Renormalization Group at finite temperature in Quantum Mechanics

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\textbf{Abstract}

We establish the exact renormalization group equation for the potential of a one quantum particle system at finite and zero temperature. As an example we use it to compute the ground state energy of the anharmonic oscillator. We comment on an improvement of the Feynman Kleinert’s variational method by the renormalization group.

\section{Introduction}

Since most of the path integrals cannot be computed exactly, different methods of approximation have been developed. The perturbation expansion is the most familiar but it diverges for all couplings strength. An another useful procedure found by Kleinert\textsuperscript{1} is the convergent variational perturbation expansion. In field theory the 'exact' Renormalization Group (RG) equations like the Wegner and Houghton one\textsuperscript{2} have led to numerous non-perturbative results. In the path integral approach a one particle system is similar to a one dimensional spin lattice\textsuperscript{3}, then the RG method could be also useful to

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extract some non-perturbative results for this system. In this paper we derive the RG equation for the potential of a quantum particle which at finite temperature is not a closed expression contrary the field theory case. We show also that we can improve the Feynman-Kleinert’s variational method, but cannot compete with the efficiency of Kleinert’s systematic variational perturbation theory.

2 Renormalization Group Equations in Quantum Mechanics

Consider the euclidean action of a quantum particle at a finite temperature

\[ S(x) = \int_0^T \left( \frac{1}{2} M \left( \frac{d}{dt} x(t) \right)^2 + V(x(t)) \right), \]

with \( M \) the mass, \( V \) the potential and \( T = \hbar \beta \).

The effective potential is defined as a constrained path integration over periodic paths with period \( T = \hbar \beta \)

\[ \exp (-\beta V_0(x_0)) = \int Dx \delta(\bar{x} - x_0) \exp \left( -\frac{1}{\hbar} S(x) \right). \]

where \( \bar{x} = \frac{1}{T} \int dt x(t) \).

The partition function is

\[ Z = \int \frac{dx_0}{\sqrt{2\pi \hbar T M}} \exp (-\beta V_0(x_0)), \]

We consider the Feynman path integral with a discretized time \( t_n = \frac{nT}{N+1} = n\epsilon \) 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

\[ x(t_n) = x_0 + \frac{1}{\sqrt{N+1}} \sum' \exp(i\omega_m t_n)x_m + H.C, \]

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 \( \omega_m^2 = \frac{2 - 2\cos \frac{Nm}{N+1}}{\epsilon^2}. \)
The discretized partition function is then
\[ Z = \int \frac{dx_0}{\sqrt{2\pi\hbar}} \int \Pi_1^N \frac{dx_m d\bar{x}_m}{2\pi\hbar} \exp \left( -\frac{1}{\hbar} S_N \right), \]
where the discretized action is given by
\[ S_N(x) = \epsilon \sum_{m=0}^{N} M \omega_m^2 |x_m|^2 - \epsilon \sum_{n=1}^{N+1} V(x(t_n)). \]

Using the fact that \( \Pi_1^N \epsilon^2 \omega_m^2 = \sqrt{N+1} \) and \( T = (N+1)\epsilon \), we define the effective potential as (see [1]):
\[ \exp (-\beta V_0(x_0)) = \int \Pi_1^N \frac{dx_m d\bar{x}_m}{\sqrt{2\pi\hbar}} \exp \left( -\frac{1}{\hbar} S_N \right). \]

Instead of evaluating (4) in one step we integrate mode after mode. Let us denote \( V_m \) the ‘running potential’ obtained after \( \frac{N}{2} - m \) integrations, and \( V_N \) the initial potential \( V \). To find the potential \( V_{m-1} \) with respect to \( V_m \) we consider paths with only one Fourier mode:
\[ x(t_n) = x_0 + \frac{1}{\sqrt{N+1}} \exp(i\omega_m t_n) x_m + H.C. \]

We thus obtain the relation:
\[ \exp (-\beta V_{m-1}(x_0)) = \int \frac{dx_m d\bar{x}_m}{\sqrt{2\pi\hbar}} \exp \left( -\frac{\epsilon}{\hbar} \left( M \omega_m^2 |x_m|^2 + \sum_{n=0}^{N+1} V_m(x_0) + \frac{\exp(i\omega_m t_n) x_m}{\sqrt{N+1}} + H.C. \right) \right) \]

Expanding the potential \( V_m \) around the point \( x_0 \) and summing over \( n \), yields the following RG equation for the potential
\[ V_{m-1}(x_0) = V_m(x_0) + \frac{1}{\beta} \log \left( 1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2 M} \right) + \frac{1}{\beta} \log \left( 1 + \sum_{n=2}^{N+1} \frac{n!}{\beta^{n-1}} \cdot \sum_{k_1 p_1 + \ldots + k_n p_n = n} (-1)^{k_1+\ldots+k_n} \frac{V_m^{(2p_1)}(x_0)^{k_1}}{k_1!(p_1!)^{2k_1}} \cdots \frac{(V_m^{(2p_n)}(x_0) k_n}{k_n!(p_n!)^{2k_n} P_m}, \]

where all the $p_i \geq 2$ are different and the propagator $P_m = \frac{1}{M\omega_m^2 + V_m^{(2)}(x_0)}$.

