma_2} \sum_{\bar{k}_1\bar{k}_2} \underbrace{a^\dagger_{\bar{k}_1\sigma_1} a^\dagger_{\bar{k}_2\sigma_2} a_{\bar{k}_2\sigma_2} a_{\bar{k}_1\sigma_1}} =$

$$= - a^\dagger_{\bar{k}_2\sigma_2} \underbrace{a^\dagger_{\bar{k}_1\sigma_1} a_{\bar{k}_2\sigma_2}} a_{\bar{k}_1\sigma_1}$$

$$= - a_{\bar{k}_2\sigma_2} a^\dagger_{\bar{k}_1\sigma_1} + \delta_{\bar{k}_1\bar{k}_2} \delta_{\sigma_1\sigma_2}$$

$$= \frac{1}{2V} \frac{4\pi\tilde{e}^2}{k^2} \sum_{\sigma_1\sigma_2} \sum_{\bar{k}_1\bar{k}_2} \left(\hat{n}_{\bar{k}_2\sigma_2} \hat{n}_{\bar{k}_1\sigma_1} - a^\dagger_{\bar{k}_2\sigma_2} a_{\bar{k}_1\sigma_1} \delta_{\bar{k}_1\bar{k}_2} \delta_{\sigma_1\sigma_2} \right) =$$

$$= \frac{1}{2V} \frac{4\pi\tilde{e}^2}{k^2} \left(\hat{N}^2 - \hat{N} \right) \sim \underbrace{\frac{\tilde{e}^2}{2} \frac{N^2}{V} \frac{4\pi}{k^2}} - \frac{\tilde{e}^2}{2} \frac{N}{V} \frac{4\pi}{k^2}$$

WHEN WE EVALUATE MATRIX ELEMENTS OF THIS ON ANY STATES OF GIVEN PARTICLE NUMBERS

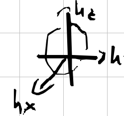
CANCELS (*) FROM PREVIOUS PAGE !!

THE SECOND TERM ABOVE GIVES 0 AFTER THERMODYNAMIC LIMIT.

NOW WE WANT TO IMPLEMENT P.T. TO ANALYZE THE IMPACT OF INTERACTIONS ON THE GROUND STATE ENERGY OF THE SYSTEM.

IN ABSENCE OF INTERACTIONS WE KNOW THE GS $= |FS\rangle$
$\rightarrow$ 1-PARTICLE STATES FILLED UP TO THE FERMI ENERGY ϵ_F.

AND EMPTY ABOVE , $\epsilon_F = \frac{\hbar^2 k_F^2}{2m}$



FOR THE NON-INTERACTING SYSTEM WE RECALL: $E = T = \frac{3}{5} N \epsilon_F$

ALSO RECALL: $\epsilon_F \sim n^{\frac{2}{3}}$.

UNDER WHAT CIRCUMSTANCES P.T IN H_{INT} MAKES SENSE?

THE KINETIC ENERGY SHOULD DOMINATE THE INTERACTION ENERGY.

WE HAVE $\frac{T}{N} \sim n^{\frac{2}{3}}$

CAN WE CRUDELY ESTIMATE H_{INT} AS SOME POWER OF n?

$$\frac{V}{N} \sim \frac{\tilde{e}^2}{\bar{d}}$$

"AVERAGE" DISTANCE BETWEEN PARTICLES $\quad \bar{d} \sim \left(\frac{V}{N}\right)^{\frac{1}{3}} = n^{\frac{1}{3}}$

$$\frac{V}{T} \sim \frac{n^{\frac{1}{3}}}{n^{\frac{2}{3}}} = n^{-\frac{1}{3}} \xrightarrow{n \to \infty} 0$$

T DOMINATES OVER V IN THE LIMIT OF LARGE DENSITIES

WE COULD USE THE DIAGRAMMATIC TOOLS TO SET UP P.T. (AT $T \to 0$ $\quad \Omega = U - \mu N = E - \epsilon_F N$). WE WILL INSTEAD USE HERE TRADITIONAL P.T. TO SEE WE GET THE SAME DIAGRAMS AND VISUALIZE THEIR MEANING IN THE PRESENT CONTEXT. (FOR THIS CASE THIS IS ALSO A BIT FASTER)

1ST ORDER P.T.: $\qquad \sum_q{}' \stackrel{df}{=} \sum_{q \neq 0}$

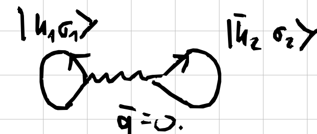
$$\frac{E^{(1)}}{N} = \langle FS | V_{el-el} | FS \rangle = \frac{1}{2VN} \sum_{q k_1 k_2}{}' \sum_{\sigma_1 \sigma_2} \frac{4\pi \tilde{e}^2}{q^2 + \mu^2} \cdot$$

$$\cdot \langle FS | a^{\dagger}_{k_1+q\sigma_1} a^{\dagger}_{k_2-q\sigma_2} a_{k_2\sigma_2} a_{k_1\sigma_1} | FS \rangle$$

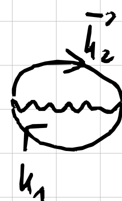
OBSERVE: • $a_{\bar k_2 \sigma_2} a_{\bar k_1 \sigma_1} |FS\rangle \neq 0$ ONLY IF $\bar k_2, \bar k_1$ ARE BELOW THE FERMI LEVEL.

• $\langle FS|$ $\Rightarrow$ THEREFORE $a^+_{\bar k_1 + \bar q \sigma_1} a^+_{\bar k_2 - \bar q \sigma_2}$ MUST BRING THE STATE OF THE SYSTEM AGAIN TO $|FS\rangle$.

$\Rightarrow$ EITHER $\left.\begin{array}{l} \bar k_1 + \bar q = \bar k_1 \\ \bar k_2 - \bar q = \bar k_2 \end{array}\right\} \Rightarrow \bar q = 0$



OR $\vec k_1 = \bar k_2 - \bar q$
$\vec k_2 = \bar k_1 + \bar q$
$\sigma_1 = \sigma_2$
(COMPARE "CONTRACTIONS")



$\vec q = \bar k_2 - \bar k_1$

$\longrightarrow$ THE TWO FAMILIAR DIAGRAM FROM EXPANSION OF Ω !

