Outline of lectures : refresher in many-body theory

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0.1 Prologue

Below, I make reference to the following free lecture notes. If you feel you are missing some prerequisites, everything is in these lecture notes.

http://www.physique.usherbrooke.ca/tremblay/cours/phy-892/N-corps.pdf

Many of these lectures are on YouTube

https://www.youtube.com/playlist?list=PL9IKDS79pLpNJS9KLrAZU0zw_Tin4E6ed

0.2 Lecture 1 (45 minutes) the formalism

Chapter 87 : Handeling many-interacting particles : Second quantization

87.1 Fock space : Creation-annihilation operators

Number operator

87.2 Change of basis

87.2.1 Position and momentum basis

87.2.2 Wave functions

87.3 One-body operators

87.4 Two-body operators

0.3 Lecture 2 (45 minutes) Hubbard model, Green functions

Chapter 82 The Hubbard model to illustrate some of the concepts

82.1 The Hubbard model

$$H = \sum_{\sigma} \sum_{i,j} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \sum_{i} U n_{i\downarrow} n_{i\uparrow} \tag{1}$$

Chapter 83 Perturbation theory (interaction representation)

$$e^{-\beta \widehat{K}} = e^{-\beta \widehat{K}_0} \widehat{U}(\beta) \tag{2}$$

$$\widehat{U}(\beta) \equiv T_\tau \left[e^{-\int_0^\beta \widehat{K}_1(\tau) d\tau} \right] \tag{3}$$

$$\widehat{K}_1(\tau) \equiv e^{\widehat{K}_0 \tau} \widehat{K}_1 e^{-\widehat{K}_0 \tau}. \tag{4}$$

Chapter 84 Green Functions contain useful information

84.1 Photoemission and fermion correlation functions

$$\frac{\partial^2 \sigma}{\partial \Omega \partial \omega} \propto \sum_{mn} e^{-\beta K_m} \langle m | c_{\mathbf{k}_{||}}^{\dagger} | n \rangle \langle n | c_{\mathbf{k}_{||}} | m \rangle \delta(\omega - (K_m - K_n)) \tag{5}$$

84.2 Definition of the Matsubara Green function

$$\mathcal{G}_{\alpha\beta}(\tau) = -\left\langle T_\tau c_\alpha(\tau) c_\beta^{\dagger}(0) \right\rangle \tag{6}$$

$$= -\left\langle c_\alpha(\tau) c_\beta^{\dagger}(0) \right\rangle \theta(\tau) + \left\langle c_\beta^{\dagger}(0) c_\alpha(\tau) \right\rangle \theta(-\tau). \tag{7}$$

84.3 The Matsubara frequency representation is convenient

$$\mathcal{G}_{\alpha\beta}\left(ik_n\right) = \int_0^\beta d\tau e^{ik_n\tau}\mathcal{G}_{\alpha\beta}\left(\tau\right) \tag{8}$$

84.5 Green function for $U = 0$

$$\mathcal{G}_{\mathbf{k}}\left(ik_n\right) = \frac{1}{ik_n - \zeta_{\mathbf{k}}} \tag{9}$$

0.4 Lecture 3 (90 minutes) Spectral weight, Self-energy

84.4 Spectral weight and how it is related to $\mathcal{G}_{\mathbf{k}}(ik_n)$ and to photoemission

$$\frac{\partial^2\sigma}{\partial\Omega\partial\omega} \propto A_{\mathbf{k}}\left(\omega\right) f\left(\omega\right) \tag{10}$$

84.6 Obtaining the spectral weight from $\mathcal{G}_{\mathbf{k}}(ik_n)$, the problem of analytic continuation

$$\mathcal{G}_{\mathbf{k}}\left(ik_n\right) = \int \frac{d\omega'}{2\pi}\frac{A_{\mathbf{k}}\left(\omega'\right)}{ik_n - \omega'} \tag{11}$$

$$G^R_{\mathbf{k}}\left(\omega\right) = \int \frac{d\omega'}{2\pi}\frac{A_{\mathbf{k}}\left(\omega'\right)}{\omega + i\eta - \omega'} \tag{12}$$

