Leiðin frá „hálf-sígildum" rafeindum í storku til skammtalíkana

frá einnar agnar líkönum til víxlverkandi fjöleinda líkana

Rafeindahreyfing <-> flutningur

Nálgun samkvæmt slökunar tíma

úr 13 kafla AM

Einu skrefi lengra..., Bolzmanns flutn osfr.

16 kafli AM

fjöleinda líkön skammtafræði (einföld H, HF, Corr.)

17 kafli AM

Viðbót við 17 kafla

línuleg svörun og svörunarföll <-> flutningar

Í 17 kafla er litið á skýlingu og svörunarföll

hér mætti bæta við samanburði um skýlingu í 2 og 3 víðum kerfum eða athuga borðareikninga, ... allt eftir tíma

4 vikur

Hvers vegna ekki beint yfir í fjöleinda líkön skammtafræðinnar?

- * Aðrar nálganir eru oft notaðar ⟺ þurfum að geta lesið greinar
- * Hollur samanburður til þess að skilja betur fjöleindalíkönin
- * Hvenær og hversvegna gilda hálfsígild fræði ekki alltaf við
- * ykkur vantar bakgrunn í fjöleindafr

stundum var þetta ástæðan

framhald í skammtafr. II undirbúnin
Kennilegri eðlisfr. þett.

Flutningur samkvæmt nálgun slökunartíma

- * Sígilda Drude líkanið

$$d_t \bar{p} = -e\left(\bar{E} + \frac{\bar{p}}{mc} \times \bar{B}\right) - \frac{\bar{p}}{\tau}$$

↑ slökunartími

- * Bohr-Sommerfeld líkanið

Fermidreifing + slökunartími
á einfaldan hátt

Athugum betur hugmyndir um slökunartíma

Nú eru allar upplýsingar um borðabyggingu teknar með.

Góður undirbúningur væru kaflar ① + ② + ⑫ í AM.

Rafeindadreifing í jafnvægi

$$f(E) = \frac{1}{e^{(E-\mu)/kT}+1} \qquad \text{fermi}$$

Ef ekki jafnvægi þá er
fjöldi rafeinda í borða n við tímann t
í hálf-sígilda fasarúminu $d\bar{r}d\bar{k}$
um punktinn $\bar{r},\bar{k}$

$$g_n(\bar{r},\bar{k},t)\,\frac{d\bar{r}\,d\bar{k}}{4\pi^3} \longleftarrow 2\,\frac{1}{(2\pi)^3}$$

→ í jafnvægi verður

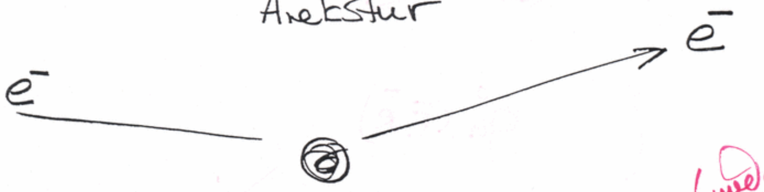
$$g_n(\bar{r},\bar{k},t) \to f(\mathcal{E}_n(\bar{k}))$$

(*) upplýsingar tapast!

(**) gerum ráð fyrir

smásætt líkan þurfi
að sýna þennan eiginleika

Árekstur



Gerum ráð fyrir

á tímabilinu dt eru árekstrarlíkur $dt/\tau_n(\bar{r},\bar{k})$

(meðal aldur ástands) (meðal tími milli árekstra)

Árekstrar beina kerfinu að jafnvægi (staðbu

- * dreifingin eftir er óháð dreifingunni fyri (*)
- * Ef rafeindirnar á svæði um $\bar{r}$ hafa jafnvægisdreifingu með staðbundna hitastigið $T(\bar{r})$ (**) þá breyta árekstrar ekki dreifingunni

Nægir til að ákvarða $dg_n(\bar{r},\bar{k},t)$: dreifingu rafeinda sem koma frá árekstri nærri $\bar{r}$ á bilinu dt um t

Jafnvægi ástands $\bar{k},n$ í hluta fasarúms

$g^0_n(\bar{r},\bar{k})$

út er tekið með árekstrum

$$\frac{dt}{\tau_n(\bar{r},\bar{k})} g^0_n(\bar{r},\bar{k})$$

inn kemur vegna árekstra

$dg_n(\bar{r},\bar{k},t)$

og er ekki í jafnvægi

fjöldi

nægir til að finna

$g_n(\bar{r},\bar{k},t)$

Ef $g_n(\bar{r},\bar{k},t) = g_n^0(\bar{r},\bar{k})$ hefur jafnvægisformið

→ dreifingin breytist ekki

(i)

$$\to \underbrace{dg_n(\bar{r},\bar{k},t)}_{\text{inn}} = \underbrace{\frac{dt}{\tau_n(\bar{r},\bar{k})}\, g_n^0(\bar{r},\bar{k})}_{\text{út}}$$

Ef $g_n(\bar{r},\bar{k},t)$ er ekki jafnvægisdreifing

fjöldi rafeinda í rúmmálinu $d\bar{r}d\bar{k}$ er

$$dN = g_n(\bar{r},\bar{k},t)\,\frac{d\bar{r}d\bar{k}}{4\pi^3} \qquad \text{(ii)}$$

$\bar{r}_n(t')$ og $\bar{k}_n(t')$ eru lausnir hreyfingajafnanna sem gefa

$$\bar{r}_n(t) = \bar{r}\,,\quad \bar{k}_n(t) = \bar{k} \quad \text{þ. } t' = t$$

síðasti árekstur þessara rafeinda var í dt' um t', þá komu þær í rúmmálið $d\bar{r}'d\bar{k}'$ þaðan sem hreyfingarjöfnurnar tóku þær

nú segir (i) að rafeindirnar sem komi frá árekstrum um $r_n(t'), k_n(t')$ inn í rúmmálið $d\bar{r}'\,d\bar{k}'$ í dt' um t' sé

$$\frac{dt'}{\tau_n(\bar{r}_n(t'),\bar{k}_n(t'))}\, g_n^0(\bar{r}_n(t'),\bar{k}_n(t'))\,\frac{d\bar{r}d\bar{k}}{4\pi^3}$$

$$\text{því} \quad d\bar{r}'d\bar{k}' = d\bar{r}d\bar{k} \quad \left(\begin{array}{c}\text{Liouville}\\ \text{viðh. M}\end{array}\right)$$

af þessum fjölda kemst aðeins brot $P_n(\bar{r},\bar{k},t;t')$ frá t' til t án frekari áreksturs

dN finnst því með að summa yfir alla mögulega t'

$$dN = \frac{d\bar{r}d\bar{k}}{4\pi^3}\int_{-\infty}^{t} \frac{dt'\, g_n^0(\bar{r}_n(t'),\bar{k}_n(t'))\, P_n(\bar{r},\bar{k},t;t')}{\tau_n(\bar{r}_n(t'),\bar{k}_n(t'))}$$

$$g(t) = \int_{-\infty}^{t} \frac{dt'}{\tau(t')} g^0(t') P(t,t')$$

summa yfir t'

fjöldi rafeinda sem koma inn á svæðið kl. t'

fjöldi sem kemst frá t' til t í sama „ástandi"

Samanburður við (ii) gefur

$$g_u(\bar{r},\bar{k},t) = \int_{-\infty}^{t} \frac{dt' \, g_u^0(\bar{r}_u(t'),\bar{k}_u(t')) P_u(\bar{r},\bar{k},t;t')}{\tau_u(\bar{r}_u(t'),\bar{k}_u(t'))}$$

Stytta táknum

$$g_u(\bar{r},\bar{k},t) \to g(t)$$

$$g_u^0(\bar{r}_u(t'),\bar{k}_u(t')) \to g^0(t')$$

$$\tau_u(\bar{r}_u(t'),\bar{k}_u(t')) \to \tau(t')$$

$$P_u(\bar{r},\bar{k},t;t') \to P(t,t')$$

$$\to \boxed{g(t) = \int_{-\infty}^{t} \frac{dt'}{\tau(t')} g^0(t') P(t,t')}$$

---

finna $P(t,t')$

$P(t,t')$ er minna en $P(t,t'+dt')$ sem nemur $\left\{1 - \frac{dt'}{\tau(t')}\right\}$

$$\to P(t,t') = P(t,t'+dt')\left\{1 - \frac{dt'}{\tau(t')}\right\}$$

$$\frac{P(t,t') - P(t,t'+dt')}{dt'} = -\frac{P(t,t'+dt')}{\tau(t')}$$

$dt' \rightarrow 0$

$$\rightarrow \quad \frac{\partial}{\partial t'} P(t,t') = \frac{P(t,t')}{\tau(t')}$$

upphafsgildi : $P(t',t') = 1$

$\rightarrow$ lausn er $P(t,t') = \exp\left\{ -\int_{t'}^{t} \frac{dt''}{\tau(t'')} \right\}$

og því

$$g(t) = \int_{-\infty}^{t} dt' \, g^0(t') \frac{\partial}{\partial t'} P(t,t')$$

hlutheildun með $P(t,-\infty) = 0$

$$\boxed{g(t) = g^0(t) - \int_{-\infty}^{t} dt' \, P(t,t') \frac{d}{dt'} g^0(t')}$$

$$\frac{d}{dt'} g^0(t') = \frac{\partial g^0}{\partial E_n} \frac{\partial E_n}{\partial \bar{k}} \cdot \frac{d\bar{k}_n}{dt'} + \frac{\partial g^0}{\partial T} \frac{\partial T}{\partial \bar{r}} \cdot \frac{d\bar{r}_n}{dt'}$$

$$+ \frac{\partial g^0}{\partial \mu} \frac{\partial \mu}{\partial \bar{r}} \cdot \frac{d\bar{r}_n}{dt'}$$

nota

$$\dot{\bar{r}}_n = \bar{v}_n(\bar{k}) = \frac{1}{\hbar} \frac{\partial E_n(\bar{k})}{\partial \bar{k}}$$

$$\hbar \dot{\bar{k}}_n = -e \left\{ \bar{E}(\bar{r},t) + \frac{1}{c} \bar{v}_n(\bar{k}) \times \bar{B}(\bar{r},t) \right\}$$

$$\frac{\partial g^0}{\partial E_n} = \frac{\partial f}{\partial \varepsilon} \qquad \frac{\partial g^0}{\partial \mu} = -\frac{\partial f}{\partial \varepsilon}$$

$$\frac{\partial g^0}{\partial T} = \frac{-1}{\left(e^{(\varepsilon-\mu)/kT} + 1\right)^2} e^{(\varepsilon-\mu)/kT} \cdot \frac{(\varepsilon-\mu)}{kT^2} (-1)$$

$$= -\frac{\partial f}{\partial \varepsilon} \frac{(\varepsilon-\mu)}{T}$$

$$\bar{v}_n \cdot \left(\bar{v}_n \times \bar{B} \right) = 0$$

Því fæst

$$g(t) = g^0 + \int_{-\infty}^{t} dt'\, P(t,t') \left\{ \left(-\frac{\partial f}{\partial \varepsilon}\right) \bar{v} \cdot \left(-e\bar{E} - \bar{\nabla}\mu - \left(\frac{\varepsilon-\mu}{T}\right)\bar{\nabla}T\right) \right. \qquad \text{(iii)}$$

$\uparrow$

háð t' í gegnum $\bar{r}_n(t')$ og $\bar{k}_n(t')$

athugum sér tilfelli

Veik svið

líkindi þess að rafeind verði ekki fyrir árekstri á milli t og t' snarminnka ef $|t-t'| > \tau$

því hefur $\bar{E}$ og $\bar{\nabla}T$ mjög lítinn tíma til þess að verka (og eru veik í mörgum til

→ span straumar eru línulegir í $\bar{E}$ og $\bar{\nabla}T$

þar sem (iii) er línuleg í $\bar{E}$ og $\bar{\nabla}T$ er því línuleg nálgun þ.a. sleppa má áhrifum $\bar{E}$ og $\bar{\nabla}T$ í öðrum hlutum fallsins sem heilda á

---

fast svið í tíma

→ óháð $r_n(t')$ $\quad$ $\bar{B}$ fasti í tíma $\varepsilon_n(\bar{k})$: ~~fasti~~ geymin stærð

$k_n(t')$ háð t' vegna $\bar{B}$

tíma verður að eins að finna í $P(t,t')$, $\bar{v}(k_n(t'))$ og $\bar{E}$, T

τ einungis háð $\varepsilon_n(\bar{k})$

→ τ er óháð t'

→ $P(t,t') = e^{-(t-t')/\tau_n(\bar{k})}$

$$g(\bar{k},t) = g^0(\bar{k}) + \int_{-\infty}^{t} dt'\, e^{-(t-t')/\tau(\varepsilon(\bar{k}))} \left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$\cdot\ \bar{v}(\bar{k}(t')) \bullet \left\{ -e\bar{E}(t') - \bar{\nabla}\mu(t') - \frac{\varepsilon(\bar{k})-\mu}{T} \nabla T \right.$$

$$\frac{\partial f}{\partial \varepsilon} \sim \dots f(1-f)$$

$\uparrow$

tómur eða fylltur borði leiðir ekki!

DC – leiðni

$\overline{B} = 0$, $\overline{\nabla} T = 0$, τ háð $\overline{k}$ í gegnum $\varepsilon_n(\overline{k})$

$$g(\overline{k}) = g^0(\overline{k}) - e\overline{E}\cdot v(\overline{k})\,\tau(\varepsilon(\overline{k}))\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

í einingarrúmmáli og rafeinda þéttleikinn í $d\overline{k}$ er $g(\overline{k})\frac{d\overline{k}}{4\pi^3}$

→ straumþéttleikinn í borða n er

$$J^n = -e\int \frac{d\overline{k}}{4\pi^3} v(\overline{k})\, g(\overline{k})$$

$$J^n_\mu = -e\int \frac{d\overline{k}}{4\pi^3} v_\mu(\overline{k})\, g^0 + e^2 \overline{E}_\mu \int \frac{d\overline{k}}{4\pi^3} v_\nu(\overline{k})\, v_\mu(\overline{k})\, \tau(\varepsilon(\overline{k}))\left(-\frac{\partial f}{\partial \varepsilon}\right)$$

$$\rightarrow \boxed{\sigma^{(n)} = e^2 \int \frac{d\overline{k}}{4\pi^3} \tau_n(\varepsilon(\overline{k}))\, v_n(\overline{k})\, v_n(\overline{k})\left(-\frac{\partial f}{\partial \varepsilon}\right)}$$

fyrir fylltan borða er $\frac{\partial f}{\partial \varepsilon} \neq 0$ aðeins þar sem enginn ástandsþéttleiki er

→ fylltir borðar leiða ekki

Í málmi $T_F >> T$

ef $T \sim 0$ $\rightarrow \left(-\frac{\partial f}{\partial \varepsilon}\right) \approx \delta(\varepsilon - \varepsilon_F)$

$$\rightarrow \sigma^{(u)} \simeq e^2 \tau(\varepsilon_F) \int \frac{d\bar{k}}{4\pi^3} v_u(\bar{k}) \boxed{v_u(\bar{k}) \left(-\frac{\partial f}{\partial \varepsilon}\right)}$$

$\bar{v}_u(\bar{k}) = \frac{1}{\hbar}\frac{\partial \varepsilon_u}{\partial \bar{k}}$ → heyfijafna

$= -\frac{1}{\hbar}\frac{\partial}{\partial \bar{k}} f(\varepsilon(\bar{k}))$

hlutheildun

$$\rightarrow \sigma^{(u)} \simeq e^2 \tau(\varepsilon_F) \int \frac{d\bar{k}}{4\pi^3 \hbar} \left[\frac{\partial}{\partial \bar{k}} v(\bar{k})\right] f(\varepsilon(\bar{k}))$$

$$\frac{1}{\hbar}\frac{\partial}{\partial \bar{k}} v(\bar{k}) = \frac{\partial}{\partial \bar{k}}\left(\frac{\partial \varepsilon_n}{\partial \bar{k}}\right)\frac{1}{\hbar^2} = M^{-1}(\bar{k})$$

$$\rightarrow \sigma^{(u)} \simeq e^2 \tau(\varepsilon_F) \underbrace{\int \frac{d\bar{k}}{4\pi^3} M^{-1}(\bar{k})}_{\text{setin ástönd}}$$

$M^{-1}(\bar{k})$ er afleiða lotubundins falls $(\varepsilon(\bar{k}))$
á einingarsellunni → heildið yfir ↑
alla selluna hverfur

bls 772
I.9

$$\rightarrow \sigma = e^2 \tau(\varepsilon_F) \underbrace{\int \frac{d\bar{k}}{4\pi^2} \left(-M^{-1}(\bar{k})\right)}_{\text{ósetin ástönd}}$$

Því má lita sem svo á að

Straumurinn komi frá setnu ástöndunum — rafeindir

eða

frá ósetnu ástöndunum með massa $-m$ — holur

Frjálsar rafeindir $M^{-1}_{\mu\nu} = \frac{1}{m^*}\delta_{\mu\nu}$

$$\rightarrow \sigma_{\mu\nu} = \frac{ne^2\tau}{m^*} \quad \text{(Drude)}$$

Í burtu frá slökunartíma

* Lögun ójafnvægisdreifingarinnar getur haft áhrif á tíðni árekstra vissrar rafeindar

* Hún hefur einnig áhrif á dreifinguna eftir árekstur

nálganir notaðar vegna einfaldleika í slökunartímanálgun

* Einsetning ástanda, er völ á loka ástandi?

fylgni hrif

leiðréttingar við slökunartímanálgunina eru venjulega háðar τ

Drude hugmyndin um árekstra rafeinda og jóna stenst ekki

Bloch rafeindir rekast á óreglur í lotubundna mættinum

punktveilur hljóðeindir

línur + sléttur

mismunandi T-hrif

Rafeinda-rafeinda árekstrar eru ekki mikilvægir fyrir leiðni vegna ástæðna sem koma síðar í ljós.