Note that in this derivation we have ignored the evolution of higher derivative interactions. The equation (6) has not the closed form of the ‘exact’ WH differential equation in field theory [2] which takes into account only the one loop contributions resumed in a logarithm term. In field theory the higher order loop terms are negligible even at finite temperature [4] but their influence is taken into account through the running of the parameters of the theory. In (6) the one loop contributions are resumed in the first logarithm term but the second one contains the higher loop terms. To compare with the usual perturbation expansion we can rewrite the RG equation in the familiar cumulant expansion. Let us define

$$A_m = \epsilon \sum_{n=0}^{N+1} \left( V_m(x(t_n)) - V_m(x_0) - \frac{1}{2} V_m^{(2)}(x_0)x^2(t_n) \right),$$

and denote the expectation value with respect to the gaussian weight $M\omega_m^2 + V_m^{(2)}(x_0)$ by $< >_m$. It is straightforward to derive:

$$\frac{1}{l!}(-\frac{1}{h})^l < A_m^l >_m = \sum_{n \geq 2} \frac{n!}{\beta^{n-1}}$$

$$\sum_{k_1p_1 + \ldots + (l-k_1-\ldots-k_{n-1})p_n = n} (-1)^{k_1+\ldots+k_n} \left( \frac{V_m^{(2p_1)}(x_0)}{k_1!(p_1!)^{2k_1}} \right) \ldots \left( \frac{V_m^{(2p_n)}(x_0)}{k_n!(p_n!)^{2k_n}} \right) P_m^n.$$

Then defining the cumulants by

$$< A_m^n >_{m,c} = < (A_m - < A_m >_m)^n >_m,$$

the Renormalization Group equation becomes:

$$V_{m-1}(x_0) = V_m(x_0) + \frac{1}{\beta} \log \left( 1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2 M} \right) + \frac{1}{h\beta} < A_m >_m$$

$$- \frac{1}{\beta} \sum_{l \geq 2} \frac{l!}{h^l} (-\frac{1}{h})^l < A_m^l >_{m,c}$$

(7)

In this formulation the equation has the disadvantage to mix the powers of $\frac{1}{\beta}$.

Clearly the RG equation seems not to be useful to extract nonperturbative results. Actually it contains an infinite number of terms, negligible only if $(\frac{V_m}{\beta})^p$ are small (for finite temperature the coupling constants must be small). Nevertheless it is interesting to discuss the various limiting cases.
2.1 Infinite temperature

For a large temperature the quantum fluctuations are small and the system is close to the classical one. The flow of the potential stays near the classical one (the potential energy of the action) and will be obtained after a relatively small number of iterations of the RG equation. In particular in the limit $\beta \to 0$, $\frac{V_m^{(2)}(x_0)}{\omega^2_m M}$ and $P$ are of order $\beta^2$ and we obtain

$$V_{m-1}(x_0) = V_m(x_0)$$

a running potential constant along the flow. As a consequence the quantum partition function reduces to the classical one.

2.2 Zero temperature

In this opposite case due to quantum fluctuations the effective potential is expected to be different from the classical one and will be obtained after a huge number of iterations of the RG equation (typically $10^8$ for $\beta = 10^5$). The higher loop contributions are negligible, then we can extract informations for large coupling constants. In particular, in the limit $\beta \to \infty$ the propagator $P_m$ is of order $\frac{1}{V_m^{(2)}(x_0)}$. Then keeping only the one loop contributions in (6) we obtain the closed form:

$$V_{m-1}(x_0) = V_m(x_0) + \frac{1}{\beta} \log \left( 1 + \frac{V_m^{(2)}(x_0)}{\omega^2_m M} \right).$$

(8)

Recall that for large $N$, $\omega^2_m$ is equivalent to $\left( \frac{2 \pi m}{\hbar \beta} \right)^2$ and then runs from $0$ to $(\frac{\pi}{\epsilon})^2$. Rewriting (8) as

$$V_{m-1}(x_0) = V_m(x_0) + \frac{\hbar \pi}{2 \pi \epsilon N + 1} \log \left( 1 + \frac{V_m^{(2)}(x_0)}{\left( \frac{\pi m}{\epsilon N+1} \right)^2 M} \right),$$

the limit $N \to \infty$ gives a continuous equation

$$V_{k-\Delta_k}(x_0) = V_k(x_0) + \frac{\hbar \Delta_k}{2 \pi} \log (1 + \frac{V_k^{(2)}(x_0)}{Mk^2}),$$

(9)
where we have introduced the notations \( k^2 = \omega_m^2 \), \( \Delta k = \frac{2\pi m}{e(N+1)} \), and neglected the higher loop contributions which are of order \( (\Delta k)^2 \). This equation is the one dimensional Wegner Houghton equation for the effective potential \([4]\). It is useful to extract informations even for very large coupling constants as shown below.

