Lecture XII: Weakly Interacting Electron Gas: Plasma Theory

▷ How are the properties of an electron gas influenced by weak Coulomb interaction?

$$\hat{H} = \sum_{i=1}^{N} \frac{\hat{\mathbf{p}}_i^2}{2m} + \sum_{i<j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|}$$

▷ Qualitative considerations:

With $r_0 = n^{-1/3}$ the average electron separation, typical p.e. e^2/r_0 and k.e. $\hbar^2/mr_0$

i.e. dimensionless ratio: $r_s = \dfrac{e^2}{r_0}\dfrac{mr_0^2}{\hbar^2} \equiv \dfrac{r_0}{a_0}$ — a_0 is Bohr radius

i.e. Coulomb effects dominate at low density!

At $r_s \sim 35$ there is (believed to be) a transition to an electron solid phase (QMC)
known as a Wigner crystal (cf. Mott-Hubbard insulator)

For most metals ($2 < r_s < 6$), k.e. and p.e. comparable;
fortunately (recall FLT) "weak coupling" theory valid even for intermediate r_s

▷ Motivates consideration of weak coupling theory $r_s \ll 1$:

$$\hat{H} = \int d\mathbf{r} c_\sigma^\dagger(\mathbf{r}) \frac{\hat{\mathbf{p}}^2}{2m} c_\sigma(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' c_\sigma^\dagger(\mathbf{r}) c_{\sigma'}^\dagger(\mathbf{r}') \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} c_{\sigma'}(\mathbf{r}') c_\sigma(\mathbf{r})$$

Σ-convention on spin

Aim: to explore dielectric properties and ground state energy of electron gas through...

▷ Quantum partition function:

$$\begin{aligned}
\mathcal{Z} \equiv \text{tr } e^{-\beta\hat{H}} &= \int_{\substack{\bar\psi_\sigma(0) = -\zeta\bar\psi_\sigma(\beta) \\ \psi_\sigma(0) = -\zeta\psi_\sigma(\beta)}} D(\bar\psi_\sigma, \psi_\sigma) e^{-S[\bar\psi_\sigma, \psi_\sigma]} \\
S[\bar\psi_\sigma, \psi_\sigma] &= \int_0^\beta d\tau \left[\int d\mathbf{r}\, \bar\psi_\sigma(\mathbf{r},\tau) \left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu \right) psi_\sigma(\mathbf{r},\tau) \right. \\
&\qquad \left. + \frac{1}{2}\int d\mathbf{r} \int d\mathbf{r}' \bar\psi_\sigma(\mathbf{r},\tau) \bar\psi_{\sigma'}(\mathbf{r}',\tau) \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \psi_{\sigma'}(\mathbf{r}',\tau) \psi_\sigma(\mathbf{r},\tau) \right]
\end{aligned}$$

Expressed in Fourier basis: $\psi_\sigma(\mathbf{r},\tau) = \dfrac{1}{\sqrt{L^3\beta}} \sum_{\mathbf{k},\omega_n} e^{i(\mathbf{k}\cdot\mathbf{r} - \omega_n\tau)} \psi_{\mathbf{k},\omega_n,\sigma}$

$$S[\bar\psi_\sigma, \psi_\sigma] = \int_0^\beta d\tau \left[\sum_{\mathbf{k}} \bar\psi_{\mathbf{k}\sigma}(\tau) \left(\partial_\tau + \epsilon_{\mathbf{k}} - \mu \right) \psi_{\mathbf{k}\sigma} + \frac{1}{2} \sum_{\mathbf{q}\neq 0} \frac{2\pi e^2}{\mathbf{q}^2} \rho_{\mathbf{q}}(\tau) \rho_{-\mathbf{q}}(\tau) \right]$$

where $\epsilon_{\mathbf{k}} = \mathbf{k}^2/2m$ and $\rho_{\mathbf{q}} = \int d\mathbf{r}\, e^{-i\mathbf{q}\cdot\mathbf{r}} \rho(\mathbf{r}) \equiv \sum_{\mathbf{k}} \bar\psi_{\mathbf{k}\sigma} \psi_{\mathbf{k}+\mathbf{q},\sigma}$

Neutralising background $\rightsquigarrow$ exclusion of $\mathbf{q} = 0$ from sum

Being quartic in the fermionic fields, $\mathcal{Z}$ can not be evaluated exactly

For weak interaction, $r_s \ll 1$, could expand in Coulomb interaction:
Feynman diagram expansion (cf. Gell-Mann Brückner theory)

Alternative — use field integral to isolate leading diagrammatic series contributions

▷ General principle:

When confronted with interacting field theory, seek decomposition of interaction through auxiliary field which captures low-energy content of the theory

In some cases, these fields will be identified with the elementary particles that mediate the interaction (see below);

in others, these fields will encode the low-energy collective modes of the system (cf. superconductor)

Decoupling facilitated using the...