Chapter 85 Self-energy and the effect of interactions

85.1 The atomic limit $t = 0$

$$G^R_{\mathbf{k}\uparrow}\left(\omega\right) = \left[\frac{1-\langle n_\downarrow\rangle}{\omega + i\eta + \mu} + \frac{\langle n_\downarrow\rangle}{\omega + i\eta + \mu - U}\right] \tag{13}$$

85.2 The self-energy and the atomic limit example (Mott insulators)

Dyson's equation

$$G^R_{\mathbf{k}\uparrow}\left(\omega\right)^{-1} = G^{(0)R}_{\mathbf{k}\uparrow}\left(\omega\right)^{-1} - \Sigma^R_{\mathbf{k}\uparrow}\left(\omega\right) \tag{14}$$

85.3 A few properties of the self-energy

$$\mathrm{Im}\,\Sigma^R_{\mathbf{k}\uparrow}\left(\omega\right) < 0 \tag{15}$$

85.4 Anderson Impurity problem, hybridization function

$$G^R_{\uparrow}\left(\omega\right)^{-1} = G^{(0)R}_{\uparrow}\left(\omega\right)^{-1} - \Delta^R_{\uparrow}\left(\omega\right) - \Sigma^R_{\uparrow}\left(\omega\right). \tag{16}$$

0.5 Lecture 4 (90 minutes) Coherent states for fermions

Chapter 79 Coherent states for fermions

79.1 Grassmann variables for fermions

$$c\left|\eta\right\rangle = \eta\left|\eta\right\rangle \ ; \ \left|\eta\right\rangle = e^{-\eta c^{\dagger}}\left|0\right\rangle \tag{17}$$

79.2 Grassmann integrals

$$\int d\eta = 0\ ;\ \int d\eta\eta = 1 \tag{18}$$

79.3 Change of variables in Grassmann integrals

$$\psi_i = \sum_{j=1}^{N} U_{ij}\eta_j\ ;\ \prod_{i=1}^{N}\int d\psi_i = \det\left[U\right]\prod_{k=1}^{N}\int d\eta_k \tag{19}$$

79.4 Grassmann Gaussian Integrals

$$\int \mathcal{D}\eta^{\dagger}\int \mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\mathbf{A}\boldsymbol{\eta}-\boldsymbol{\eta}^{\dagger}\mathbf{J}-\mathbf{J}^{\dagger}\boldsymbol{\eta}} = \det\left(A\right)\exp\left(\mathbf{J}^{\dagger}\mathbf{A}^{-1}\mathbf{J}\right) \tag{20}$$

79.5 Closure, overcompleteness, trace formula

$$\mathrm{Tr}[O] = \int d\eta^{\dagger}\int d\eta e^{-\eta^{\dagger}\eta}\left\langle -\eta\right| O\left|\eta\right\rangle \tag{21}$$

Chapter 80 The coherent-state functional integral for fermions

80.1 and 80.2 A simple example with a single fermion

$$Z = \int \mathcal{D}\eta^{\dagger}\int \mathcal{D}\eta\exp\left(-S\right) \tag{22}$$

$$S = \int_0^{\beta} d\tau\left(\eta^{\dagger}\left(\tau\right)\frac{\partial}{\partial\tau}\eta\left(\tau\right)+\varepsilon\left(\tau\right)\eta^{\dagger}\left(\tau\right)\eta\left(\tau\right)\right) \tag{23}$$

80.3 Wick's theorem

$$\left(-1\right)^n\left\langle T_{\tau}c\left(\tau_n\right)c^{\dagger}\left(\tau_n'\right)\cdots c\left(\tau_2\right)c^{\dagger}\left(\tau_2'\right)c\left(\tau_1\right)c^{\dagger}\left(\tau_1'\right)\right\rangle \tag{24}$$

$$= \left(-1\right)^n\frac{1}{Z}\int \mathcal{D}\eta^{\dagger}\int \mathcal{D}\eta e^{-\boldsymbol{\eta}^{\dagger}\left(-\mathcal{G}^{-1}\right)\boldsymbol{\eta}}\eta\left(\tau_n\right)\eta^{\dagger}\left(\tau_n'\right)\cdots\eta\left(\tau_2\right)\eta^{\dagger}\left(\tau_2'\right)\eta\left(\tau_1\right)\eta^{\dagger}\left(\tau_1'\right)$$