—— —— —— ——

Í stað slökunartíma

er notuð

árekstrarlíkindi á einingartíma

fjöllum um einn borða

mjög staðbundnir árekstrar

Líkindi þess að rafeind með $\bar{k}$ fari í ástand með $(\bar{k}', \bar{k}'+d\bar{k}')$ á tímanum dt er

$$\frac{W_{\bar{k},\bar{k}'}\,dt\,d\bar{k}'}{(2\pi)^3}$$

hliðstætt við venjulega framsetningu á dreififræði

Ef loka ástandið er tómt og spuninn er varðveittur

$W_{\bar k,\bar k'}$ má reikna með smásæjum aðferðum (t.d. tímaháð-truflun)

gerð árekstrar hornháðing …… er hér inni

Ef bæði $W_{\bar k,\bar k'}$ og $g(\bar k)$ eru þekkt má reikna líkindi þess að rafeind með $\bar k$ verði fyrir árekstri (í eitthvert ástand)

→ jafngilt $\frac{1}{\tau(\bar k)}$

summað yfir $\bar k'$

möguleg $\bar k'$

$$\frac{1}{\tau(\bar k)} = \int \frac{d\bar k'}{(2\pi)^3} W_{\bar k,\bar k'} \{\underbrace{1-g(\bar k')}_{}\}$$

ósetin lokaástönd

$$\longrightarrow \boxed{\frac{1}{\tau(\bar k)} \text{ er í raun háð } g(\bar k)}$$

Hvernig er $g(\bar k)$ reiknað

$\left(\frac{dg}{dt}\right)_{out}$ er skilgreint þ.a.

fjöldi rafeinda á einingar rúmmál með $\bar k$ sem rekast á á dt er

$$-\left(\frac{dg}{dt}\right)_{out} \frac{d\bar k}{(2\pi)^3} dt$$

teknar út með árekstri úr $d\bar k$

En við vitum að fjöldi rafeinda/ein.rúm sem verður fyrir árekstri er

$$\frac{dt}{\tau(\bar k)} \cdot g(\bar k) \frac{d\bar k}{(2\pi)^3}$$

$$\longrightarrow \boxed{\left(\frac{dg(\bar k)}{dt}\right)_{out} = - \frac{g(\bar k)}{\tau(\bar k)} = - g(\bar k) \int \frac{d\bar k'}{(2\pi)^3} W_{\bar k\bar k'} (1-g(\bar k'))}$$

Rafeindir koma líka inn vegna árekstra í sama rúmmál

$$\boxed{\left(\frac{dg(\bar{k})}{dt}\right)_{in} \frac{d\bar{k}}{(2\pi)^3}\, dt}$$

heildarfjöldi rafeinda sem kemur inn á svæðið um $\bar{k}$ (á rúmeiningu) vegna árekstra um $\bar{k}'$ á tímabili dt er

$$\underbrace{\left\{ g(\bar{k}') \frac{d\bar{k}'}{(2\pi)^3} \right\}}_{\substack{\text{árekstrar} \\ \text{um } \bar{k}'}} \underbrace{\left\{ W_{\bar{k}'\bar{k}} \frac{d\bar{k}}{(2\pi)^3} dt \right\}}_{\substack{\text{berast inn} \\ \text{á svæði} \\ \text{um } \bar{k}}} \underbrace{(1-g(\bar{k}))}_{\substack{\text{laus} \\ \text{ástönd}}}$$

mögulegir → árekstrar um $\bar{k}'$

upphafsástönd — lokaástönd

$$\to \boxed{\left(\frac{dg(\bar{k})}{dt}\right)_{in} = (1-g(\bar{k})) \int \frac{d\bar{k}'}{(2\pi)^3} W_{\bar{k}'\bar{k}}\, g(\bar{k}')}$$

líta á töflu 16.1.

hún sýnir ljóslega áhrif $g(\bar{k})$

Breytingar á g vegna árekstra eru því

$$\boxed{\left(\frac{dg(\bar{k})}{dt}\right)_{coll} = -\int \frac{d\bar{k}'}{(2\pi)^3} \left\{ W_{\bar{k}\bar{k}'}\, g(\bar{k})(1-g(\bar{k}')) - W_{\bar{k}'\bar{k}}\, g(\bar{k}')(1-g(\bar{k})) \right\}}$$

út - inn

heildis-afleiðujafna

á meðan slökunartíma nálgunin gefur

$$\left(\frac{dg(\bar{k})}{dt}\right)_{coll} = -\frac{\{g(\bar{k}) - g^0(\bar{k})\}}{\tau(\bar{k})}$$

Hreyfijöfnur — Aflfræði?

En rafeindir koma ekki og fara aðeins úr svæðinu um $\bar{k}$ vegna árekstra

sumar koma og fara vegna hreyfingar jafnanna

$$\dot{\bar{r}} = \bar{v}(\bar{k}) \quad , \hbar\dot{\bar{k}} = \bar{F}(\bar{r},\bar{k})$$

$$\bar{F}(\bar{r},\bar{k}) = -e\left(\bar{E} + \frac{1}{c}\bar{v}\times\bar{B}\right)$$

setjum fyrst sem svo að enginn árekstur verði á bilinu $(t-dt, t)$ þá hafa allar rafeindir sem eru um $\bar{r}, \bar{k}$ á t komið frá

$$\bar{r}-\bar{v}(\bar{k})dt \;,\; \bar{k}-\bar{F}\frac{dt}{\hbar} \;,\; \text{á } t-dt$$

$$\rightarrow\; g(\bar{r},\bar{k},t) = g(\bar{r}-v(\bar{k})dt, \bar{k}-\bar{F}\tfrac{dt}{\hbar}, t-dt)$$

en hér vantar árekstra

sem koma í veg fyrir að allar rafeindir frá ... komist á $\bar{r}, \bar{k}, t$

og síðan koma aðrar annarsstaðar frá vegna árekstra

$$\rightarrow$$

$$g(\bar{r},\bar{k},t) = g(\bar{r}-v(\bar{k})dt, \bar{k}-\bar{F}\tfrac{dt}{\hbar}, t-dt) + \left(\frac{\partial g(\bar{r},\bar{k},t)}{\partial t}\right)_{out} dt + \left(\frac{\partial g(\bar{r},\bar{k},t)}{\partial t}\right)_{in} dt$$

athugum markgildið fyrir $dt \to 0$

$$g(\bar{r},\bar{k},t) = g(\bar{r},\bar{k},t) + \frac{\partial}{\partial t} g(\bar{r},\bar{k},t)(-dt) + \bar{\nabla} g(\bar{r},\bar{k},t)\cdot\bar{v}\,(-dt) + \bar{\nabla}_k g(\bar{r},\bar{k},t)\cdot\frac{\bar{F}}{\hbar}(-dt) + \left(\frac{\partial g}{\partial t}\right)_{coll} dt$$

Boltzmanns jafnan

$$\rightarrow\; \boxed{\underbrace{\frac{\partial}{\partial t} g + \bar{v}\cdot\frac{\partial}{\partial \bar{r}} g + \bar{F}\cdot\frac{1}{\hbar}\frac{\partial}{\partial \bar{k}} g}_{\text{rek liðir}} = \underbrace{\left(\frac{\partial g}{\partial t}\right)_{coll}}_{\text{árekstrar liður}}}$$

jafnan verður því ólínuleg hlutafleiðuheildis jafna

ef slökunartíma nálgunin er notuð fyrir árekstraliðinn

$$\left(\frac{\partial g}{\partial t}\right)_{col} = -\frac{(g(\bar{k}) - g^{\circ}(\bar{k}))}{\tau(\bar{k})}$$

þá er $g(t) = g^{\circ}(t) - \int_{-\infty}^{t} dt' P(t,t')\frac{d}{dt'}g^{\circ}(t')$

er lausn B-jöfnunnar

efni dæma 2 og 3

!

Við munum athuga einhver einföld tilfelli

Hægt er að sýna að Boltzmanns jafnan varðveitir N_s og skriðþunga og orku

↙

orkan er hreyfiorka. (þetta er þó hægt að útvíkka)

⇕

þar sem stöðuorku vantar er Boltzmanns jafnan aðeins í lagi fyrir veikt víxlverkandi kerfi

(Sjá Quantum Statistical Mech.
L. P. Kadanoff, G. Baym)

↑

skammtaaðferðirnar sem athugaðar verða seinna leyfa miklu meiri fjölbreytni

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Boltzmann : Phenomenology

Árekstrar við veilur

* verða ráðandi við lágt hitastig
* árekstrarnir verða fjaðrandi ef orkugeilin á milli grunnástands og næsta örvaða ástands veilunnar er stór miðað við k_BT
* veilurnar eru nógu dreifðar til þess að rafeind víxlverkast við eina í einu

$$\longrightarrow W_{\bar{k},\bar{k}'} = \frac{2\pi}{\hbar} n_i \delta(\varepsilon(\bar{k}) - \varepsilon(\bar{k}'))|\langle\bar{k}|U|\bar{k}'$$

samkvæmt Gullnu reglu Fermis

$$\langle\bar{k}|U|\bar{k}'\rangle = \int d\bar{r}\, \psi^*_{n\bar{k}'}(\bar{r})\, U(\bar{r})\, \psi_{n\bar{k}}(\bar{r})$$

$$\int_{cell} dr\, |\psi_{n\bar{k}}(\bar{r})|^2 = v_{cell}$$

Gullnaregla Fermis

fjaðrandi

$W_{\bar{k},\bar{k}'}$ er hér óháð g („óháðar rafeindir")

U er Hermite virki $\rightarrow$ $W_{\bar{k},\bar{k}'} = W_{\bar{k}',\bar{k}}$

var kallað „detailed balancing"

$$\rightarrow \boxed{\left(\frac{dg(\bar{k})}{dt}\right)_{coll} = -\int \frac{d\bar{k}'}{(2\pi)^3} W_{\bar{k}\bar{k}'} \left\{ g(\bar{k}) - g(\bar{k}') \right\}}$$

Regla Matthiessens

Ef um tvær mismunandi árekstra tegunda er t.d. að ræða. Rafeindir ↔ Rafeindir
Rafeindir ↔ veilur þ.a. hvorug tegund hafi áhrif á hina

$$\rightarrow W = W^{(1)} + W^{(2)}$$

Sem í slökunartímanálguninni þýðir

$$\frac{1}{\tau} = \frac{1}{\tau^{(1)}} + \frac{1}{\tau^{(2)}}$$

Ef τ er óháð $\bar{k}$ þá fæst fyrir viðnámið

$$\rho = \frac{m}{ne^2\tau} = \frac{m}{ne^2\tau^{(1)}} + \frac{m}{ne^2\tau^{(2)}}$$

$$= \rho^{(1)} + \rho^{(2)}$$

Matthiessens Regla

t.d. veilu árekstrar óháðir T
en rafeinda árekstrar háðir T^2

$$\rightarrow \rho \simeq A + BT^2$$

Ef $\tau(\bar{k})$ er háð $\bar{k}$ þá er þetta ekki lengur hægt

Árekstrartegundir oft ekki óháðar
Almennar má sanna

$$\rho \geq \rho^{(1)} + \rho^{(2)}$$

Einsleit efni

Slökunartímanálgun má réttlæta ef:

a) $\Sigma = \Sigma(|\bar{k}|)$

b) líkindi árekstra milli $\bar{k}$ og $\bar{k}'$ hverfur nema $|\bar{k}| = |\bar{k}'|$ og eru einungis háð Σ og θ

þá fæst fyrir einsleitt efni og fjaðrandi veiluárekstra í föstu einsleitu rafsviði

$$g(\bar{k}) = g^0(\bar{k}) + \bar{a}(\Sigma)\cdot\bar{k} \qquad (1)$$

samkvæmt slökunartímanálgun og Boltzmannsjöfnu

sýna þarf að þegar (1) heldur þá megi finna $\tau(\bar{k})$ sem er óháð g

$$\int \frac{d\bar{k}'}{(2\pi)^3} W_{\bar{k},\bar{k}'}\left(g(\bar{k}) - g(\bar{k}')\right) = \frac{1}{\tau(\bar{k})}\left(g(\bar{k}) - g^0(\bar{k})\right)$$

þ.e. (16.9) = (16.18)

fjaðrandi → $W_{\bar{k}\bar{k}'} = 0$ ef $\Sigma(\bar{k}) \neq \Sigma(\bar{k}')$

nota (1) →

$$\bar{a}(\Sigma)\cdot\int \frac{d\bar{k}'}{(2\pi)^3} W_{\bar{k}\bar{k}'}(\bar{k} - \bar{k}') = \frac{1}{\tau(\bar{k})}\bar{a}(\Sigma)\cdot\bar{k}$$

$$\bar{k}' = \underset{\substack{\uparrow \\ \text{samsíða } \bar{k}}}{\bar{k}'_{\parallel}} + \bar{k}'_{\perp} = (\hat{k}\cdot\bar{k}')\hat{k} + k'_{\perp}$$

fjaðrandi → $W_{\bar{k},\bar{k}'}$ er aðeins háð horninu á milli $\bar{k}$ og $\bar{k}'$

→ $W_{\bar{k},\bar{k}'}$ er óháð $\bar{k}'_{\perp}$

$$\rightarrow \int d\bar{k}'\, W_{\bar{k}\bar{k}'}\,\bar{k}'_{\perp} = 0$$

→

$$\int d\bar{k}'\, W_{\bar{k}\bar{k}'}\,\bar{k}' = \int d\bar{k}'\, W_{\bar{k}\bar{k}'}\,\bar{k}'_{\parallel}$$

$$= \hat{k}\int d\bar{k}'\, W_{\bar{k}\bar{k}'}(\hat{k}\cdot\hat{k}')\underset{\overset{\parallel}{k}}{k'}$$

$$= \bar{k}\int d\bar{k}'\, W_{\bar{k},\bar{k}'}\, (\hat{k}\cdot\hat{k}')$$

$$\rightarrow \int d\bar{k}'\, W_{\bar{k}\bar{k}'}\, \bar{k}' = \bar{k}\int d\bar{k}'\, W_{\bar{k}\bar{k}'}\, (\hat{k}\cdot\hat{k}')$$

bera saman við

$$\bar{a}\cdot\int \frac{d\bar{k}'}{(2\pi)^3}\, W_{\bar{k}\bar{k}'}\, (\bar{k}-\bar{k}') = \frac{1}{\tau(k)}\,\bar{a}(\varepsilon)\cdot\bar{k}$$

$$\rightarrow \frac{1}{\tau(k)} = \int \frac{d\bar{k}'}{(2\pi)^3}\, W_{\bar{k},\bar{k}'}\, (1-\hat{k}\cdot\hat{k}')$$

sem er óháð $g(\bar{k})$

Fjöleindalíkön rafeinda í storku

Þyrftum að leysa

jónir

$$H\Psi = \sum_{i=1}^{N}\Big\{-\frac{\hbar^2}{2m}\nabla_i^2 + Ze^2\sum_{\bar{R}}\frac{1}{|\bar{r}_i-\bar{R}|} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\bar{r}_i-\bar{r}_j|}\Big\}\Psi = E\Psi$$

← rafeinda víxlv.

