Broken Scale Invariance Ward Identities for the Homogeneous Electron Gas

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Abstract

We derive exact equations for a broken scale invariance of the homogeneous electron gas HEG, and show that they lead to a closed non-linear integral equation for the density-density correlation function when evaluated to leading order in the $1/N$ expansion. More generally, the identity leads to a sequence of more refined systems of equations, which close on a finite number of one plasmon irreducible (1PLI) correlation functions.

1 Introduction

The homogeneous electron gas (HEG) lies at the foundation of atomic and condensed matter physics. The Schwinger Effective Action of the plasmon field\[1\] for this model is a time-dependent generalization of the Density Functional of Hohenberg and Kohn\[2\]. If one knew it, it could be used to compute the ground state energy of the gas in an arbitrary background potential. Choosing that potential to be that of a collection of static nuclei, and adding the Coulomb repulsion of the nuclei, one has reduced the Born-Oppenheimer approximation to atoms, molecules and solids to a classical variational problem. The HEG is not just a toy problem.

2 The Effective Action and Broken Scale Invariance

In [3], the author proposed a computation of the effective action in a systematic $1/N$ expansion. We will work in units where distances are measured in Bohr radii and energies are measured in Rydbergs. All coordinates, fields and parameters in this paper are dimensionless. The classical
imaginary time action for the HEG is

\[
S = \int dt d^3 x \left[ \Psi_a^\dagger \left( \frac{\partial_t}{2} - \nabla^2 - \mu + i \Phi(x, t) \right) \Psi_a - \frac{1}{2} \Phi(\nabla^2) \Phi \right].
\]  

(1)

This action is believed to be ultraviolet finite, except for normal ordering, which is equivalent to an additive shift in \( \mu \). We will always compute things in terms of the renormalized chemical potential. In using this action to compute the energy density of the model as a functional integral, we must divide through by the Gaussian functional integral over the plasmon field \( \Phi \), in order to get the proper Hubbard-Stratonovich transformation. This has no effect on correlation functions, which are a ratio of two functional integrals.

The large \( N \) expansion is generated by enlarging the number of fermion spin components from 2 to \( N \), and multiplying the purely plasmon term in the action by \( N/2 \). For large \( N \), the quantum fluctuations of the plasmon field are small and the leading term in the expansion comes from integrating out the fermions and solving the classical equations for \( \Phi \). In [2] I argued that this approximation yielded a first order phase transition between a homogeneous gas and a Wigner crystal. The spin polarized gas phase expected in three dimensions from Quantum Monte Carlo simulations does not make an appearance: there is no spontaneous breakdown of \( SU(N) \).

In this paper we will exhibit a broken scale invariance Ward identity, which may turn out to be useful in search for second order phase transitions in this model. We’ll see that in the large \( N \) approximation it leads to an infinite sequence of more and more refined closed systems of integro-differential equations, each of which involves only a finite number of correlation functions. It may come as a surprise that our model has any remnant of scale invariance, since everything is written in terms of dimensionless variables. Nonetheless, it is easy to exhibit the broken symmetry. The fermionic terms in the effective action are invariant under the simultaneous transformations

\[
t \to e^{-2s} t,
\]

(2)

\[
x \to e^{-s} x,
\]

(3)

\[
\mu \to e^{2s} \mu,
\]

(4)

\[
\Phi(x, t) \to e^{2s} \Phi(e^{-s} x, e^{-2s} t),
\]

(5)

\[
\Psi(x, t) \to e^{-3s/2} \Psi(e^{-s} x, e^{-2s} t).
\]

(6)

Note of course that we’re rescaling the coupling \( \mu \), so \( \mu \) breaks the Lifshitz scale invariance of the model.

This transformation does not leave the bare plasmon Lagrangian invariant. Instead, for infinitesimal rescalings we have an equation

\[
[D + 2 \Phi(x, t)] \frac{\delta S}{\delta \Phi(x, t)} = -\frac{1}{2} \int dtd^3 x \, \Phi(\nabla^2) \Phi,
\]

(7)

where \( D = \mu \partial_t - \partial_t - 2x \cdot \nabla \). We define the generating functional of Green’s functions as the functional integral ratio

\[
Z[J] = \frac{\int [d\Phi] e^{-S + \int J \Phi} \Phi J}{\int [d\Phi] e^{-S}}.
\]

(8)
We give $J$ weight 3 under rescaling and do a change of variables equal to a rescaling transformation on the numerator integral.

