Correlation effects in Fermion Systems
Lecture I

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Outlines

1) Correlations in Electron Liquid
   - Introduction
   - Dyson equation and self-energy
   - Effective mass
   - Fermi Liquid & non-Fermi Liquid
   - Luttinger Liquid, Bosonization

2) Hubbard Model
   - Introduction
   - Spin-charge separation
   - Mott insulators
   - Phase diagram

Many-body systems

$$\left\{-\frac{\hbar^2}{2m}\sum_{j=1}^{N}\nabla_j^2+\sum_{i<j}V(\vec{x}_i-\vec{x}_j)+\sum_j U(\vec{x}_j)\right\}\Psi=i\hbar\frac{\partial\Psi}{\partial t}$$

$$\Psi(\vec{x}_1,\vec{x}_2\ldots\vec{x}_N,t)$$

$$V(\vec{x})=\frac{e^2}{4\pi\epsilon_o}\frac{1}{|\vec{x}|}.$$

Microscopic and Macroscopic

- Time scale
- Length scale
- Number of particles
- Complexity

$$\Delta\tau \sim \frac{\hbar}{[1eV]} \sim \frac{\hbar}{10^{-19}J} \sim 10^{-15}s,$$

$$L_{Quantum} \sim 10^{-10}m,$$

$$N_{Macroscopic} = 6 \times 10^{23} \sim (100 \text{ million})^3$$

Many-body systems: Concepts

$$
\begin{aligned}
H_{\mathrm{e}} &= \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} V_{\mathrm{ee}}(\mathbf{r}_i - \mathbf{r}_j), \\
H_{\mathrm{i}} &= \sum_I \frac{\mathbf{P}_I^2}{2M} + \sum_{I<J} V_{\mathrm{ii}}(\mathbf{R}_I - \mathbf{R}_J) \\
H_{\mathrm{ei}} &= \sum_{iI} V_{\mathrm{ei}}(\mathbf{R}_I - \mathbf{r}_i).
\end{aligned}
$$

- Structural reducibility
- Low energy physics: Universality
- Large number of particles and concept of statistics
- Number of intrinsic symmetries

Strongly correlated systems

Electrons in Solids

$$E_{\rm int} \sim 1 \div 4 \ {\rm eV} \sim 10^4 \ {\rm K}$$

$$E_{\rm kin} \sim 1 \div 10 \ {\rm eV} \sim 10^5 \ {\rm K}$$

Atoms in optical lattices

$$E_{\rm int} \sim E_{\rm kin} \sim 10 \ {\rm kHz} \sim 10^{-6} \ {\rm K}$$

Simple metals $E_{\rm int} < E_{\rm kin}$

Perturbation theory in Coulomb interaction applies.
Band structure methods wotk

Strongly Correlated Electron Systems $E_{\rm int} \geq E_{\rm kin}$

Band structure methods fail.

Novel phenomena in strongly correlated electron systems:

Quantum magnetism, phase separation, unconventional superconductivity, high temperature superconductivity, fractionalization of electrons ...

Some examples

1) Correlations in Electron Liquid
   - Low density
   - Low Dimensionality
   - Transports effects
2) Bose Einstein Condensation in Low dimension
   - 1D cold atom in optical lattice
   - BEC-BCS Crossover
3) Localization in correlated disorder Low dimension
   - disorder/interaction?
   - dimensionality and Anderson impurity
4) Strongly correlated in electronic structure
   - L(S)DFT (Weakly interaction)
   - DMFT , LDA+DMFT (Mediate interaction)
   - LDA+U (Insulator system)

General Properties of EL

Total Hamiltonian

$$\hat{H} = \sum_i \frac{\hat{p}_i^2}{2m} + \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\hat{\vec{r}}_i - \hat{\vec{r}}_j|} + \hat{H}_{e-b} + \hat{H}_{b-b} .$$

