Lecture 5 - Hubbard-Stratonovich transformation.

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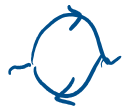
Last time:

$\Pi_0 =$  for high density electrons when

$|\underline{q}| \ll p_F, \quad |\omega| \ll \varepsilon_F.$

It can be calculated exactly,

as $\Pi_0(\underline{q}, \omega) = I(\underline{q}, \omega) + I(-\underline{q}, -\omega)$,

with $$I(\underline{q}, \omega) = 2\int \frac{n_{\underline{p}}}{\omega + \xi_{\underline{p}} - \xi_{\underline{p}+\underline{q}} + i\delta \operatorname{sgn}\omega} \frac{d^3p}{(2\pi)^3}$$

The result is called Lindhardt formula.

In the static case, $\omega = 0$, we have

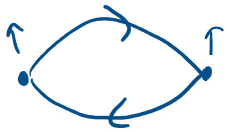
$$\Pi_0(\underline{q}, \omega=0) = -\frac{\nu_0}{2} - \frac{\nu_0}{2p_F q}\left(p_F^2 - \frac{q^2}{4}\right) \ln\left|\frac{q+2p_F}{q-2p_F}\right|$$

$$V_{eff} = \frac{4\pi e^2}{q^2 - 4\pi e^2 \Pi_0} \equiv \frac{4\pi e^2}{\varepsilon(q) q^2}$$

↑ dielectric function

$$\varepsilon(\underline{q}) = 1 + 4\pi \chi(\underline{q}) \quad ; \quad \rightarrow \chi = -e^2 \Pi_0(\underline{q})$$

↑ polarisability



In real space, $\chi(\underline{r}) = -e^2 \int e^{i\underline{q}\cdot\underline{r}} \Pi_0(\underline{q}) \, d\vec{q}$

Usually, we state that when $r \to \infty$, only $q \to 0$ contribution matters, since fast oscillation kills the integral.

Not true if $\Pi_0(q)$ has essential singularity.

When $q \to 0$, it's easy to check that

$$\Pi_0 \to -\frac{\nu_0}{2} - \frac{\nu_0}{2} = -\nu_0 \to \text{Thomas-Fermi screening.}$$

When $q \to \infty$, $\Pi_0 \to \frac{1}{q^2} \quad \left(\sim \frac{4}{3}\frac{p_F^2}{q^2}\right)$

The only unremoveable singularity (but not divergence) is at $|q| \to 2p_F$.

Rewriting $\Pi_0(q,0) \equiv -\frac{1}{2}\nu_0 f(q)$. Then

$$\psi(\underline{r}) = \tfrac{1}{2}\nu e^2 \int f(q)\, e^{i\underline{q}\cdot\underline{r}}\, d\vec{q} \quad ; \qquad d\vec{q} = \frac{d^d q}{(2\pi)^d}$$

where $f(q) = 1 + \frac{4p_F^2 - q^2}{4p_F q} \ln\left|\frac{q + 2p_F}{q - 2p_F}\right|$

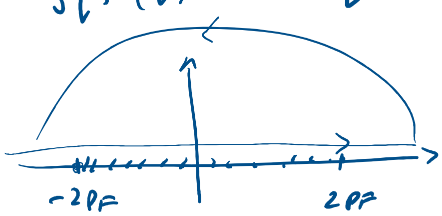
[Peirls]

$$\tilde{f}(q) = 1 + \frac{4p_F^2 - q^2}{4p_F q} \ln\left(\frac{q + 2p_F}{q - 2p_F}\right)$$

$$\psi(\underline{r}) = \frac{\nu_0 e^2}{8\pi^2} \int_0^\infty q^2 f(q)\, dq \int_{-1}^{1} e^{iqr\mu}\, d\mu$$

$$= \frac{\nu_0 e^2}{8\pi^2} \int_{-\infty}^{\infty} q f(q)\, e^{iqr}\, dq$$

$$\int q\tilde{f}(q)\, e^{iqr}\, dq = 0$$ as $\tilde{f} \sim \frac{1}{q}$ is regular above the cut.



As usual, $\ln z = \ln|z| + i \arg z \quad \left(z = |z| e^{i\arg z}\right)$

$$\tilde{f}(q) = f(q) - i\pi\,\theta(2p_F - |q|)\,\frac{4p_F^2 - q^2}{4p_F q}$$

$\Rightarrow$ Hence, $\int f(q)\, q\, e^{iqr}\, dq$ is contributed by the imaginary part only:

$$\chi(r) = \frac{\nu_0 e^2}{8\pi r \cdot 4p_F} \int_{-2p_F}^{2p_F} (4p_F^2 - q^2)\, e^{iqr}\, dq$$

$$= -\frac{\nu_0 e^2}{4\pi r^3}\left[\underbrace{\cos(2p_F r)}_{\text{dominates}} - \frac{\sin(2p_F r)}{2p_F r}\right]$$

Friedel oscillations (lead to RKKY interaction).