HERE THEY HAVE AN INTERPRETATION VIA "INTERACTION PROCESSES". (THE TWO HERE – SO CALLED "DIRECT" AND "EXCHANGE".)

THE FIRST DIAGRAM GIVES NO CONTRIBUTION FOR $\bar q \neq 0$. AS WE HAVE ALREADY SHOWN THE $\bar q = 0$ TERMS SERVE ONLY TO CANCEL THE BACKGROUND. WE CAN RESTRICT TO $\bar q \neq 0$.

$$\circledast \overset{\bar q \neq 0}{=} \delta_{k_2, k_1 + \bar q}\, \delta_{\sigma_1 \sigma_2} \langle FS| a^+_{\bar k_1 + \bar q, \sigma_1} \underbrace{a^+_{\bar k_1 \sigma_1} a_{\bar k_1 + \bar q\, \sigma_1}}_{= -a_{\bar k_1 + \bar q \sigma_1} a^+_{\bar k_1 \sigma_1}} a_{\bar k_1 \sigma_1} |FS\rangle =$$

$$= -\delta_{\bar k_2, \bar k_1 + \bar q}\, \delta_{\sigma_1 \sigma_2} \langle FS| \hat n_{\bar k_1 + \bar q \sigma_1} \hat n_{\bar k_1 \sigma_1} |FS\rangle =$$

$$= -\delta_{\bar k_2, \bar k_1 + \bar q}\, \delta_{\sigma_1 \sigma_2}\, \Theta\left(k_F - |\bar k_1|\right) \Theta\left(k_F - |\bar k_1 + \bar q|\right)$$

THE σ-SUMMATIONS IS TRIVIAL $\rightarrow$ GIVES A FACTOR OF 2.
WE INTRODUCE $\vec k_1 = \vec k$, AND FIND:

$$\frac{E^{(1)}}{N} = -\frac{1}{2NV}\sum_{\vec{q}\neq 0}\sum_{\vec{k}}\sum_{\sigma}\frac{4\pi\tilde{e}^2}{q^2+\kappa^2}\,\Theta\left(k_F-|\vec{k}+\vec{q}|\right)\Theta\left(k_F-|\vec{k}|\right) =$$

NEGATIVE IN SIGN!

$$\sum_{\vec{q}\neq 0} \to \frac{V}{(2\pi)^3}\int d\vec{q} \qquad \sum_{\vec{k}} \to \frac{V}{(2\pi)^3}\int d\vec{k} \qquad \sum_{\sigma} \to 2$$

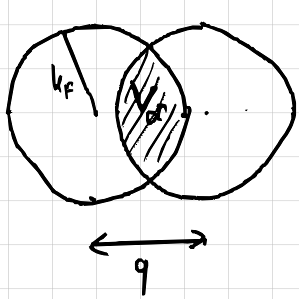
$$\overset{V\to\infty}{=} -\frac{2}{2NV}\frac{V^2}{(2\pi)^6}\left(4\pi\tilde{e}^2\right)\int d\vec{q}\int d\vec{k}\,\frac{1}{q^2+\kappa^2}\,\Theta\left(k_F-|\vec{k}+\vec{q}|\right)\Theta\left(k_F-|\vec{k}|\right)$$

IS IT SAFE TO PUT $\kappa = 0$? YES! THE INTEGRAL CONVERGES.

INTEGRATION: FIRST OVER $d\vec{k}$

THIS IS V_α!

(NONZERO ONLY FOR $q < 2k_F$)



RESULT: $V_\alpha = \frac{4}{3}\pi k_F^3\left[1-\frac{3}{2}\frac{q}{2k_F}+\frac{1}{2}\left(\frac{q}{2k_F}\right)^3\right]\Theta\left(2k_F-|\vec{q}|\right)$

$\to$ HOMEWORK SEE NEXT PAGE $\to$

THEN OVER $d\vec{q}$

RESULT: $\frac{E^{(1)}}{N} = -\frac{\tilde{e}^2}{2\pi^3}\frac{1}{n}\frac{k_F^4}{2}$

COLLECTING: $\frac{E}{N} \simeq \frac{E^{(0)}+E^{(1)}}{N} = \left(\frac{2.211}{r_s^2} - \frac{0.916}{r_s}\right)Ry$

$\simeq$: 1ST ORDER P.T! $\to$ AT HIGH DENSITIES

$\frac{2.211}{r_s^2}$: KINETIC ENERGY

$\frac{0.916}{r_s}$: EXCHANGE ENERGY.

{ FOR THE PROBLEM OF INTERACTING CHARGES RELEVANT ENERGY AND LENGTH SCALES:

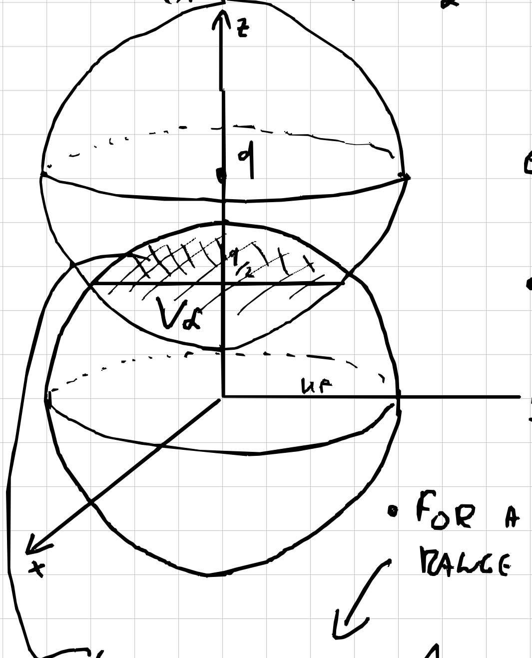
$a_0 = \frac{\hbar^2}{m\tilde{e}^2} \simeq 0.053\ \mathrm{nm}$ (BOHR RADIUS)

$E_0 = -\frac{\tilde{e}^2}{2a_0} = -13.6\,eV = -1\,Ry$ }

$r_s := \frac{V}{\left(\frac{4}{3}\pi a_0\right)^3} = N$ $\to$ {RADIUS OF A BALL CONTAINING 1 electron IN UNITS OF a_0.}

$$\left(r_s = \left(\frac{9\pi}{4}\right)^{\frac{1}{3}}\frac{1}{a_0 k_F}\right)$$