Ekki hægt nákvæmlega

→ ýmsar nálganir til innan fjöleindafræði

Athugum tvær hér

Hartree
Hartree-Fock

Vel skilgreindar nálganir „sjálfsamkvæmar" sem leiða til einnarögnar Schrödinger jöfnu þar sem tillit er tekið til hinna agnanna

Hartree

Gerum ráð fyrir að bylgjufall N einda (N þarf ekki að vera heildar fjöldi einda) megi skrifa sem

$$\Psi_N(\bar{r}_1 \cdots \bar{r}_N) = \phi_1(\bar{r}_1)\,\phi_2(\bar{r}_2) \cdots \phi_N(\bar{r}_N)$$

þegar frjálsa orkan fyrir líkindavirkja einnar fermieindar tekur lággildi fæst hreyfingarjafnan

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + U_{ion}(\bar{r}) + V_H(\bar{r})\right\}\phi_i(\bar{r}) = \varepsilon_i \phi_i(\bar{r})$$

með

$$V_H(\bar{r}) = e^2 \int d\bar{r}' \, \frac{n_s(\bar{r}')}{|\bar{r} - \bar{r}'|}$$

$$n_s(\bar{r}) = \sum_j |\phi_j(\bar{r})|^2 f(\varepsilon_j - \mu)$$

↑ fermi

mættið sem hver rafeind sér vegna heildar hleðsluþéttleika rafeindanna

---

* $\Psi(\bar{r}_1 \cdots \bar{r}_N)$ er ekki andsamhverft

* Vantar fylgni : hver rafeind hreyfist eins og óháð eind í ytra mætti sem er þó vegna heildar hleðsluþéttleikans.

Hér sést ekki sá möguleiki að tvær eindir t.d. með skriðþunga $\bar{P}_1$ og $\bar{P}_2$ „rekist á" og hafi eftir árekstur $\bar{P}_1' \neq \bar{P}_1$ og $\bar{P}_2' \neq \bar{P}_2$

Hartree-Fock

Gerum ráð fyrir að bylgjufallið fyrir N-eindir sé slater ákveða

$$\Psi(\bar{r}_1 \cdots \bar{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\bar{r}_1) & \cdots & \phi_N(\bar{r}_1) \\ \vdots & & \vdots \\ \phi_1(\bar{r}_N) & \cdots & \phi_N(\bar{r}_N) \end{vmatrix}$$

óaðgreinanlegar Fermi eindir

þegar frjálsa orkan er nú í lágmarki fæst

Hartree mætti

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + U_{ion}(\bar{r}) + V_H(r)\right\}\phi_i(\bar{r})$$

$$+\int d\bar{r}'\Delta(\bar{r},\bar{r}')\phi_i(\bar{r}') = \varepsilon_i\phi_i(\bar{r})$$

óstaðbundið Fock mætti

berum saman mættin

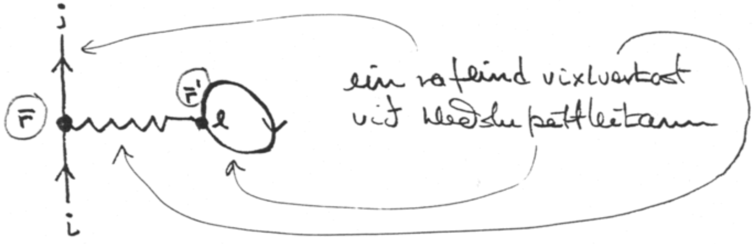
$$(V_F)_{ji} = \int d\bar{r}d\bar{r}'\,\Delta(\bar{r},\bar{r}')\,\phi_j^*(\bar{r})\phi_i(\bar{r}')$$

$$= -e^2\sum_{\substack{l \\ \parallel\ \mathrm{spin}}} f(\varepsilon_l-\mu)\int d\bar{r}d\bar{r}'\,\frac{\phi_l^*(\bar{r}')\phi_l(\bar{r})}{|\bar{r}-\bar{r}'|}\,\phi_j^*(\bar{r})\phi_i(\bar{r}$$

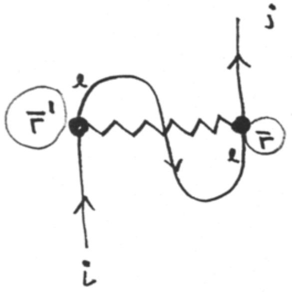
$$(V_H)_{ji} = \int d\bar{r}\,\phi_j^*(\bar{r})\,V_H(\bar{r})\phi_i(\bar{r})$$

$$= +e^2\sum_l f(\varepsilon_l-\mu)\int d\bar{r}d\bar{r}'\,\frac{|\phi_l(\bar{r}')|^2}{|\bar{r}-\bar{r}'|}\,\phi_j^*(\bar{r})\phi_i(\bar{r})$$

Talað er um að Fock liðurinn valdi skiptakrafti því Hartree liðurinn (eða beini liðurinn) má tákna sem



en Fock liðurinn verður þá



Fock liðurinn eyðir „sjálfsvíxlverkunni" og veikir fráhrindikraftinn á milli rafeindanna (vegna formerkis hans)

HF-Schrödinger jöfnuna verður að leysa með ítrun í fallagrunni eigintalla

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + U_{ion}(\bar{r})\right\}\varphi_i(\bar{r}) = \epsilon_i\,\varphi_i(\bar{r})$$

Sýna má að planbylgjur eru nákvæm
lausn HF-jöfnunnar
fyrir „gel"-líkanið
Af þeirri lausn má læra nokkuð.

$$\psi_i(\bar r) = \frac{1}{(2\pi)^{3/2}} e^{i\bar k_i\cdot\bar r} \chi_{\sigma_i} \leftarrow \text{spunafall}$$

eða normað með $\frac{1}{\sqrt V}$ ef $\sum_k$ í stað $\int\frac{d\bar k}{(2\pi)^3}$ síðar $V \to \infty$

→ rafeinda þéttleikinn er einsleitur og fastur

Efnið er óhlaðið út á við

Jónirnar í grindinni eru hugsaðar
sem jákvætt hlaðinn einsleitur
bakgrunnur

$$\to \quad U_{ion} + \overset{\swarrow}{V_H} = 0$$

aðeins skiptikrafturinn lifir
(hann er ekki fall af n_s)

notum

$$\frac{e^2}{|\bar r - \bar r'|} = 4\pi e^2 \int \frac{d\bar q}{(2\pi)^3}\frac{1}{q^2} e^{i\bar q\cdot(\bar r - \bar r')}$$

til þess að reikna skiptiliðinn við $\boxed{T=0}$

$$\int d\bar r' \Delta(\bar r, \bar r')\phi_i(\bar r') \qquad\qquad \frac{1}{V}\sum_k \to \int\frac{d\bar k}{(2\pi)^3}$$

$$= -\sum_{\substack{l \\ \parallel\text{spin}}} \theta(k_F - k_l)\int d\bar r' \frac{e^2}{|\bar r - \bar r'|}\phi_l^*(\bar r')\phi_l(\bar r)\phi_i(\bar r')$$

$$= -4\pi e^2 \int_{\parallel\text{spin}} \frac{dk_l}{(2\pi)^3}\,\theta(k_F - k_l)\int d\bar r' d\bar q\,\frac{1}{q^2} e^{i\bar q\cdot(\bar r - \bar r') - i\bar k_l\cdot\bar r' + i\bar k_l\cdot\bar r}$$

$$\cdot\, e^{i\bar k_i\cdot\bar r'}\frac{1}{(2\pi)^3}\frac{1}{(2\pi)^{3/2}}$$

$$= -4\pi e^2 \int_{\parallel\text{spin}} \frac{d\bar k_l}{(2\pi)^3}\theta(k_F - k_l)\int d\bar q\,\frac{1}{q^2} e^{i\bar q\cdot\bar r + i\bar k_l\cdot\bar r}\delta(\bar q - \bar k_i + \bar k_l)$$

$$\cdot\,\frac{1}{(2\pi)^{3/2}}$$

$$= -4\pi e^2 \int_{\parallel\text{spin}} \frac{d\bar k_l}{(2\pi)^3}\,\theta(k_F - k_l)\,\frac{1}{|\bar k_i - \bar k_l|^2} e^{i\bar k_i\cdot\bar r}\frac{1}{(2\pi)^{3/2}}$$

$$= -4\pi e^2 \int_{\parallel \text{spin}} \frac{d\bar{k}_l}{(2\pi)^3}\,\Theta(k_F - k_l)\,\frac{1}{|\bar{k}_i - \bar{k}_l|^2}\,\phi_i(\bar{r})$$

$$= -4\pi e^2 \int_{k'<k_F} \frac{d\bar{k}'}{(2\pi)^3}\,\frac{1}{|\bar{k}_i - \bar{k}'|^2}\cdot\phi_i(\bar{r})$$

því verður öll vinstrihlið Hartree-Fock schrödinger jöfnunnar

$$\longrightarrow \Sigma(\bar{k}_i)\,\phi_i(\bar{r})$$

með

$$\Sigma(\bar{k}) = \frac{\hbar^2 k^2}{2m} - \int_{k'<k_F} \frac{d\bar{k}'}{(2\pi)^3}\,\frac{4\pi e^2}{|\bar{k}-\bar{k}'|^2}$$

$$= \frac{\hbar^2 k^2}{2m} - \frac{2e^2}{\pi}\,k_F\,F\!\left(\frac{k}{k_F}\right)$$

flatar bylgjur uppfylla jöfnuna

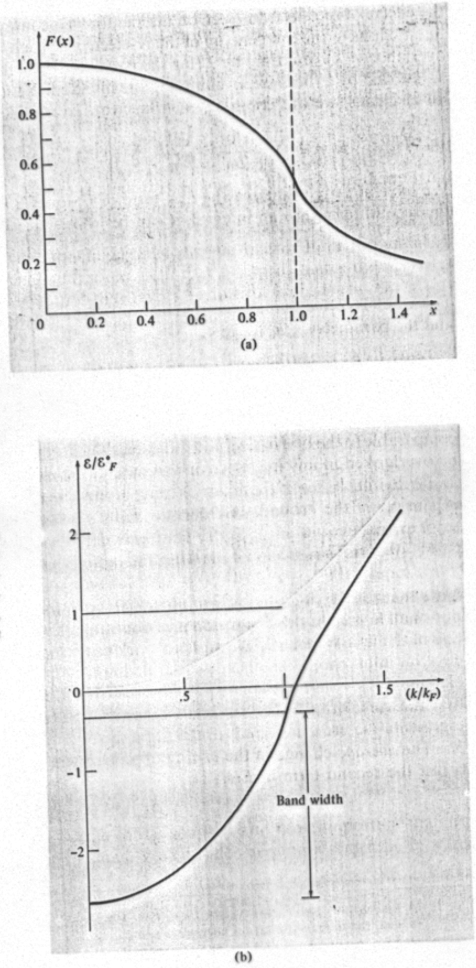
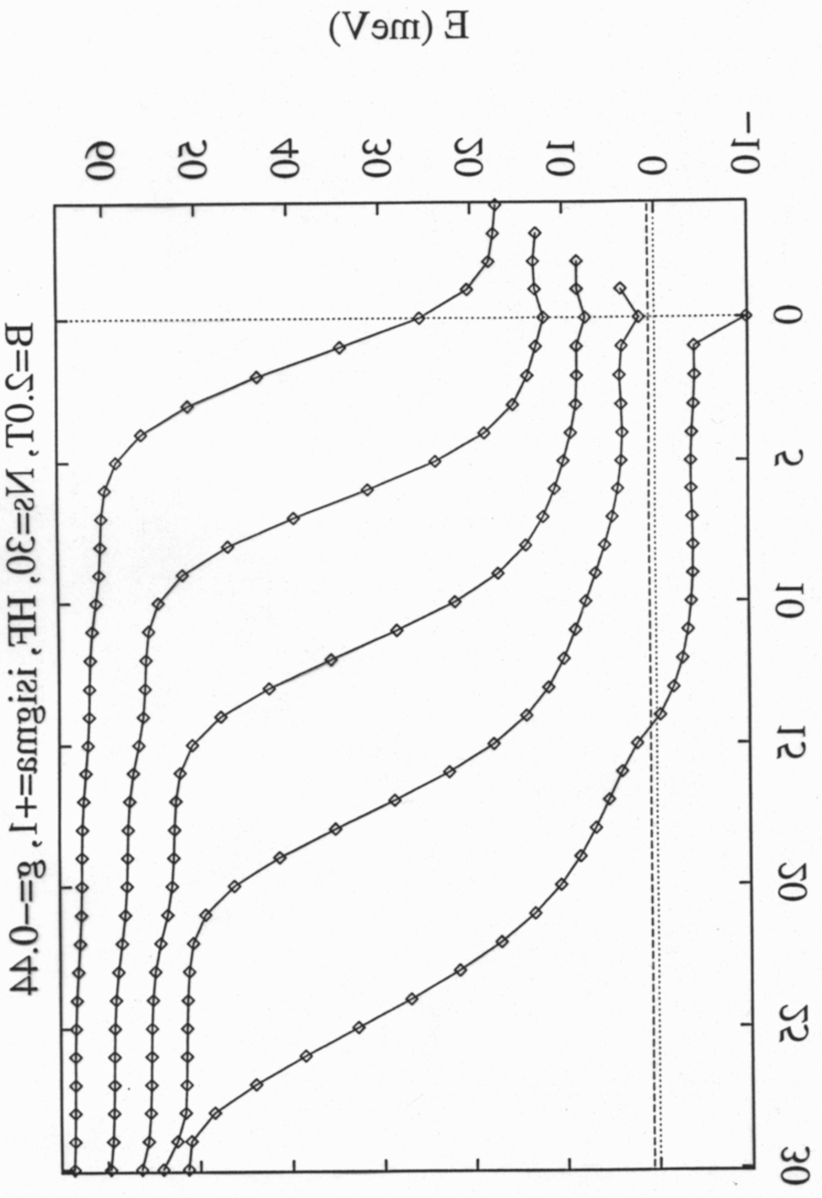
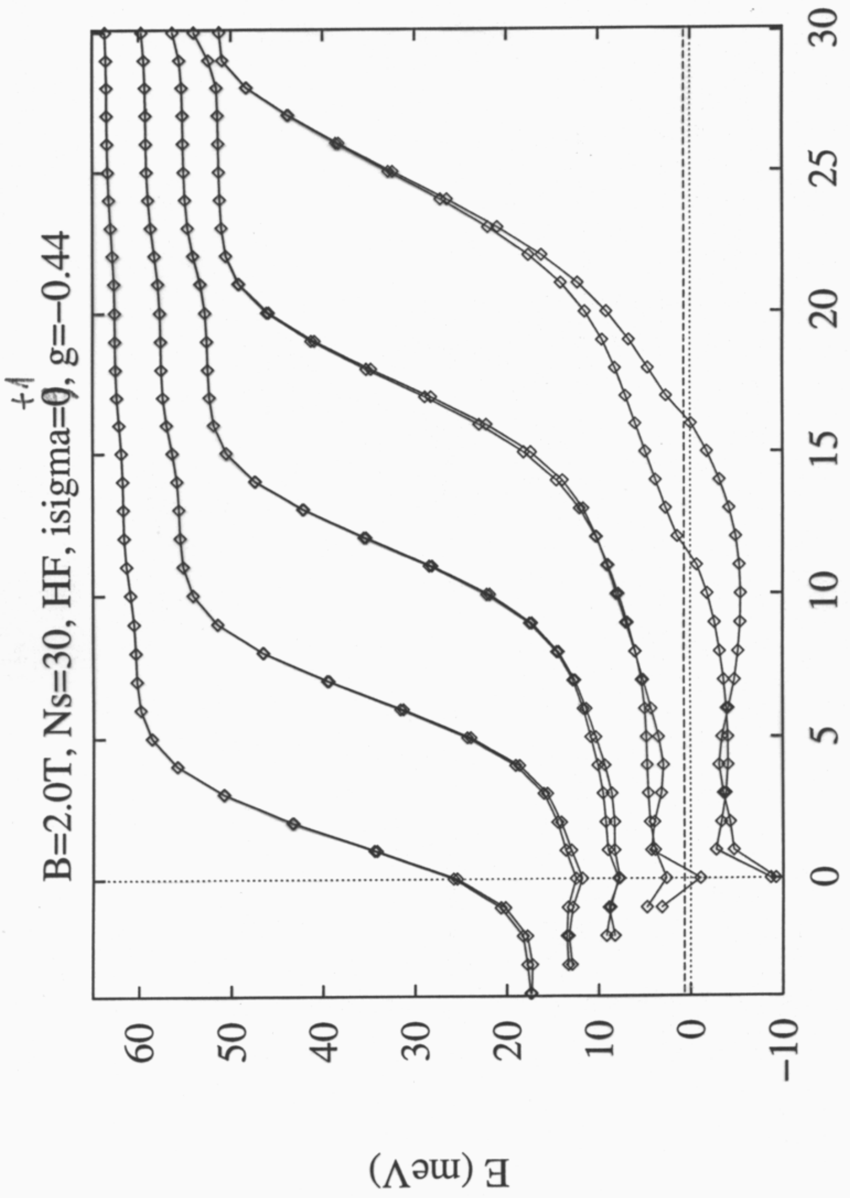