All the results for V_{eff} & Π_0 came from the perturbative expansion of the functional integral.

Let's avoid the expansion. Our action:

$$S = S_0 + S_{int}$$

$$S_0 = \int dx\, \bar{\psi}(x)\,(i\partial_t - \hat{H}_0 - \mu)\,\psi(x)$$

$$S_{int} = \frac{1}{2}\int dx\, dx'\, \rho(x)\rho(x')\, V(x - x')$$

where $\rho(x) = \bar{\psi}(x)\psi(x)$

Let's make the FT assuming a finite size:

$$\int d\vec{q} \equiv \int \frac{d^d q}{(2\pi)^d} = \frac{1}{L^d} \sum_q \quad , \text{ where } q$$

is quantised, so that $q_x = \frac{2\pi}{L} n_x$, etc

Then $S_{int} = \frac{1}{2} \int \rho_q e^{-i\underline{q}\cdot\underline{r}} \rho_{q'} e^{-i\underline{q}'\cdot\underline{r}'} V_{q_1} e^{-i\underline{q}_1\cdot(\underline{r}-\underline{r}')} d\underline{r}\, d\underline{r}'\, d\underline{q}\, d\underline{q}'\, d\underline{q}_1$

$\underline{r}$ integrations give $\delta(\underline{q}+\underline{q}_1)\,\delta(\underline{q}'-\underline{q}_1)\,(2\pi)^6$

Hence, we have

$$S_{int} = \frac{1}{2} \int \rho_{\underline{q}}\, \rho_{-\underline{q}}\, V_{\underline{q}}\, d\vec{q}$$

$$= \frac{1}{L^d} \sum_q \rho_q \rho_{-q} \frac{2\pi e^2}{q^2}$$

As $\rho(\underline{r})$ is real, then $\rho_{-\underline{q}} = \rho_{\underline{q}}^*$

$$\frac{2\pi e^2}{L^d q^2} \rho_{\underline{q}} \rho_{-\underline{q}} \equiv \underbrace{\frac{e}{2L^d}\rho_q}_{\zeta_q} \; \underbrace{\frac{e}{2L^d}\rho_{-q}}_{\zeta_{-q}} \cdot \underbrace{\frac{8\pi \; L^d}{q^2}}_{a_q}$$

$$e^{iS_{int}} = e^{i\sum_q \zeta_q \zeta_{-q} a_q} = \prod_q e^{i\zeta_q \zeta_{-q} a_q}$$

The aim: to represent each $e^{i\zeta_q \zeta_{-q} a_q}$ as a Gaussian integral over some auxiliary field, φ_q, which behaves like ζ_q.

↓

bosonic as ζ is bilinear in fermionic operators.

The aim: to integrate out fermionic $\bar{\psi}\,\psi$ and have a "bosonic" action in terms of φ.

$$Z_q \equiv \underline{I_0} \equiv \int d\bar{\varphi}_q d\varphi_q \, e^{-\frac{1}{a_q}\varphi_q \varphi_{-q}} \qquad \varphi_{-q} = \overline{\varphi_q}, \quad a_q = a_{-q}$$

make a shift of variables

$$= \int d\bar{\varphi}_q d\varphi_q \, e^{-\frac{1}{a_q}(\varphi_q - i a_q \xi_q)(\varphi_{-q} - i a_{-q}\xi_{-q})}$$

$$= \int d\bar{\varphi}_q d\varphi_q \, \underbrace{e^{-\frac{1}{a_q}\bar{\varphi}_q \varphi_q + i(\varphi_q \xi_{-q} + \varphi_{-q}\xi_q) + a_q \xi_q \xi_{-q}}}$$

$$= e^{a_q \xi_q \xi_{-q}} \int \ldots\ldots$$

Hence

$$\prod_q e^{-a_q \xi_q \xi_{-q}} = \frac{\prod_q \int d\varphi_q d\varphi_{-q} \, e^{-\frac{1}{a_q}\varphi_q \varphi_{-q} + i(\varphi_q \xi_{-q} + \varphi_{-q}\xi_q)}}{Z}$$

