

AN INTRODUCTION TO FUNCTIONAL METHODS

for many-body Green functions

Luca G Molinari

Dipartimento di Fisica and INFN, Milano

Abstract

This an introduction to Grassmann coherent states and the path-integral representation of the generating functional of time-ordered thermal correlators. Dyson's equations, and the effective potential are discussed for electrons with Coulomb interaction.

- The generating functional of thermal correlators
- Grassmann coherent states and path-integral
- Electron gas: functional relations, effective action

CECAM workshop "Green's function methods: the next generation"

Toulouse, june 4 2013

Operators or Path-integral?

Q.M.: **Schrödinger**'s equation or **Feynman**'s path integral?

The first relies on well established theory of differential eqs & linear operators.

The path integral is difficult for bound systems (see **Kleinert**'s book).

A beautiful application is **Gutzwiller**'s trace-formula for chaotic systems.

Q.F.T.: **Schwinger**'s S-matrix or **Feynman**'s path-integral?

Path integral: sum over particle histories/ configurations/ fields.

- critical phenomena (Amit, **Zinn-Justin**, Le Bellac, Kardar,)
- particle physics: gauge theories and renormalization (Ramond, Zee ...)
- superconductivity, superfluidity, condensates (Popov; Kapusta-Gale; Stoof-Gubbels-Dickerscheid, *Ultracold quantum fields*, Springer (2009).)
- Disordered systems: spin-glass, Anderson localization, random matrices ... (Efetov, Brezin, Parisi-Mezard).
- Numerical evaluations (lattice, Montecarlo sampling).

Julian Schwinger (1918 - 2011)

During world war II J.S. was at the Radiation Lab. at MIT with Uhlenbeck, for the development of radars, and was the expert in Green functions.

1950-54: foundation of QFT with functional methods, Green functions, sources, in 4 papers on PNAS.

1965: Nobel prize with Richard Feynman and Sin-Itiro Tomonaga for the foundation of QED (Freeman Dyson proved equivalence of path-integral and functional approaches in 1949).

He was PhD advisor of four Nobel laureates: Roy Glauber, Ben Mottelson, Sheldon Lee Glashow, **Walter Kohn**, and the advisor of **Gordon Baym**, ...



1 Thermal correlators

Fermions with Hamiltonian $\hat{K} = \hat{H} - \mu\hat{N}$, in thermal equilibrium at inverse temperature β . Thermal average and imaginary time evolution:

$$\langle \dots \rangle = \frac{1}{Z} \text{tr}(e^{-\beta\hat{K}} \dots), \quad \hat{O}(x) = e^{\frac{1}{\hbar}\tau\hat{K}} \hat{O}(\vec{x}) e^{-\frac{1}{\hbar}\tau\hat{K}}, \quad 0 \leq \tau \leq \hbar\beta$$

\vec{x} = set of quantum numbers (e.g. position, spin, ...).

$Z(T, \mu, \dots) = \text{tr} e^{-\beta\hat{K}}$: partition function, \Rightarrow Thermodynamics .

Imaginary-time-ordered correlators: $\langle T \hat{O}_1(x_1) \dots \hat{O}_n(x_n) \rangle$

Operators of interest are coupled linearly to external “sources”:

$$\hat{K}[\varphi_i] = \hat{K} + \int d\mathbf{x} \sum_i \varphi_i(\mathbf{x}, \tau) \hat{O}_i(\mathbf{x})$$

Interaction picture: $\hat{\mathcal{U}}(\tau, 0) = e^{-\frac{1}{\hbar}\tau\hat{K}} \hat{\mathcal{U}}_I(\tau, 0)$

Generating functional = Partition function with sources

1.1 The generator of T-correlators

$$\mathbf{Z}[\varphi] =: \text{tr } \mathcal{U}(\hbar\beta, \mathbf{0}) = \mathbf{Z} \langle \hat{\mathcal{U}}_I(\hbar\beta, \mathbf{0}) \rangle$$

Dyson's expansion:

$$\begin{aligned} \frac{\mathbf{Z}[\varphi]}{\mathbf{Z}} &= \left\langle \mathbf{T} \exp \left[-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \int d\mathbf{x} \varphi(\mathbf{x}) \hat{\mathbf{O}}(\mathbf{x}) \right] \right\rangle \\ &= 1 + \sum_r \frac{\pm 1}{r!} \left(-\frac{1}{\hbar} \right)^r \int dx_1 \dots dx_r \langle T \hat{\mathbf{O}}(x_1) \dots \hat{\mathbf{O}}(x_r) \rangle \varphi(x_1) \dots \varphi(x_r) \end{aligned}$$

$$\begin{aligned} \langle T \hat{\mathbf{O}}(x_1) \dots \hat{\mathbf{O}}(x_r) \rangle_\varphi &= \frac{(-\hbar)^r}{Z[\varphi]} \frac{\delta^r Z[\varphi]}{\delta\varphi(x_1) \dots \delta\varphi(x_r)} \\ &= \frac{\langle T \hat{\mathcal{U}}_I(\hbar\beta, 0) \hat{\mathbf{O}}(x_1) \dots \hat{\mathbf{O}}(x_r) \rangle}{\langle \hat{\mathcal{U}}_I(\hbar\beta, 0) \rangle} \end{aligned}$$

- sources break symmetries (which may not restore as $s \rightarrow 0$)
- for Fermi operators derivatives must anticommute (Grassmann fields)

