Determination of the one-body Green function:

Freedom and constraints

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GDR General Meeting, Paris, November 2013

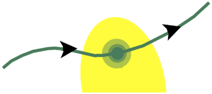
Outline

Calculation of the one-body Green function

- Recap of widely used approaches

Exploring an alternative route

- Model framework
- Functional framework



$$G(1,2) = -i\langle\Psi|\mathbf{T}[\hat{\psi}_H(1)\hat{\psi}_H^\dagger(2)]|\Psi\rangle$$
$$(1) \rightarrow (r_1, \sigma_1, t_1)$$

Observables

- Spectral function

$$A(\omega) = \frac{1}{\pi}|\mathcal{I}m\, G(\omega)|$$

- Expectation value of single-particle operators (e.g. $\langle\hat{n}\rangle$)
- Ground state total energy[1,2]

[1] V. M. Galitskii and A. B. Migdal, JETP 34 (1958)
[2] J. M. Luttinger and J. C. Ward, Phys. Rev. 118 (1960)

How to calculate G?

- Straightforward diagrammatic expansion[2]
  - Diagrams are intuitive (visual)
  - When to truncate?
- Self-energy based methods (e.g. GW approximation[3])
  - Dyson equation
  - Approximations for Σ are intuitive
  - Difficult to improve systematically (vertex corrections)
- Non perturbative solution to a simplified problem (DMFT[4], cumulant expansion approximation[5,6])
- **Any alternative?**

[2] A. Fetter and J. D. Walecka, *Quantum Theory of Many Particle Systems*, (2003)
[3] L. Hedin, Phys. Rev. 139 (1965)
[4] A. Georges and G. Kotliar, Phys. Rev. B, 45 (1992)
[5] B. I. Lundqvist, Phys. Kondensierten Materie, 9 (1969)
[6] D. C. Langreth, Phys. Rev. B, 1 (1970)

Yet another route

i. EOM for G_1

ii. Hierarchy of GFs: $G_2 \leftrightarrow G_3 \leftrightarrow ... \leftrightarrow G_n$

iii. Closure with Schwinger's technique: $G_2 \leftrightarrow \frac{\delta G_1[\varphi]}{\delta \varphi}$

Schwinger's integro-differential equations

$$
\begin{aligned}
G(1,2;[\varphi]) = G_0(1,2) &+ \int d3 G_0(1,3) V_H(3;[\varphi]) G(3,2;[\varphi]) \\
&+ \int d3 G_0(1,3) \varphi(3) G(3,2;[\varphi]) \\
&+ i \int d4 d3 G_0(1,3) v(3^+,4) \frac{\delta G(3,2;[\varphi])}{\delta \varphi(4)}
\end{aligned}
$$

Unfortunately there exist no practical techniques for solving such functional differential equations exactly.

[7] G. Baym and L. P. Kadanoff, *Quantum Statistical Mechanics*

Linearization

$$V_H(3;[\varphi]) \approx -i\int d4 v(3^+,4)G(4,4^+;[\varphi])\Big|_{\varphi=0} - i\int d45\, v(3^+,4)\frac{\delta G(4,4^+;[\varphi])}{\delta\varphi(5)}\Big|_{\varphi=0}\varphi(5)+\cdots$$

Linearized integro-differential equations

$$\begin{aligned} G(1,2;[\bar\varphi]) = G_H^0(1,2) &+ \int d3d5 G_H^0(1,3)\bar\varphi(3)G(3,2;[\bar\varphi]) \\ &+ i\int d3d5 G_H^0(1,3)W(3^+,5)\frac{\delta G(3,2;[\bar\varphi])}{\delta\bar\varphi(5)} \end{aligned}$$

- $\bar\varphi = \varphi\cdot\epsilon^{-1}$, $W = v\cdot\epsilon^{-1}$ and G_H^0 Hartree G @ $\varphi\to 0$

Retrieving known approximations

- Recast Lin. DE introducing $\Sigma \to \dfrac{\delta\Sigma}{\delta\bar\varphi} = 0 \to$ **GW Green function**
- G and G_H^0 diag. on same basis $\to$ **cumulant Green function**[8]

[8] M. Guzzo, GL, *et al.*, Phys. Rev. Lett. 107, 166401 (2011)

1-point model[9,10]

$$\underbrace{y_u(x) = y_0 + y_0 x y_u(x) - u y_0 \frac{d\, y_u(x)}{dx}}_{G([\varphi]) = G_H^0 + G_H^0 \varphi G([\varphi]) + iWG_H^0 \frac{\delta G([\varphi])}{\delta \varphi}}$$

Ansatz: $y_u(x) = A(x) \cdot \mathcal{J}(x)$

General non-equilibrium solution[11]

$$y_u(x) = \sqrt{\frac{\pi}{2u}} e^{\left[\frac{x^2}{2u} - \frac{x}{u y_0} + \frac{1}{2 u y_0^2}\right]} \left\{ erf\left[(x - \frac{1}{y_0}) \sqrt{\frac{1}{2u}} \right] - C(y_0, u) \right\}$$