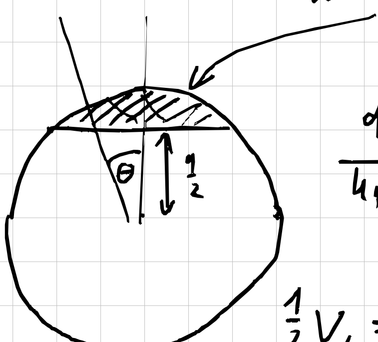
Calculation of V_α (spherical coordinates)



θ_{MAX}: $\cos\theta_{MAX} = \frac{q/2}{k_F}$

- $\theta \in [0, \theta_{MAX}[$
- $\varphi \in [0, 2\pi[$
- For a given θ what is the range of integration over k?

We calculate $\frac{1}{2} V_\alpha$



$$\frac{q/2}{k_{MIN}} = \cos\theta \to k_{MIN} = \frac{q}{2\cos\theta}$$

$$k_{MAX} = k_F$$

$$\frac{1}{2} V_\alpha = \int_0^{2\pi} d\varphi \int_0^{\theta_{MAX}} d\theta \int_{\frac{q}{2\cos\theta}}^{k_F} dk \, \sin\theta \, k^2 =$$

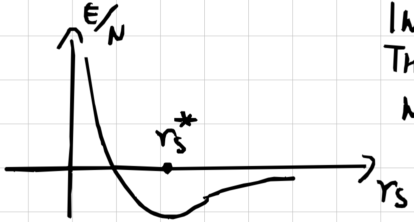
$$= 2\pi \int_0^{\theta_{MAX}} d\theta \, \sin\theta \, \frac{1}{3}\left[k_F^3 - \frac{q^3}{8\cos^3\theta}\right] = \left\{ \begin{array}{l} u = +\cos\theta \\ du = -\sin\theta \, d\theta \end{array} \right\}$$

$$= -\frac{2}{3}\pi \int_1^{q/2k_F} du \left[k_F^3 - \frac{q^3}{8} u^{-3}\right] = -\frac{2}{3}\pi \left[k_F^3\left(\frac{q}{2k_F} - 1\right) - \frac{q^3}{8}\frac{1}{-2}\left(\left(\frac{q}{2k_F}\right)^{-2} - 1\right)\right]$$

$$= -\frac{2}{3}\pi k_F^3\left[\frac{q}{2k_F} - 1 + \frac{q^3}{16k_F^3}\frac{4k_F^2}{q^2} - \frac{q^3}{16k_F^3}\right] = \frac{2}{3}\pi k_F^3\left[1 - \frac{3}{4}\frac{q}{k_F} + \frac{q^3}{16k_F^3}\right]$$

$$\Rightarrow V_\alpha = \frac{4}{3}\pi k_F^3\left[1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3\right]\Theta(2k_F - |q|)$$

NICE RESULT!



INTERACTIONS STABILIZE THE SYSTEM. THE EXTERNAL POTENTIAL IS NOT NECESSARY TO KEEP THE SYSTEM STABLE.

THERE EXISTS AN OPTIMAL r_s^* (OR n^*), WHICH MINIMIZES E.

$$r_s^* = 4.83.$$

$$\frac{E^*}{N} = -0.095\ Ry$$

EXPERIMENT E.G. Na $r_s = 3.96$

$$\frac{E}{N} = -0.083\ Ry$$

NOT SO BAD! (CONSIDERING THE LOW LEVEL OF THE CALCULATION).

ENCOURAGING!

PERHAPS WE MIGHT STILL IMPROVE BY GOING TO SECOND ORDER IN P.T. LET'S SEE...

$\bar{q} = 0$ EXCLUDED.

$$\frac{E^{(2)}}{N} = \frac{1}{N} \sum_{|\nu\rangle \neq |FS\rangle} \frac{\langle FS | V_{el-el} | \nu \rangle \langle \nu | V_{el-el} | FS \rangle}{E^{(0)} - E_\nu}$$

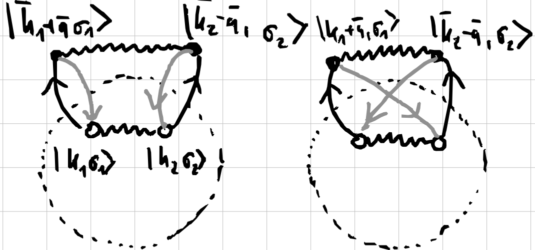
$|\nu\rangle \neq |FS\rangle \rightarrow$ INTERMEDIATE STATES, WHERE TWO ELECTRONS ARE EJECTED OUT OF THE FERMI SPHERE.

FROM SUCH INTERMEDIATE STATES THE $|FS\rangle$ IS RESTORED BY PUTTING THE EXCITED ELECTRONS BACK INTO THE HOLES.

$$|\nu\rangle = \Theta(|\bar{k}_1 + \bar{q}| - k_F)\,\Theta(|\bar{k}_2 - \bar{q}| - k_F)\,\Theta(k_F - |\bar{k}_1|)\,\Theta(k_F - |\bar{k}_2|) \cdot$$

$$\cdot\, a^\dagger_{\bar{k}_1+\bar{q}\sigma_1} a^\dagger_{\bar{k}_2-\bar{q}\sigma_2} a_{\bar{k}_2\sigma_2} a_{\bar{k}_1\sigma_1} |FS\rangle$$

THERE ARE TWO DIFFERENT CONTRIBUTIONS:



(DIRECT) (EXCHANGE)