The (Schwinger) effective action of the plasmon field is defined as the functional Legendre transform of $W[J]$.

$$W[J] = \Gamma[\phi] + \int dt d^3 x \phi(t, x) J(t, x).$$  \hfill (9)

The connected $n$-point correlation functions are

$$W[J] = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^4 x_1 \ldots d^4 x_n J(x_1) \ldots J(x_n) W_n(x_1, \ldots x_n).$$ \hfill (10)

The one plasmon irreducible correlation functions are

$$\Gamma[\phi] = \sum_{n=0}^{\infty} \frac{1}{n!} \int d^4 x_1 \ldots d^4 x_n \phi(x_1) \ldots \phi(x_n) \Gamma_n(x_1, \ldots x_n).$$ \hfill (11)

Now note that for a static external source, $J(t, x) = V(x)$, $W[J] = TE[iV(x)]$, where $E$ is the ground state energy of the interacting electron gas in the presence of an external potential, and $T$ is the length of the imaginary time interval. Thus, knowledge of the effective action, like that of the Density Functional, reduces the Born-Oppenheimer approximation to a classical variational exercise. The effective action approach to electron dynamics has been championed by [1]. It is similar in spirit to Dynamical Mean Field Theory for lattice models in that the effective action contains information about the excitation spectrum of the model, which is not captured by the Density Functional. The connection between $\Gamma[\phi]$ and the density functional was explained in [3]. The plasmon field is connected to the fermion charge density by Gauss’ law

$$\nabla^2 \Phi = \Psi^\dagger_a \Psi_a,$$ \hfill (12)

so its connected two point function in momentum space is just $\frac{1}{p^2}$ times the time dependent density density correlation function. This two point function is the algebraic inverse (in momentum space) of the function $\Gamma_2$, for which we will eventually find a closed equation.

It is possible to derive the equations for broken scale invariance by functional manipulations using these definitions, but in the interests of clarity I will present the derivation in the next section in the language of Feynman diagrams of the $1/N$ expansion for the correlation functions of the plasmon field.

It is a well known consequence of the algebraic properties of Legendre transforms that $W_n(p_1, \ldots p_n)$ is a sum of all tree diagrams with vertices made from $\Gamma_m$ with $m \leq n$, and limbs made from the full propagator $W_2(p)$. Written in terms of $\Gamma_m$, the scaling Ward identity is a highly non-linear equation relating 1PLI vertices to those with more legs. In this, it’s similar to the Schwinger-Dyson equations. We’ll see however that this hierarchy truncates in an interesting way in the $1/N$ expansion.

### 3 $1/N$ Expansion of the Scaling Ward Identity

It is clear that for large $N$, $\Phi$ is a semi-classical variable. In the gas phase the classical configuration around which we expand is $\Phi = 0$. Note that the transformation $\Phi(x, t) \to$
\( \Phi(x, t) + \lambda(t) \) is a gauge transformation. That is, the zero wave number mode of \( \Phi \) decouples from the fermion determinant. To do this carefully, we should work on a spatial torus and simply discard the discrete zero mode. We will simply make sure that our calculations are consistent with gauge invariance. Thus, we write \( \Phi = \frac{\zeta}{\sqrt{N}} \) and perform the functional integral over \( \zeta \) in terms of Feynman diagrams. The \( k \) point terms in the action, \( S_k[\zeta] = \Gamma_k[\zeta] \) scales like \( N^{-(k-2)/2} \). The scale transformations described in the previous section enable us to extract the \( \mu \) dependence of \( S_k \) in a straightforward manner.