Figure 17.1
(a) A plot of the function $F(x)$, defined by Eq. (17.20). Although the slope of this function diverges at $x = 1$, the divergence is logarithmic, and cannot be revealed by changing the scale of the plot. At large values of x the behavior is $F(x) \rightarrow 1/3x^2$. (b) The Hartree-Fock energy (17.19) may be written

$$\frac{\mathcal{E}_k}{\mathcal{E}_F^0} = [\text{illegible}]^2 - 0.663\left(\frac{r_s}{a_0}\right)F(x)\Big],$$

where $x = k/k_F$. This function is plotted here for $r_s/a_0 = 4$, and may be compared with the free electron energy (white line). Note that in addition to depressing the free electron energy substantially, the exchange term has led to a considerable increase in the bandwidth (in these units from 1 to 2.33), an effect not corroborated by experiments such as soft X-ray emission or photoelectron emission from metals, which purport to measure such bandwidths.


B=2.0T, Ns=30, HF, isigma=+1, g=−0.44
E (meV)
M
60
50
40
30
20
10
0
−10
0
5
10
15
20
25
30


B=2.0T, Ns=30, HF, isigma=~~0~~+1, g=−0.44
E (meV)
M
60
50
40
30
20
10
0
−10
0
5
10
15
20
25
30

með

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x}\ln\left|\frac{1+x}{1-x}\right|$$

Athuga Myndir 17.1

Logariþma sérstöðupunktur við $k=k_F$ í afleiðu $F(x)$

Fockliðurinn dregur úr fráhrindinga

---

heildarorkan er

$$E = \underset{\substack{\uparrow\\ \text{spuni}}}{2}\sum_{k<k_F}\frac{\hbar^2k^2}{2m} - \underset{\substack{\uparrow\\ 1 = 2\cdot\frac{1}{2} = \text{spuni}\,\frac{1}{\text{tvítalning para}}}}{\frac{e^2k_F}{\pi}}\sum_{k<k_F}\left\{1+\frac{k_F^2-k^2}{2kk_F}\ln\left|\frac{k_F+k}{k_F-k}\right|\right.$$

Summur aftur í heildi

$$E = N\left\{\frac{3}{5}\Sigma_F - \frac{3}{4}\frac{e^2k_F}{\pi}\right\}$$

$$\frac{V}{N} = \frac{1}{n_s} = \frac{4\pi r_s^3}{3}$$ rúmmál á rafeind

$$\rightarrow\ r_s = \left(\frac{3}{4\pi n}\right)^{1/3}$$

$$\frac{e^2}{2a_0} = 1Ry = 13.6eV$$ a_0: Bohrradius

$$a_0 = \frac{\hbar^2}{2me^2} \qquad \Sigma_F = \frac{\hbar^2k_F^2}{2m}$$

$$\rightarrow\ \frac{E}{N} = \frac{e^2}{2a_0}\left\{\frac{3}{5}(k_Fa_0)^2 - \frac{3}{2\pi}(k_Fa_0)\right\}$$

$$k_F^3 = 3\pi^2 n \qquad n = \frac{3}{4\pi r_s^3}$$

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

$$\rightarrow\ \frac{E}{N} = \left\{\frac{2{,}21}{(r_s/a_0)^2} - \frac{0{,}916}{(r_s/a_0)}\right\}Ry$$

fyrir málma er $r_s/a_0 \sim 2-6$

→ Coulomb hrif skipta máli

$\frac{E}{N} \longrightarrow E_{kin}$ þegar $\frac{r_s}{a_0} \longrightarrow 0$

mjög þétt gas

$\frac{E}{N} \longrightarrow E_{pot}$ þegar $\frac{r_s}{a_0} \longrightarrow \infty$

mjög lítill þéttleiki

truflanareikningur verður beti
með vaxandi þéttleika

Hærri liðir í E/N eru nefndir fylgniliði
sjá (17.24)

{ í 2D-kerfum má breyta $\frac{r_s}{a_0}$ }

$\frac{r_s}{a_0}$ er í raun truflanastikill

* $\langle \Sigma^{exch} \rangle = -\frac{0,916}{(r_s/a_0)} Ry = -2.95(a_0^3 n_s)^{1/3} Ry$

því er sú nálgun oft notuð að
í stað Fock liðsins er notað

$$V_{\neq}(\bar{r}) = -2.95(a_0^3 n_s(\bar{r}))^{1/3} Ry$$

Síðan hefur byggst upp
LDA „Local density Approximation"
með endurbótum á þessu

---

* sérstöðupunkturinn í F(x) kemur
aðeins vegna Coulombmættisins

hann hverfur í smáu (endanlegu) kerfi

hann hverfur ef hærri nálganir eru
notaðar

eða

ef mættinu er breytt, t.d. veikt
með skýlingu

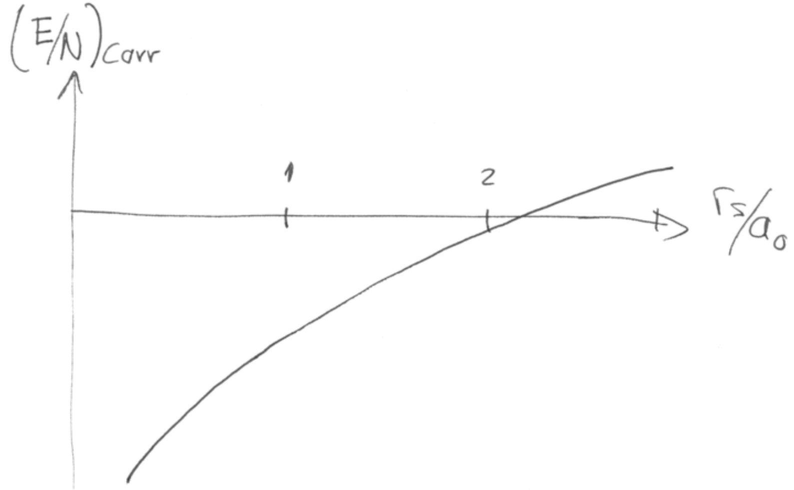
Hvenar gildir truflunaraðf. ? fyrir hvaða (r_s/a_0)

Smár stikill, gildir f. $(r_s/a_0) < 1$

En málmar hafa $1{,}8 < \frac{r_s}{a_0} < 6$

Er fáguð framlenging í lagi ?

Nei (algeng ástæða .....)



Einfaldar hugmyndir um fylgni

→ fylgniorkan < 0

Wigner (1934) fann að rafeindir við $\left(\frac{r_s}{a_0}\right) >> 1$ eru ekki gas, heldur raðast saman í kristall $(T \to 0)$

Allt annað grunnástand! (hvernig reiknað)

fyrir málma er gripið til brúunar

$$\frac{E_{corr}}{N} \simeq -0{,}115 + 0{,}031 \ln\left(\frac{r_s}{a_0}\right)$$

---

fyrir $r_s/a_0 \to 0$ fékkst

$$\left(\frac{E}{N}\right)_{corr} = -0{,}094 + 0{,}0622 \ln\left(\frac{r_s}{a_0}\right) + 0{,}018\left(\frac{r_s}{a_0}\right)\ln\left(\frac{r_s}{a_0}\right)$$

$$+ a r_s + O\left(\frac{r_s^2}{a_0^2}\right)$$

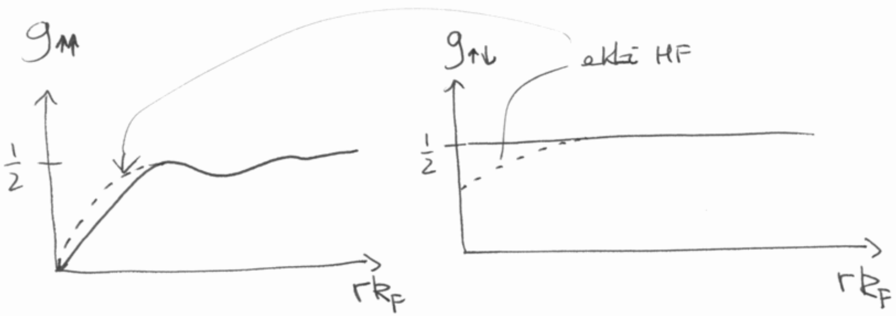
Fylgniföll

Para fylgni

$$g(\bar{r}_1,\bar{r}_2) = V^2\int d\bar{r}_3\cdots d\bar{r}_N \left|\Psi_{\lambda_1\cdots\lambda_N}(\bar{r}_1\cdots\bar{r}_N)\right|^2$$

$$g_{ss'}(\bar{r}_1,\bar{r}_2) = \frac{V^2}{N(N-1)}\sum_{\lambda_i\lambda_j}\begin{vmatrix}\phi_{\lambda_i}(\bar{r}_1) & \phi_{\lambda_i}(\bar{r}_2)\\ \phi_{\lambda_j}(\bar{r}_1) & \phi_{\lambda_j}(\bar{r}_2)\end{vmatrix}^2$$

flatar bylgjur $\quad g_{ss'}(\bar{r}_1-\bar{r}_2)$



HF

$$g_{\uparrow\downarrow}(\bar{r}_1-\bar{r}_2) = \frac{1}{2}$$

$$g_{\uparrow\uparrow}(\bar{r}_1-\bar{r}_2) = \cancel{\frac{1}{2}\left(1-\phi^2(\bar{r}_1-\bar{r}_2)\right)}$$

Skýling

Inngangur að línulegri svörun

Auka hleðslu $\rho^{ext}(\bar{r})$ er komið fyrir núna eða í rafeindakerfið

-> ytra mætti skoðast

$$-\nabla^2\phi^{ext}(\bar{r}) = 4\pi\rho^{ext}(\bar{r})$$

(ϕ^{ext} samsvarar $\bar{D}$)

heildar mættið í kerfinu er $\phi(\bar{r})$

$$-\nabla^2\phi(\bar{r}) = 4\pi\rho(\bar{r})$$

með

$$\rho(\bar{r}) = \rho^{ext}(\bar{r}) + \rho^{ind}(\bar{r})$$

þar ρ^{ind} er „spanað" af ρ^{ext} í kerfinu

(ϕ samsvarar $\bar{E}$)

Skautast

Síðan er gert ráð fyrir að

$$\phi^{ext}(\bar{r}) = \int d\bar{r}' \, \epsilon(\bar{r}, \bar{r}')\phi(\bar{r}')$$

(línuleg tengsl)

Í einsleitukerfi fæst $\epsilon = \epsilon(\bar{r} - \bar{r}')$

$$\rightarrow \phi^{ext}(\bar{q}) = \epsilon(q)\phi(\bar{q})$$

Eða öllu heldur

$$\boxed{\phi(\bar{q}) = \frac{1}{\epsilon(\bar{q})}\phi^{ext}(\bar{q})}$$

þar sem ϕ^{ext} var þekkt

Síðan má eins og gert er í bókinni tengja $\epsilon(\bar{q})$, rafsvörunarfallið við rafviðtakið $\chi(\bar{q})$

$$\boxed{\epsilon(\bar{q}) = 1 - \frac{4\pi}{q^2}\chi(\bar{q})}$$

$$\rho^{ind}(\bar{q}) = \chi(\bar{q})\phi(\bar{q})$$

Spurningin er því

Hvernig er hægt að reikna $\epsilon(\bar{q})$ eða $\chi(\bar{q})$ fyrir eitthvert kerfi.