▷ Hubbard-Stratonovich transformation:

$$e^{-\int_0^\beta d\tau \sum_{\mathbf{q}\neq 0} \frac{2\pi e^2}{\mathbf{q}^2} \rho_{\mathbf{q}}(\tau)\rho_{-\mathbf{q}}(\tau)} = \int D\phi \; e^{-\int_0^\beta d\tau \sum_{\mathbf{q}\neq 0} \left[\frac{\mathbf{q}^2}{8\pi}\phi_{\mathbf{q}}(\tau)\phi_{-\mathbf{q}}(\tau) + \frac{ie}{2}(\phi_{\mathbf{q}}(\tau)\rho_{-\mathbf{q}}(\tau) + \rho_{\mathbf{q}}(\tau)\phi_{-\mathbf{q}}(\tau)) \right]}$$

▷ Physically, ϕ represents (scalar) photon field which mediates Coulomb interaction

$$\mathcal{Z} = \int D(\bar{\psi}_\sigma, \psi_\sigma) \int D\phi \; e^{-\int_0^\beta d\tau \int d\mathbf{r} \left[\frac{1}{8\pi}(\partial\phi)^2 + \bar{\psi}_\sigma \left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi \right) \psi_\sigma \right]}$$

quadratic in Grassmann fields, field integral may be performed straightforwardly:

Using identity $\int D[\bar{\psi}, \psi] \exp[-\bar{\psi} M \psi] = \det M = \exp[\ln \det M]$

$$\mathcal{Z} = \int D\phi \exp\left[-\int_0^\beta d\tau \int d\mathbf{r} \frac{1}{8\pi} (\partial\phi)^2 + \overbrace{2}^{\text{spin}} \ln \det \left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi \right) \right]$$

Setting $e = 0$, photon field decouples from determinant
recovers partition function of non-interacting electron gas

Philosophy: All HS decouplings (including this one) are exact. So which to choose? — the one that exposes the low-energy degrees of freedom of the theory — usually signalled by the appearance of some symmetry breaking (although not in this case) and the proliferation of massless degrees of freedom, e.g. magnetisation and superconuductivity

▷ Perturbation Theory in e:

Define free particle Green function: $\hat{G}_0 = [-\partial_\tau - \frac{\hat{\mathbf{p}}^2}{2m} + \mu]^{-1}$ and expand: $\ln(1-x) = -\sum_{n=1} x^n/n$

$$\begin{aligned}\ln\det\left(\partial_\tau + \frac{\hat{\mathbf{p}}^2}{2m} - \mu + ie\phi\right) &\equiv \mathrm{tr}\ln\left(\hat{G}_0^{-1} - ie\phi\right) = \mathrm{tr}\ln\hat{G}_0^{-1} + \mathrm{tr}\ln\left[1 - ie\hat{G}_0\phi\right] \\ &= \mathrm{tr}\ln\hat{G}_0^{-1} - \mathrm{tr}\left[ie\hat{G}_0\phi + \frac{1}{2}\left(ie\hat{G}_0\phi\right)^2 + \cdots\right]\end{aligned}$$

First order term:for convenience, set $k \equiv (\mathbf{k}, \omega_n)$, etc.

$$2\mathrm{tr}[\hat{G}_0\phi] = 2\sum_k \overbrace{\langle k|\hat{G}_0|k\rangle}^{G_0(k)} \overbrace{\frac{1}{\sqrt{L^3\beta}}\phi_{k=0}}^{\langle k|\phi|k\rangle} = \frac{2}{\sqrt{L^3\beta}}\sum_k \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} + \mu}\phi_0 = 0$$

$\phi_0 = 0$ due to neutralising background

Second order term:

$$2\frac{e^2}{2}\mathrm{tr}[\hat{G}_0\phi]^2 = e^2\sum_{k,q} G_0(k)\frac{\phi_q}{\sqrt{\beta L^3}}G_0(k+q)\frac{\phi_{-q}}{\sqrt{\beta L^3}} = \frac{e^2}{2}\sum_q \chi(q)\phi_{-q}\phi_q$$

where density-density response function

$$\chi(q) = \frac{2}{\beta L^3}\sum_k \frac{1}{i\omega_n - \epsilon_{\mathbf{k}} + \mu}\,\frac{1}{i\omega_n + i\omega_m - \epsilon_{\mathbf{k+q}} + \mu}$$

