AN INTRODUCTION TO FUNCTIONAL METHODS

for many-body Green functions

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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

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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 hystories/ 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 matries ... (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:

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

$\vec{x}$ = set of quantum numbers (e.g. position, spin, ...).
$Z(T, \mu, \ldots) = \mathrm{tr} e^{-\beta \hat{K}}$: partition function, $\Rightarrow$ Thermodynamics .

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

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

Generating functional = Partition function with sources

1.1 The generator of T-correlators

$$\mathbf{Z}[\varphi] =: \mathrm{tr}\, \mathscr{U}(\hbar\beta, \mathbf{0}) = \mathbf{Z}\, \langle \hat{\mathscr{U}}_{\mathbf{I}}(\hbar\beta, \mathbf{0}) \rangle$$

Dyson's expansion:

$$\frac{\mathbf{Z}[\varphi]}{\mathbf{Z}} = \left\langle \mathbf{T} \exp\left[-\frac{\mathbf{1}}{\hbar} \int_{\mathbf{0}}^{\hbar\beta} \mathbf{d}\tau \int \mathbf{dx}\, \varphi(\mathbf{x}) \hat{\mathbf{O}}(\mathbf{x}) \right] \right\rangle$$

$$= 1 + \sum_r \frac{\pm 1}{r!} \left(-\frac{1}{\hbar} \right)^r \int dx_1 \dots dx_r \langle T\hat{O}(x_1) \dots \hat{O}(x_r) \rangle \varphi(x_1) \dots \varphi(x_r)$$

$$\langle T\hat{O}(x_1) \dots \hat{O}(x_r) \rangle_\varphi = \frac{(-\hbar)^r}{Z[\varphi]} \frac{\delta^r Z[\varphi]}{\delta\varphi(x_1) \dots \delta\varphi(x_r)}$$

$$= \frac{\langle T\hat{\mathscr{U}}_I(\hbar\beta, 0) \hat{O}(x_1) \dots \hat{O}(x_r) \rangle}{\langle \hat{\mathscr{U}}_I(\hbar\beta, 0) \rangle}$$

- sources break symmetries (which may not restore as $s \to 0$)

- for Fermi operators derivatives must anticommute (Grassmann fields)

1.2 Green functions

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

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

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

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

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

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

[a] bilocal 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

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

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

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

If $\hat{K} = \hat{K}_0 + g\hat{V}$, the expansion of $Z[\overline{\eta}, \eta; g]/Z[g]$ 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 resumm to a connected correlator, the others produce of lower-order connected parts:

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

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

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

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 $\hat{\mathbf{a}}_{\mathbf{r}}\hat{\mathbf{a}}_{\mathbf{s}}^{\dagger} \mp \hat{\mathbf{a}}_{\mathbf{s}}^{\dagger}\hat{\mathbf{a}}_{\mathbf{r}} = \delta_{\mathbf{rs}}$

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

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

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)

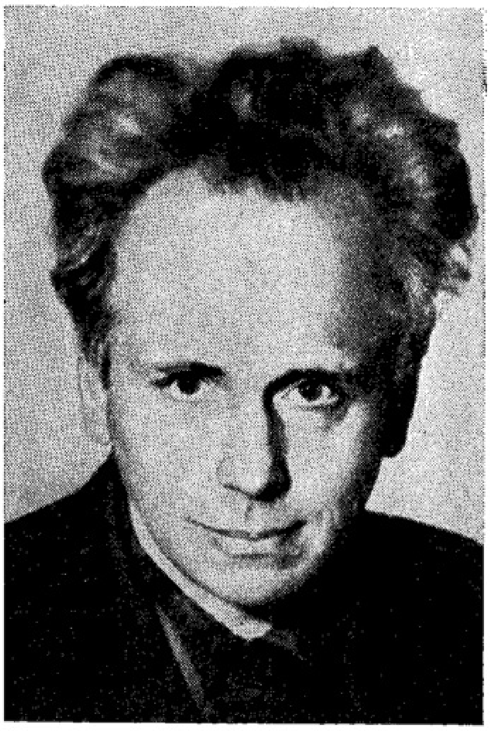
REFS:
- L. D. Faddeev, *Introduction to functional methods*, Les Houches 1975, session XXVIII (Methods in Field Theory), World Scientific (Singapore 1981);
- J. Negele and H. Orland, *Quantum Many-Particle Systems*, Perseus Books;
- J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena*, Oxford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