Electron-electron interaction

$$\begin{aligned}\hat{H}_{e-e} &\equiv \frac{1}{2}\sum_{i\neq j}\frac{e^2}{|\hat{\vec{r}}_i - \hat{\vec{r}}_j|} \\ &= \frac{1}{2L^d}\sum_{\vec{q}} v_q(\kappa)\left[\hat{n}_{-\vec{q}}\hat{n}_{\vec{q}} - \hat{N}\right]\end{aligned}$$

$$v_q = \begin{cases} \frac{4\pi e^2}{q^2}, & 3D, \\ \frac{2\pi e^2}{q}, & 2D, \end{cases}$$

$$v_q(a) = -e^2 e^{q^2 a^2}\,\mathrm{Ei}\left(-q^2 a^2\right) , \quad 1D .$$

Fourier transformation of the Coulomb potentials

General Properties

Density in D dimension

$$\frac{1}{n} = \begin{cases} \frac{4\pi}{3}(r_s a_B)^3 \,, & 3D, \\ \pi(r_s a_B)^2 \,, & 2D, \\ 2 r_s a_B \,, & 1D \,, \end{cases}$$

Fermi wave vector

$$k_F = \begin{cases} (3\pi^2 n)^{\frac{1}{3}}, & 3D, \\ (2\pi n)^{\frac{1}{2}}, & 2D, \\ \frac{\pi}{2} n, & 1D. \end{cases}$$

Giuliani & Vignale's book

General Properties

K.E :

$$E_0 = \sum_{|\vec{k}|\le k_F,\sigma} \frac{\hbar^2 k^2}{2m} = \frac{2\Omega_d L^d}{(2\pi)^d} \int_0^{k_F} dk k^{d-1} \frac{\hbar^2 k^2}{2m} ,$$

$$\boxed{\epsilon_0(r_s) = \begin{cases} \frac{3}{5}\epsilon_F \simeq \frac{2.21}{r_s^2}\ Ry, & 3D, \\ \frac{1}{2}\epsilon_F = \frac{1}{r_s^2}\ Ry, & 2D, \\ \frac{1}{3}\epsilon_F \simeq \frac{0.205}{r_s^2}\ Ry, & 1D. \end{cases}}$$

$$\boxed{E_1 \equiv E_x = -\frac{1}{2L^d} \sum_{\vec{q}\neq 0} v_q \sum_{\vec{k}\sigma} n_{\vec{k}+\vec{q}\ \sigma} n_{\vec{k}\sigma} .}$$

$$\boxed{\epsilon_x(r_s) = \begin{cases} -\frac{3}{2\pi\alpha_3 r_s} \simeq -\frac{0.916}{r_s}\ Ry, & 3D , \\ -\frac{8\sqrt{2}}{3\pi r_s} \simeq -\frac{1.200}{r_s}\ Ry, & 2D . \end{cases}}$$

Virial theorem $\boxed{2t + u = d\frac{p}{n}}$

Second quantization

Field operator

$$\boxed{\hat{\Psi}_\sigma(\vec{r}) = \sum_\alpha \phi_\alpha(\vec{r},\sigma)\,\hat{a}_\alpha}$$

$$\{\hat{a}_\alpha, \hat{a}_\beta\} = \{\hat{a}^\dagger_\alpha, \hat{a}^\dagger_\beta\} = 0\,, \qquad \{\hat{a}_\alpha, \hat{a}^\dagger_\beta\} = \delta_{\alpha,\beta}$$

One body operator

$$\boxed{\hat{V}^{(1)} = \sum_{i=1}^{N} \hat{V}_i = \sum_{\alpha,\beta} V_{\beta\alpha}\hat{a}^\dagger_\beta \hat{a}_\alpha}$$

Two body operator

$$\boxed{\hat{V}^{(2)} = \frac{1}{2}\sum_{i\neq j} \hat{V}_{ij} = \frac{1}{2}\sum_{\alpha,\beta,\gamma,\delta} V_{\alpha\beta\gamma\delta}\hat{a}^\dagger_\alpha \hat{a}^\dagger_\beta \hat{a}_\gamma \hat{a}_\delta}$$