1.2 Green functions

$$S[\text{sources}] = \int dx \left[\bar{\eta}(x) \hat{\psi}(x) + \hat{\psi}^\dagger(x) \eta(x) \right] + \int dx dy \hat{\psi}^\dagger(x) \hat{\psi}(x) \theta(x) + \dots$$

$\eta(x)$ and $\bar{\eta}(x)$ are independent anti-commuting source-fields

$$\langle T \hat{\psi}(1) \dots \hat{\psi}(r) \hat{\psi}^\dagger(s') \dots \hat{\psi}^\dagger(1') \rangle_{\bar{\eta}, \eta, \theta, \dots} = (-1)^r \frac{\hbar^{r+s}}{Z[\dots]} \frac{\delta^{r+s} Z[\bar{\eta}, \eta, \theta, \dots]}{\delta \bar{\eta}(1) \dots \delta \eta(1')}$$

$\theta(x)$ is a commuting source for composite fields^a.

$$\langle \hat{\psi}^\dagger(x) \hat{\psi}(x) \rangle_{\text{sources}} = -\hbar \frac{1}{Z[\dots]} \frac{\delta Z[\dots]}{\delta \theta(x)},$$

$$\langle T \hat{\psi}^\dagger(x) \hat{\psi}(x) \hat{\psi}^\dagger(x') \hat{\psi}(x') \rangle_{\text{sources}} = \hbar^2 \frac{1}{Z[\dots]} \frac{\delta^2 Z[\dots]}{\delta \theta(x) \delta \theta(x')}, \quad \dots$$

^abilocal sources $\theta(x, y)$: Cornwall, Jackiw and Tomboulis (1974), Rebei and Hitchon (1994); R. Chitra and G. Kotliar (2001)

1.3 Independent fermions & perturbative expansion

$$\langle T e^{-\frac{1}{\hbar} \int dx \bar{\eta} \psi + \bar{\psi} \eta} \rangle = e^{-\frac{1}{\hbar^2} \int dx dy \bar{\eta}(x) \mathcal{G}_0(x, y) \eta(y)}$$

$\hat{K}_0 = \int d\vec{x} \bar{\psi}(\vec{x})(h(\vec{x}) - \mu)\psi(\vec{x})$. Expansion in $\bar{\eta}, \eta$ gives:

$$(-1)^r \langle \psi_1 \dots \psi_r \bar{\psi}_{r'} \dots \bar{\psi}_{1'} \rangle_0 = \sum_P (-1)^P \mathcal{G}_0(1, i'_1) \dots \mathcal{G}_0(r, i'_r)$$

If $\hat{K} = \hat{K}_0 + g\hat{V}$, the expansion of $Z[\bar{\eta}, \eta; g]/Z[g]$ in the sources and g produces the perturbative expansion of all Green functions (Feynman diagrams with vacuum sub-diagrams removed).

1.4 Generator of connected correlators

The perturbative expansion of a correlator is the sum of connected and non-connected diagrams. The first ones resum to a connected correlator, the others produce of lower-order connected parts:

$$\langle T\hat{O}_1\hat{O}_2 \rangle = \langle T\hat{O}_1\hat{O}_2 \rangle_c + \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle,$$

$$\langle T\hat{O}_1\hat{O}_2\hat{O}_3 \rangle = \langle T\hat{O}_1\hat{O}_2\hat{O}_3 \rangle_c + \langle T\hat{O}_1\hat{O}_2 \rangle_c \langle \hat{O}_3 \rangle + \dots + \langle \hat{O}_1 \rangle \langle \hat{O}_2 \rangle \langle \hat{O}_3 \rangle,$$

$$\boxed{\frac{Z[\varphi]}{Z} = \exp \left[-\frac{1}{\hbar} W[\varphi] \right]}$$

$$\frac{1}{\hbar} W[\varphi] = \sum_r \frac{\pm 1}{r!} \left(-\frac{1}{\hbar} \right)^r \int d1 \dots r \langle T\hat{O}(1) \dots \hat{O}(r) \rangle_c \varphi(1) \dots \varphi(r)$$

Locality implies the cluster property: if $\varphi = \varphi_1 + \varphi_2$ with disjoint supports, then $W[\varphi_1 + \varphi_2] \approx W[\varphi_1] + W[\varphi_2]$, and connected correlators vanish if arguments belong to two or more regions far apart.

2 Functional integral for Z

Feynman integral (1948): a sum over particle trajectories (Slater states of positions at each time-slice).

Summation over anticommuting fields first done in: P. T. Matthews and A. Salam, *Propagators of quantized fields*, Il Nuovo Cimento 11 n.1 (1956) 120.

Holomorphic representation of $\hat{\mathbf{a}}_r \hat{\mathbf{a}}_s^\dagger \mp \hat{\mathbf{a}}_s^\dagger \hat{\mathbf{a}}_r = \delta_{rs}$

CCR (V. Bargmann, I. Segal, 1961) H-space of entire functions

$$\int \frac{d^2 z}{\pi} e^{-|z|^2} |f(z)|^2 < \infty, \quad \hat{\mathbf{a}}^\dagger = z, \quad \hat{\mathbf{a}} = \frac{d}{dz}$$

Path integral: S. S. Schweber, J. Math. Phys. 3 (1962) 831; A. Casher, D. Lurié and M. Revzen, *Functional integral for many-boson systems*, J. Math. Phys. 9 (1968) 1312.

CAR (F. Berezin, 1961 in Russian) functions of Grassmann variables.