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

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

$$\int d\theta_2 d\theta_1 f = -\int d\theta_2 d\theta_1 f = f_{12}$$

Example (change of symbols):

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

2.3 Gaussian integral

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

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: $\langle G(1) \dots G(k) \rangle \to$ 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

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

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_as generated by:

$$(1+\theta_1)(1+\theta_2)\ldots(1+\theta_N) = \sum_\alpha \Theta_\alpha(\theta)$$

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

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

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

2.5 The reproducing kernel

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

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

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

$I_{\overline{\theta}}(\eta) =: I(\eta,\overline{\theta})$ as a function of η, is not an element of the Hilbert space of holomorphic functions (coefficients of expansion $\Theta_\alpha(\overline{\theta})$ 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 $\mathscr{H}_N$ through isomorphism:

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

Accordingly

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

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

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

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

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

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

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

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

3) **Completeness in $\mathscr{H}_N$:**

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

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

$$\boxed{\int \prod_a d\overline{\theta}_a d\theta_a e^{-\sum_a \overline{\theta}_a \theta_a} \langle\theta|\hat{O}| - \theta\rangle \;=\; \mathrm{tr}\, \hat{O}}$$

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

2.7 A functional integral for 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 $\hbar\beta = \tau_n < \ldots < \tau_0 = 0$,

$$\mathbf{Z} = \mathrm{tr}\,[e^{-\beta \hat{K}}] = \mathrm{tr}\left[e^{-\frac{1}{\hbar}(\tau_n - \tau_{n-1})\hat{K}} I_{n-1} \ldots e^{-\frac{1}{\hbar}(\tau_2-\tau_1)\hat{K}} I_1 e^{-\frac{1}{\hbar}(\tau_1-\tau_0)\hat{K}}\right]$$
$$= \int d\overline{\theta}_r(n) d\theta_r(n) e^{-\overline{\theta}_r(n)\theta_r(n)} \langle \theta(n)| e^{-\frac{1}{\hbar}(\tau_n-\tau_{n-1})\hat{K}} I_{n-1} \ldots I_1 e^{-\frac{1}{\hbar}(\tau_1-\tau_0)\hat{K}} |\theta(0)\rangle$$

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

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

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

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

"continuum limit": $2N$ Grassmann fields $\theta_r(\tau)$, $\overline{\theta}_r(\tau)$ with b.c. $\theta_r(\hbar\beta) = -\theta(0)$,

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

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

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

3 The Electron Gas (path integral description)

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

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

3.1 The "Coulomb field"

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

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

3.2 The electron propagator

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

An infinitesimal shift $\overline{\psi} \to \overline{\psi} + \delta\overline{\psi}$ leaves $\mathscr{D}\overline{\psi}$ 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:

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

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

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

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

3.3 Coulomb propagator and polarization

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

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

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

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

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

$$\mathbf{U(x,y) = U_0(x,y) + U_0(x,x')\Pi(x',y')U_0(y',y)}$$

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

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

4 The effective action Γ

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

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

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

$$e^{-\frac{1}{\hbar}W[\rho,\overline{\eta},\eta]} = e^{-\frac{1}{\hbar}\int dx\,[e\rho\,\varphi_{c\ell}+\overline{\eta}\psi_{c\ell}+\overline{\psi}_{c\ell}\eta]}$$
$$\int \mathscr{D}[\varphi',\overline{\psi}',\psi']e^{-\frac{1}{\hbar}S[\varphi'+\varphi_{c\ell},\ldots]-\frac{1}{\hbar}\int dx\,[\rho\,\varphi'+\overline{\eta}\psi'+\overline{\psi}'\eta]}$$

$$\boxed{\Gamma[\varphi_{c\ell},\psi_{c\ell},\overline{\psi}_{c\ell}] \;=\; W[\rho,\overline{\eta},\eta] - \frac{1}{\hbar}\int dx\;\left[e\rho\,\varphi_{c\ell} + \overline{\eta}\psi_{c\ell} + \overline{\psi}_{c\ell}\eta\right]}$$