LET US FIRST <u>EXAMINE THE DIRECT ONE.</u>

TO GO BACK TO $|FS\rangle$ FROM $|\nu\rangle$ WE MUST HAVE THE SAME $\bar q$ INVOLVED BOTH IN $\langle\nu|V_{ee-ee}|FS\rangle$ AND IN $\langle FS|V_{ee-ee}|\nu\rangle$ AND WE OBTAIN:

$$\frac{E^{(2)}_{DIR}}{N} = \frac{1}{N}\sum_{\bar q}\sum_{\bar k_1 \bar k_2}\sum_{\sigma_1\sigma_2}\frac{1}{(2V)^2}\frac{(V_q)^2}{E^{(0)}-E_\nu}\Theta(|\bar k_1+\bar q|-k_F)\Theta(|\bar k_2-\bar q|-k_F)\cdot$$
$$\cdot\,\Theta(k_F-|\bar k_1|)\Theta(k_F-|\bar k_2|)$$

$$V_q \sim \frac{1}{q^2+\kappa^2} \overset{\kappa=0}{=} \frac{1}{q^2}$$

$$\sum_{k_1/k_2} \longrightarrow \int\frac{d\bar k_{1/2}}{(2\pi)^3}$$

$$\sum_q \longrightarrow \int\frac{d^3q}{(2\pi)^3}$$

LIMIT $\kappa\to 0^+$

POWER counting at q SMALL:

$$V_q^2 \sim \frac{1}{q^4}$$

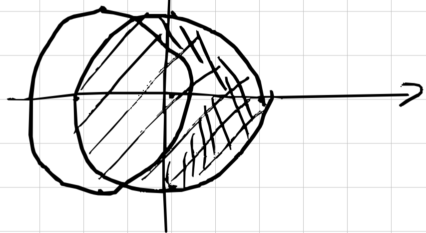
$$E^{(0)}-E_\nu \sim k_1^2+k_2^2-(\bar k_1+\bar q)^2-(k_2-\bar q)^2$$
$$\sim q$$

SEE NEXT PAGE $\circledast \longrightarrow$

$$\sum_{k_1}\Theta(|k_1+q|-k_F)\Theta(k_F-\bar k_1) \sim q$$

$$\frac{E^{(2)}_{DIR}}{N} \sim \int_0 \underbrace{dq\,q^2}_{\text{JACOBIAN}}\ \overbrace{\frac{1}{q^4}}^{\sim V_q^2}\ \overbrace{\frac{1}{q}}^{E_0-E_\nu}\ \underbrace{q}_{\sum_{k_1}}\ \underbrace{q}_{\sum_{k_2}} \sim \int_0 dq\,\frac{1}{q} = \infty$$

$$\int d\bar{k}\, \Theta(k_F - |\bar{k}|)\, \Theta(|\bar{k}+\bar{q}| - k_F) \ldots$$



RESTRICTS THE REGION OF INTEGRATION TO VOLUME OF ONE SPHERE MINUS THE VOLUME OF THE OVERLAP REGION WHICH WE ALREADY CALCULATED. The resulting volume:

$$\to V_{\Gamma_k} = \frac{4}{3} k_F^3 - \frac{4}{3}\pi k_F^3 \left[1 - \frac{3}{2}\frac{q}{2k_F} + \frac{1}{2}\left(\frac{q}{2k_F}\right)^3\right] \sim q$$

FOR THE EXCHANGE TERM IT IS SIMILAR, BUT

$$\left(V_{\bar{q}}\right)^2 \longrightarrow V_{\bar{q}}\, V_{\bar{k}_2-\bar{k}_1-\bar{q}} \sim \frac{1}{q^2}$$

AND THE INTEGRAL CONVERGES...

THIS IS A SURPRISE. AT 1ST ORDER P.T GIVES PHYSICALLY APPEALING RESULT, BUT THE 2ND ORDER CORRECTION IS INFINITE! $E^{(2)}_{dir} \sim \int_0 dq\, q^2 \frac{1}{(q^2+k^2)^2} \frac{1}{q} q q \sim -\ln k$

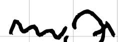
ALL IS FINITE FOR $k>0$. → THE REASON FOR DIVERGENCIES COMES FROM LONG-RANGE (COULOMB) INTERACTIONS.

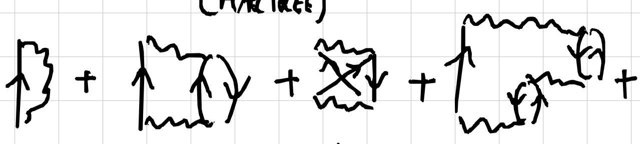
PERHAPS THERE ARE CANCELLATIONS BETWEEN DIVERGENT TERMS IF WE CONSIDER P.T AT HIGHER ORDER?
TO DIAGNOSE THIS WE NEED TO BETTER UNDERSTAND THE ENTIRE STRUCTURE OF THE P.T. FOR THIS CASE.

KEEP THE PROBLEM IN MIND. THERE EXISTS A WAY OF CONNECTING THE SYSTEM'S INTERNAL ENERGY (GS ENERGY FOR $T=0$) TO THE SELF-ENERGY. LET US NOW EXAMINE THE PT. FOR THE SELF-ENERGY OF THE ELECTRONIC GAS:

RECALL $\Sigma_\sigma(i\omega_n, \vec{k})$ = SUM OF IRREDUCIBLE DIAGRAMS WITH THE EXTERNAL LINES REMOVED.

WE EXCLUDE $\vec{q}=0$ (THIS CANCELS THE BACKGROUND.)

THEREFORE THE  DIAGRAM VANISHES.
(HARTREE)

$\Sigma_\sigma(i\omega_n, \vec{k}) =$  $+ \ldots$

AT EACH ORDER IN INTERACTION V WE WILL IDENTIFY THE MOST IMPORTANT TERMS AND RESUM THE EXPANSION TAKING ONLY THESE TERMS INTO ACCOUNT.

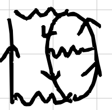
• DENSITY DEPENDENCE OF SELF-ENERGY DIAGRAMS

TAKE AN ARBITRARY SELF-ENERGY DIAGRAM OF ORDER n in V.

NOTATION: $(i\omega_n, \vec{k}) \to k$.

$$\Sigma^{(n)}(k) \sim \underbrace{\int dk_1 \dots \int dk_n}_{n \text{ internal momenta / frequencies}} \underbrace{V() \dots V()}_{n \text{ interaction vertices}} \underbrace{g_0() \dots g_0()}_{2n-1 \text{ (noninteracting) G. functions}}$$

E.G.



BECAUSE WE HAVE:

- $2n-1$ g_0s
- n momentum-conserving δs AT VERTICES, ONE OF THEM REDUNDANT.