Path integral: Faddeev-Slavnov (1977 in Russian, 1980); Y. Ohnuki and T. Kashiwa, PTP 60 (1978); D. Soper, PRD 18 (1978) 4590.

Non-Grassmann coherent states, for fermions: J. Klauder, *The action option and a Feynman quantization of spinor fields in terms of ordinary c - numbers*, Ann. Phys. 11 (1960) 123.

(see also Perelomov)

REFS:

- L. D. Faddeev, *Introduction to functional methods*, Les Houches 1975, session XXVIII (Methods in Field Theory), World Scientific (Singapore 1981);
- J. Negele and H. Orland, *Quantum Many-Particle Systems*, Perseus Books;
- J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, Oxford (1980);

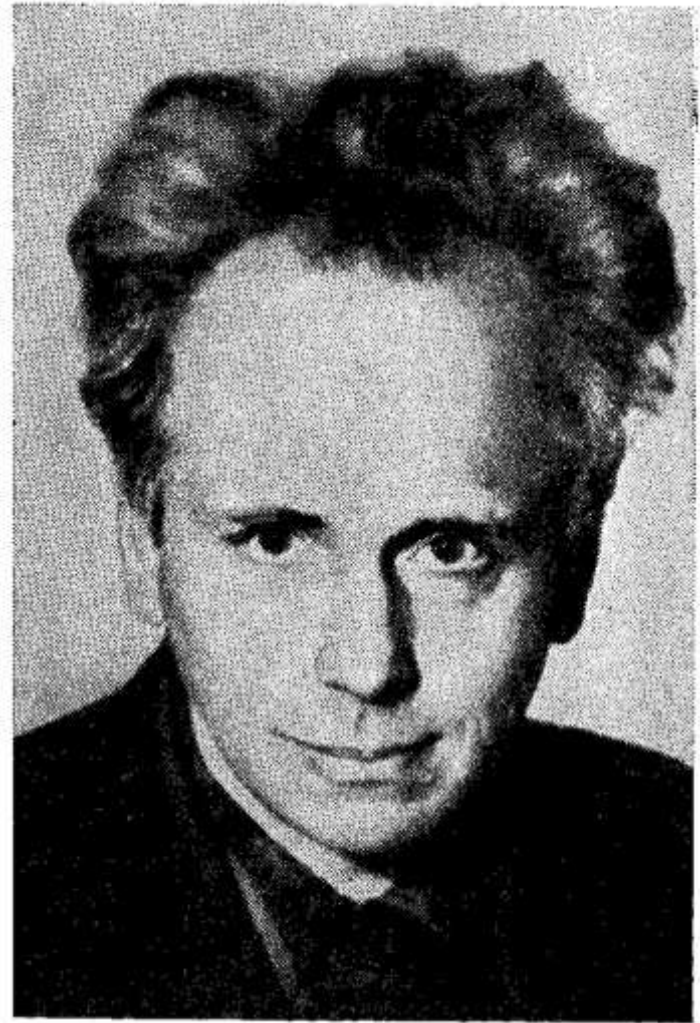
2.1 Grassmann calculus

Hermann Grassmann
(1809 - 1877)



Axioms for exterior algebra. Unrecognized by Möbius, Kummer. Dispute with Saint-Venant.

Felix Berezin (1931- 1980)



The method of second quantisation (1966), super analysis.

2.2 Grassmann algebra with units θ_1, θ_2 .

$$\theta_1^2 = 0, \quad \theta_2^2 = 0, \quad \theta_1\theta_2 = -\theta_2\theta_1$$

A “function” has expansion: $f(\theta_1, \theta_2) = f_0 + \theta_1 f_1 + \theta_2 f_2 + \theta_1\theta_2 f_{12}$.

Derivatives and integrals are defined by the rules:

$$\frac{\partial f}{\partial \theta_1} = f_1 + \theta_2 f_{12}, \quad \frac{\partial f}{\partial \theta_2} = f_2 - \theta_1 f_{12} \Rightarrow \frac{\partial^2 f}{\partial \theta_2 \partial \theta_1} = f_{12} = -\frac{\partial^2 f}{\partial \theta_1 \partial \theta_2}$$

$$\int d\theta_i = 0, \quad \int d\theta_i \theta_i = 1 \Rightarrow \int d\theta_1 f = f_1 + \theta_2 f_{12}, \quad \int d\theta_2 f = f_2 - \theta_1 f_{12}$$
$$\int d\theta_2 d\theta_1 f = -\int d\theta_2 d\theta_1 f = f_{12}$$

Example (change of symbols):

$$\int d\theta d\bar{\theta} e^{-\bar{\theta}\theta} f(\theta, \bar{\theta}) = \int d\theta d\bar{\theta} (1 - \bar{\theta}\theta)(f_0 + f_1\theta + f_2\bar{\theta} + f_{12}\theta\bar{\theta}) = -f_0 - f_{12}$$

2.3 Gaussian integral

$$\int \prod_r \frac{d\bar{z}_r dz_r}{\pi} e^{-\bar{z}_r H_{rs} z_s} = \frac{1}{\det H}, \quad \int \prod_r d\bar{\theta}_r d\theta_r e^{-\bar{\theta}_r H_{rs} \theta_s} = \det H$$

Resolvent $G(E) = (E - H)^{-1}$ as a “super-integral”:

$$G(E)_{ij} = \int \prod_r \frac{d\bar{\theta}_r d\theta_r d\bar{z}_r dz_r}{\pi} e^{-\bar{\theta}(E-H)\theta - \bar{z}(E-H)z} \bar{z}_j z_i$$

Average on random H : $\langle G(1) \dots G(k) \rangle \rightarrow$ effective theory for auxiliary fields.