\[
S_k(p_1, \ldots, p_{k-1}) = \int \frac{d^4p}{(2\pi)^4} \prod_{i=0}^{k-1} \frac{1}{i(\omega - \Omega_i) - \frac{(p - P_i)^2}{2} + \mu},
\]

where \( \Omega_i = \sum_{j=0}^i \omega_j \) and \( \omega_0 = 0 \). \( P_i \) is defined in a similar manner. We’ve also given the fourth component of each momentum the name \( \omega \). If we define, for both loop and external momenta \( p = \mu^{1/2}q \) and \( \omega = \mu \omega_q \) then

\[
S_k(p_1 \ldots p_{k-1}) = \mu^{5/2-n} \tilde{S}_k(q_1, \ldots, q_n).
\]

This is valid for \( k \geq 2 \). The Coulomb term spoils this relation for the two point function, but this means that all non-trivial dependence on \( \mu \) has to do with the plasmon propagator.

Now let’s consider the 1PLI correlation functions and write

\[
\Gamma_k(p_1 \ldots p_{k-1}) = \mu^{5/2-n} \tilde{\Gamma}_k(q_1, \ldots, q_n).
\]

The \( 1/N \) expansion of \( \tilde{\Gamma}_k(q) \) in the homogeneous phase consists of all \( k \) point Feynman diagrams, with vertices given by the \( S_l \) and propagator

\[
W_2^0(q) = \frac{1}{(q^2)^{\mu^{1/2} + \tilde{S}_2(q)}}.
\]

\( \tilde{S}_2(q) \) is the familiar Lindhard function, with chemical potential set equal to 1. The dependence of \( \tilde{\Gamma}_k(q) \) on \( \mu \) for fixed \( q_i \) comes only from differentiating the internal propagators as shown in the Figure.

\[
\mu^{-1/2} \partial_{\mu^{-1/2}}[W_2^0(q)] = -\frac{\mu^{1/2}}{[(q^2)^{\mu^{1/2} + \tilde{S}_2(q)}]^2}(q^2)^2/2.
\]

This differentiated propagator is integrated against a \( k + 2 \) point function, with momenta \( q, -q \) and \( q_1 \ldots q_k \). This function is connected, but not necessarily 1PLI, because the derivative has broken open one internal propagator. In fact, every diagram for the connected \( k + 2 \) point function contributes to the scaling derivative of the 1PLI two point function. However, one must be careful about the propagators on the external legs of the \( k + 2 \) point function. On the \( k \) legs of the original 1PLI vertex, there are no propagators, so, in the popular jargon, these legs are truncated. On the integrated legs, with momentum \( q \) and \( -q \), we resum the Dyson series and get

\[
-\mu^{1/2}q^2/2 \frac{1}{[\mu^{1/2}q^2/2 + \Pi(q)]^2},
\]

where \( \Pi \) is the full polarization function, summed to all orders in the \( 1/N \) expansion. The easiest way to see that the combinatorics works out is to go through the functional derivation in the appendix. Defining \( s = -\frac{1}{2} \ln \mu \) we get an exact equation

\[
\partial_s \tilde{\Gamma}_k(q_1, \ldots, q_{k-1}) = -e^{-s/2} \int \frac{d^4q}{(2\pi)^4} \frac{(q^2)}{2} \frac{1}{[e^{-s/2}q^2/2 + \Pi(q)]^2} W_{k+2}^T(q, -q, q_1 \ldots q_{k-1}).
\]
The Sum is over all possible insertions of $P^2$ (X) into propagator lines

Figure 1: Differentiating $\tilde{\Gamma}_k$ Gives an Insertion into $W_{2+k}^T$

In this equation, the connected correlator has all of its legs truncated.

Like the Schwinger-Dyson equations, this equation relates 1PLI correlators with $k$ points to those with a larger number of points.