BECAUSE n VERTICES $\Rightarrow 4n-2$ legs, EACH g_0 TAKES CARE OF 2 LEGS.

$$(2n-1)-(n-1) = n \to \text{NUMBER OF } \int dk$$

WE CAN MAKE THE INTEGRAL DIMENSIONLESS: AND PULL OUT THE FACTORS OF k_F.

MEASURE MOMENTA AND FREQUENCIES IN POWERS OF k_F

$$\left.\begin{aligned} |\vec{k}| &\sim k_F \\ \varepsilon &= \frac{k_F^2}{2m} \sim k_F^2 \\ \beta^{-1} &= k_B T \sim k_F^2 . \end{aligned}\right\} \to \begin{aligned} \int dk_1 &\sim \frac{1}{\beta} \sum_{\omega_n} \int \frac{d^3k}{(2\pi)^3} \sim k_F^{2+3} = k_F^5 \\ V(q) &\sim \frac{1}{q^2+k^2} \sim k_F^{-2} \\ g_0 &= \frac{1}{i\omega_n - \varepsilon_k} \sim k_F^{-2} \end{aligned}$$

$$\Sigma^{(n)}(k) \sim (k_F^5)^n (k_F^{-2})^n (k_F^{-2})^{2n-1} = k_F^{-n+2} \sim r_s^{n-2}$$

$$r_s = \left(\frac{9\pi}{4}\right)^{\frac{1}{3}} \Big/ a_0 k_F .$$

WE ARE WORKING WITH PT (MEANING IN THE HIGH-DENSITY LIMIT) $\Rightarrow r_s \ll 1$. $(k_F \to \infty)$

WE FOUND $n < n' \Rightarrow |\Sigma_\sigma^{(n)}(k)| \gg |\Sigma_\sigma^{(n')}(k)|$ FOR $r_s \to 0$.

$\to$ ALSO NOTE THAT THIS AGREES WITH THE PREVIOUS RESULTS AT 0-TH $(n=0)$ AND 1ST $(n=1)$ ORDER of P.T.

- THE DIVERGENCE NUMBER OF SELF-ENERGY DIAGRAMS

RECALL THE DIVERGENCE OF THE 2^{nd} order energy correction

$$E^{(2)}_{div} \sim \int \frac{1}{q} \, dq \to \infty \qquad \left(\frac{1}{(q^2+\mu^2)^2} \right)$$

THE MORE INTERACTION LINES CARRYING THE SAME MOMENTUM THERE ARE IN A DIAGRAM THE MORE DIVERGENT IS THE DIAGRAM.

E.G. $(\mu=0)$ TWO LINES WITH MOMENTUM $\bar{q}$ CONTRIBUTE $V(\bar{q})^2 \sim \frac{1}{q^4}$. IN CONTRAST, TWO LINES WITH DIFFERENT MOMENTA $\bar{q}$ AND $\bar{p}$ CONTRIBUTE $V(\bar{q})V(\bar{p}) \sim \frac{1}{\bar{q}^2 \bar{p}^2}$

DEFINE A DIVERGENCE NUMBER $\delta^{(n)}$ OF ANY SELF-ENERGY DIAGRAM AS

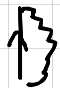
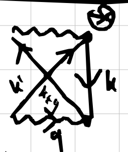
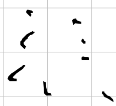
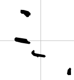
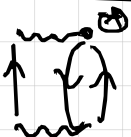
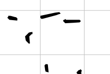
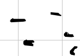
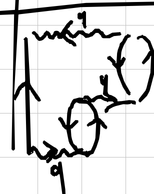
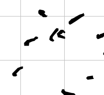
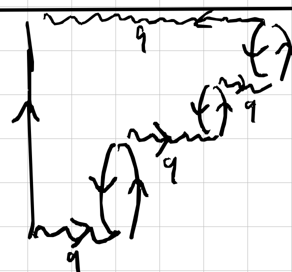
$$\delta^{(n)} = \text{THE LARGEST NUMBER OF INTERACTION LINES IN } \Sigma_\sigma^{(n)}(k) \text{ having the same momentum } \bar{q}.$$

RPA RESUMMATION OF THE SELF-ENERGY

AT GIVEN ORDER IN P.T. THE MOST IMPORTANT TERMS ARE THE ONES WITH THE LARGEST DIVERGENCE NUMBER.

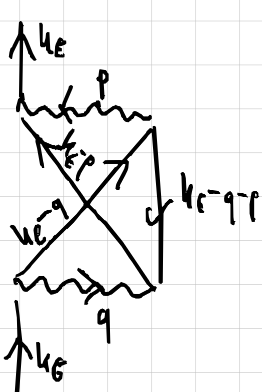
LETS DRAW A TABLE ILLUSTRATING THE SITUATION

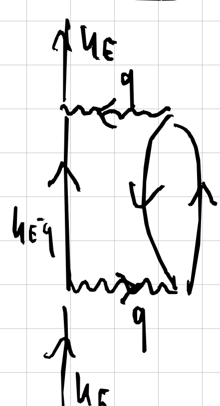
OF COURSE $\delta \leq n$

	$n=1$	$n=2$	$n=3$	$n=4$
$\delta=1$				
$\delta=2$	—			
$\delta=3$	—	—		
$\delta=4$	—	—	—	

AT GIVEN ORDER THE DIAGRAMS WITH THE HIGHEST DIVERGENCE NUMBER ARE THE MOST IMPORTANT.

⊛ RESOLVE THIS:

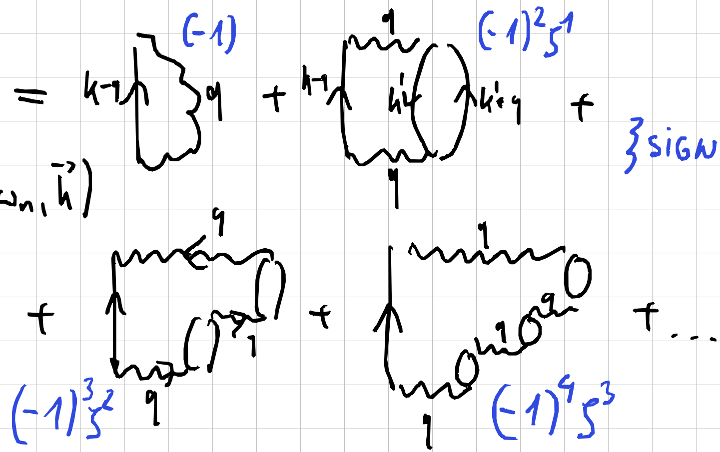




SELF-ENERGY IN THE RANDOM PHASE APPROXIMATION

→ CONSIDER P.T. AT INFINITE ORDER, BUT AT EACH ORDER RETAIN ONLY THE MOST IMPORTANT DIAGRAM.