- Anderson localization (Efetov, Mirlin, Spencer)
- Nuclear resonances, 1-P transport (Weidenmüller)
- Random Matrices (Brézin, Zirnbauer, Fyodorov)

2.4 Holomorphic representation of CAR

$$\{\hat{a}_r, \hat{a}_s^\dagger\} = \delta_{rs}, \quad \{\hat{a}_r^\dagger, \hat{a}_s^\dagger\} = 0, \quad \{\hat{a}_r, \hat{a}_s\} = 0 \quad (\text{N modes}).$$

Linear space of functions of N Grassmann variables $\{\theta_r, \theta_s\} = 0$:

$$f(\theta) = \sum_{\alpha} f_{\alpha} \Theta_{\alpha}(\theta)$$

$\Theta_{\alpha}(\theta)$: basis of 2^N independent products of θ_a s generated by:

$$(1 + \theta_1)(1 + \theta_2) \dots (1 + \theta_N) = \sum_{\alpha} \Theta_{\alpha}(\theta)$$

A **Hilbert space** with inner product $\langle f|g\rangle = \sum_{\alpha} f_{\alpha}^* g_{\alpha}$, i.e. $\langle \Theta_{\alpha}|\Theta_{\beta}\rangle = \delta_{\alpha\beta}$

$$\langle f|g\rangle = \int \prod_{r=1}^N d\theta_r d\bar{\theta}_r e^{\sum_r \bar{\theta}_r \theta_r} \overline{f(\theta)} g(\theta)$$

$$\hat{a}_r = \frac{\partial}{\partial \theta_r}, \quad \hat{a}_r^\dagger = \theta_r, \quad r = 1 \dots N$$

2.5 The reproducing kernel

Completeness: $f(\theta) = \sum_{\alpha} \Theta_{\alpha}(\theta) \langle \Theta_{\alpha} | f \rangle$.

$$I(\theta, \bar{\eta}) =: \sum_{\alpha} \Theta_{\alpha}(\theta) \overline{\Theta_{\alpha}(\eta)} = \prod_r (1 + \theta_r \bar{\eta}_r) = \exp \sum_r \theta_r \bar{\eta}_r$$

$$\begin{aligned} f(\theta) &= \int \prod_r d\eta_r d\bar{\eta}_r e^{\sum_r \bar{\eta}_r \eta_r} I(\theta, \bar{\eta}) f(\eta) \\ &= \int \prod_r d\eta_r d\bar{\eta}_r e^{\sum_r \bar{\eta}_r \eta_r} \overline{I(\eta, \bar{\theta})} f(\eta) \\ &= \langle I_{\bar{\theta}} | f \rangle \end{aligned}$$

$I_{\bar{\theta}}(\eta) =: I(\eta, \bar{\theta})$ as a function of η , is not an element of the Hilbert space of holomorphic functions (coefficients of expansion $\Theta_{\alpha}(\bar{\theta})$ are Grassmann numbers) but the formal inner product is well defined.

2.6 Abstract Hilbert space

We wish to export the features of the reproducing kernel to an abstract Hilbert space \mathcal{H}_N through isomorphism:

$$\Theta_\alpha(\theta) =: \theta_b \theta_c \dots \theta_r \quad \iff \quad |\Theta_\alpha\rangle =: \hat{a}_b^\dagger \hat{a}_c^\dagger \dots \hat{a}_r^\dagger |0\rangle, \quad b < c < \dots < r$$

Accordingly

$$I_{\bar{\theta}}(\eta) = \exp \left[- \sum_r \bar{\theta}_r \eta_r \right] \Rightarrow |\bar{\theta}\rangle = \exp \left[- \sum_r \bar{\theta}_r \hat{a}_r^\dagger \right] |0\rangle \notin \mathcal{H}_N$$

An extension is needed to give meaning to formal steps with Grassmann variables:

Graded-Hilbert space $\mathcal{H}_{\Lambda, N} \supset \mathcal{H}_N$:

$$|\Psi\rangle = \sum_\alpha \Theta_\alpha(\theta) |\psi_\alpha\rangle, \quad |\psi_\alpha\rangle \in \mathcal{H}_N$$

Inner product: $\langle \Psi' | \Psi \rangle = \sum_\alpha \langle \psi'_\alpha | \psi_\alpha \rangle$. Ladder operators act on $|\psi_\alpha\rangle$ and anticommute (by def) with Grassmann units θ_r .

1) If $|\psi\rangle \in \mathcal{H}_N \Leftrightarrow \psi(\theta)$ (holomorphic function), then:

$$\psi(\theta) = \langle \bar{\theta} | \psi \rangle$$

2) $|\theta\rangle = \exp \left[- \sum_r \theta_r \hat{a}_r^\dagger \right] |0\rangle$ is a **coherent state** in $\mathcal{H}_{\Lambda, N}$:

$$\boxed{\hat{a}_r |\theta\rangle = \theta_r |\theta\rangle} \quad r = 1 \dots N.$$

3) **Completeness in \mathcal{H}_N :**

$$\boxed{\int \prod_a d\bar{\theta}_a d\theta_a e^{-\sum_a \bar{\theta}_a \theta_a} |\theta\rangle \langle \theta| \psi\rangle = |\psi\rangle}$$

4) **Trace of operators in \mathcal{H}_N :**

$$\boxed{\int \prod_a d\bar{\theta}_a d\theta_a e^{-\sum_a \bar{\theta}_a \theta_a} \langle \theta | \hat{O} | -\theta \rangle = \text{tr } \hat{O}}$$

where $\langle \theta | \hat{a}_r^\dagger \dots \hat{a}_s | \eta \rangle = \langle \theta | \eta \rangle \bar{\theta}_r \dots \eta_s$.