Jellium model

$$\mathcal{H} = \sum_{p,\sigma} \varepsilon_p c^\dagger_{p,\sigma} c_{p,\sigma} + \sum_{pq,\sigma} \tilde{v}(q)\, c^\dagger_{p+q,\sigma}\, c_{p,\sigma}$$

$$+ \frac{1}{2\Omega} \sum_{pp'q,\sigma\sigma'} V(q)\, c^\dagger_{p+q,\sigma}\, c^\dagger_{p'-q,\sigma'}\, c_{p',\sigma'}\, c_{p,\sigma} \; .$$

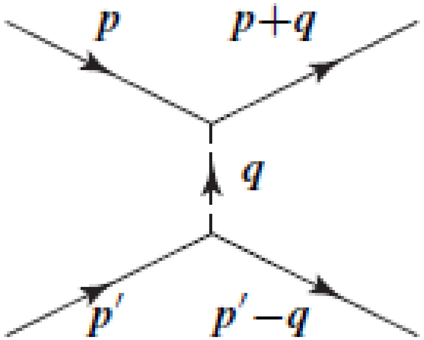
$$\boxed{\hat{H} = \left(\frac{1}{r_s^2} \sum_i \hat{\vec{p}}_i^{\,2} + \frac{1}{r_s L^d} \sum_{\vec{q}\neq 0} v_{\vec{q}} \left[\hat{n}_{-\vec{q}} \hat{n}_{\vec{q}} - \hat{N} \right] \right) \mathrm{Ry}}$$

$$T \sim 1/r_s^2$$

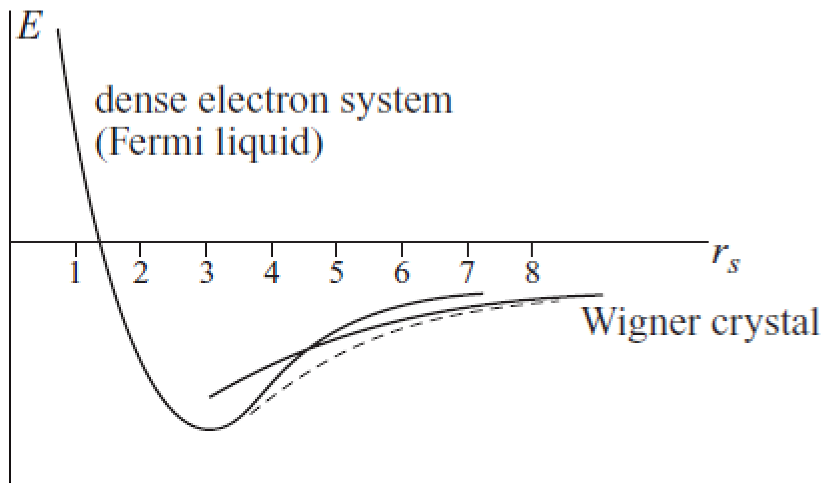
$$V \sim 1/r_s$$

Electron density operator

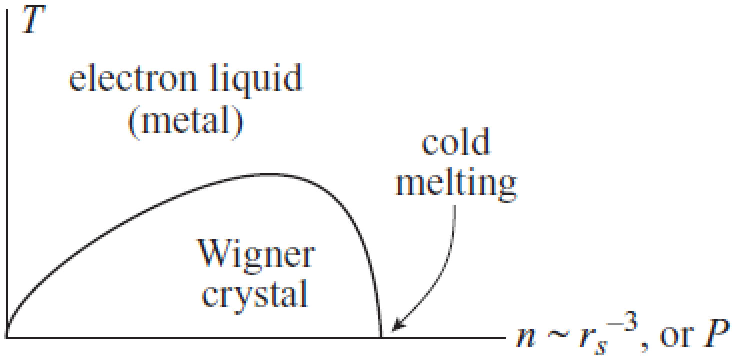
$$\rho(q) = \sum_{p,\sigma} c^\dagger_{p,\sigma}\, c_{p+q,\sigma} \; .$$