Since the action for plasmon field contains vertices of all orders in $\Phi$, the SD equations are much more complicated. In principle the scaling equation involves $\Gamma_{k+1}$ and $\Gamma_{k+2}$, and so does not truncate. Recall however, that $\Gamma_k \sim N^{1-k/2}$, plus higher orders in $1/N$. This suggests an approximation scheme in which we replace $\Gamma_{k+1}$ and $\Gamma_{k+2}$ by their leading large $N$ approximation and get a closed system of scaling equations involving only $\Gamma_m$ with $m \leq k$. The simplest such approximation is a closed equation for $\tilde{\Gamma}_2$:

$$\partial_s \tilde{\Gamma}_2(q_1) = -e^{-s/2} \int \frac{d^q}{(2\pi)^4} \frac{(q)^2}{2} \frac{1}{N(\Gamma_2(q))^2} [\tilde{S}_4(q, -q, q_1, -q_1) + (\tilde{S}_3(q, q_1))^2 \tilde{\Gamma}^{-1}_2(q + q_1)].$$  (19)

The action for the Plasmon field is non-polynomial so its S-D equations are extremely complicated. The scaling equation is more analogous to the coupled boson-fermion S-D equations, but purely in terms of bosonic correlators.
This is supplemented by the large \( \mu \) boundary condition that \( \tilde{\Gamma}_2 \to \mu^{1/2} q_1^2 \). We also know that

\[
\Gamma_2(q_1) = \mu^{1/2} q_1^2 / 2 + \Pi_0(q_1),
\]

as \( N \to \infty \). The solution of the scaling equation with these boundary conditions is a complicated function of \( N \) and \( s \) and might capture some of the phase structure of the model at finite \( N \).

It would be particularly interesting to explore the question of whether the solution can have zero frequency singularities as the spatial momentum vanishes, since these would indicate the existence of a gapless plasmon excitation, and would be a likely sign of a quantum critical point.

The equations for \( \tilde{\Gamma}_3,4 \) involve \( \tilde{\Gamma}_5,6 \) and one can obtain a more refined approximation by making the substitution \( \tilde{\Gamma}_{5,6} \to S_{5,6} \). This gives a highly non-linear set of coupled equations for \( \tilde{\Gamma}_{2,3,4} \). One would imagine that this second set of equations captures much of the low energy dynamics of the HEG. High point correlation functions contain only rather complicated multi-plasmon interactions, and probably do not contribute much to the coarse grained properties studied in experiment. Approximating them by their leading order large \( N \), behavior which is also dominant in the high density limit, seems quite innocuous.

Once one has chosen one of these approximation schemes, one computes the plasmon effective action by using the solutions to compute the first few terms in the \( \phi \) expansion and approximating the rest by their leading large \( N \) behavior. One then has a classical variational problem to solve in order to find the Born-Oppenheimer potential. It seems clear that any serious attack on these equations will have to be numerical, but perhaps analytical insight can be gained by looking for solutions with some kind of scaling behavior.

4 Conclusions

We’ve proposed a sequence of approximation schemes, each a refinement of the \( 1/N \) expansion for the HEG. The simplest of these, which is a closed equation for the two point function of the plasmon field, simply related to the density density correlation function, deserves the most attention. One should try to analyze the possibility of a gapless plasmon and or scale invariant behavior. More straightforwardly, one can try to solve the equation numerically. The unknown function depends on three variables, and is a simple evolution equation in one of them. It remains to be seen how difficult a numerical challenge this will be.

It’s also important to find the corresponding set of equations in the Wigner crystal phase of the model. The background classical solution provides an additional breaking of the scale symmetry we’ve used, and various contributions to the scaling equations that vanished because of exact moment conservation will now have umklapp contributions. The equations will be much more complex, but might be revealing. We could also try to generalize our analysis to phases of the system with \( SU(N) \) breaking, since quantum Monte Carlo Methods seem to indicate that such phases occur for \( N = 2 \). There’s a very general argument that breaking to \( SU(M) \times SU(N - M) \) is only possible at large \( N \) when \( M \) is of order 1. The free energy of the model scales like \( N \) at large \( N \), so the system cannot have more than \( o(N) \) Goldstone bosons. Large \( N \) semi-classical analysis does not show any instability in these Goldstone directions. If the approximate scaling identities \( do \) detect the broken symmetry phase, that would be strong evidence for their utility.
5 Appendix: Functional Derivation of the Scaling Equations