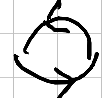
$\Sigma_\sigma^{RPA}(k) =$



$k = (i\omega_n, \vec{k})$

$\}\ \text{SIGN} = (-1)^n \xi^{n_e}$

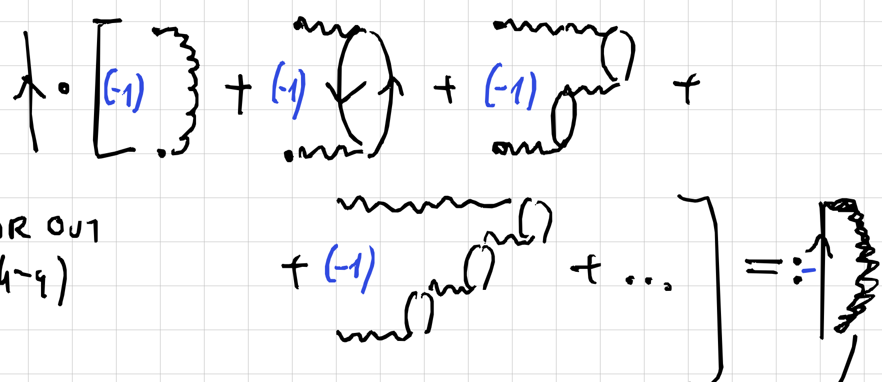
IMPORTANT CONSTITUENT: PAIR BUBBLE $\Pi^0(iq_n, \vec{q}) =$

$\equiv$ 

(EXPLICIT EVALUATION LATER ON)

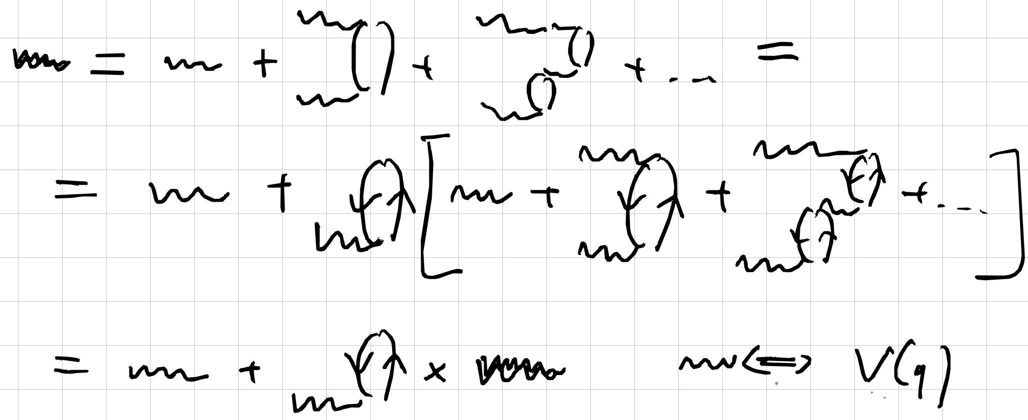
LET US ANALYZE THIS FURTHER (DIAGRAMMATICALLY)

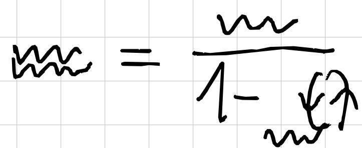
$\Sigma_\sigma^{RPA} =$



FACTOR OUT $g_0(k-q)$

RENORMALIZED $V^{RPA}(q)$ INTERACTION LINE



 $\to \quad V^{RPA}(q) = \dfrac{V(q)}{1 - V(q)\Pi_0(q)}$

$\Pi_0(q) =$  $\quad V(q) = \dfrac{4\pi \tilde{e}^2}{q^2 + \kappa^2}$

$$V^{RPA}(q) = \frac{\frac{4\pi\tilde{e}^2}{q^2+\kappa^2}}{1 - \frac{4\pi\tilde{e}^2}{q^2+\kappa^2}\Pi_0(q)} \xrightarrow[\text{SAFE!}]{\kappa \to 0} \frac{4\pi\tilde{e}^2}{q^2 - 4\pi\tilde{e}^2\Pi_0(q)}$$

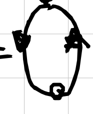
$V^{RPA}(q)$ HAS A FORM SIMILAR TO $V(q)$ BUT THE ARTIFICIAL PARAMETER κ BECAME REPLACED BY THE PAIR-BUBBLE FUNCTION!

PAIR BUBBLE $\to \Pi_0(q) = \Pi_0(\underbrace{iq_n}_{\text{FREQUENCY}}, \vec{q})$

FOR $q \to 0$ (IN Π_0) $\quad V^{RPA} \xrightarrow{q \to 0} \dfrac{4\pi\tilde{e}^2}{\vec{q}^2 + k_s^2}$ { k_s - Thomas-Fermi SCREENING WAVENUMBER } (SEE IN A WHILE)

$k_s^2 = \dfrac{4k_F}{\pi a_0}$ $\qquad$ METALS: $k_s \approx 0.1 \dfrac{1}{nm}$

THE PHYSICS OF SCREENING CAPTURED BY THE INFINITE RESUMMATION OF THE PERTURBATIVE SERIES

$\Pi_0(\vec{q}, iq_n) =$ 

$$= \frac{\overset{\text{SPIN}}{2}}{\beta}\sum_{ip_n}\int\frac{d^3p}{(2\pi)^3}\frac{1}{i(q_n+p_n) - \xi_{\vec{p}+\vec{q}}}\frac{1}{ip_n - \xi_{\vec{p}}}$$