2.7 A functional integral for \mathbf{Z}

$$\hat{K} = \sum_{mn} \hat{a}_m^\dagger k_{mn} \hat{a}_n + \frac{1}{2} \sum_{mnpq} \hat{a}_m^\dagger \hat{a}_n^\dagger v_{mnpq} \hat{a}_q \hat{a}_p$$

Let $\hbar\beta = \tau_n < \dots < \tau_0 = 0$,

$$\begin{aligned} \mathbf{Z} &= \text{tr} [e^{-\beta\hat{K}}] = \text{tr} \left[e^{-\frac{1}{\hbar}(\tau_n - \tau_{n-1})\hat{K}} I_{n-1} \dots e^{-\frac{1}{\hbar}(\tau_2 - \tau_1)\hat{K}} I_1 e^{-\frac{1}{\hbar}(\tau_1 - \tau_0)\hat{K}} \right] \\ &= \int d\bar{\theta}_r(n) d\theta_r(n) e^{-\bar{\theta}_r(n)\theta_r(n)} \langle \theta(n) | e^{-\frac{1}{\hbar}(\tau_n - \tau_{n-1})\hat{K}} I_{n-1} \dots I_1 e^{-\frac{1}{\hbar}(\tau_1 - \tau_0)\hat{K}} | \theta(0) \rangle \end{aligned}$$

$\theta_r(0) =: -\theta_r(n)$, I_k identity insertion with coherent states $|\theta(k)\rangle$,

$$\begin{aligned} \langle \theta(j+1) | e^{-\frac{1}{\hbar}(\tau_{j+1} - \tau_j)\hat{K}} | \theta(j) \rangle &= \langle \theta(j+1) | \theta(j) \rangle \left[1 - \frac{1}{\hbar}(\tau_{j+1} - \tau_j)K(\bar{\theta}(j+1), \theta(j)) \right] \\ &= \exp \left[\bar{\theta}(j+1)\theta(j) - \frac{1}{\hbar}(\tau_{j+1} - \tau_j)K(\bar{\theta}(j+1), \theta(j)) \right] \end{aligned}$$

$$K(\bar{\theta}, \theta') = \sum_{mn} \bar{\theta}_m k_{mn} \theta'_m + \frac{1}{2} \sum_{mnpq} \bar{\theta}_m \bar{\theta}_n v_{mnpq} \theta'_q \theta'_p$$

$$Z = \int \prod_{j,r} d\bar{\theta}_r(j) d\theta_r(j) e^{-\sum_{j=0}^{n-1} [\bar{\theta}(j+1)(\theta(j+1) - \theta(j)) + \frac{1}{\hbar}(\tau_{j+1} - \tau_j)K(\bar{\theta}(j+1), \theta(j))]}$$

“continuum limit”: $2N$ Grassmann fields $\theta_r(\tau)$, $\bar{\theta}_r(\tau)$ with b.c.

$$\theta_r(\hbar\beta) = -\theta_r(0),$$

$$Z = \int \mathcal{D}[\bar{\theta}_r(\tau)\theta_r(\tau)] \exp \left[-\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \bar{\theta}(\tau) \hbar \frac{d}{d\tau} \theta(\tau) + K(\bar{\theta}(\tau), \theta(\tau)) \right]$$

Generating functional for $\psi, \bar{\psi}$ -correlators:

$$Z[\bar{\eta}, \eta] = \int \mathcal{D}[\bar{\psi}(x)\psi(x)] \exp \left[-\frac{1}{\hbar} S - \frac{1}{\hbar} \int dx \bar{\eta}(x)\psi(x) + \bar{\psi}(x)\eta(x) \right]$$

3 The Electron Gas (path integral description)

$$S[\bar{\psi}, \psi] = \int dx \bar{\psi}(x) k(x) \psi(x) + \frac{1}{2} \int dx dx' \bar{\psi}(x) \psi(x) U_0(x - x') \bar{\psi}(x') \psi(x')$$

$$k(x) = \hbar \partial_\tau - \frac{\hbar^2}{2m} \nabla^2 + V(\vec{x}), \quad U_0(x - x') = e^2 \frac{\delta(\tau - \tau')}{|\vec{x} - \vec{x}'|}, \quad \nabla^2 U^0(x - y) = -4\pi e^2 \delta_{x,y}.$$

3.1 The "Coulomb field"

$$\begin{aligned} & \exp \left[-\frac{1}{2\hbar} \int dx dy n(x) U_0(x - x') n(x') \right] \\ &= \frac{1}{Z_C} \int \mathcal{D}\varphi e^{-\frac{1}{\hbar} \int dx \left[\frac{1}{8\pi} \varphi \nabla^2 \varphi - e n(x) \varphi(x) \right]} \\ &= \frac{1}{Z'_C} \int \mathcal{D}\varphi e^{\frac{1}{\hbar} \int dx \left[\frac{1}{8\pi} \varphi \nabla^2 \varphi - i e n(x) \varphi(x) \right]} \end{aligned}$$

$$S[\bar{\psi}, \psi, \varphi] = \int dx \bar{\psi}(x) [k(\vec{x}) - e\varphi(x)] \psi(x) + \frac{1}{8\pi} \varphi(x) \nabla^2 \varphi(x)$$