$$= \det\left[\begin{array}{cccc} \mathcal{G}\left(\tau_1,\tau_1'\right) & \mathcal{G}\left(\tau_1,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_1,\tau_n'\right) \\ \mathcal{G}\left(\tau_2,\tau_1'\right) & \mathcal{G}\left(\tau_2,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_2,\tau_n'\right) \\ \cdots & \cdots & \cdots & \cdots \\ \mathcal{G}\left(\tau_n,\tau_1'\right) & \mathcal{G}\left(\tau_n,\tau_2'\right) & \cdots & \mathcal{G}\left(\tau_n,\tau_n'\right) \end{array}\right]. \tag{25}$$

80.5 Interactions and quantum impurities

$$\Delta\left(ik_n\right) \equiv \sum_{\mathbf{k}} V_{i\mathbf{k}}^{*}\frac{1}{ik_n-\varepsilon\left(\mathbf{k}\right)}V_{\mathbf{k}i} \tag{26}$$

0.6 Lecture 5 (90 minutes) Many-body perturbation theory

Chapter 87 Source fields for Many-Body Green's function

87.1 A simple example in classical statistical mechanics

$$\frac{\delta^2 \ln Z[h]}{\beta^2 \delta h(\mathbf{x}_1)\, \delta h(\mathbf{x}_2)} = \langle M(\mathbf{x}_1)\, M(\mathbf{x}_2)\rangle_h - \langle M(\mathbf{x}_1)\rangle_h \langle M(\mathbf{x}_2)\rangle_h \tag{27}$$

87.2 Green's functions and higher order correlation functions

$$Z[\phi] = \mathrm{Tr}\left[e^{-\beta K} T_\tau \exp\left(-\psi^\dagger(\overline{1})\, \phi(\overline{1},\overline{2})\, \psi(\overline{2})\right)\right] \; ; \; \mathcal{G}(1,2)_\phi = -\frac{\delta \ln Z[\phi]}{\delta \phi(2,1)} \tag{28}$$

Chapter 88 Equations of motion to find $\mathcal{G}(1,2)_\phi$ and $\Sigma(1,2)_\phi$

88.1 Equation of motion for $\psi(1)$

$$\frac{\partial \psi(1)}{\partial \tau_1} = \frac{\nabla_1^2}{2m}\psi(1) + \mu\psi(1) - \psi^\dagger(\overline{2})\, \psi(\overline{2})\; V(\overline{2}-1)\, \psi(1) \tag{29}$$

88.2 Equation of motion for $\mathcal{G}(1,2)_\phi$ and definition of $\Sigma(1,2)_\phi$

$$\left(\mathcal{G}_0^{-1}(1,\overline{2}) - \phi(1,\overline{2}) - \Sigma(1,\overline{2})_\phi\right) \mathcal{G}(\overline{2},2)_\phi = \delta(1-2) \tag{30}$$

$$\Sigma(\overline{1},\overline{1'})\, \mathcal{G}\left(\overline{1'},\overline{1^+}\right) = 2\langle V\rangle \beta = \left\langle T_\tau\left[\psi^\dagger\left(\overline{1^+}\right) \psi^\dagger\left(\overline{1'^+}\right)\, V(\overline{1'}-1)\, \psi(\overline{1'})\, \psi(\overline{1})\right]\right\rangle \tag{31}$$

Chapter 72 Luttinger Ward Functional

72.3 Luttinger Ward functional and the Legendre transform of $-T \ln Z[\phi]$

$$\Omega[\mathcal{G}] = F[\phi] - \mathrm{Tr}[\phi\mathcal{G}] \; ; \; \frac{1}{T}\frac{\delta \Omega[\mathcal{G}]}{\delta \mathcal{G}(1,2)} = 0 \text{ in equilibrium} \tag{32}$$