EVALUATION OF THE PAIR BUBBLE

$$\chi_0(\vec{q}, iq_n) = \frac{2}{\beta} \sum_{ik_n} \int \frac{d^3k}{(2\pi)^3} \frac{1}{iq_n + ik_n - \xi_{\vec{q}+\vec{k}}} \frac{1}{ik_n - \xi_{\vec{k}}}$$

RECALL: $\displaystyle \frac{1}{\beta} \sum_{ik_n} \underbrace{\left(\prod_j \frac{1}{ik_n - z_j} \right)}_{f(ik_n)} e^{ik_n \epsilon} = \sum_j \operatorname*{Res}_{z = z_j} \left[f(z) \right] n_f(z_j) e^{z_j \epsilon}$

$f(z) = \prod_j \frac{1}{z - z_j}$ $\qquad n_f(x) = \frac{1}{e^{\beta x} + 1}$

OUR CASE: $\displaystyle \operatorname*{Res}_{\xi_{\vec{k}}} \left[\frac{1}{iq_n + ik_n - \xi_{\vec{q}+\vec{k}}} \frac{1}{iq_n - \xi_{\vec{k}}} \right] = \frac{1}{\xi_{\vec{k}} - \xi_{\vec{q}+\vec{k}} + iq_n}$

$$\operatorname*{Res}_{\xi_{\vec{k}+\vec{q}} - iq_n} \left[- \;\; " \;\; - \right] = \frac{1}{\xi_{\vec{k}+\vec{q}} - \xi_{\vec{q}} - iq_n}$$

$$\chi_0(iq_n, \vec{q}) = 2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{\xi_{\vec{k}} - \xi_{\vec{k}+\vec{q}} + iq_n} \left(n_f(\xi_{\vec{k}}) - n_f(\xi_{\vec{k}+\vec{q}} - iq_n) \right)$$

$$\left\{ q_n = \frac{2\pi n}{\beta} \qquad n_f(x - iq_n) = \frac{1}{e^{\beta x} e^{-i 2\pi n} + 1} = n(x) \right\}$$

$$\chi_0 = 2 \int \frac{d^3k}{(2\pi)^3} \frac{n_f(\xi_{\vec{k}+\vec{q}}) - n_f(\xi_{\vec{k}})}{\xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}} - iq_n}$$

STATIC LIMIT $\displaystyle \chi_0(0, \vec{q}) = 2 \int \frac{d^3k}{(2\pi)^3} \frac{n_f(\xi_{\vec{k}+\vec{q}}) - n_f(\xi_{\vec{k}})}{\xi_{\vec{k}+\vec{q}} - \xi_{\vec{k}}}$

STATIC AND LONG-WAVELENGTH LIMIT: $\qquad \approx \delta(\epsilon_F)$

$$\chi_0 \overset{\vec{q}^2 \to 0}{\simeq} 2 \int \frac{d^3k}{(2\pi)^3} \frac{\partial n_f}{\partial \xi_{\vec{k}}} = - \int d\xi_{\vec{k}} \, D(\epsilon_{\vec{k}}) \left(- \frac{\partial n_f}{\partial \xi_{\vec{k}}} \right) = -D(\epsilon_F)$$

$\displaystyle \sum_{k\sigma} \longrightarrow \int d\epsilon_k \, D(\epsilon_{\vec{k}})$ $\qquad$ CHANGE INTEGRATION TO $d\xi$, $k_B T \ll \epsilon_F$

RECALL:

$$V^{RPA} = \frac{4\pi\tilde{e}^2}{q^2 - 4\pi\tilde{e}^2\Pi_0(q)} \underset{q\to 0}{\downarrow} = \frac{4\pi\tilde{e}^2}{q^2 + \underbrace{4\pi\tilde{e}^2 \mathcal{D}(\epsilon_F)}_{k_s^2}}$$

Relates the screening length k_s^{-1} to microscopic parameters

For continuum Fermi gas $\left(\epsilon_k = \frac{\hbar^2 k^2}{2m}\right)$

$$k_s^2 = \frac{4}{\pi}\frac{k_F}{a_0}.$$

Connection between the GS energy and the 1-particle Green's function:

Consider $\lambda \in [0,1]$ and define $H_\lambda := \hat{H}_0 - \mu \hat{N} + \lambda \underbrace{\hat{V}}_{\text{COULOMB INT.}}$

$\lambda = 0 \rightarrow$ NONINTERACTING EL. GAS

$\lambda = 1 \rightarrow$ FULL COULOMB - INT

(VALID FOR ANY $\hat{V}$)

$$\Omega = U - TS - \mu N \qquad \Omega(\lambda) = -\frac{1}{\beta} \ln \mathrm{Tr}\left[e^{-\beta(\hat{H}_0 - \mu\hat{N} + \lambda\hat{V})}\right]$$

$$\frac{\partial \Omega}{\partial \lambda} = -\frac{1}{\beta} \frac{\mathrm{Tr}\left[-\beta\hat{V} e^{-\beta(\hat{H}_0 - \mu\hat{N} + \lambda\hat{V})}\right]}{\mathrm{Tr}\left[e^{-\beta(\hat{H}_0 - \mu\hat{N} + \lambda\hat{V})}\right]} = \langle \hat{V} \rangle_\lambda = \frac{1}{\lambda} \langle \lambda \hat{V} \rangle_\lambda$$

INTEGRATE OVER λ: $\Omega(1) - \Omega(0) = \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda \hat{V} \rangle_\lambda$

AT $T = 0$ WE HAVE $\Delta\Omega = \Delta E$

AND THE GS ENERGY FOLLOWS FROM $E = E^0 + \lim_{T \to 0} \int_0^1 \frac{d\lambda}{\lambda} \langle \lambda \hat{V} \rangle_\lambda$