3.2 The electron propagator

$$e^{-\frac{1}{\hbar}W[\bar{\eta},\eta,\rho]} = \int \mathcal{D}[\bar{\psi},\psi,\varphi] e^{-\frac{1}{\hbar} \int [\bar{\psi}(k-e\varphi)\psi + \frac{1}{8\pi}\varphi\nabla^2\varphi + \bar{\psi}\eta + \eta\varphi + e\rho\varphi]}$$

An infinitesimal shift $\bar{\psi} \rightarrow \bar{\psi} + \delta\bar{\psi}$ leaves $\mathcal{D}\bar{\psi}$ and W invariant, but changes the action arbitrarily. This gives $k_x\langle\psi(x)\rangle_s - e\langle\varphi(x)\psi(x)\rangle_s + \eta(x) = 0$ i.e. a **Ward identity** for W :

$$\left[k_x - \frac{\delta W}{\delta\rho(x)} \right] \frac{\delta W}{\delta\bar{\eta}(x)} + \hbar \frac{\delta^2 W}{\delta\rho(x)\delta\bar{\eta}(x)} + \eta(x) = 0$$

Take functional derivative in $\eta(y)$ and put sources=0:

$$[k_x - e\langle\varphi\rangle] \mathcal{G}(x,y) + \hbar \frac{\delta}{\delta\rho(x)} \mathcal{G}(x,y) = -\hbar\delta_{x,y}$$

$$\mathcal{G}(x,y) := -\langle T\psi(x)\bar{\psi}(y)\rangle = -\hbar \frac{\delta^2 W}{\delta\bar{\eta}(x)\delta\eta(y)} \Big|_{s=0}$$

3.3 Coulomb propagator and polarization

$$e^{-\frac{1}{\hbar}W[\theta, \rho]} = \int \mathcal{D}[\bar{\psi}, \psi, \varphi] e^{-\frac{1}{\hbar} \int [\bar{\psi}(k - e\varphi)\psi + \frac{1}{8\pi} \varphi \nabla^2 \varphi + \bar{\psi}\psi\theta + e\rho\varphi]}$$

An infinitesimal shift of φ gives $\nabla^2 \langle \varphi(x) \rangle_s = -4\pi e [\rho(x) - \langle \bar{\psi}(x)\psi(x) \rangle_s]$, i.e.

$$\boxed{\frac{\delta W}{\delta \rho(x)} = U^0(x, x') \left[\rho(x') - \frac{\delta W}{\delta \theta(x')} \right]}$$

$$\frac{\delta^2 W}{\delta \rho(x) \delta \rho(y)} = U^0(x, x') \left[\delta(x' - y) - \frac{\delta^2 W}{\delta \theta(x') \delta \rho(y)} \right]$$

$$\frac{\delta^2 W}{\delta \rho(x) \delta \theta(y)} = -U^0(x, x') \frac{\delta^2 W}{\delta \theta(x') \delta \theta(y)}$$

$$\mathbf{U}(\mathbf{x}, \mathbf{y}) = \mathbf{U}_0(\mathbf{x}, \mathbf{y}) + \mathbf{U}_0(\mathbf{x}, \mathbf{x}') \mathbf{\Pi}(\mathbf{x}', \mathbf{y}') \mathbf{U}_0(\mathbf{y}', \mathbf{y})$$

$$\boxed{U(x, y) := \left. \frac{\delta^2 W}{\delta \rho(x) \delta \rho(y)} \right|_{s=0} = -\frac{e^2}{\hbar} \langle T \varphi(x) \varphi(y) \rangle_{conn}}$$

$$\boxed{\Pi(x, y) := \left. \frac{\delta^2 W}{\delta \theta(x) \delta \theta(y)} \right|_{s=0} = -\frac{1}{\hbar} \langle T n(x) n(y) \rangle_{conn}}$$

4 The effective action Γ

In presence of sources, fields have non-zero expectation:

$$\varphi_{cl}(x) =: \langle \varphi(x) \rangle_s = \frac{1}{e} \frac{\delta W}{\delta \rho(x)}, \quad \psi_{cl}(x) = \frac{\delta W}{\delta \bar{\eta}(x)}, \quad \bar{\psi}_{cl}(x) = -\frac{\delta W}{\delta \eta(x)}$$

Let's make the shifts $\varphi = \varphi_{cl} + \varphi'$ etc. of integrated fields:

$$e^{-\frac{1}{\hbar} W[\rho, \bar{\eta}, \eta]} = e^{-\frac{1}{\hbar} \int dx [e\rho \varphi_{cl} + \bar{\eta} \psi_{cl} + \bar{\psi}_{cl} \eta]}$$

$$\int \mathcal{D}[\varphi', \bar{\psi}', \psi'] e^{-\frac{1}{\hbar} S[\varphi' + \varphi_{cl}, \dots]} e^{-\frac{1}{\hbar} \int dx [\rho \varphi' + \bar{\eta} \psi' + \bar{\psi}' \eta]}$$

$$\Gamma[\varphi_{cl}, \psi_{cl}, \bar{\psi}_{cl}] = W[\rho, \bar{\eta}, \eta] - \frac{1}{\hbar} \int dx [e\rho \varphi_{cl} + \bar{\eta} \psi_{cl} + \bar{\psi}_{cl} \eta]$$