$\epsilon(\bar{q})$ og $\chi(\bar{q})$ lýsa svörun kerfisins við ytra rafmætti ϕ^{ext}

eða

$T_{ij}(\bar{q})$ sem lýsir svöruninni við ytra vigursviði $\bar{A}^{ext}$

Línuleg svörun við ytra rafmætti ϕ^{ext}

aðferðin sem hér verður sýnd jafngildir Lindhard fræðinni

eða RPA - random phase approximation slembifasanálgun

eða Hartree tímaháðri nálgun

og er því gersamlega samkvæmt skammtafræði

Byrjum með hreyfingarjöfnu

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + U_{ion} + V_H + V_{imp}\right\}\phi_i(\bar{r}) = \varepsilon_i\,\phi_i(\bar{r})$$

veilur þegar þær eiga við

$$H_0\phi_i = \varepsilon_i\phi_i$$

síðan er bætt við truflun

$$H_I = \delta V^{ext}(t) = e^{-i(\omega+i\eta)t}\,\delta V(\bar{r})$$

$$= e^{-i(\omega+i\eta)t}\left(-e\phi^{ext}(\bar{r})\right)$$

einföld hreintóna truflun, $\eta \to 0^+$

η: veldur því að kveikt er hægt á trufluninni

því $H_I \xrightarrow[t\to-\infty]{} 0$

Í skammtasafneðlisfræði er unnið með líkindafylkið ρ_{ij} eða líkindavirkjann $\hat{\rho}$ í stað ójafnvægisdreifingarinnar $g(\bar{k},t)$ áður

$$\hat{\rho}(t\to-\infty) = \hat{\rho}^0 = \underset{\substack{\uparrow\\ \text{Fermi dreifing}}}{f(\hat{H}_0)}$$

síðan má hugsa sér að truflunin valdi breytingu á $\hat{\rho}$

$$\hat{\rho}(t) = \rho^0 + \delta\hat{\rho}(t)$$

þessa breytingu $\delta\hat{\rho}(t)$ má reikna samkvæmt línulegri nálgun m.t.t. ϕ^{ext}

{ sjá skammtafræði I eða II
eða viðbót A hér að aftan }

Þá fæst fyrir fylkjastökin

$$\boxed{\begin{aligned}\delta\varrho_{\alpha\beta}(t) &= \delta\varrho_{\alpha\beta}\, e^{-i\omega t + \eta t}\\ \delta\varrho_{\alpha\beta} &= -\frac{e}{\hbar}\left\{\frac{f_\beta - f_\alpha}{\omega + \omega_{\beta\alpha} + i\eta}\right\}\langle\alpha|\phi^{ext}|\beta\rangle\end{aligned}}$$

með

$$\omega_{\beta\alpha} = \omega_\beta - \omega_\alpha = \frac{1}{\hbar}\left\{\varepsilon_\beta - \varepsilon_\alpha\right\}$$

$f_\beta = f(\varepsilon_\beta)$: fermidreifing

$|\alpha\rangle$ er ástand H_0 og ε_α er eigingildi H_0

{Þessi jafna samsvarar hálfsígildu jöfnunni fyrir $g(\bar{k},t)$ (13.19), lausn (16.13)}

Í viðbót A (aftast) er einnig sýnt að

$$\boxed{\begin{aligned}n_s(\bar r) &= \sum_\alpha |\phi_\alpha(\bar r)|^2 f(\varepsilon_\alpha)\\ &= tr\left\{\delta(\underset{\uparrow\atop\text{Virki}}{\hat{\bar r}} - \bar r)\,\hat\varrho^0\right\}\end{aligned}}$$

truflunin ϕ^{ext} veldur því þéttleikahvikun

$$\delta n_s(\bar r) \equiv n_s^{ind}(\bar r) = tr\left\{\delta(\hat{\bar r} - \bar r)\,\delta\hat\varrho\right\}$$

$$= \sum_\alpha \langle\alpha|\delta(\hat{\bar r} - \bar r)\,\delta\hat\varrho|\alpha\rangle$$

$$= \sum_\alpha \int d\bar r'\, \langle\alpha|\bar r'\rangle\langle\bar r'|\delta(\hat{\bar r} - \bar r)\,\delta\hat\varrho|\alpha\rangle$$

$$= \sum_{\alpha\beta} \int d\bar r'\, \phi^*_\alpha(\bar r')\,\delta(\bar r' - \bar r)\,\phi_\beta(\bar r')\,\delta\varrho_{\beta\alpha}$$

$$= \sum_{\alpha\beta} \phi^*_\alpha(\bar r)\,\phi_\beta(\bar r)\,\delta\varrho_{\beta\alpha}$$

því fæst

$$\boxed{n_s^{ind}(\bar r) = -\frac{e}{\hbar}\sum_{\alpha\beta}\phi^*_\alpha(\bar r)\,\phi_\beta(\bar r)\left\{\frac{f_\alpha - f_\beta}{\omega + \omega_{\alpha\beta} + i\eta}\right\}\phi^{ext}_{\cancel{\alpha\beta}\;\beta\alpha}}$$

Þessa jöfnu má umskrifa sem

$$n_s^{ind}(\bar r) = -\frac{e}{\hbar}\sum_{\alpha\beta}\int d\bar r'\, \phi^*_\alpha(\bar r)\phi_\beta(\bar r)\phi^*_\alpha(\bar r')\phi_\beta(\bar r')\left\{\frac{f_\alpha - f_\beta}{\omega+\omega_{\alpha\beta}+i\eta}\right\}\phi^{ext}(\bar r'$$

$$\rightarrow \boxed{n_s^{ind}(\bar r) = -\frac{e}{\hbar}\int d\bar r'\, D(\bar r,\bar r';\omega)\,\phi^{ext}(\bar r')}$$

þar sem

$$\boxed{D(\bar r,\bar r';\omega) = \sum_{\alpha\beta}\phi^*_\alpha(\bar r)\phi_\beta(\bar r)\phi^*_\alpha(\bar r')\phi_\beta(\bar r') \cdot \left\{\frac{f_\alpha - f_\beta}{\omega+\omega_{\alpha\beta}+i\eta}\right\}}$$

er þéttleika svörunarfallið, sem við munum nú tengja við ϵ, rafsvörunarfallið

nú má nota

$$\phi^{ind}(\bar r'') = -e\int d\bar r\, \frac{n_s^{ind}(\bar r)}{|\bar r'' - \bar r|}$$ (muna Hartree)

og

$$\phi(\bar r) = \phi^{ext}(\bar r) + \phi^{ind}(\bar r)$$

$$\rightarrow \phi(\bar r'') - \phi^{ext}(\bar r'') = \frac{e^2}{\hbar}\int d\bar r' d\bar r\, \frac{D(\bar r,\bar r';\omega)}{|\bar r'' - \bar r|}\phi(\bar r'$$

$$\rightarrow \phi(\bar r'') = \int d\bar r' \left\{\delta(\bar r' - \bar r'') + \frac{e^2}{\hbar}\int d\bar r\, \frac{D(\bar r,\bar r';\omega)}{|\bar r'' - \bar r|}\right\}\phi^{ext}(\bar r$$

þetta þarf að bera saman við

$$\phi(\bar r) = \int d\bar r'\, \epsilon^{-1}(\bar r,\bar r')\,\phi^{ext}(\bar r')$$

til þess að fá

$$\boxed{\epsilon^{-1}(\bar r,\bar r') = \delta(\bar r' - \bar r) + \frac{e^2}{\hbar}\int d\bar r''\, \frac{D(\bar r'',\bar r';\omega)}{|\bar r - \bar r''|}}$$

Ef

$$D(\bar{r}'',\bar{r}',\omega) = D(\bar{r}''-\bar{r},\omega)$$

þá fæst

$$\epsilon^{-1}(\bar{q},\omega) = 1 + \frac{4\pi e^2}{q^2}\underbrace{\left(\frac{D(\bar{q},\omega)}{\hbar}\right)}_{=\chi(\bar{q}\omega)}$$

Við höfum því aðferð til þess að reikna $\epsilon^{-1}(\bar{q},\omega)$ fyrir Hartree víxlverkandi kerfi

$$\boxed{\begin{array}{l}\underline{\epsilon^{-1}\text{ og }\chi}\text{ ákvarða svörun kerfisins}\\ \text{við }\underline{\text{ytra}}\text{ mætti }\phi^{ext}\\ \qquad\phi(\bar{r}) = \int d\bar{r}'\epsilon^{-1}(\bar{r},\bar{r}')\phi^{ext}(\bar{r}')\end{array}}$$

Ef litið er til baka á

$$n_s^{ind}(\bar{r}) = -\frac{e}{\hbar}\int d\bar{r}' D(\bar{r},\bar{r}',\omega)\phi^{ext}(\bar{r}')$$

þá má gera <u>svörunina sjálfsamkvæma</u> með því að segja að ϕ en ekki ϕ^{ext} valdi $n_s^{ind}(\bar{r})$. (þetta má skýra betur í fjöleindafr.

$$\longrightarrow \quad n_s^{ind}(\bar{r}) = -\frac{e}{\hbar}\int d\bar{r}' D(\bar{r},\bar{r}',\omega)\phi(\bar{r})$$

nota síðan aftur

$$\phi^{ind}(\bar{r}'') = -e\int d\bar{r}\,\frac{n_s^{ind}(\bar{r})}{|\bar{r}''-\bar{r}|}$$

og

$$\phi(\bar{r}) = \phi^{ext}(\bar{r}) + \phi^{ind}(\bar{r})$$

$$\longrightarrow \quad \phi(\bar{r}'') - \phi^{ext}(\bar{r}'') = \frac{e^2}{\hbar}\int d\bar{r}'d\bar{r}\,\frac{D(\bar{r},\bar{r}',\omega)}{|\bar{r}''-\bar{r}|}\phi(\bar{r}') \qquad (*)$$

$$\longrightarrow \quad \phi^{ext}(\bar{r}'') = \int d\bar{r}'\left\{\delta(\bar{r}'-\bar{r}'') - \frac{e^2}{\hbar}\int d\bar{r}\,\frac{D(\bar{r},\bar{r}',\omega)}{|\bar{r}''-\bar{r}|}\right\}\phi(\bar{r}$$

$$\longrightarrow \quad \boxed{\epsilon(\bar{r},\bar{r}') = \delta(\bar{r}'-\bar{r}) - \frac{e^2}{\hbar}\int d\bar{r}''\,\frac{D(\bar{r}'',\bar{r}',\omega)}{|\bar{r}-\bar{r}''|}}$$

RPA eða Lindhard

Ef $D(\bar r'', \bar r', \omega) = D(\bar r'' - \bar r', \omega)$

þá fæst

$$\epsilon(\bar q, \omega) = 1 - \frac{4\pi e^2}{q^2}\underbrace{\left(\frac{D(\bar q,\omega)}{\hbar}\right)}_{= \chi_{sc}(\bar q\omega)}$$

Ef notaðar eru hér flatar bylgjur í D fæst niðurstaða $\underline{\underline{(17.60)}}$

Eins má endurskrifa (*) sem heildis jöfnu fyrir ϕ

$$\phi(\bar r'') = \phi^{ext}(\bar r'') + \frac{e^2}{\hbar}\int d\bar r' d\bar r \, \frac{D(\bar r, \bar r', \omega)}{|\bar r'' - \bar r|}\phi(\bar r')$$

eða þegar $D(\bar r'', \bar r', \omega) = D(\bar r'' - \bar r', \omega)$

$$\phi(\bar q\omega) = \phi^{ext}(\bar q\omega) + \frac{4\pi e^2}{q^2}\frac{D(\bar q,\omega)}{\hbar}\phi(\bar q\omega)$$

$$\longrightarrow \phi(\bar q\omega) = \frac{\phi^{ext}(\bar q\omega)}{1 - \frac{4\pi e^2}{q^2}\frac{D(\bar q,\omega)}{\hbar}} = \frac{\phi^{ext}(\bar q\omega)}{\epsilon(\bar q\omega)}$$

þannig að núllstöð í $\epsilon(q\omega)$ leiðir til bylgja í rafeindagasinu sem geta borist um : <u>rafgasbylgjur</u>

↑ þær hefðu ekki fundist þegar hin nálgunin var notuð

ϵ ákvarðar svörun kerfisins við sjálf samkvæma mættinu $\phi = \phi^{ind} + \phi^{ext}$

Leiðni

Nú má reikna leiðni hliðstætt því sem að framan var lýst

Notum línulegasvörun til þess að reikna strauminn sem vigurmætti veldur m. línulegri nálgun m.t.t. A

$$H_I = -\frac{e}{c}\int d\bar{r}\, \bar{A}(\bar{r}t)\cdot \bar{J}(\bar{r}t)$$

$$J(\bar{r}) = \frac{1}{2m}\left\{\hat{p}\,\delta(\hat{r}-\bar{r}) + \delta(\hat{r}-\bar{r})\,\hat{p}\right\} - \frac{e^2}{mc}\bar{A}(\bar{r}\,t)\,\delta(\hat{r}-\bar{r})$$

Þá fæst

$$\sigma_{kl}(\bar{r},\bar{r}',\omega) = \frac{ie^2}{\hbar}\,\frac{D_{kl}(\bar{r},\bar{r}',\omega)}{\omega} - \frac{ie^2 n(\bar{r})}{\omega m}\delta_{kl}\cdot\delta(\bar{r}-\bar{r}')$$

þ.s.

$$J_i(\bar{x}\omega) = \int d\bar{x}'\,\sigma_{ij}(\bar{r},\bar{r}',\omega)\,\bar{E}_j(\bar{r}'\omega)$$

og

$$\bar{E}(\bar{r}t) = -\frac{1}{c}\partial_t \bar{A}(\bar{r}t)$$

þar sem straumsvörunarfallið er

$$D_{ij}(\bar{r},\bar{r}',\omega) = -\frac{\hbar^2}{4m^2}\sum_{\alpha\beta}\left(\phi^*_\alpha(\bar{r})\overleftrightarrow{\nabla}\phi_\beta(\bar{r})\right)\left(\phi^*_\alpha(\bar{r}')\overleftrightarrow{\nabla}'\phi_\beta(\bar{r}')\right)\cdot\left\{\frac{f_\alpha - f_\beta}{\omega+\omega_{\alpha\beta}+i\eta}\right\}$$

Málið flækist mjög þegar V_{imp} er tekið með fyrir slembidreifðar veilur

Þá er venja að nota truflanareikning með tilliti til V_{imp} til þess að smíða D_{ij} .....

Slíkt verður reynt í "Kennilegri eðlisfræði þéttefnis"

Fermi vökvar

$T<<T_F$ án víxlverkunar

Rafeindirnar sitja í fermikúlu
Einsetulögmálið kemur í veg fyrir árekstra

Kveikt á víxlverkun rafeindir með
$\Sigma \sim \Sigma_F$ geta víxlverkast við (eða rekist á
rafeindir með $\Sigma \sim (\Sigma_F - kT, \Sigma_F + kT)$

Víxlverkunin breytir eiginleikum þessara
rafeinda :

Halda skammtatölum
en m^*, g^* og K^* eru breytt
og $\Sigma(\bar{k})$

-> sýndareindir

Hér er gert ráð fyrir að þær séu
Fermi eindir (þarf ekki að vera, og
þær þurfa ekki að samsvara
upphaflegu rafeindunum)

þær ráða flestum stórsæjum eiginleikum
„málmsins" -> mikilvægi fermiyfirb.

Fáar sýndareindir, lítill þéttleiki
lítið um árekstra

Líftími eindar í ástandi með $\Sigma = \Sigma_1 > \Sigma_F$
er

$$\frac{1}{\tau} = a(\Sigma_1 - \Sigma_F)^2 + b(k_B T)^2$$

verður ∞ við $T=0$ á fermiyfirb.

Þegar rafeindir verða fyrir ytri áhrifum
er venja að líta svo á að $\Sigma(\bar{k})$ breytist
ekki en í stað f^0 kemur $g(k\ldots)$

Sýndareindir orsakast af rafeindavíxlverkun
sem breytist með setni ástanda

-> $\Sigma(\bar{k})$ breytist vegna ytri áhrifa

$$\delta\Sigma(\bar{k}) = \frac{1}{V}\sum_{\bar{k}'} f(\bar{k},\bar{k}')\,\delta n(\bar{k}')$$

samkvæmt HF væri $\left(\delta n(\bar{k}) = g(\bar{k}) - f(\bar{k})\right)$

$$f(\bar{k},\bar{k}') = \frac{4\pi e^2}{(\bar{k}-\bar{k}')^2}$$

en $f(\bar{k},\bar{k}')$ er víxlverkun sýndareindanna

Síðan er venja að leiða út jöfnu í líkingu við Boltzmann jöfnuna fyrir $\delta n(\bar{k})$.
Í henni kemur $f(\bar{k},\bar{k}')$ fyrir
$\nearrow$
má finna í einhverri nálgun skv.
Greens falla aðferðum fjöleindafr.