WE WILL NOW RELATE $\langle \lambda \hat{V} \rangle_\lambda$ TO $G_\sigma^\lambda(\vec{k}, ik_n)$ VIA THE E.O.M. FOR G_σ^λ

$$\partial_\tau A(\tau) = \partial_\tau \left(e^{\tau H} A e^{-\tau H}\right) = e^{\tau H} [H, A] e^{-\tau H} = ([H, A])(\tau)$$

$$G(\nu\tau\, \nu'\tau') = -\left\langle T_\tau \left(a_\nu(\tau) a^\dagger_{\nu'}(\tau')\right)\right\rangle$$

$$-\partial_\tau G(\nu\tau, \nu'\tau') = \delta(\tau - \tau')\delta_{\nu\nu'} + \left\langle T_\tau \left\{ [H, a_\nu](\tau), a^\dagger_{\nu'}(\tau') \right\} \right\rangle$$

$$\Rightarrow -\partial_\tau \frac{1}{V} \sum_{\vec{k}\sigma} G_\sigma^\lambda(\vec{k}, \tau) = \frac{1}{V}\sum_{\vec{k}\sigma} \delta(\tau) + \frac{1}{V} \sum_{\vec{k}\sigma} \left\langle T_\tau \left\{ [H_\lambda, a_{\vec{k}\sigma}](\tau), a^\dagger_{\vec{k}\sigma} \right\} \right\rangle_\lambda$$

$$= \frac{1}{V}\sum_{\vec{k}\sigma} \delta(\tau) + \frac{1}{V} \sum_{\vec{k}\sigma} \left\{ \epsilon_{\vec{k}} G_\sigma^\lambda(\vec{k}, \tau) - 2 \sum_{\vec{k}'\sigma'\vec{q}} \frac{\lambda}{2} V(q) \left\langle T_\tau a^\dagger_{\vec{k}'\sigma'}(\tau) a_{\vec{k}'+\vec{q}\sigma'}(\tau) \cdot a_{\vec{k}-\vec{q}\sigma}(\tau) a^\dagger_{\vec{k}\sigma} \right\rangle_\lambda \right\}$$

PUT $\tau = 0^-$ AND NOTE THAT THE LAST TERM IS $\langle \lambda \hat{V} \rangle_\lambda$.

PUTTING $\tau = -\eta = -0^+$ WRITE $G_\sigma^\lambda(\vec{k}, -\eta) = \frac{1}{\beta} \sum_{ik_n} G_\sigma^\lambda(\vec{k}, ik_n) e^{ik_n \eta}$

$$\delta(-\eta) = \frac{1}{\beta} \sum_{ik_n} e^{ik_n \eta}$$

$$\rightarrow \frac{1}{\beta V} \sum_{ik_n} \sum_{\vec{k}\sigma} (ik_n - \varepsilon_{\vec{k}}) G_\sigma^\lambda(\vec{k}, ik_n) e^{ik_n \eta} = \frac{1}{\beta V} \sum_{ik_n, \vec{k}\sigma} e^{ik_n \eta} + 2\langle \lambda \hat{V} \rangle_\lambda$$

$$\rightarrow \frac{1}{\beta V} \sum_{ik_n} \sum_{\vec{k}\sigma} \Big[\underbrace{(ik_n - \varepsilon_{\vec{k}})}_{= G_\sigma^0(\vec{k}, ik_n)^{-1} = \Sigma_\sigma^\lambda + G_\sigma^{\lambda\,-1}} G_\sigma^\lambda(\vec{k}, ik_n) - 1 \Big] e^{ik_n \eta} = 2\langle \lambda \hat{V} \rangle_\lambda$$

$$\frac{1}{\beta V} \sum_{ik_n} \sum_{\vec{k}\sigma} \Sigma_\sigma^\lambda(\vec{k}, ik_n) G_\sigma^\lambda(\vec{k}, ik_n) e^{ik_n \eta} = 2\langle \lambda \hat{V} \rangle_\lambda$$

THIS LEADS TO

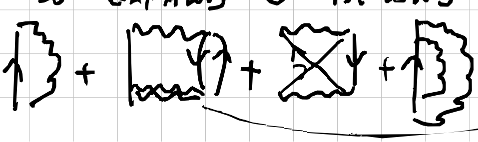
$$\boxed{E = E^0 + \lim_{T \to 0} \frac{1}{2\beta V} \sum_{ik_n} \sum_{\vec{k}\sigma} \int_0^\lambda \frac{d\lambda}{\lambda} \Sigma_\sigma^\lambda(\vec{k}, ik_n) G_\sigma^\lambda(\vec{k}, ik_n) e^{ik_n \eta} \quad \circledast}$$

REMARKABLE RESULT $\rightarrow$ RELATES THE GS ENERGY TO ONE-BODY G.F OF AN INTERACTING SYSTEM.

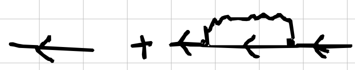
TO IMPROVE THE HIGH-DENSITY 2ND ORDER P.T, INCLUDE IN $\circledast$ ALL DIAGRAMS UP TO 2ND ORDER AND, THROUGH RPA, THE MOST DIVERGENT DIAGRAM OF EACH OF THE HIGHER ORDERS.

Σ CONTAINS DIAGRAMS FROM 1ST ORDER UP

$\Rightarrow$ NO NEED TO EXPAND G BEYOND 1ST ORDER.

$\Sigma_\sigma^\lambda(\vec{k}, ik_n) \simeq$ 

THE ONLY DIVERGENT DIAGRAM

$G^{\lambda}_{\sigma}(\vec{k}, ik_n) \simeq$ 

$E - E^0 \simeq \lim_{T\to 0} \int_0^1 \frac{d\lambda}{\lambda}$ 

$N \cdot \frac{2.211}{r_s^2}$

$-N \cdot \frac{0.916}{r_s}$

THOMAS-FERMI WAVENUMBER k_s REPLACES Λ AS MOMENTUM CUTOFF $\Rightarrow$ CONTRIBUTION PROPORTIONAL TO $\log k_s$

$N \cdot 0.0622 \log r_s$

$-N \cdot 0.094$

$$\frac{E}{N} \overset{r_s \to 0}{\simeq} \left(\frac{2.211}{r_s^2} - \frac{0.916}{r_s} + 0.0622 \log r_s - 0.094 \right) Ry.$$

The RPA resummation solves the problem of failed 2ND ORDER P.T.

RECALL

$k_s = \sqrt{\frac{4}{\pi} \frac{k_F}{a_0}}$, $r_s = \left(\frac{9\pi}{4}\right)^{1/3} \frac{1}{a_0 k_F}$ $\rightarrow \log k_s \sim \log r_s$.

HIGH DENSITY EXPANSION: r_s SMALL, k_F LARGE