$W \rightarrow \Gamma$ is a Legendre transform (Jona-Lasinio). By the chain rule obtain:

$$\frac{\delta \Gamma}{\delta \varphi_{cl}(x)} = -e\rho(x), \quad \frac{\delta \Gamma}{\delta \bar{\psi}_{cl}(x)} = -\eta(x), \quad \frac{\delta \Gamma}{\delta \psi_{cl}(x)} = \bar{\eta}(x)$$

4.1 1-P irreducible correlators

A functional derivative and sources = 0 give the basic identities:

$$\hbar\delta_{x,y} = \int dz \frac{\delta^2\Gamma}{\delta\bar{\psi}_{cl}(x)\delta\psi_{cl}(z)} \mathcal{G}(z,y) \Rightarrow \frac{\delta^2\Gamma}{\delta\psi_{cl}(x)\delta\bar{\psi}_{cl}(y)} = -\delta_{x,y}k(y) - \hbar\Sigma^*(x,y)$$

$$-e^2\delta_{x,y} = \int dz \frac{\delta^2\Gamma}{\delta\varphi_{cl}(x)\delta\varphi_{cl}(z)} U(z,y) \Rightarrow \frac{\delta^2\Gamma}{\delta\varphi_{cl}(x)\delta\varphi_{cl}(y)} = \delta_{x,y} \frac{1}{4\pi} \nabla_y^2 + \Pi^*(x,y)$$

Non-interacting electrons and Coulomb field:

$$\Gamma^0[\bar{\psi}_{cl}, \psi_{cl}, \varphi_{cl}] = \exp - \int dx \left[\bar{\psi}_{cl} k(x) \psi_{cl} + \varphi_{cl} \frac{\nabla^2}{8\pi} \varphi_{cl} \right]$$

4.2 The effective action - main properties

- 1) Γ_{xx} removes propagators from connected diagrams $W_{yy\dots}$
- 2) $\Gamma - \Gamma^0$ is the generator of 1-P irreducible correlators (vertex correlators).
- 3) A connected diagram is a **tree** of vertices and propagators.
(renormalisation of vertices)
- 4) Fields φ_{cl} etc. minimize Γ when sources $\rho = 0$ etc.
- 5) At minimum (zero sources): $e^{-\frac{1}{\hbar}\Gamma} = e^{-\beta\Omega} \rightarrow e^{-\beta E_{GS}}$ for $\beta \rightarrow \infty$ (and non-degenerate ground-state)

4.3 The proper polarisation

With sources ρ and θ , the effective action is the functional $\Gamma[\varphi_{cl}, n_{cl}]$. The Ward identity for φ , $\nabla^2 \langle \varphi(x) \rangle_s = -4\pi e [\rho(x) - \langle \bar{\psi}(x)\psi(x) \rangle_s]$ is

$$\frac{1}{4\pi} \nabla^2 \varphi_{cl} - e \left(n_{cl} + \frac{\partial \Gamma}{\partial \varphi_{cl}} \right) = 0$$

is solved by $\Gamma[\varphi_{cl}, n_{cl}] = \int dx dy \left[\frac{1}{8\pi} \varphi_{cl} \nabla^2 \varphi_{cl} - e n_{cl} \varphi_{cl} \right] + \Gamma[n_{cl}]$. The general identity for second derivatives

$$\int dz \begin{bmatrix} \frac{1}{e} W_{\rho_x \rho_z} & W_{\rho_x \theta_z} \\ \frac{1}{e} W_{\theta_x \rho_z} & W_{\theta_x \theta_z} \end{bmatrix} \begin{bmatrix} \Gamma_{\varphi_z \varphi_y} & \Gamma_{\varphi_z n_y} \\ \Gamma_{n_z \varphi_y} & \Gamma_{n_z n_y} \end{bmatrix} = \begin{bmatrix} -e \delta_{xy} & 0 \\ 0 & -\delta_{xy} \end{bmatrix}$$

simplifies and gives the eqs of motion of W and:

$$\boxed{\frac{\delta^2 \Gamma}{\delta n_x \delta n_y} = \Pi^*(x, y)^{-1}}$$

$$\mathbf{\Pi}(\mathbf{x}, \mathbf{y}) = \mathbf{\Pi}^*(\mathbf{x}, \mathbf{y}) + \mathbf{\Pi}^*(\mathbf{x}, \mathbf{z}) \mathbf{U}^0(\mathbf{z}, \mathbf{z}') \mathbf{\Pi}(\mathbf{z}', \mathbf{y})$$

4.4 Skeleton structure of Σ^*

Ward's identity for the electron gives:

$$\Sigma^*(x, z)\mathcal{G}(z, y) = -\hbar \frac{\delta}{\delta\rho(x)} \frac{\delta^2 W}{\delta\eta(y)\delta\bar{\eta}(x)}$$