Þessi Fermi vökvafræði gildir ekki alltaf
því sýndareindirnar geta verið flóknari
hlutir

Cooper pör í ofurleiðurum
hér bætist við áhrif hljóðeinda
á rafeinda víxlverkunina

Mörg önnur dæmi

Járnseglum
kristöllum
⋮
1D

A1

Viðbót við línulegasvörun, A

$$H_0 |\alpha\rangle = E^0_\alpha |\alpha\rangle$$

Við H_0 bætist tímaháð truflun

$$\delta V(t) = \delta V e^{-i(\omega+i\eta)t} \qquad \eta \to 0^+$$

$$\to \lim_{t\to-\infty} \delta V(t) = 0$$

það er sem sé kveikt hægt á truflunni

þ.a.

$$\rho(t \to -\infty) = \rho^0$$

Fyrir Fermi eindir þá getur safnmeðalstæðin gefið

$$\rho^0 = f(H_0)$$

því samkvæmt stóru kórdreifingu

$$\rho^0 = Z^{-1} e^{-H_0/kT}$$

$$Z = tr\{e^{-H_0/kT}\}$$

A2

Hreyfijafna $\rho(t)$

$$i\hbar\dot{\rho}(t) = [H(t), \rho(t)]$$

sem við viljum leysa línulega með tilliti til δV

$$i\hbar\dot{\rho}(t) = [H_0, \rho(t)] + [\delta V(t), \rho(t)]$$

athuga fylkisstök

$$\langle\alpha|\rho(t)|\beta\rangle = \rho_{\alpha\beta}(t)$$

og nota $\rho(t) = \rho^0 + \delta\rho(t)$

þá fæst í línulegri nálgun:

$$i\hbar\delta\dot{\rho}(t) = [H_0, \delta\rho(t)] + [\delta V(t), \rho^0]$$

þ.a.

$$i\hbar\delta\dot{\rho}_{\alpha\beta}(t) = (E^0_\alpha - E^0_\beta)\delta\rho_{\alpha\beta}(t) + \langle\alpha|[\delta V(t), \rho^0]|\beta$$

því fæst

$$i\hbar\delta\dot{\varrho}_{\alpha\beta}(t) = \hbar\omega_{\alpha\beta}\delta\varrho_{\alpha\beta}(t) + (n_\beta - n_\alpha)\langle\alpha|\delta V(t)|\beta$$

því

$$\boxed{\begin{aligned}\varrho_0|\beta\rangle &= f(H_0)|\beta\rangle = f(E_\beta)|\beta\rangle \\ &\equiv n_\beta|\beta\rangle\end{aligned}}$$

Notum Fourier umformun

tryggja samleitn.

$$\delta\varrho(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega'\, e^{-i\omega' t + \eta t}\,\delta\varrho(\omega')$$

$$\delta V(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\omega'\, e^{-i(\omega' + i\eta)t}\,\delta V(\omega')$$

því verður hreyfijafnan

$$\hbar(\omega' + i\eta)\delta\varrho_{\alpha\beta}(\omega') = \hbar\omega_{\alpha\beta}\delta\varrho_{\alpha\beta}(\omega') + (n_\beta - n_\alpha)\langle\alpha|\delta V(\omega$$

$$\rightarrow \delta\varrho_{\alpha\beta}(\omega') = \frac{1}{\hbar}\left\{\frac{n_\beta - n_\alpha}{\omega' + (\omega_\beta - \omega_\alpha) + i\eta}\right\}\langle\alpha|\delta V(\omega')|\beta$$

Fourier umformun tilbaka

$$\delta V(\omega') = \int_{-\infty}^{\infty} dt\, e^{i\omega' t}\,\delta V(t) = \int_{-\infty}^{\infty} dt\, e^{i(\omega - \omega')t}\,\delta V$$

$$= 2\pi\delta(\omega - \omega')\delta V$$

$$\rightarrow \delta\varrho_{\alpha\beta}(\omega') = \frac{1}{\hbar}\left\{\frac{n_\beta - n_\alpha}{\omega' + (\omega_\beta - \omega_\alpha) + i\eta}\right\} 2\pi\delta(\omega - \omega')\langle\alpha|\delta V|\beta\rangle$$

$$\rightarrow \delta\varrho_{\alpha\beta}(t) = \frac{1}{\hbar}\left\{\frac{n_\beta - n_\alpha}{\omega' + \omega_{\beta\alpha} + i\eta}\right\}\langle\alpha|\delta V|\beta\rangle e^{-i\omega t + \eta t}$$

---

eða

$$\delta\varrho_{\alpha\beta}(t) = \delta\varrho_{\alpha\beta}\, e^{-i\omega t + \eta t}$$

og

$$\delta\varrho_{\alpha\beta} = \frac{1}{\hbar}\left\{\frac{n_\beta - n_\alpha}{\omega + \omega_{\beta\alpha} + i\eta}\right\}\langle\alpha|\delta V|\beta\rangle$$

(A5)

þéttleiki $n(\bar{r})$

Í kerfi frjálsra agna er þéttleikinn

$$n(\bar{r}) = \mathrm{tr}\{\delta(\hat{r}-\bar{r})\rho^{\circ}\}$$

$$= \sum_{\alpha} \langle\alpha|\delta(\hat{r}-\bar{r})f(H_0)|\alpha\rangle$$

$$= \sum_{\alpha}\int d\bar{r}'\langle\alpha|\bar{r}'\rangle\langle\bar{r}'|\delta(\hat{r}-\bar{r})f(H_0)|\alpha\rangle$$

$$= \sum_{\alpha\beta}\int d\bar{r}'\langle\alpha|\bar{r}'\rangle\langle\bar{r}'|\delta(\hat{r}-\bar{r})|\beta\rangle\langle\beta|f(H_0)|\alpha\rangle$$

$$= \sum_{\alpha}\int d\bar{r}'\,\phi_{\alpha}^{*}(\bar{r}')\,\delta(\bar{r}'-\bar{r})\,\phi_{\beta}(\bar{r}')\,f(E_{\alpha})$$

$$= \sum_{\alpha}|\phi_{\alpha}(\bar{r})|^{2}f(E_{\alpha})$$

---

(1)

(2)

Einsleitt $\bar{E}$ og $\bar{\nabla}T$

leysa B-jöfnuna línul. m.t.t. $\bar{E}$ og $\bar{\nabla}T$

$$g_0(\bar{k}) = f(n(\bar{r})) \leftarrow \text{stöðb. jafn. dreif.}$$

$$f(\Sigma) = f(\bar{n}) \leftarrow \text{jafnv. dreif. samkv. meðal þéttl.}$$

veljum $g(\bar{k}) = f(\Sigma) + g_1(\bar{k})$

Jafnan er
$$\boxed{\frac{\partial g}{\partial t} + \bar{v}\frac{\partial g}{\partial \bar{r}} + \bar{F}\cdot\frac{1}{\hbar}\frac{\partial g}{\partial \bar{k}} = \left(\frac{\partial g}{\partial t}\right)_{coll}}$$

slökunartímanálgun

$$\left(\frac{\partial g}{\partial t}\right)_{coll} = -\frac{g(\bar{k})-g_0(\bar{k})}{\tau}$$

Setjum jöfnuna á línulegt form

$$\frac{\partial g_1}{\partial t} + \bar{v}\cdot\frac{\partial g_1}{\partial \bar{r}} + \bar{F}\cdot\frac{1}{\hbar}\frac{\partial f}{\partial \bar{k}} = -\frac{g_1}{\tau} + \frac{\delta_n f}{\tau}$$

m. $\delta_n f = g_0(\bar{k}) - f(\Sigma)$

athugum einungis $\bar{E}$, $(\bar\nabla T \neq 0$ í raun$)$ $\bar\nabla T = 0$

$$\rightarrow \quad \bar{F} = -e\bar{E}$$

$\bar{E}$ óháð t, leitum sístæðs ástands $\frac{\partial g}{\partial t} = 0$

$g_0(\bar{k})$ og $g(\bar{k})$ eru óháð $\bar{r}$

$$\rightarrow \quad \boxed{\bar{F}\cdot\frac{1}{\hbar}\frac{\partial f}{\partial \bar{k}} = -\frac{g_1}{\tau}}$$

$$\frac{1}{\hbar}\frac{\partial f}{\partial \bar{k}} = \frac{\partial f}{\partial \Sigma}\frac{1}{\hbar}\frac{\partial \Sigma}{\partial \bar{k}} = \frac{\partial f}{\partial \Sigma}\bar{v}$$

$$\rightarrow \quad \rightarrow \quad g_1(\bar{k}) = \tau e \bar{E}\cdot\bar{v}\left(\frac{\partial f}{\partial \Sigma}\right)$$

$$= -e\tau\left(-\frac{\partial f}{\partial \Sigma}\right)\bar{E}\cdot\bar{v}$$

$\bar\nabla T \neq 0 \rightarrow$ gerum ráð fyrir

$$g(\bar{k}) = f\left(\frac{\Sigma - \mu(x)}{k_B T(x)}\right) + g_1(\bar{k})$$

sístætt ástand

$$\bar{v}\cdot\frac{\partial g}{\partial \bar{r}} + \bar{F}\cdot\frac{1}{\hbar}\frac{\partial g}{\partial \bar{k}} + \frac{g-f}{\tau} = 0$$

Höldum fyrsta stig stigli at g m.t.t. $\bar{r}$

$$\rightarrow \quad -e\bar{E}\cdot\frac{\partial f}{\partial \Sigma}\frac{1}{\hbar}\frac{\partial \Sigma}{\partial \bar{k}} + \frac{\partial f}{\partial \Sigma}\frac{\partial \Sigma}{\partial \bar{r}}\cdot\bar{v} + \frac{g_1}{\tau} = 0$$

$$(-e\bar{E})\cdot\bar{v}\,\frac{\partial f}{\partial \Sigma} + \frac{\partial f}{\partial \Sigma}\left(-\frac{d\mu}{d\bar{r}} - \frac{\Sigma-\mu(x)}{T}\frac{dT}{d\bar{r}}\right)\cdot\bar{v}$$

$$+ \frac{g_1}{\tau} = 0$$

$$\rightarrow \quad g_1(\bar{k}) = \tau\vec{v}\cdot\left(-\frac{\partial f}{\partial \Sigma}\right)\left\{-e\bar{E} - \bar\nabla\mu + \frac{\Sigma-\mu}{T}\left(-\bar\nabla T\right)\right\}$$

Einvíðar rafgasbylgjur

$$\phi_\alpha(x) = \frac{1}{\sqrt{L}}\, e^{-iqx} , \quad L \to \infty$$

$$\frac{1}{L}\sum f(q) \to \frac{1}{2\pi}\int dq\, f(q)$$

$$D(x,x';\omega) = \sum_{\alpha\beta} \phi^*_\alpha(x)\phi_\beta(x)\phi^*_\beta(x')\phi_\alpha(x') \cdot \left\{\frac{f_\alpha - f_\beta}{\omega + \omega_{\alpha\beta} + i\eta}\right\}$$

$$\to \frac{1}{(2\pi)^2}\int dq\,dk \exp\left\{iq(x-x') - ik(x-x')\right\} \cdot \left\{\frac{f_q - f_k}{\omega + \omega_q - \omega_k + i\eta}\right\}$$

$$= D(x-x';\omega)$$

Fourier umformun

$$D(q,\omega) = \int d(x-x')\, e^{i(x-x')q}\, D(x-x';\omega)$$

$$= \int d(x-x') \frac{dq'dk}{(2\pi)^2} \exp\left\{iq(x-x') + iq'(x-x') - ik(x-x')\right\} \cdot \left\{\frac{f_{q'} - f_k}{\omega + \omega_{q'} - \omega_k + i\eta}\right\}$$

$$= \int \frac{dq'dk}{(2\pi)}\, \delta(q+q'-k) \left\{\frac{f_{q'} - f_k}{\omega + \omega_{q'} - \omega_k + i\eta}\right\}$$

$$= \int \frac{dk}{(2\pi)} \left\{\frac{f_{k-q} - f_k}{\omega + \omega_{k-q} - \omega_k + i\eta}\right\}$$

$$D(q,\omega) = \int \frac{dk}{(2\pi)} \left[\frac{\theta(k_F-|k+q|) - \theta(k_F-|k|)}{\omega + \omega_{k-q} - \omega_k + i\eta} \right]$$

$$= \int \frac{dk}{(2\pi)} \theta(k_F-k) \left\{ \frac{1}{\omega + \omega_k - \omega_{k+q} + i\eta} - \frac{1}{\omega + \omega_{k-q} - \omega_k + i\eta} \right\}$$

$$\frac{1}{\omega + \frac{\hbar k^2}{2m} - \frac{\hbar (k+q)^2}{2m} + i\eta}$$

$$\omega_k - \omega_{k+q} = -\frac{\hbar}{2m} 2qk - \frac{\hbar}{2m} q^2$$

$$\omega_{k-q} - \omega_k = -\frac{\hbar}{2m} 2qk + \frac{\hbar}{2m} q^2$$

---

notum

$$\frac{1}{1+x} \simeq 1 - x + x^2 + \cdots$$

$$\frac{1}{\omega - \frac{\hbar}{2m} 2qk - \frac{\hbar}{2m} q^2 + i\eta} - \frac{1}{\omega - \frac{\hbar}{2m} 2qk + \frac{\hbar}{2m} q^2 + i\eta}$$

$$= \frac{1}{(\omega+i\eta)\left\{1 - \frac{\hbar}{m}\frac{qk}{(\omega+i\eta)} - \frac{\hbar}{2m}\frac{q^2}{(\omega+i\eta)}\right\}} - \frac{1}{(\omega+i\eta)\left\{1 - \frac{\hbar}{m}\frac{qk}{(\omega+i\eta)} + \frac{\hbar}{2m}\frac{q^2}{(\omega+i\eta)}\right\}}$$

$$= \frac{1}{(\omega+i\eta)} \left\{ \left(\frac{\hbar}{m}\frac{qk}{(\omega+i\eta)} + \frac{\hbar}{2m}\frac{q^2}{(\omega+i\eta)}\right) - \left(+\frac{\hbar}{m}\frac{qk}{\omega+i\eta} - \frac{\hbar}{2m}\frac{q^2}{(\omega+i\eta)}\right) \right.$$
$$\left. + \left(\frac{\hbar}{m}\frac{qk}{(\omega+i\eta)} + \frac{\hbar}{2m}\frac{q^2}{(\omega+i\eta)}\right)^2 - \left(\frac{\hbar}{m}\frac{qk}{(\omega+i\eta)} - \frac{\hbar}{2m}\frac{q^2}{(\omega+i\eta)}\right)^2 \right\}$$

$$\simeq \frac{1}{(\omega+i\eta)} \left\{ \frac{\hbar}{m}\frac{q^2}{(\omega+i\eta)} + O(q^3) \right\}$$

$$D(q,\omega) = \int_{-k_F}^{k_F} \frac{dk}{(2\pi)} \frac{\hbar}{m} \frac{q^2}{(\omega+i\eta)^2}$$

$$= n_s^{1D} \frac{\hbar}{m} \frac{q^2}{(\omega+i\eta)^2} \cdot 2$$

þ. munað er eftir spuna

$$\epsilon(q,\omega) = 1 - V(q)\, n_s^{1D} \frac{q^2 \cdot 2}{m(\omega+i\eta)^2} = 0$$

$$\to (\omega+i\eta)^2 = V(q)\, n_s^{1D} \frac{q^2}{m} \cdot 2$$

~~$= \cdot \frac{4e^2}{K}\left\{-\ln\left(\frac{|q|l_0}{2}\right)+\gamma\right\} \frac{n_s^{1D}}{m} q^2$~~

~~$= \frac{2e^2}{K} \frac{n_s^{1D}}{m} \left\{-q^2\left(2\ln\left(\frac{|q|l_0}{2}\right)+\gamma\right)\right\}$~~