Call $\prod_q \int d\varphi_q d\varphi_{-q} \equiv \int \mathcal{D}\varphi$

$$e^{iS_{int}} = \frac{1}{Z}\int \underbrace{\mathcal{D}\varphi} \exp\left[\frac{i}{L^d}\sum_q \int dt \, \frac{\bar{\varphi}_q \varphi_q}{a_q} - \underbrace{\underbrace{\frac{ie}{2}(\varphi_q \rho_{-q} + \varphi_{-q}\rho_q)}_{-ie\,\varphi_q \rho_{-q}}}\right]$$

$\rho(\underline{r}) = \bar{\psi}(\underline{r})\psi(\underline{r})$; ρ_q is the FT

Hense $S_{int} = \int d\vec{q}\, dt \, \frac{q^2}{8\pi} \underline{\varphi_q \varphi_{-q}} = \int dx \, \varphi(x)\left(\frac{-\nabla^2}{8\pi}\right)\varphi(x)$

while $\varphi_q \rho_{-q}$ is absorbed by S_0 so that

$$S_0 = \int dx \, \bar{\psi}(x)\left[i\partial_t - (\hat{H}_0 - \mu) - ie\,\varphi(x)\right]\psi(x)$$

S_0 is bilinear over $\bar{\psi}, \psi$ and we can use

$$\int \bar{\psi}\, \hat{A}\, \psi\, dx = \left[\det \hat{A}\right] = e^{\ln\det A}$$

(would be $\frac{1}{\det A}$ for bosons.

Hence, we arrived at the bosonic action

$$S[\varphi] = \int dx \left\{ \frac{(\nabla\varphi)^2}{8\pi} + \mathrm{tr}\ln\Big[\underbrace{i\partial_t - (\hat{H}_0-\mu)}_{\hat{G}_0^{-1}} - ie\varphi\Big]\right\}$$

$$\left[\ \ln\det\hat{A} = \mathrm{Tr}\ln\hat{A}\ \right]$$

Then we have $\mathrm{Tr}\ln\hat{A} = \int dx\ \mathrm{tr}\ln\hat{A}$.

Tr is a "functional trace" including $\int dx$ or $\int dq$.

The task is to expand Tr ln, hopefully with a small parameter.

Reminder: $\left[i\partial_t - (\hat{H}_0-\mu)\right] G_0(x-x') = \delta(x-x')$

$$\left[\ \equiv \delta(t-t')\,\delta(\underline{r}-\underline{r}')\ \right]$$

$$S_0 = \mathrm{Tr}\ln\left[G_0^{-1} - ie\varphi\right] = \mathrm{Tr}\ln\left\{G_0^{-1}\left[1 - ieG_0\varphi\right]\right\}$$

$$= \underbrace{\mathrm{Tr}\ln G_0^{-1}}_{\text{no } \varphi} + \mathrm{Tr}\ln\left(1 - ieG_0\varphi\right) \quad !$$

Hubbard-Str.

cancels with $\frac{1}{Z}$ in any observable

$$\mathrm{Tr}\ln\left(1 - ie G_0 \varphi\right) = \mathrm{Tr}\sum_{n=1}^{\infty} \frac{\left(ie\hat{G}_0\varphi\right)^n}{n}$$

The $n=1$ term disappears upon integration due to the $x \to -x$ symmetry.

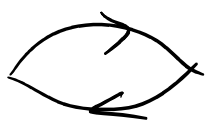
The lowest contributing term is

$$-\frac{e^2}{2}\mathrm{Tr}\,\hat{G}_0\varphi\,\hat{G}_0\varphi \quad (+\text{ higher orders}).$$

$$= -\frac{e^2}{2}\int dx\, dx'\, G_0(x-x')\,\varphi(x')\,G_0(x'-x)\,\varphi(x)$$

$$= -\frac{e^2}{2}\int dp\; \varphi(p)\varphi(-p)\,\Pi_0(p)$$

Here $\Pi_0(p) = 2\int G_0(q)\,G_0(p-q)\,dq$

 — the polarisation operator.

The full action is

$$S = \underbrace{\int dx \frac{(\nabla\varphi)^2}{8\pi}}_{\int dq\, \varphi_q v_q^{-1} \varphi_q} - \int \frac{e^2}{2}\varphi(p)\varphi(-p)\,\Pi_0(p)\,dp$$

$$= \frac{1}{2}\int \bar{\varphi}_q\left(\frac{q^2}{4\pi} - e^2\Pi_0(q)\right)\varphi_q\, dq$$

$$= \frac{1}{2}\int \bar{\varphi}_q\, \mathcal{D}_q^{-1}\,\varphi_q$$

$$\mathcal{D}_q = \mathcal{D}(\omega, \vec{q}) = \left[\frac{q}{4\pi} - e^2\Pi_0\right]^{-1}$$