Renormalization Group Computation of Correlation Functions and Particle Densities

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Abstract

We show that the Renormalization Group formalism allows to compute with accuracy the zero temperature correlation functions and particle densities of quantum systems.

In [1] we showed that the Renormalization Group is an efficient tool to compute the ground state and first excited energy levels of a one quantum particle system. The method is the following: instead of computing directly the effective potential $V_0(x_0)$ defined as a path integral on the Fourier modes:

$$\exp \left( -\beta V_0(x_0) \right) = \int \frac{N^2}{2\pi} \prod dx_m d\bar{x}_m \exp \left( -\frac{1}{\hbar} S_{\frac{N^2}{2}} \right), \quad (1)$$

we compute recursively a running potential by integrating each modes after the other. Note that the Feynman path integral is considered here with a discretized time $t_n = \frac{n\epsilon}{N+1} = n\epsilon$, with $N$ an arbitrary large number, and $n = 0, \ldots, N+1$. The Fourier decomposition of a periodic path $x(t_n)$ contains only a finite number of Fourier modes

$$x(t_n) = x_0 + \frac{1}{\sqrt{N+1}} \sum' \exp(i\omega_m t_n) x_m + c.c., \quad (2)$$

where $\sum'$ is from 1 to $\frac{N}{2}$ if $N$ is even and from 1 to $\frac{N-1}{2}$ if $N$ is odd. The $x_m$ are the Fourier modes and $\omega_m^2 = \frac{2-\cos\frac{2\pi m}{N}}{\epsilon^2}$. The discrete action is:

$$S_{\frac{N}{2}}(x) = \epsilon \sum_0^{\frac{N}{2}} M \omega_m^2 |x_m|^2 + \epsilon \sum_{n=1}^{N+1} V_{\frac{N}{2}}(x(t_n)) \quad (3)$$
In the Local Potential Approximation \[1\], \[2\], the potential at scale \(m^{-1}\) is given by the Wegner-Houghton equation:

\[
V_{m-1}(x_0) = V_m(x_0) + \frac{1}{\beta} \log(1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2}) + O\left(\frac{1}{\beta^2}\right) \quad (4)
\]

In the present work we consider only the zero temperature case and neglect as a consequence terms of order \(\frac{1}{\beta^2}\). Our experience tells us that the finite temperature case is more difficult to handle with this equation \[4\] and gives less good results than the Feynman-Kleinert variational method \[3\]. In order to use this method to get the correlation functions we have to compute the partition function in the presence of a source term:

\[
Z(j) = \int D\xi e^{-\beta (\xi \xi + V_m^{(2)}(\xi \xi)) - |j\xi| + \text{c.c.}} \quad (5)
\]

Note that the expression is written in the continuum only for convenience. As in \[1\], we define recursively the effective potential \(V_{m-1}^j(x_0)\) (which is now \(j\) dependent) at scale \(m-1\) for a constant background path \(x_0 = \frac{1}{\beta} \int_0^\infty dt x(t)\), as a path integration on the modes \(x_m\) and \(x_{m-1}:\)

\[
e^{-\beta V_{m-1}^j(x_0)} = e^{-\beta V_m^j(x_0)} \int \frac{dx m dx_{m-1}}{2\pi \varepsilon \omega_m^2} e^{-\varepsilon \left(\omega_m^2 + V_m^{(2)}(x_0)\right) |x_m|^2 + \left(\varepsilon \sum_{n=1}^{N+1} j(t_n) e^{\omega_m (t_n - t_p)} + \text{c.c.}\right)} \quad (6)
\]

At the end of the flow of \(V_m^{j}(x_0)\), formula \(4\) reduces to a classical partition function with a source term:

\[
Z(j) = \int \frac{dx_0}{2\pi \beta} e^{-\beta (V_0^j(x_0) - j_0 x_0)}.
\]