The action for the large $N$ fluctuation field $\zeta$ is

$$S = \int \frac{d^4p}{(2\pi)^4} \zeta(p)[p^2/4\zeta(p)] + \int d^4x \ \Psi_a^\dagger(x)(\partial_t + \nabla^2/2 + \mu + i\frac{\zeta(x)}{\sqrt{N}})\Psi_a(x). \quad (21)$$

Now perform the functional change of variables

$$\zeta(t, x) = \mu \tilde{\zeta}(\mu t, \mu^{1/2}x), \quad (22)$$

$$\Psi(t, x) \mu^{3/4} \tilde{\Psi}(\mu t, \mu^{1/2}x). \quad (23)$$

The action is now

$$S = \mu^{1/2} \int \frac{d^4q}{(2\pi)^4} \tilde{\zeta}(q)[q^2/4]\tilde{\zeta}(q) + \int d^4\tilde{x} \ \tilde{\Psi}_a^\dagger(\tilde{x})(\partial_t + \tilde{\nabla}^2/2 + 1 + i\frac{\tilde{\zeta}(\tilde{x})}{\sqrt{N}})\tilde{\Psi}_a(\tilde{x}). \quad (24)$$

$q$ is the Fourier conjugate variable to $\tilde{x}$. We’ve kept the new names for position and momentum space variables and new fields, because experiments are done in Rydberg units, and measure the charge density correlations in these units. This change of variables shows that we can eliminate the dimensionless chemical potential from the equations of the HEG by a simple change of units, except for a rescaling of the Coulomb interaction. We introduce $s = -\frac{\ln \mu}{2}$ and $s \rightarrow -\infty$ manifestly gives us a theory of weakly coupled fermions.

The derivation of the scaling equations is now straightforward. We write the generating functional of correlations as a ratio of functional integrals, and perform the above change of variables only. This gives us

$$\partial_s Z[\tilde{J}] = \int \frac{d^4q}{(2\pi)^4}[q^2/4]\frac{\delta^2 Z}{\delta \tilde{J}(q)\delta \tilde{J}(-q)}. \quad (25)$$

Writing $Z = e^{-W}$ we get

$$\partial_s W[\tilde{J}] = \int \frac{d^4q}{(2\pi)^4}[q^2/4][\frac{\delta^2 W}{\delta \tilde{J}(q)\delta \tilde{J}(-q)} - \frac{\delta W}{\delta \tilde{J}(q)}\frac{\delta W}{\delta \tilde{J}(-q)}]. \quad (26)$$

Knowledgeable readers will notice the structural relation between these equations and the Wegner-Wilson-Polchinski exact renormalization group equations. We note that there is an extra term in the equation, $\partial_s EZ$, which comes from the $\mu$ dependence of the ground state energy. However, when we write the equation for the connected generating functional, this just leads to a constant and does not contribute to the equations for correlation functions.

We can now pass to the effective action defined by

$$W[\tilde{J}] = \Gamma[\tilde{\zeta}] + \int \tilde{\zeta}\tilde{J}, \quad (27)$$

where for fixed $\tilde{\zeta}$,

$$\tilde{J} \equiv -\frac{\delta \Gamma}{\delta \tilde{\zeta}}.$$
Then the left hand side of the scaling equation is just $\partial_\zeta \Gamma$, at fixed $\tilde{\zeta}$. The second term on the right hand side is proportional to $\zeta(q)\zeta(-q)$ and, in the homogeneous phase, contributes only to the two point function. In the crystalline phase this term is more complicated, because there are $1/N$ corrections to the density profile of the background crystal. We see that the truncation of the unintegrated legs of $W_{2+k}$ in the equation for $\Gamma_k$ comes about because we are differentiating with respect to $\zeta$ instead of $J$. 
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References

[1] Yi-Kuo Yu, “Derivation of the Density Functional via Effective Action” arXiv:09100670v3[cond-matt.other] .

[2] Hohenberg, P.; Kohn, W. (1964). ”Inhomogeneous Electron Gas”. Physical Review. 136 (3B): B864. Bibcode:1964PhRv..136..864H. doi:10.1103/PhysRev.136.B864.

[3] T. Banks, “Density Functional Theory for Field Theorists I,” arXiv:1503.02925 [cond-mat.mtrl-sci].