Chapter 76 The constraining-field method

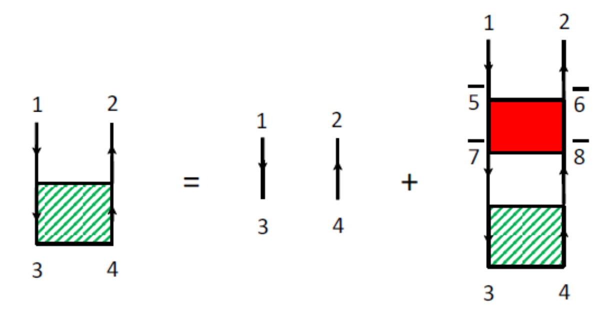
76.1 Another derivation of the Baym-Kadanoff functional

$$\Omega[\mathcal{G}] = \Phi[\mathcal{G}] - \mathrm{Tr}\left[\left(\mathcal{G}_0^{-1} - \mathcal{G}^{-1}\right)\mathcal{G}\right] + \mathrm{Tr}\left[\ln\left(\frac{-\mathcal{G}}{-\mathcal{G}_\infty}\right)\right] \tag{33}$$

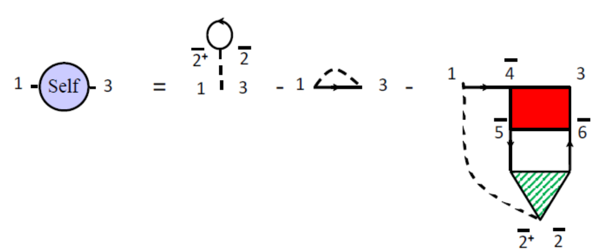
$$\frac{1}{T}\frac{\delta \Phi[\mathcal{G}]}{\delta \mathcal{G}(1,2)} = \Sigma(2,1) \; ; \; \Phi_{\lambda=1}[\mathcal{G}] = \int_0^1 d\lambda \frac{1}{\lambda}\left\langle \lambda \hat{V}\right\rangle_\lambda \tag{34}$$

Chapter 36 Equations of motion for $\mathcal{G}$ in the presence of source fields

36.3 An integral equation for the 4-point function

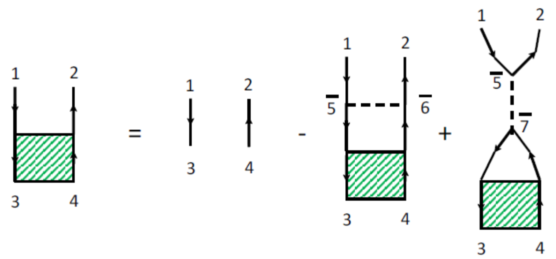


36.4 Self-energy from functional derivative

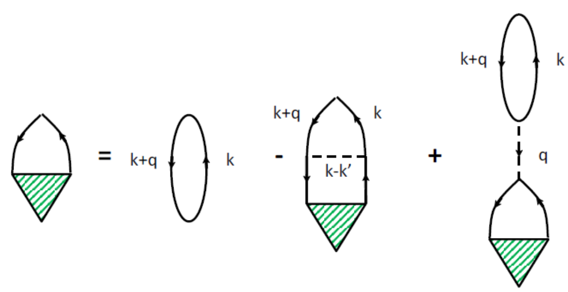


0.7 Lecture 6 (90 minutes) GW + TPSC

Chapter 37 First steps with functional derivatives, Hartree-Fock and RPA
37.2 Hartree-Fock and RPA in space-time



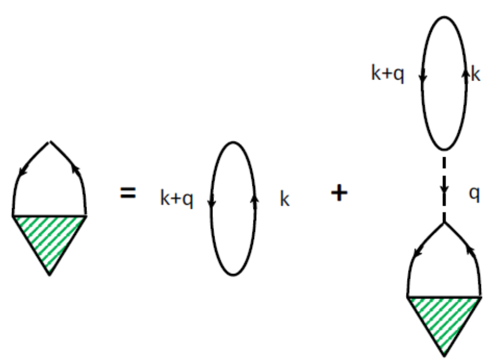
37.3 Hartree-Fock and RPA in momentum-Matsubara space