Combined with bare term, to leading order in e,

$$\mathcal{Z} = \mathcal{Z}_0\int D\phi\, e^{-S[\phi]}, \qquad S[\phi] = \frac{1}{2}\sum_q \overbrace{\left(\frac{\mathbf{q}^2}{4\pi} - e^2\chi(q)\right)}^{e^2 D^{-1}(q)}|\phi_q|^2 + O(e^4)$$

$\mathcal{Z}_0$ denotes partition function of non-interacting gas

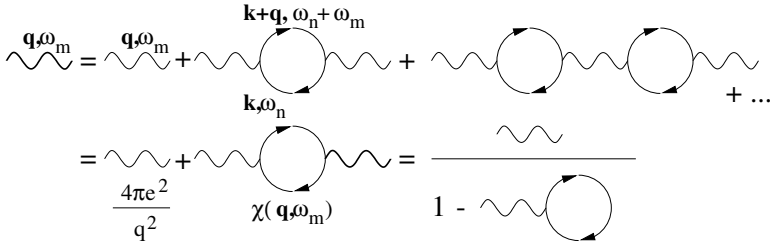
▷ Physically, $D^{-1}(q)$ denotes dynamically screened Coulomb interaction

$$D^{-1}(q) = \epsilon(q)\frac{\mathbf{q}^2}{4\pi e^2}, \qquad \epsilon(q) = 1 - \frac{4\pi e^2}{\mathbf{q}^2}\chi(q)$$

where $\epsilon(q)$ is the energy and momentum dependent effective dielectric function

This result, known as the Random Phase Approximation, amounts to treating the long-range part of the Coulomb interaction as an "external" polarisation field, with screened polarisability:

$$\frac{4\pi e^2}{\mathbf{q}^2}\chi(q)$$



Diagrammatic interpretation:

$$D(q) = \frac{4\pi e^2}{\mathbf{q}^2} \frac{1}{1 - \frac{4\pi e^2}{\mathbf{q}^2}\chi(q)}$$

Dielectric properties: $\chi(q)$?

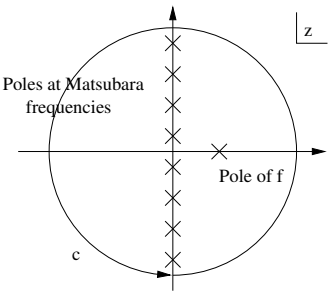
▷ Digression: Matsubara Summations

Basic idea: introduce auxilliary function $g(z)$ that has simple poles at $z = i\omega_n$

$$\sum_{\omega_n} f(i\omega_n) = \oint_C dz g(z) f(z)$$

For example:

$$g(z) = \begin{cases} \dfrac{\beta}{\exp(\beta z) - 1}, & \text{bosons} \\ \dfrac{\beta}{\exp(\beta z) + 1}, & \text{fermions} \end{cases}, \text{ and } \quad g(z) = \begin{cases} \dfrac{\beta}{2}\coth(\beta z/2), & \text{bosons} \\ \dfrac{\beta}{2}\tanh(\beta z/2), & \text{fermions} \end{cases}$$



Applied to density-density response function,

$$I \equiv \oint_C dz \overbrace{\frac{\beta}{\exp(\beta z) + 1}}^{g(z)} \overbrace{\frac{1}{z - \mu + \epsilon} \frac{1}{z - \mu + \epsilon'}}^{f(z)}$$

(i) Integral exists *(the integrand decays sufficiently fast)*

(ii) $I = 0$

Residue integral:

$$0 = \int_C dz (fg)(z) = 2\pi i \left(\sum_n \overbrace{\text{Res } (fg)(i\omega_n)}^{-f(i\omega_n)} + \overbrace{\text{Res } (fg)(\mu - \epsilon)}^{g(\mu-\epsilon)/(\epsilon'-\epsilon)} + \text{Res } (fg)(\mu - \epsilon') \right)$$

Using $e^{i\beta\omega_n} = 1$

$$\chi(\omega_m, \mathbf{q}) = \frac{2}{L^3} \sum_{\mathbf{k}} \frac{n_F(\epsilon_{\mathbf{k}-\mathbf{q}}) - n_F(\epsilon_{\mathbf{k}})}{i\omega_m + \epsilon_{\mathbf{k}-\mathbf{q}} - \epsilon_{\mathbf{k}}}, \qquad n_F(\epsilon) = \frac{1}{e^{\beta(\epsilon-\mu)} + 1}$$