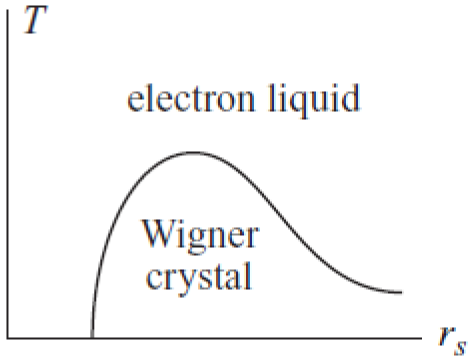


Wigner crystal



$$E_W = -\frac{1.8}{r_s}\,\mathrm{Ry}$$





Green's function

Time order operator

$$G_{\sigma\sigma'}(\boldsymbol{r}_1, t_1; \boldsymbol{r}_2, t_2) = -i\,\langle 0|\mathrm{T}\Big\{\hat{\Psi}_{\sigma}(\boldsymbol{r}_1, t_1)\,\hat{\Psi}^{\dagger}_{\sigma'}(\boldsymbol{r}_2, t_2)\Big\}|0\rangle\ .$$

$$G_{\sigma\sigma'}(\boldsymbol{r}_1, t_1; \boldsymbol{r}_2, t_2) = \begin{cases} -i\,\langle 0|\hat{\Psi}_{\sigma}(\boldsymbol{r}_1, t_1)\,\hat{\Psi}^{\dagger}_{\sigma'}(\boldsymbol{r}_2, t_2)|0\rangle & \text{for } t_1 > t_2 \\ i\,\langle 0|\hat{\Psi}^{\dagger}_{\sigma'}(\boldsymbol{r}_2, t_2)\,\hat{\Psi}_{\sigma}(\boldsymbol{r}_1, t_1)|0\rangle & \text{for } t_1 < t_2\,. \end{cases}$$

Density distribution

$$\boxed{n(\boldsymbol{r}) = -2i \lim_{\substack{\boldsymbol{r}=\boldsymbol{r}' \\ t'\to t+0}} G(\boldsymbol{r}, t; \boldsymbol{r}', t')}$$

$$n(\boldsymbol{p}) = -i \lim_{t\to -0} \int G(\boldsymbol{p}, \omega)\, e^{-i\omega t}\, \frac{d\omega}{2\pi}$$

Mahan's book

Wick's theorem

$$
\begin{aligned}
&{}_0\langle|T\hat{C}_\alpha(t)\hat{C}^\dagger_\beta(t_1)\hat{C}_\gamma(t_2)\hat{C}^\dagger_\delta(t')|\rangle_0 \\
&= {}_0\langle|T\hat{C}_\alpha(t)\hat{C}^\dagger_\beta(t_1)|\rangle_{00}\langle|T\hat{C}_\gamma(t_2)\hat{C}^\dagger_\delta(t')|\rangle_0 \\
&\quad - {}_0\langle|T\hat{C}_\alpha(t)\hat{C}^\dagger_\delta(t')|\rangle_{00}\langle|T\hat{C}_\gamma(t_2)\hat{C}^\dagger_\beta(t_1)|\rangle_0 \\
&= \delta_{\alpha\beta}\delta_{\gamma\delta}\,{}_0\langle|T\hat{C}_\alpha(t)\hat{C}^\dagger_\alpha(t_1)|\rangle_{00}\langle|T\hat{C}_\gamma(t_2)\hat{C}^\dagger_\gamma(t')|\rangle_0 \\
&\quad - \delta_{\alpha\delta}\delta_{\beta\gamma}\,{}_0\langle|T\hat{C}_\alpha(t)\hat{C}^\dagger_\alpha(t')|\rangle_{00}\langle|T\hat{C}_\gamma(t_2)\hat{C}^\dagger_\gamma(t_1)|\rangle_0
\end{aligned}
$$

$$
\boxed{
\begin{aligned}
G(\mathbf{p}, t-t') = -i\sum_{n=0}^{\infty}(-i)^n\int_{-\infty}^{\infty} dt_1 \cdots \int_{-\infty}^{\infty} dt_n\,{}_0\langle|T\hat{C}_{\mathbf{p}\sigma}(t)\hat{C}^\dagger_{\mathbf{p}\sigma}(t') \\
\times \hat{V}(t_1)\cdots\hat{V}(t_n)|\rangle_0 \ (\text{different connected})
\end{aligned}
}
$$