39.3 Density response in the non-interacting limit: Lindhard function

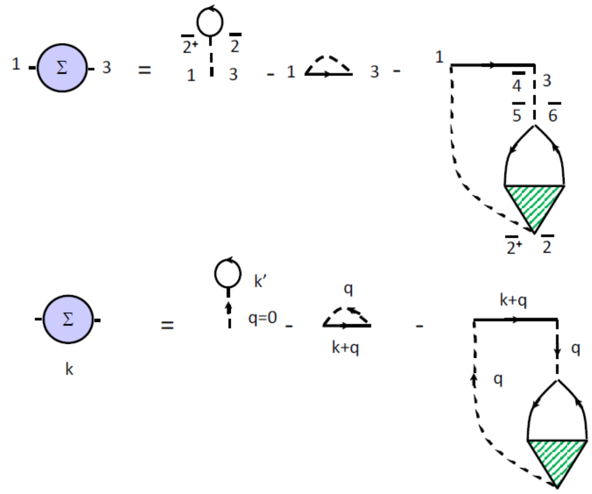
$$\chi_{nn}^{0R}(\mathbf{q},\omega) = -2\int \frac{d^3\mathbf{k}}{(2\pi)^3}\frac{f(\zeta_{\mathbf{k}}) - f(\zeta_{\mathbf{k+q}})}{\omega + i\eta + \zeta_{\mathbf{k}} - \zeta_{\mathbf{k+q}}} \tag{35}$$

41.1.2 RPA



$$\chi_{nn}(q) = \frac{\chi_{nn}^0(q)}{1 + V_{\mathbf{q}}\chi_{nn}^0(q)} \tag{36}$$

Chapter 44 Second step of the approximation, GW curing Hartree-Fock
44.2 Self-energy and screening, GW



Chapter 56 Hubbard model in the footsteps of the electron gas
56.2 Response functions

$$U_{sp} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} - \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow} \tag{37}$$

$$U_{ch} = \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\downarrow} + \frac{\delta\Sigma_\uparrow}{\delta\mathcal{G}_\uparrow} \tag{38}$$

56.3 Hartree-Fock and RPA

$$\chi_{sp}(q) = \frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} \tag{39}$$

$$\chi_{ch}(q) = \frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)} \tag{40}$$

56.4 RPA and violation of the Pauli exclusion principle

$$\frac{T}{N}\sum_q \left(\frac{\chi_0(q)}{1-\frac{1}{2}U\chi_0(q)} + \frac{\chi_0(q)}{1+\frac{1}{2}U\chi_0(q)}\right) \neq 2n-n^2 \tag{41}$$

56.6 RPA, phase transitions and the Mermin-Wagner theorem

$$\mathbf{q}^2 \left\langle \phi_{\mathbf{q}}\phi_{-\mathbf{q}}\right\rangle = \frac{T}{2}\ ;\ \left\langle \phi^2\right\rangle = \int_0^\infty \frac{d^2q}{q^2}\frac{T}{2} = \infty \tag{42}$$

Chapter 57 The two-particle self-consistent approach TPSC
57.1 TPSC first step, spin and charge fluctuations

$$U_{sp} = U\frac{\langle n_\uparrow n_\downarrow\rangle}{\langle n_\uparrow\rangle\langle n_\downarrow\rangle}\ ;\ U_{ch} \text{ from Pauli} \tag{43}$$

57.2 An improved self-energy

$$\Sigma_\sigma^{(2)}(k) = Un_{-\sigma} + \frac{U}{8}\frac{T}{N}\sum_q \left[3U_{sp}\chi_{sp}(q) + U_{ch}\chi_{ch}(q)\right]\mathcal{G}_\sigma^{(1)}(k+q) \tag{44}$$

57.3 An internal consistency check

$$\Sigma_\sigma\left(1,\overline{1}\right)\mathcal{G}_\sigma\left(\overline{1},1^+\right) \equiv \frac{1}{2}\mathrm{Tr}\left(\Sigma\mathcal{G}\right) = U\langle n_\uparrow n_\downarrow\rangle \tag{45}$$

$$\frac{1}{2}\mathrm{Tr}\left(\Sigma^{(2)}\mathcal{G}^{(1)}\right) = U\langle n_\uparrow n_\downarrow\rangle \tag{46}$$