Apply the functional inverse

$$\frac{\delta^2 \Gamma}{\delta\bar{\psi}_{cl}(y)\delta\psi_{cl}(x')}$$

and obtain:

$$\hbar\Sigma^*(x, x') = -\hbar \frac{\delta}{\delta\rho(x)} (\dots) + \hbar \frac{\delta^2 W}{\delta\eta(y)\delta\bar{\eta}(x)} \frac{\delta\varphi_{cl}(y')}{\delta\rho(x)} \frac{\delta^3 \Gamma}{\delta\varphi_{cl}(y')\delta\bar{\psi}_{cl}(y)\delta\psi_{cl}(x')}$$

$$\Sigma^*(x, x') = \frac{1}{e} \mathcal{G}(x, y) U(x, y') \frac{\delta^3 \Gamma}{\delta\varphi_{cl}(y')\delta\bar{\psi}_{cl}(y)\delta\psi_{cl}(x')}$$

4.5 Effective theory

With Coulomb decoupling, the integration of Grassmann fields is exact and produces an effective theory. We include a source $\theta(x)$ coupled to the density

$$\begin{aligned} e^{-\frac{1}{\hbar}W[\theta]} &\approx \int \mathcal{D}\varphi \det[k + \theta - e\varphi]^2 e^{-\frac{1}{8\pi\hbar} \int dx \varphi(x) \nabla^2 \varphi(x)} \\ &\approx \int \mathcal{D}\varphi e^{-\frac{1}{\hbar}S_{\text{eff}}[\varphi, \theta]} \end{aligned}$$

$$S_{\text{eff}} = (\varphi + \frac{1}{e}\theta) \frac{\nabla^2}{8\pi} (\varphi + \frac{1}{e}\theta) + 2\hbar \text{tr} \log[1 + \frac{e}{\hbar} \mathcal{G}^0 \varphi]$$

$$\det[k - e\varphi] = \det[k] \det[1 + \frac{e}{\hbar} \mathcal{G}^0 \varphi].$$

R.P.A. Expansion in e

$$\text{tr} \log \left[\delta_{x,y} + \frac{e}{\hbar} \mathcal{G}_{x,y}^0 \varphi_y \right] \approx \exp \left\{ \frac{e}{\hbar} \int dx \mathcal{G}_{x,x}^0 \varphi_x - \frac{e^2}{2\hbar^2} \int dx dy \mathcal{G}_{x,y}^0 \varphi_y \mathcal{G}_{y,x}^0 \varphi_x + \dots \right\}$$

The quadratic part of the Coulomb action is $U^{-1}(x, y)_{RPA}$:

$$S[\varphi] = \frac{e^2}{2} \int dx dy \varphi(x) \left[U^0(x, y)^{-1} - \Pi^{(0)}(x, y) \right] \varphi(y)$$

Beyond R.P.A.

Steepest descent evaluation:

$$0 = \frac{\delta}{\delta\varphi} S_{\text{eff}}[\varphi, \theta] \quad \Rightarrow \quad \varphi_m[\theta]$$

$$W[\theta] = S_{\text{eff}}[\varphi_m, \theta] + \frac{\hbar}{2} \text{tr} \log S''_{\text{eff}}[\varphi_m, \theta] + \dots$$

$$n_{cl} := \langle \bar{\psi}\psi \rangle_{\theta} = \frac{\delta W}{\delta\theta} = \left[\frac{\delta}{\delta\theta} + \frac{\delta\varphi_m}{\delta\theta} \frac{\delta}{\delta\varphi_m} \right] W$$

$$\Gamma[n] = W[\theta] - \int dx \theta(x) n_{cl}(x)$$

$$\frac{\delta\Gamma}{\delta n_{cl}} = -\theta.$$

Put $\theta = 0$, the density minimizes the density functional $\Gamma[n]$.

$$\det(1 - sK) = \exp[\text{tr} \log(1 - sK)] = \sum \frac{(-s)^n}{n!} d_n$$

$$d_n = \begin{bmatrix} \text{tr}(K) & n-1 & & & \\ \text{tr}(K^2) & \text{tr}(K) & \ddots & & \\ \vdots & & & 2 & \\ \vdots & & & & \text{tr}(K) & 1 \\ \text{tr}(K^n) & \dots & \dots & \text{tr}(K^2) & \text{tr}(K) \end{bmatrix}$$

The series converges if $\text{tr}K$ and $\text{tr}(K^\dagger K)$ are finite. The proof is based on $x + \log(1 - x) \leq 0$ if $x < 1$, and remains valid for infinite size of K .

RPA: N. Nagaosa, *Quantum Field Theory in Condensed Matter Physics*, Springer TMP (1999); V. N. Popov, *Functional integrals and collective excitations*, Cambridge (1990); Altland and Simon, Kapusta-Gale

Correlation energy: A. Rebei and W. N. G. Hitchon, *An expression for the correlation energy of an electron gas*, Phys. Lett. A 196 (1994);
Correlation energy of an electron gas: a functional approach, Int. J. Mod. Phys. B 17 (2003).

DFT: M. Valiev and G. Fernando, *Path-integral analysis of the xc-energy and potential in DFT: unpolarized systems*, Phys. Rev. B 54 (1996); J. Polonyi and K. Sailer, *Effective action and density functional theory*, Phys. Rev. B 66 (2002); R. Chitra and G. Kotliar, *Effective action approach to strongly correlated fermion systems*, Phys. Rev. B 63 (2001) and Rev. Mod. Phys. 78 (2006)

conclusions:

The Feynman path-integral with source-fields is the natural *path* to correlations and functional relations among them.

The path integral offers some freedoms/advantages:

- Source-fields and fields stand on the same level.
- Change of integration variables,
- Inclusion of constraints as functional delta,
- The saddle point expansion.

In any case, *it is another tool for difficult tasks. :-)*