Non-interacting Green's functions

$$\Psi(\boldsymbol{r}, t) = \frac{1}{\sqrt{\Omega}} \sum_{\boldsymbol{p}} c_{\boldsymbol{p}} e^{i[\boldsymbol{p}\cdot\boldsymbol{r} - \varepsilon_0(\boldsymbol{p})t]}$$

$$G_0(\boldsymbol{p}, \omega) = \frac{1}{\omega - \xi_{\boldsymbol{p}} + i\delta_{\boldsymbol{p}}}$$

$$\delta_{\boldsymbol{p}} = \delta \operatorname{sign} \xi_{\boldsymbol{p}}$$

$$\xi_{\boldsymbol{p}} = \varepsilon_{\boldsymbol{p}} - \mu$$

Linear response function

External field

$$\boxed{\hat{H}_F(t) = \hat{H} + F(t)\hat{B}}$$

$$\int V_{ext}(\vec{r}, t)\hat{n}(\vec{r})d\vec{r}$$

$$\hat{B} = \sum_{i=1}^{N} \hat{B}_i = \sum_{\alpha\beta} B_{\alpha\beta}\hat{a}_\alpha^\dagger \hat{a}_\beta$$

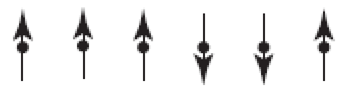
$$\hat{A} = \sum_{i=1}^{N} \hat{A}_i = \sum_{\alpha\beta} A_{\alpha\beta}\hat{a}_\alpha^\dagger \hat{a}_\beta$$

$$\langle \hat{A}\rangle_F(t) - \langle \hat{A}\rangle_0 = -\frac{i}{\hbar}\int_{t_0}^{t} \langle [\hat{A}(t), \hat{B}(t')]\rangle_0 F(t')dt' = \int_0^{t-t_0} \chi_{AB}(\tau)F(t-\tau)d\tau$$

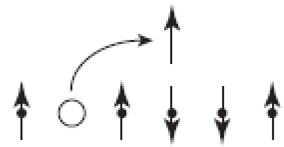
$$\boxed{\chi_{AB}(\tau) \equiv -\frac{i}{\hbar}\Theta(\tau)\langle [\hat{A}(\tau), \hat{B}]\rangle_0}$$

Mott Insulator

$2zt$ (z is the number of nearest neighbours)



$U \gg t$



$|0\rangle, |\uparrow\rangle, |\downarrow\rangle \; |\uparrow\downarrow\rangle$

Energy gap

$$E_g \simeq U - 2zt$$

Thus the ground state of the Hubbard model for U>>t and n=1 is an insulating

$$\mathcal{H}_0 = U \sum_i n_{i\uparrow} n_{i\downarrow} \, ,$$

$$\mathcal{H}' = -t \sum_{\langle ij \rangle, \sigma} c_{i\sigma}^{\dagger} c_{j\sigma}$$

$$\mathcal{H} = \sum_{ij} t_{ij} \, \tilde{c}_{i\sigma}^{\dagger} \, \tilde{c}_{j\sigma} + J \sum_{ij} S_i \cdot S_j$$

$$c_{i\uparrow}^{\dagger} c_{i\uparrow} = n_{i\uparrow} = \tfrac{1}{2} + S_i^z, \quad c_{i\downarrow}^{\dagger} c_{i\downarrow} = n_{i\downarrow} = \tfrac{1}{2} - S_i^z, \quad c_{i\uparrow}^{\dagger} c_{i\downarrow} = S_i^+, \quad c_{i\downarrow}^{\dagger} c_{i\uparrow} = S_i^-$$