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

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

4.1 1-P irreducible correlators

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

$$\hbar\delta_{x,y} = \int dz \frac{\delta^2\Gamma}{\delta\overline{\psi}_{c\ell}(x)\delta\psi_{c\ell}(z)}\mathscr{G}(z,y) \Rightarrow \frac{\delta^2\Gamma}{\delta\psi_{c\ell}(x)\delta\overline{\psi}_{c\ell}(y)} = -\delta_{x,y}k(y) - \hbar\Sigma^\star(x,y)$$

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

Non-interacting electrons and Coulomb field:

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

4.2 The effective action - main properties

1) Γ_{xx} removes propagators from connected diagrams $W_{yy\ldots}$

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 $\varphi_{c\ell}$ etc. minimize Γ when sources $\rho = 0$ etc.

5) At minimum (zero sources): $e^{-\frac{1}{\hbar}\Gamma} = e^{-\beta\Omega} \to e^{-\beta E_{GS}}$ for $\beta \to \infty$ (and non-degenerate ground-state)

4.3 The proper polarisation

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

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

is solved by $\Gamma[\varphi_{c\ell}, n_{c\ell}] = \int dx dy \left[\frac{1}{8\pi} \varphi_{c\ell} \nabla^2 \varphi_{c\ell} - e n_{c\ell} \varphi_{c\ell} \right] + \Gamma[n_{c\ell}]$. 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:

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

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

4.4 Skeleton structure of $\Sigma^\star$

Ward's identity for the electron gives:

$$\Sigma^\star(x,z)\mathscr{G}(z,y) = -\hbar\frac{\delta}{\delta\rho(x)}\frac{\delta^2 W}{\delta\eta(y)\delta\overline{\eta}(x)}$$

Apply the functional inverse

$$\frac{\delta^2\Gamma}{\delta\overline{\psi}_{c\ell}(y)\delta\psi_{c\ell}(x')}$$

and obtain:

$$\hbar\Sigma^\star(x,x') = -\hbar\frac{\delta}{\delta\rho(x)}(\ldots) + \hbar\frac{\delta^2 W}{\delta\eta(y)\delta\overline{\eta}(x)}\frac{\delta\varphi_{c\ell}(y')}{\delta\rho(x)}\frac{\delta^3\Gamma}{\delta\varphi_{c\ell}(y')\delta\overline{\psi}_{c\ell}(y)\delta\psi_{c\ell}(x')}$$

$$\boxed{\Sigma^\star(x,x') = \frac{1}{e}\mathscr{G}(x,y)U(x,y')\frac{\delta^3\Gamma}{\delta\varphi_{c\ell}(y')\delta\overline{\psi}_{c\ell}(y)\delta\psi_{c\ell}(x')}}$$

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

$$e^{-\frac{1}{\hbar}W[\theta]} \approx \int \mathscr{D}\varphi \, \det[k+\theta-e\varphi]^2 \, e^{-\frac{1}{8\pi\hbar}\int dx\, \varphi(x)\nabla^2\varphi(x)}$$

$$\approx \int \mathscr{D}\varphi \, e^{-\frac{1}{\hbar}S_{\text{eff}}[\varphi,\theta]}$$

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

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

R.P.A. Expansion in e

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

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

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

Beyond R.P.A.

Steepest descent evaluation:

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

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

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

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

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

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

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

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

The series converges if $\operatorname{tr}K$ and $\operatorname{tr}(K^\dagger K)$ 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 Consended 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. :-)