The gaussian integration in \(5\) leads to:

\[
V_{m-1}^j(x_0) = V_m^j(x_0) + \frac{1}{\beta} \log(1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2}) - \frac{1}{\beta^2} \sum_n \varepsilon j(t_n) \sum_p \varepsilon j(t_p) e^{\omega_m (t_n - t_p)} \frac{\omega_m^2 + V_m^{(2)}(x_0)}{\omega_m^2 + V_m^{(2)}(x_0)}, \quad (7)
\]

or in terms of the Fourier transform of the source:

\[
V_{m-1}^j(x_0) = V_m^j(x_0) + \frac{1}{\beta} \log(1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2}) - \frac{j_m j_{m-1}}{\omega_m^2 + V_m^{(2)}(x_0)}. \quad (8)
\]
By neglecting the source term dependence in the right hand side of equation (7), we obtain the following approximate relation:

\[ V_{m-1}^j(x_0) = V_m(x_0) + \frac{1}{\beta} \log(1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2}) - \frac{1}{\beta^2} \frac{\sum_{m} \varepsilon j(t_n) \sum_{p} \varepsilon j(t_p)e^{i\omega_m(t_n-t_p)}}{\omega_m^2 + V_m^{(2)}(x_0)} \tag{9} \]

where now \( V_m(x_0) \) is the running potential without source term defined in equation (4). It will be shown below, when computing the particle density, that this approximation is quite good. Note that the double sum in the left hand side of (9) is of order \( \beta^2 \) so that the whole source contribution is of order \( \beta^0 \).

After iteration, (9) leads to the effective potential \( V_0^j(x_0) \) in terms of the effective potential without source \( V_0(x_0) \):

\[ V_0^j(x_0) = V_0(x_0) - \frac{1}{\beta^2} \sum_{m=1}^{N} \int_0^\beta dt_j(t) \int_0^\beta dt'_j(t') \frac{e^{i\omega_m(t-t')}}{\omega_m^2 + V_m^{(2)}(x_0)} \tag{10} \]

where for convenience we have replaced the double sum by integrals. It’s then easy to compute the correlation functions using the following relation:

\[ \langle x(t_1)...x(t_n) \rangle = \frac{1}{Z(j=0)} \frac{\delta}{\delta j(t_1)}...\frac{\delta}{\delta j(t_n)} \int dx_0 e^{-\beta V_0^j(x_0)+x_0} \int_0^\beta dt_j(t) \tag{11} \]

Since we consider only the zero temperature limit, the integral in (11) is dominated by the minimum of the effective potential \( V(x_0) \) so that:

\[ \langle x(t_1)...x(t_n) \rangle = \frac{\delta}{\delta j(t_1)}...\frac{\delta}{\delta j(t_n)} e^{\frac{1}{\beta} \sum_{m=1}^{N} \int_0^\beta dt_j(t) \int_0^\beta dt'_j(t') e^{i\omega_m(t-t')}} + \lim_{\beta \to 0} \int_0^\beta dt_j(t) \tag{12} \]

As an example the two point correlation function is easily deduced:

\[ \langle x(t_1)x(t_2) \rangle_{j=0} = x_0^2 - \frac{1}{\beta V_0^{(2)}(x_0)} + \frac{1}{\beta} \sum_{m=-N}^{N} \frac{e^{i\omega_m(t-t')}}{\omega_m^2 + V_m^{(2)}(x_0)} \tag{13} \]

In a similar manner we will now compute the particle density which is defined as:

\[ \rho(x_a) = Z^{-1} \int dx \langle x | e^{-\beta H} | x \rangle \delta(x - x_a) = \frac{1}{\sum_n e^{-\beta E_n}} \sum_n |\psi_n(x_a)|^2 e^{-\beta E_n}, \tag{14} \]

In the limit \( \beta \to \infty \):
\[\rho(x_a) = |\psi_0(x_a)|^2 \tag{15}\]

where \(\psi_0(x_a)\) is the ground state wave function. In terms of the path integral the density is:

\[
\rho(x_a) = \int \mathcal{D} \bar{\phi}(\bar{\phi})(\bar{\phi} - \bar{\phi}_0) \exp \left\{ - \int_\tau^\beta \left[ \sum_{E} \phi_0^E + \mathcal{V}(\phi_0) \right] \right\} \tag{16}\]

valuable for any value of \(\tau\). These expressions can also be written:

\[
\rho(x_a) = Z^{-1} \int \frac{dx_0}{\sqrt{2\pi M}} \int \frac{dk}{2\pi} e^{-ikx_a} \int \mathcal{D} \bar{\phi} \bar{\phi} \mathcal{D} \phi \exp \left\{ -S_{\phi} \right\} \tag{17}\]