- Static Limit: $(|\omega_m| \ll k_F|\mathbf{q}|/m)$

  For frequencies small as compared to the momentum transfer
  (and temperatures $T \ll \mu$)

$$\chi(0, \mathbf{q}) \simeq \frac{2}{L^3} \sum_{\mathbf{k}} \frac{\mathbf{q} \cdot \partial_{\mathbf{k}} n_F(\epsilon_{\mathbf{k}})}{\mathbf{q} \cdot \partial_{\mathbf{k}} \epsilon_{\mathbf{k}}} \simeq 2 \int \frac{d\mathbf{k}}{(2\pi)^3} \partial_{\epsilon_{\mathbf{k}}} n_F(\epsilon_{\mathbf{k}}) = -2\nu(\mu),$$

  where $\nu(\mu)$ is DoS at Fermi level, i.e.

$$D(0, \mathbf{q}) \simeq \frac{4\pi e^2}{\mathbf{q}^2} \frac{1}{1 + 2\frac{4\pi e^2}{\mathbf{q}^2}\nu(\mu)}$$

  Fourier transformed, one obtains the static screened Coulomb interaction

$$V_{\text{screen}}(\mathbf{r}) = \frac{e^2}{|\mathbf{r}|} e^{-|\mathbf{r}|/\lambda_{\text{TF}}}$$

  where $\lambda_{\text{TF}} = 2 \times 4\pi e^2 \nu(\mu)$ denotes the Thomas-Fermi screening length

  At long time scales, the Coulomb interaction is screened by fluctuations
  in the neighbouring charge

- High Frequency Limit: $(|\omega_n| \gg k_F|\mathbf{q}|/m)$

$$\begin{aligned} \chi(\omega_m, \mathbf{q}) &\simeq -\frac{2}{L^3} \sum_{\mathbf{k}} \frac{\mathbf{q} \cdot \partial_{\mathbf{k}} n_F(\epsilon_{\mathbf{k}})}{i\omega_m - \mathbf{q} \cdot \partial_{\mathbf{k}} \epsilon_{\mathbf{k}}} \simeq -2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{1}{i\omega_m} \left(1 + \frac{\mathbf{q} \cdot \mathbf{k}}{im\omega_m} \right) \mathbf{q} \cdot \partial_{\mathbf{k}} n_F(\epsilon_{\mathbf{k}}) \\ &\simeq -2 \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{\mathbf{q}^2}{m\omega_m^2} n_F(\epsilon_{\mathbf{k}}) = -\frac{\mathbf{q}^2}{m\omega_m^2} n \end{aligned}$$

  where $n = N/L^3$ is the total number density (including spin)

$$D(q) = \frac{4\pi e^2}{\mathbf{q}^2} \frac{1}{1 + \frac{4\pi e^2 n}{m\omega_m^2}}$$

Analytic continuation to real frequencies, $i\omega_m \to \omega + i0$

$$\lim_{m\omega/k_F|\mathbf{q}|\to\infty} D^R(\omega,\mathbf{q}) = \frac{4\pi e^2}{\mathbf{q}^2}\frac{1}{1-\frac{\omega_p^2}{\omega^2}}$$

pole at $\omega_p = 4\pi e^2 n/m$ corresponds to the Plasma frequency

Generally, for $|\mathbf{q}| \ll k_F$,

$$\begin{aligned}\chi(q) &\simeq -2\nu(\mu)\left(1+\frac{\omega_m}{2v_F|\mathbf{q}|}\ln\left[\frac{i\omega_m - v_F|\mathbf{q}|}{i\omega_m + v_F|\mathbf{q}|}\right]\right)\\ &= -2\nu(\mu)\left(1-\frac{\omega_m}{v_F|\mathbf{q}|}\tan^{-1}\left[\frac{v_F|\mathbf{q}|}{\omega_m}\right]\right)\end{aligned}$$

Lindhard function

For $|\omega_m| \ll v_F|\mathbf{q}|$,

$$\chi(q) \simeq -2\nu(\mu)\left[1-\frac{\pi}{2}\frac{|\omega_m}{v_F|\mathbf{q}|}\right]$$

correction due to Landau damping:

Excitation of particle/hole pairs $\rightsquigarrow$ finite lifetime for ϕ

- Ground State Energy

$$\lim_{\beta\to\infty} \mathcal{Z} \sim e^{-\beta E_{\text{g.s.}}}.$$

In the RPA approximation, integ. over ϕ

$$E_{\text{g.s.}} = E_{\text{g.s.}}(e=0) - \frac{1}{2\beta}\sum_q \ln[e^2 D(q)], \qquad E_{\text{g.s.}}(e=0) \equiv -\ln\mathcal{Z}_0/\beta = 3n\mu/5$$

High density ($r_s \ll 1$) expansion

$$E_{\text{g.s.}} \simeq n\left(\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + 0.622\ln r_s - 0.142\right)\text{Ry}.$$