~~$= \frac{2e^2 n_s^{1D}}{Km} \{-$~~

$$(\omega+i\eta)^2 = \frac{4e^2 n_s^{1D}}{Km} \left\{-q^2\left(\ln\left(\frac{|q|l_0}{2}\right)-\gamma\right)\right\}$$

$$\omega^2 = \frac{4e^2 n_s^{1D}}{Km} \left\{q^2\gamma - q^2\ln\left(\frac{|q|l_0}{2}\right)\right\}$$

1D

$$V(x) = -\frac{e^2}{\kappa}\frac{1}{\sqrt{(x^2+\ell_0^2)}}$$

$$V(q) = -\frac{e^2}{\kappa}\int_{-\infty}^{\infty} dx\, \frac{e^{-iqx}}{\sqrt{x^2+\ell_0^2}}$$

$$= -\frac{e^2}{\kappa}\left\{ \int_{-\infty}^{0} dx\, \frac{e^{-iqx}}{\sqrt{x^2+\ell_0^2}} + \int_{0}^{\infty} dx\, \frac{e^{-iqx}}{\sqrt{x^2+\ell_0^2}} \right\}$$

$$= -\frac{e^2}{\kappa}\left\{ \int_{0}^{\infty} dx\, \frac{e^{iqx}}{\sqrt{x^2+\ell_0^2}} + \int_{0}^{\infty} dx\, \frac{e^{-iqx}}{\sqrt{x^2+\ell_0^2}} \right\}$$

$$= -\frac{e^2}{\kappa} 2\int_{0}^{\infty} dx\, \frac{\cos(qx)}{\sqrt{x^2+\ell_0^2}}$$

bera saman við

$$K_0(xz) = \frac{\Gamma(\frac{1}{2})}{\Gamma(\frac{1}{2})}\int_0^\infty dt\, \frac{\cos xt}{\sqrt{t^2+z^2}} \qquad (8.432.5) \quad x>0$$

$$\rightarrow V(q) = -\frac{2e^2}{\kappa} K_0(|q|\ell_0)$$

$$K_0(z) \underset{z\to 0}{\simeq} -\left\{\ln\left(\frac{z}{2}\right)+\gamma\right\} I_0(z) + \frac{\frac{1}{4}z^2}{(1!)^2} + (1+1/2)\frac{(\frac{1}{4}z^2)^2}{(2!)^2} + \cdots$$

$$I_0(z) = 1 + \frac{\frac{1}{4}z^2}{(1!)^2} + \cdots$$

$V(q) = V_0$ fasti .....

$V(q) = \frac{2}{3}\frac{e^2 k_F^2}{q^2}$ ....

⑤

Hvernig lítur skýlda mættið út fyrir púnkt hleðslu : $\boxed{V_{ext}(r) = -\frac{e^2}{\kappa r}}$

punkthleðsla $\longrightarrow \delta n_{ext}(\tilde{k}) = 1$

$$\longrightarrow \quad V_{ext}(\tilde{k}) = -\frac{2\pi e^2}{\kappa|\tilde{k}|}$$

en ef punkt hleðslan er fyrir utan 2D-kerfið þá er: $(z \neq 0)$

$$V_{ext}(\tilde{r}) = -\frac{e^2}{\kappa}\frac{1}{\sqrt{\tilde{r}^2+z_0^2}}$$

finnum $V_{ext}(\tilde{k})$

$$V_{ext}(\tilde{k}) = -\frac{e^2}{\kappa}\int d\tilde{r}\,\frac{e^{-i\tilde{r}\cdot\tilde{k}}}{\sqrt{\tilde{r}^2+z_0^2}}$$

$$= -\frac{e^2}{\kappa}\int r\,dr\,d\varphi\,\frac{e^{-irk\cos\varphi}}{\sqrt{r^2+z_0^2}}$$

⑥

nota
$$J_0(kr) = \frac{1}{2\pi}\int_0^{2\pi} d\varphi\, e^{ikr\cos\varphi} \qquad \text{Bessel}$$

því fæst

$$V_{ext}(\tilde{k}) = -2\pi\frac{e^2}{\kappa}\int r\,dr\,\frac{J_0(rk)}{\sqrt{r^2+z_0^2}}$$

$$= -2\pi\frac{e^2}{\kappa|\tilde{k}|}e^{-z_0|\tilde{k}|}$$

heilda mættið verður því

$$V(\tilde{k}) = V_{ext}(\tilde{k})/\epsilon(\tilde{k})$$

$$= -\frac{2\pi e^2}{\kappa|\tilde{k}|}\frac{1}{1+\frac{Q}{|\tilde{k}|}}e^{-z_0|\tilde{k}|}$$

svo heilda mættið í r-rúmi er:

$$V(\tilde{r}) = \frac{1}{(2\pi)^2}\int_0^{\infty} k\,dk\int_0^{2\pi} d\varphi\,\frac{e^{ikr\cos\varphi}}{k+Q}\left(-\frac{2\pi e^2}{\kappa}\right)e^{-z_0 k}$$

$k = |\tilde{k}|$

④

$$\Sigma(\bar{k}) = \frac{\hbar^2k^2}{2m} - \frac{2e^2}{\pi}k_F\left\{\frac{1}{2} + \frac{1-(k/k_F)^2}{4k/k_F}\ln\left|\frac{1+k/k_F}{1-k/k_F}\right|\right\}$$

nærri $k=0$

$$\Sigma(\bar{k}) \simeq \frac{\hbar^2k^2}{2m} - \frac{2e^2}{\pi}k_F\left\{1 - \frac{1}{3}\frac{k^2}{k_F^2} - \frac{1}{15}\frac{k^4}{k_F^4}\right\}$$

$$\simeq -\frac{2e^2k_F}{\pi} + \frac{\hbar^2k^2}{2m} + \frac{2}{3\pi}\frac{e^2k^2}{k_F}$$

Stílgreinum

$$\Sigma(k) \simeq \frac{\hbar^2k^2}{2m}\left\{1 + \frac{2e^2\,2m}{3\pi k_F\hbar^2}\right\}$$

$$= \frac{\hbar^2k^2}{2m}\left\{1 + \frac{4e^2\,m}{3\pi(3\pi^2n)^{1/3}\hbar^2}\right\}$$

$$= \frac{\hbar^2k^2}{2m}\left\{1 + \frac{2\cdot 2}{3\pi(3\pi^2n)^{1/3}a_0}\right\}$$

$$= \frac{\hbar^2k^2}{2m}\left\{1 + \frac{2\cdot 2}{3\pi(3\pi n)^{1/3}\pi^{1/3}a_0}\right\}$$

$$\frac{\hbar^2 k^2}{2m}\left\{1+\frac{2\,4^{1/3}\,(3^{1/3})\cdot 2}{3(3\pi)^{1/3}(4\pi n)^{1/3}a_0\pi(3^{1/3})}\right\}$$

$$=\frac{\hbar^2 k^2}{2m}\left\{1+\frac{2\cdot 4^{1/3}\cdot 2}{3(3\pi)^{1/3}\pi(3)^{1/3}}\,\frac{r_s}{a_0}\right\}$$

$$=\frac{\hbar^2 k^2}{2m}\left\{1+0{,}22\,\frac{r_s}{a_0}\right\}$$

$$\Rightarrow\ m\left\{1+0{,}22\,\frac{r_s}{a_0}\right\}^{-1}=m^*$$

$$\rightarrow\ \frac{m^*}{m}=\frac{1}{1+0{,}11\left(\frac{r_s}{a_0}\right)}$$

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

$$\Sigma\simeq\frac{\hbar^2 k^2}{2m}\left\{1+\frac{2\cdot 2\,r_s}{3\pi\left(\frac{9\pi}{4}\right)^{1/3}a_0}\right\}$$

$$\simeq\frac{\hbar^2 k^2}{2m}\left\{1+0{,}22\,\frac{r_s}{a_0}\right\}$$

---

①

①

$$H=2\int\frac{d\bar{k}}{(2\pi)^3}\,h(\bar{k})\,g(\bar{k})$$

þéttleiki

eiginl. einvareindar

$$\left(\frac{dH}{dt}\right)_{coll}=2\int\frac{d\bar{k}}{(2\pi)^3}\,h(\bar{k})\left(\frac{\partial g}{\partial t}\right)_{coll}$$

a) sýna að $\left(\frac{dH}{dt}\right)_{coll}=0$ ef h varðveitist í öllum árekstrum

þ.e. aðeins eru til árekstrar ~~þ.a.~~.
milli $\bar{k}'$ og $\bar{k}$ með $h(\bar{k})=h(\bar{k}')$

$$\left(d_t g(\bar{k})\right)_{coll}=-\int\frac{d\bar{k}'}{(2\pi)^3}\left\{W_{\bar{k},\bar{k}'}\,g(\bar{k})\left(1-g(\bar{k}')\right)-W_{\bar{k}',\bar{k}}\,g(\bar{k}')\left(1-g(\bar{k})\right)\right\}$$

Slökunartíma nálgun

$$\left(\frac{\partial g}{dt}\right)_{coll} = -\frac{1}{\tau(\bar{k})}\left(g(\bar{k}) - g^{\circ}(\bar{k})\right)$$

$\rightarrow$

$$\left(\frac{dH}{dt}\right)_{coll} = 2\int \frac{d\bar{k}}{(2\pi)^3}\, h(\bar{k})\, \frac{\left(g^{\circ}(\bar{k}) - g(\bar{k})\right)}{\tau(\bar{k})}$$

$= 0$ aðeins ef $\mu(\bar{r},t)$ og $T(\bar{r},t)$ eru þ.a. $g^{\circ}(\mu, T, \dots) = g$

c)

$$\frac{\partial g}{\partial t} + \bar{V}\cdot\vec{\nabla} g + \vec{F}\cdot\frac{1}{\hbar}\vec{\nabla}_k g = \left(\frac{\partial g}{\partial t}\right)_{coll}$$

$$\vec{F}(\bar{r},\bar{k}) = -e\left(\bar{E} + \frac{1}{c}\bar{v}\times\bar{H}\right)$$

$$\rho = 2\int \frac{d\bar{k}}{(2\pi)^3}(-e)\,g(\bar{k})$$

$$j = -e\cdot 2\int \frac{d\bar{k}}{(2\pi)^3}\,\bar{v}(\bar{k})\,g(\bar{k})$$

$$\left(\frac{dH}{dt}\right)_{coll} = 2\int \frac{d\bar{k}\,d\bar{k}'}{(2\pi)^3(2\pi)^3}\, h(\bar{k})\left\{W_{\bar{k},\bar{k}'}\, g(\bar{k})\left(1-g(\bar{k}')\right) - W_{\bar{k}'\bar{k}}\, g(\bar{k}')\left(1-g(\bar{k})\right)\right\}$$

$$W_{\bar{k},\bar{k}'} = W_{\bar{k}',\bar{k}}$$

$$\left(\frac{dH}{\partial t}\right)_{coll} = 2\int \frac{d\bar{k}\,d\bar{k}'}{(2\pi)^6}\left\{h(\bar{k}')\, W_{\bar{k}\bar{k}'}\, g(\bar{k})\left(1-g(\bar{k}')\right) - h(\bar{k})\, W_{\bar{k}'\bar{k}}\, g(\bar{k}')\left(1-g(\bar{k})\right)\right\}$$

$= 0$ ef skipt er á $\bar{k}$ og $\bar{k}'$ breytunum í síðari liðnum

$$\frac{\partial}{\partial t}\rho = -2e\int\frac{d\bar{k}}{(2\pi)^3}\frac{\partial}{\partial t}g(\bar{k})$$

$$= -2e\int\frac{d\bar{k}}{(2\pi)^3}\left\{\left(\frac{\partial g}{\partial t}\right)_{coll} - \bar{v}\cdot\frac{\partial g}{\partial \bar{r}} - \bar{F}\cdot\frac{1}{\hbar}\frac{\partial g}{\partial \bar{k}}\right\}$$

$$= \underbrace{\left(\frac{\partial \rho}{\partial t}\right)_{coll}}_{=0} - (-2e)\int\frac{d\bar{k}}{(2\pi)^3}\,\bar{v}(\bar{k})\cdot\frac{\partial}{\partial \bar{r}}g(\bar{k})$$

$$+ \frac{(2e)}{\hbar}\int\frac{d\bar{k}}{(2\pi)^3}\,\bar{F}\cdot\frac{\partial g(\bar{k})}{\partial \bar{k}}$$

$$\frac{\partial}{\partial t}\rho + \bar{\nabla}\cdot\left\{(-2e)\int\frac{d\bar{k}}{(2\pi)^3}\,\bar{v}(\bar{k})g(\bar{k})\right\}$$

$$= (-2e)\int\frac{d\bar{k}}{(2\pi)^3}\left(\bar{\nabla}\cdot\bar{v}(k)\right)g(\bar{k})$$

$$+ \frac{(-2e)}{\hbar}\int\frac{d\bar{k}}{(2\pi)^3}\,\bar{F}\cdot\frac{\partial}{\partial \bar{k}}g(\bar{k})$$

want fost

$$\frac{\partial}{\partial t}\rho + \bar{\nabla}\cdot\bar{j} = 0$$

but

$$\int d\bar{k}\;\bar{F}\cdot\frac{\partial}{\partial \bar{k}}g(\bar{k}) = \bar{F}\cdot\int d\bar{k}\,\frac{\partial}{\partial \bar{k}}g(\bar{k})$$

$$= \bar{F}\cdot\int_{S\to\infty} d\bar{S}\;g(\bar{k}) = 0$$

$$\int d\bar{k}\;\underbrace{\left(\bar{\nabla}\cdot\bar{v}(k)\right)}_{}g(\bar{k}) = \cancel{\bar{\nabla}\cdot\int d\bar{k}\;\bar{v}(\bar{k})g(\bar{k})}$$

~~$= \bar{\nabla}\cdot$~~

scattering angles Ω can be immediately effected to yield

$$Z = \int d^3v_1 \int d^3v_2\, \sigma_{\text{tot}}\, |\mathbf{v}_1 - \mathbf{v}_2|\, f(\mathbf{r}, \mathbf{v}_1, t)(\mathbf{r}, \mathbf{v}_2, t) \tag{5.1}$$

A free path is defined as the distance traveled by a molecule between two successive collisions. Since it takes two molecules to make a collision, every collision terminates two free paths. The total number of free paths occurring per second per unit volume is therefore $2Z$. Since there are n molecues per unit volume, the average number of free paths traveled by a molecule per second is $2Z/n$. The *mean free path*, which is the average length of a free path, is given by

$$\lambda = \frac{n}{2Z}\bar{v} \tag{5.2}$$

where $\bar{v} = \sqrt{2kT/m}$ is the most probable speed of a molecule. The average duration of a free path is called the *collision time* and is given by

$$\tau = \frac{\lambda}{\bar{v}} \tag{5.3}$$

For a gas in equilibrium, $f(\mathbf{r}, \mathbf{v}, t)$ is the Maxwell-Boltzmann distribution. Assume for an order-of-magnitude estimate that σ_{tot} is insensitive to the energy of the colliding molecules and may be replaced by a constant of the order of πa^2 where a is the molecular diameter. Then we have

$$\begin{aligned} Z &= \sigma_{\text{tot}} \int d^3v_1 \int d^3v_2 |\mathbf{v}_1 - \mathbf{v}_2|\, f(\mathbf{v}_1) f(\mathbf{v}_2) \\ &= \sigma_{\text{tot}} n^2 \left(\frac{m}{2\pi kT}\right)^3 \int d^3v_1 \int d^3v_2\, |\mathbf{v}_1 - \mathbf{v}_2| \exp\left[-\frac{m}{2kT}(v_1^2 + v_2^2)\right] \\ &= \sigma_{\text{tot}} n^2 \left(\frac{m}{2\pi kT}\right)^3 \int d^3V \int d^3v\, |\mathbf{v}| \exp\left[-\frac{m}{2kT}(2V^2 + \tfrac{1}{2}v^2)\right] \end{aligned}$$

where $\mathbf{V} = \frac{1}{2}(\mathbf{v}_1 + \mathbf{v}_2)$, $\mathbf{v} = \mathbf{v}_2 - \mathbf{v}_1$. The integrations are elementary and give

$$Z = 4n^2 \sigma_{\text{tot}} \sqrt{\frac{kT}{\pi m}} = 4n^2\, \sigma_{\text{tot}} \frac{\bar{v}}{\sqrt{2\pi}} \tag{5.4}$$

Therefore

$$\lambda = \frac{1}{4}\sqrt{\frac{\pi}{2}} \frac{1}{n\sigma_{\text{tot}}} \tag{5.5}$$

$$\tau = \frac{1}{4}\sqrt{\frac{\pi}{2}} \frac{1}{n\sigma_{\text{tot}}\bar{v}} \tag{5.6}$$

where $\bar{v} = \sqrt{2kT/m}$. We see that the mean free path is independent of the temperature and is inversely proportional to the density times the total cross section. The numbers (5.5) and (5.6) are also good estimates for a gas not far from equilibrium, which is the only case we discuss further.