Setting \(j(t) = -ik\delta(t - \tau)\) allows to use the previous formula (10) to directly write:

\[
\rho(x_a) = Z^{-1} \int \frac{dx_0}{\sqrt{2\pi M}} \int \frac{dk}{2\pi} e^{-k^2a^2/2+ikx_a} e^{-\beta V_0(x_0)} \tag{18}\]

where:

\[a^2(x_0) = \frac{2}{\beta} \sum_{m=1}^{N} \frac{1}{\omega_m^2 + V_m^{(2)}(x_0)} \tag{19}\]

after integrating out \(k\), we obtain:

\[
\rho(x_a) = Z^{-1} \int \frac{dx_0}{\sqrt{2\pi M}} \frac{e^{-(x_a-x_0)^2/2a^2(x_0)}}{\sqrt{2\pi a^2(x_0)}} e^{-\beta V_0(x_0)} \tag{20}\]

So that in the limit \(\beta \to \infty\):

\[
\rho(x) = \frac{e^{-(x-x_0)^2/2a^2(x_0)}}{\sqrt{2\pi a^2(x_0)}} \tag{21}\]

is a gaussian distribution. The procedure is now very simple. We just have to determine the flow of the second derivative of the effective potential. Note that the distribution (21) is the same as the variational Kleinert’s one except that for him \(a^2(x_0) = \frac{2}{M\beta} \sum_{m=0}^{N} \frac{1}{M\omega_m^2 + H(x_0)}\)

where \(\Omega\) is the variational parameter [3].

As an example consider the anharmonic oscillator. In [1] we showed that the running potential at scale \(m\) is best approximated by a polynomial of order six:

\[V_m(x) = g_0^m + \frac{g_2^m}{2} x^2 + \frac{g_4^m}{4!} x^4 + \frac{g_6^m}{6!} x^6 \tag{22}\]

where the initial potential is chosen to be:
\[ V_N(x) = \frac{1}{2} x_0^2 + \frac{240}{4!} x_0^4 \]  
(23)

Since the minimum of the effective potential is located at \( x_0 = 0 \) it is then easy to see that \( a^2(0) = \frac{2}{M \beta} \sum_{m=1}^{N} \frac{1}{M^2 + g_m} \). From the properties of the correlation function we can also deduce that the first excited energy level is given by: \( E_1 - E_0 = \sqrt{g_0^2} \).

From [1] we have:

\[
\begin{array}{|c|c|c|c|c|c|c|c|}
\hline
\lambda & E_{RG} & E_{var} & E_{ex} & E_{1, RG} & E_{1, var} & E_{1, ex} & a^2 & a_{var}^2 \\
\hline
240 & 1.4982 & 1.5313 & 1.50497 & 5.3368 & 5.3482 & 5.3216 & 0.1472 & 0.125 \\
\hline
\end{array}
\]

A comparison between the RG density and the variational density is shown in fig1. The RG density is very near the exact density given in [3]. In particular the RG computation greatly improves the value of the density near \( x = 0, (\rho_{RG}(0) \approx \rho_{ex}(0)) \).

The double well potential case is much more involved. It is well known that the effective potential at \( T = 0 \) must be a convex quantity. For a very deep potential the truncation of the running potential is no more a good approximation of the true effective potential near zero, which is almost flat. Indeed the truncation of the running potential does not allow a positive term in the logarithm of the Wegner-Houghton equation and the approximation breaks down. We have considered the case \( \lambda = 2.4 \) where an expansion at the order 10 is necessary to get valuable results:

\[
\begin{array}{|c|c|c|c|c|c|c|c|}
\hline
\lambda & E_{RG} & E_{var} & E_{ex} & E_{1, RG} & E_{1, var} & E_{1, ex} & a^2 & a_{var}^2 \\
\hline
2.4 & 0.46498 & 0.549 & 0.4709 & 0.8285 & 1.035 & 0.7677 & 3.48 & 1.03 \\
\hline
\end{array}
\]

Another problem with our approach is that a convex effective potential is incompatible with the two picks of the true particle density [3] (it’s clear that the particle will spend most of his time around the two minima of the potential energy). In statistical mechanics language each spin fluctuates most of the time around two values (like Ising spin). In fact our approximation which relates the density to the effective potential breaks down in this case. Nevertheless, the behavior of our RG density is quite correct near zero \( (\rho_{RG}(0) \approx \rho_{ex}(0)) \) and for large values of \( x \). Moreover it is much more better than the variational computation.
(fig2.). To get a better result we must go beyond the LPA approximation, and make the computation for an arbitrary background path configuration.
FIG. 1. The RG density of the anharmonic oscillator potential as compared to the variational density (dashed line).

FIG. 2. Comparison of the particle density of the double well potential between the RG density and the variational density (dashed line). The RG density is globally much better than the variational one (to compare with exact result see [3]) but our approximation is not good enough to show the double picks structure of the true density (see text).
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