Particular equilibrium ($x = 0$) solution

$$y(x=0)\Big|_{u=0} \equiv y_0 \quad \rightarrow \quad C(y_0, u) = -1$$

$$y_u = -\sqrt{\frac{\pi}{2u}}\, e^{\frac{1}{2 u y_0^2}} \left\{ erf\left[\sqrt{\frac{1}{2 u y_0^2}} \right] - 1 \right\}$$

[9] L. G. Molinari, *Phys. Rev. B*, 71 (2005)
[10] Y. Pavlyukh and W. Hübner, *J. Math. Phys.*, 48, (2007)
[11] GL, P. Romaniello, L. Reining, *New J. Phys.*, 14, (2012)

Solving the full DE

Ansatz (general)

$$G(1,2;[\varphi]) = \int d5 A(1,5;[\varphi]) \mathcal{J}(5,2;[\varphi])$$

2 DE's

... for $A([\varphi])$ (solved with exponential ansatz)

$$A(1,5;[\varphi]) = \underbrace{j(1,5)}_{\text{arb.}} \cdot e^{\alpha([\varphi]) - \beta(5;[\varphi])}$$

$$\alpha([\varphi]) = \frac{i}{2} \int d5 d6\, W^{-1}(6,5)\varphi(5)\varphi(6)$$

$$\beta(5;[\varphi]) = -i \int d6 d7 d8\, \frac{j(8,5)}{j(7,5)} W^{-1}(6,7) G_H^{0^{-1}}(7,8)\varphi(6)$$

... and $\mathcal{J}([\varphi])$ (trickier)

$$\delta(6,2) = -i \int d4 d5 W(6,4) A(6,5;[\varphi]) \frac{\delta \mathcal{J}(5,2;[\varphi])}{\delta \varphi(4)}$$

Introducing a formal quantity: $q([\varphi])$

Family of solutions for G[14]

$$G(1,2;[\varphi]) = \int d5\, j(1,5)\, e^{\alpha([\varphi]) - \beta(5,[\varphi])}$$
$$\times \left\{ \mathcal{J}_0(5,2) + \int_0^1 d\lambda \int d7d6\, W^{-1}(7,6) \frac{q(6,5,2;[\varphi])}{A(6,5;[\varphi])} \varphi(7) \right\}$$

i. $-i \int d5 q(6,5,2;[\varphi]) = \delta(6,2)$

ii. $\int d6\, W^{-1}(7,6) \frac{q(6,5,2;[\varphi])}{A(6,5;[\varphi])} = \frac{\delta \mathcal{J}(5,2;[\varphi])}{\delta \varphi(7)} \rightarrow$ Taylor expandable

All done?

- Find a "suitable" $q([\varphi])$
- Particular solution $\Rightarrow$ set $\mathcal{J}_0(5,2)$

[14] GL, P. Romaniello, L. Reining, in preparation

A little help from...

... the Taylor expansion for $q([\varphi])$

$$q(6,5,2;[\varphi]) = q_0(6,5,2;[\varphi=0]) + \sum_{n\neq 0}\int dx_1 ... dx_n q_n(6,5,2;x_1...x_n)\varphi(x_1)...\varphi(x_n)$$

where

$$q_n(6,5,2;x_1...x_n) = \frac{\delta^n q(6,5,2;[\varphi])}{\delta\varphi(x_1)...\delta\varphi(n_n)}\Big|_{\varphi=0}$$

- Explicit constraints on $q([\varphi])$
- Explicit integration of $\int_0^1 d\lambda \int d7d6\, W^{-1}(7,6)\frac{q(6,5,2;[\varphi])}{A(6,5;[\varphi])}\varphi(7)$

Exact constraint $\#1$ and $\#2$

Sum rule

$$\delta(6,2) = -i \int d5 q_0(6,5,2)$$
$$0 = -i \int d5 q_n(6,5,2; x_1 ... x_n) \qquad \forall x_n$$

Symmetry constraint

Example @ 1^{st} order: $\left.\frac{\delta^2 \mathcal{J}(5,2;[\varphi])}{\delta\varphi(x_1)\delta\varphi(4)}\right|_{\varphi=0} = \left.\frac{\delta^2 \mathcal{J}(5,2;[\varphi])}{\delta\varphi(4)\delta\varphi(x_1)}\right|_{\varphi=0}$

$$\int d6 \frac{W^{-1}(4,6)}{j(6,5)} \left[q_1(6,5,2;x_1) + i q_0(6,5,2) \int d7 d8 \frac{j(8,5)}{j(7,5)} W^{-1}(x_1,7) {G_H^0}^{-1}(7,8) \right]$$