The following are some numerical estimates. For H_2 gas at its critical point,

$$\lambda \approx 10^{-7} \text{ cm}$$
$$\tau \approx 10^{-11} \text{ sec}$$

For H_2 gas in intergalactic space, where the density is about 1 molecule/cc,

$$\lambda \approx 10^{15} \text{ cm}$$

The diameter of H_2 has been taken to be about 1 Å.

From these qualitative estimates, it is expected that in H_2 gas under normal conditions, for example, any nonuniformity in density or temperature over distances of order 10^{-7} cm will be ironed out in the order of 10^{-11} sec. Variations in density or temperature over macroscopic distances may persist for a long time.

5.2 THE CONSERVATION LAWS

To investigate nonequilibrium phenomena, we must solve the Boltzmann transport equation, with given initial conditions, to obtain the distribution function as a function of time. Some rigorous properties of any solution to the Boltzmann equation may be obtained from the fact that in any molecular collision there are dynamical quantities that are rigorously conserved.

Let $\chi(\mathbf{r}, \mathbf{v})$ be any quantity associated with a molecule of velocity $\mathbf{v}$ located at $\mathbf{r}$, such that in any collision $\{\mathbf{v}_1, \mathbf{v}_2\} \to \{\mathbf{v}_1', \mathbf{v}_2'\}$ taking place at $\mathbf{r}$, we have

$$\chi_1 + \chi_2 = \chi_1' + \chi_2' \tag{5.7}$$

where $\chi_1 = \chi(\mathbf{r}_1, \mathbf{v}_1)$, etc. We call χ a conserved property. The following theorem holds.

THEOREM

$$\int d^3v\, \chi(\mathbf{r}, \mathbf{v}) \left[\frac{\partial f(\mathbf{r}, \mathbf{v}, t)}{\partial t}\right]_{\text{coll}} = 0 \tag{5.8}$$

where $(\partial f/\partial t)_{\text{coll}}$ is the right-hand side of (3.36).*

Proof. By definition of $(\partial f/\partial t)_{\text{coll}}$ we have

$$\int d^3v\, \chi \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} = \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\Omega)\, |\mathbf{v}_2 - \mathbf{v}_1|\, \chi_1(f_1' f_2' - f_1 f_2) \tag{5.9}$$

Making use of the properties of $\sigma(\Omega)$ discussed in Section 3.2, and proceeding in a manner similar to the proof of the H theorem, we make each

---

* Note that it is not required that f be a solution of the Boltzmann transport equation.

of the following interchanges of integration variables.

First: $\mathbf{v}_1 \rightleftarrows \mathbf{v}_2$
Next: $\mathbf{v}_1 \rightleftarrows \mathbf{v}_1'$ and $\mathbf{v}_2 \rightleftarrows \mathbf{v}_2'$
Next: $\mathbf{v}_1 \rightleftarrows \mathbf{v}_2'$ and $\mathbf{v}_2 \rightleftarrows \mathbf{v}_1'$

For each case we obtain a different form for the same integral. Adding the three new formulas so obtained to (5.9) and dividing the result by 4 we get

$$\begin{aligned} \int d^3v\, \chi \left(\frac{\partial f}{\partial t}\right)_{\text{coll}} &= \frac{1}{4} \int d^3v_1 \int d^3v_2 \int d\Omega \sigma(\Omega)\, |\mathbf{v}_1 - \mathbf{v}_2| \\ &\quad \times (f_2' f_1' - f_2 f_1)(\chi_1 + \chi_2 - \chi_1' - \chi_2') \equiv 0 \quad \text{(QED)} \end{aligned}$$

The conservation theorem relevant to the Boltzmann transport equation is obtained by multiplying the Boltzmann transport equation on both sides by χ and then integrating over $\mathbf{v}$. The collision term vanishes by virtue of (5.8), and we have*

$$\int d^3v\, \chi(\mathbf{r}, \mathbf{v}) \left(\frac{\partial}{\partial t} + v_i \frac{\partial}{\partial x_i} + \frac{1}{m} F_i \frac{\partial}{\partial v_i}\right) f(\mathbf{r}, \mathbf{v}, t) = 0 \tag{5.10}$$

We may rewrite (5.10) in the form

$$\begin{aligned} \frac{\partial}{\partial t} \int d^3v\, \chi f + \frac{\partial}{\partial x_i} \int d^3v\, \chi v_i f - \int d^3v \frac{\partial \chi}{\partial x_i} v_i f + \frac{1}{m} \int d^3v \frac{\partial}{\partial v_i}(\chi F_i f) \\ - \frac{1}{m} \int d^3v \frac{\partial \chi}{\partial v_i} F_i f - \frac{1}{m} \int d^3v\, \chi \frac{\partial F_i}{\partial v_i} f = 0 \end{aligned} \tag{5.11}$$

The fourth term vanishes if $f(\mathbf{r}, \mathbf{v}, t)$ is assumed to vanish when $|\mathbf{v}| \to \infty$. Defining the average value $\langle A \rangle$ by

$$\langle A \rangle \equiv \frac{\int d^3v\, Af}{\int d^3v\, f} = \frac{1}{n} \int d^3v\, Af \tag{5.12}$$

where

$$n(\mathbf{r}, t) \equiv \int d^3v\, f(\mathbf{r}, \mathbf{v}, t) \tag{5.13}$$

we obtain finally the desired theorem.

CONSERVATION THEOREM

$$\frac{\partial}{\partial t} \langle n\chi \rangle + \frac{\partial}{\partial x_i} \langle n v_i \chi \rangle - n \left\langle v_i \frac{\partial \chi}{\partial x_i} \right\rangle - \frac{n}{m} \left\langle F_i \frac{\partial \chi}{\partial v_i} \right\rangle - \frac{n}{m} \left\langle \frac{\partial F_i}{\partial v_i} \chi \right\rangle = 0 \tag{5.14}$$

---

* The summation convention, whereby a repeated vector index is understood to be summed from 1 to 3, is used.

where χ is any conserved property. Note that $\langle nA \rangle = n \langle A \rangle$ because n is independent of $\mathbf{v}$. From now on we restrict our attention to velocity-independent external forces so that the last term of (5.14) may be dropped.

For simple molecules the independent conserved properties are mass, momentum, and energy. For charged molecules we also include the charge, but this extension is trivial. Accordingly we set successively

$\chi = m$ (mass)
$\chi = mv_i \quad (i = 1, 2, 3)$ (momentum)
$\chi = \frac{1}{2}m\, |\mathbf{v} - \mathbf{u}(\mathbf{r}, t)|^2$ (thermal energy)

where $\mathbf{u}(\mathbf{r}, t) \equiv \langle \mathbf{v} \rangle$

We should then have three independent conservation theorems.

For $\chi = m$ we have immediately

$$\frac{\partial}{\partial t}(mn) + \frac{\partial}{\partial x_i} \langle mnv_i \rangle = 0$$

or, introducing the mass density

$$\rho(\mathbf{r}, t) \equiv mn(\mathbf{r}, t)$$

we obtain

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{5.15}$$

Next we put $\chi = mv_i$, obtaining

$$\frac{\partial}{\partial t} \langle \rho v_i \rangle + \frac{\partial}{\partial x_j} \langle \rho v_i v_j \rangle - \frac{1}{m} \rho F_i = 0 \tag{5.16}$$

To reduce this further let us write

$$\begin{aligned} \langle v_i v_j \rangle &= \langle (v_i - u_i)(v_j - u_j) \rangle + \langle v_i \rangle u_j + u_i \langle v_j \rangle - u_i u_j \\ &= \langle (v_i - u_i)(v_j - u_j) \rangle + u_i u_j \end{aligned}$$

Substituting this into (5.16) we obtain

$$\rho \left(\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j}\right) = \frac{1}{m} \rho F_i - \frac{\partial}{\partial x_j} \langle \rho (v_i - u_i)(v_j - u_j) \rangle \tag{5.17}$$

Introducing the abbreviation

$$P_{ij} \equiv \rho \langle (v_i - u_i)(v_j - u_j) \rangle$$

which is called the *pressure tensor*, we finally have

$$\left(\frac{\partial}{\partial t} + u_j \frac{\partial}{\partial x_j}\right) u_i = \frac{1}{m} F_i - \frac{1}{\rho} \frac{\partial}{\partial x_j} P_{ij} \tag{5.18}$$

Finally we set $\chi = \frac{1}{2} m \, |\mathbf{v} - \mathbf{u}|^2$. Then

$$\frac{1}{2} \frac{\partial}{\partial t} \langle \rho \, |\mathbf{v} - \mathbf{u}|^2 \rangle + \frac{1}{2} \frac{\partial}{\partial x_i} \langle \rho v_i \, |\mathbf{v} - \mathbf{u}|^2 \rangle - \frac{1}{2} \rho \left\langle v_i \frac{\partial}{\partial x_i} |\mathbf{v} - \mathbf{u}|^2 \right\rangle = 0 \tag{5.19}$$

We define the *temperature* by

$$kT \equiv \theta \equiv \tfrac{1}{3} m \langle |\mathbf{v} - \mathbf{u}|^2 \rangle$$

and the *heat flux* by

$$\mathbf{q} \equiv \tfrac{1}{2} m \rho \langle (\mathbf{v} - \mathbf{u}) \, |\mathbf{v} - \mathbf{u}|^2 \rangle$$

We then have

$$\begin{aligned} \tfrac{1}{2} m \rho \langle v_i \, |\mathbf{v} - \mathbf{u}|^2 \rangle &= \tfrac{1}{2} m \rho \langle (v_i - u_i) \, |\mathbf{v} - \mathbf{u}|^2 \rangle + \tfrac{1}{2} m \rho u_i \langle |\mathbf{v} - \mathbf{u}|^2 \rangle \\ &= q_i + \tfrac{3}{2} \rho \theta u_i \end{aligned}$$

and

$$\rho \langle v_i (v_j - u_j) \rangle = \rho \langle (v_i - u_i)(v_j - u_j) \rangle + \rho u_i \langle v_j - u_j \rangle = P_{ij}$$

Thus (5.19) can be written

$$\frac{3}{2} \frac{\partial}{\partial t} (\rho \theta) + \frac{\partial q_i}{\partial x_i} + \frac{3}{2} \frac{\partial}{\partial x_i} (\rho \theta u_i) + m P_{ij} \frac{\partial u_j}{\partial x_i} = 0$$

Since $P_{ij} = P_{ji}$

$$m P_{ij} \frac{\partial u_j}{\partial x_i} = P_{ij} \frac{m}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \equiv P_{ij} \Lambda_{ij}$$

The final form is then obtained after a few straightforward steps:

$$\rho \left(\frac{\partial}{\partial t} + u_i \frac{\partial}{\partial x_i} \right) \theta + \frac{2}{3} \frac{\partial}{\partial x_i} q_i = -\frac{2}{3} \Lambda_{ij} P_{ij} \tag{5.20}$$

The three conservation theorems are summarized in (5.21), (5.22), and (5.23).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \qquad \text{(conservation of mass)} \tag{5.21}$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = \frac{\rho}{m} \mathbf{F} - \nabla \cdot \overleftrightarrow{P} \qquad \text{(conservation of momentum)} \tag{5.22}$$

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \theta = -\tfrac{2}{3} \nabla \cdot \mathbf{q} - \tfrac{2}{3} \overleftrightarrow{P} \cdot \overleftrightarrow{\Lambda} \qquad \text{(conservation of energy)} \tag{5.23}$$

where $\overleftrightarrow{P}$ is a dyadic whose components are P_{ij}, $\nabla \cdot \overleftrightarrow{P}$ is a vector whose

ith component is $\partial P_{ij}/\partial x_j$, and $\overleftrightarrow{P} \cdot \overleftrightarrow{\Lambda}$ is the scalar $P_{ij} \Lambda_{ij}$. The auxiliary quantities are defined as follows.

$$\rho(\mathbf{r}, t) \equiv m \int d^3 v \, f(\mathbf{r}, \mathbf{v}, t) \qquad \text{(mass density)} \tag{5.24}$$

$$u(\mathbf{r}, t) \equiv \langle \mathbf{v} \rangle \qquad \text{(average velocity)} \tag{5.25}$$

$$\theta(\mathbf{r}, t) \equiv \tfrac{1}{3} m \langle |\mathbf{v} - \mathbf{u}|^2 \rangle \qquad \text{(temperature)} \tag{5.26}$$

$$\mathbf{q}(\mathbf{r}, t) \equiv \tfrac{1}{2} m \rho \langle (\mathbf{v} - \mathbf{u}) \, |\mathbf{v} - \mathbf{u}|^2 \rangle \qquad \text{(heat flux vector)} \tag{5.72}$$

$$P_{ij} \equiv \rho \langle (v_i - u_i)(v_j - u_j) \rangle \qquad \text{(pressure tensor)} \tag{5.28}$$

$$\Lambda_{ij} \equiv \tfrac{1}{2} m \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \tag{5.29}$$

Although the conservation theorems are exact, they have no practical value unless we can actually solve the Boltzmann transport equation and use the distribution function so obtained to evaluate the quantities (5.24)–(5.29). Despite the fact that these quantities have been given rather suggestive names, their physical meaning, if any, can only be ascertained after the distribution function is known. We shall see that when it is known these conservation theorems become the physically meaningful equations of hydrodynamics.

5.3 THE ZERO-ORDER APPROXIMATION

We assume that we are dealing with a gas that, although not in equilibrium, is not far from it. In particular, we assume that in the neighborhood of any point in the gas, the distribution function is locally Maxwell-Boltzmann, and that the density, temperature, and average velocity vary only slowly in space and time. For such a gas it is natural that we try the approximation

$$f(\mathbf{r}, \mathbf{v}, t) \approx f^{(0)}(\mathbf{r}, \mathbf{v}, t) \tag{5.30}$$

where

$$f^{(0)}(\mathbf{r}, \mathbf{v}, t) = n \left(\frac{m}{2\pi\theta} \right)^{3/2} \exp \left[-\frac{m}{2\theta} (\mathbf{v} - \mathbf{u})^2 \right] \tag{5.31}$$

where n, θ, $\mathbf{u}$ are all slowly varying functions of $\mathbf{r}$ and t. It is obvious that (5.30) cannot be an exact solution of the Boltzmann transport equation. It is obvious that

$$\left(\frac{\partial f^{(0)}}{\partial t} \right)_{\text{coll}} = 0 \tag{5.32}$$