Symmetric in $x_1 \leftrightarrow 4$

A more explicit expression for G

$$
\begin{aligned}
G(1,2;[\varphi]) \quad &= \int d5 e^{\alpha-\beta(5)} j(1,5) \left\{ \mathcal{J}_0(5,2) - \mathcal{T}_1(5,2;[\varphi]) \right\} \\
&+ \int d5 e^{\alpha-\beta(5)+\frac{\beta^2(5)}{4\alpha}} j(1,5) \mathcal{T}_2(5,2;[\varphi]) \left\{ erf\left(\sqrt{\alpha} - \frac{\beta(5)}{2\sqrt{\alpha}}\right) + erf\left(\frac{\beta(5)}{2\sqrt{\alpha}}\right) \right\} \\
&+ \int d5 j(1,5) \mathcal{T}_3(5,2;[\varphi])
\end{aligned}
$$

with

$$
\mathcal{T}_1(5,2;[\varphi]) = \sum_{n\neq 0} \sum_{m=1}^{n} \sum_{i=0}^{s} \binom{n}{m} \frac{1}{2^{n-m}} b_i^m \beta(5)^{n-m} \alpha^{\frac{m}{2}-n-\frac{1}{2}} \left(-\frac{\beta(5)}{2\sqrt{\alpha}}\right)^{m-(2i+1)} \hat{q}_n(5,2;[\varphi])
$$

$$
\mathcal{T}_2(5,2;[\varphi]) = \sum_{n} \sum_{m=0}^{s'} \binom{n}{2m} \frac{1}{2^{n-2m}} a_{2m} \beta(5)^{n-m} \alpha^{\frac{m}{2}-n-\frac{1}{2}} \hat{q}_n(5,2;[\varphi])
$$

$$
\mathcal{T}_3(5,2;[\varphi]) = \sum_{n\neq 0} \sum_{m=1}^{n} \sum_{i=0}^{s} \binom{n}{m} \frac{1}{2^{n-m}} b_i^m \beta(5)^{n-m} \alpha^{\frac{m}{2}-n-\frac{1}{2}} \left(\sqrt{\alpha} - \frac{\beta(5)}{2\sqrt{\alpha}}\right)^{m-(2i+1)} \hat{q}_n(5,2;[\varphi])
$$

Towards a particular solution

A well behaved solution for $W \to 0$

$$\begin{aligned} G(1,2;[\varphi]) &= \int d5 e^{\alpha-\beta(5)} j(1,5) \Big\{ \mathcal{J}_0(5,2) - \mathcal{T}_1(5,2;[\varphi]) \Big\} \\ &+ \int d5 e^{\alpha-\beta(5)+\frac{\beta^2(5)}{4\alpha}} j(1,5) \mathcal{T}_2(5,2;[\varphi]) \left\{ erf\left(\sqrt{\alpha} - \frac{\beta(5)}{2\sqrt{\alpha}}\right) + erf\left(\frac{\beta(5)}{2\sqrt{\alpha}}\right) \right\} \\ &+ \int d5 j(1,5) \mathcal{T}_3(5,2;[\varphi]) \end{aligned}$$

Conditions for a physical solution

iii. $\mathcal{T}_2 = 0 \quad \forall\varphi, \forall W$

iv. $\mathcal{T}_1 = \mathcal{J}_0(5,2) \quad \forall\varphi, \forall W$

$$G(1,2;[\varphi]) = \int d5 j(1,5)\, \mathcal{T}_3(5,2;[\varphi])$$

Exact constraints #3 and #4

$$\hat{q}_n(5,2;[\varphi]) = \int d4d6 \frac{W^{-1}(4,6)}{j(6,5)} \varphi(4) \sum_n \int dx_1...dx_n q_n(6,5,2;x_1...x_n)\varphi(x_1)...\varphi(x_n)$$

Further sum rule

$$\mathcal{T}_2 = \sum_n \sum_{m=0}^{s'} \binom{n}{2m} \frac{1}{2^{n-2m}} a_{2m} \beta(5)^{n-m} \alpha^{\frac{m}{2}-n-\frac{1}{2}} \hat{q}_n(5,2;[\varphi]) = 0$$

Independence from φ

$$\mathcal{J}_0 = \mathcal{T}_1 = \sum_{n\neq 0} \sum_{m=1}^{n} \sum_{i=0}^{s} \binom{n}{m} \frac{1}{2^{n-m}} b_i^m \beta(5)^{n-m} \alpha^{\frac{m}{2}-n-\frac{1}{2}} \left(-\frac{\beta(5)}{2\sqrt{\alpha}}\right)^{m-(2i+1)} \hat{q}_n(5,2;[\varphi])$$

What about the equilibrium ($\varphi = 0$) solution?

Prerequisite:

0. $W \to 0$ is crucial to obtain the particular non equilibrium solution

1. When $\varphi \to 0$ also $\mathcal{T}_3 \to \mathcal{T}_1$

2. Solution is uniquely fixed by $\int d5 j(1,5)\mathcal{J}_0(5,2)$

0,1,2 are consistent with findings from simplified framework*

[*] DE is diagonal in space and spin

Conclusions & Outlook

Conclusions

- We obtained a family of solutions&the particular (physical) solution for G (in terms of q)
- We showed that the physical solution is determined by $W \to 0$
- We presented a number of **exact constraints** that q should fulfil

Outlook

- Focus on simplified (DE diag. in space&spin) framework
  - What's the most important constraint (can we violate any?)
  - How many orders of q do we need?
  - Guess for q to be translated to the full functional problem