3 Examples

We solve exactly the Renormalization Group equation for some easy examples and recover known results.

3.1 The free particle

This case is trivial because \( V_{\frac{N}{2}}(x_0) = 0 \). It’s easy to show recursively that at each step \( V_{m-1}(x_0) = V_m(x_0) = 0 \). Then, the effective potential \( V_0(x_0) = 0 \).

3.2 The harmonic oscillator

As a second example, consider the case: \( V_{\frac{N}{2}}(x_0) = M^2 \Omega^2 x_0^2 \). Once again, we obtain recursively: \( V_{m-1}(x_0) = M^2 \Omega^2 x_0^2 + C_m \) with \( C_m \) a constant. Inserting this result in (6), we obtain the solution

\[
V_0(x_0) = M^2 \Omega^2 x_0^2 + \frac{1}{\beta} \log \left( \prod_{m=1}^{N} \left( \frac{\omega_m^2 + \Omega^2}{\omega_m^2} \right) \right),
\]

which gives the partition function (see [1]):

\[
Z = \frac{1}{\hbar \beta \Omega} \prod_{m=1}^{N} \left( \frac{\omega_m^2}{\omega_m^2 + \Omega^2} \right)
\]

3.3 Perturbation expansion

Replacing \( V_m \) by \( V_{\frac{N}{2}} \) in (7) one recovers the usual perturbative expansion

\[
V_0(x_0) = V_{\frac{N}{2}}(x_0) + \sum_{m=1}^{N} \frac{1}{\beta} \log \left( 1 + \frac{V_{\frac{N}{2}}(x_0)}{\omega_m^2 M} \right) + \frac{1}{\hbar \beta} \sum_{m=1}^{N} <A_{\frac{N}{2}}>_m
\]

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\[-\frac{1}{\beta} \sum_{l \geq 2} \frac{1}{l!} \left(\frac{1}{h}\right)^l \sum_{m=1}^{N} <A^l_{m,c}>_{m,c} \]

4 The anharmonic oscillator

In this part we compute the ground state energy of the anharmonic oscillator at zero temperature for various values of the coupling constant by using the RG equation, and compare with Kleinert’s [1] variational results. The ground state energy is the value of the effective potential \( V_0(x_0) \) at its minimum \( x_0 = 0 \). Unfortunately it is a hard task to use the RG equation (8) because at each step we must find the second derivative of the potential by fitting it numerically. Due to the very slow convergence we must repeat the procedure a huge number of time for each point of the potential. We leave this method for another paper and try instead to compute the flow equations for the coupling constants.

We define the n-th coupling constant at the scale \( m \) by

\[
g^{(n)}_m = \frac{d^n}{dx_0^n} |_{x_0=0} V_m(x_0). \]

We give a general formulation for the flow of the couplings where we neglect terms of higher order in \( \frac{1}{\beta} \):

\[
g^{(0)}_{m-1} = g^{(0)}_m + \frac{1}{\beta} \log \left( 1 + \frac{g^{(2)}_m}{\omega^2_m M} \right). \tag{10} \]

For \( k \neq 0 \) we have

\[
g^{(k)}_{m-1} = g^{(k)}_m + \frac{1}{\beta} \left( \sum_p (-1)^{p-1} P_m(0)^p \left( \sum_{\alpha_1+\ldots+\alpha_p=k, \alpha_i>0} \frac{k! A_p}{p!} \sum_2^{(\alpha_1+2)} \frac{g^{(\alpha_1+2)}_m}{\omega^2_m A_p^{(\alpha_1+2)}} \ldots \frac{g^{(\alpha_p+2)}_m}{\omega^2_m A_p^{(\alpha_p+2)}} \right) \right), \tag{11} \]

where \( A_p \) is the combinatorial factor of \( \frac{2^{(\alpha_1+2)}_{\alpha_1}}{\alpha_1!} \ldots \frac{2^{(\alpha_p+2)}_{\alpha_p}}{\alpha_p!} \) in the series expansion of \( \left( V^{(2)}(x_0) \right)^p \) in powers of \( x_0 \) and \( P_m(0) = \frac{1}{\omega^2_n M + g^{(2)}_m} \).

For the initial potential we choose

\[
V_N(x) = \frac{1}{2} M \Omega^2 x^2 + \frac{\lambda}{4!} x^4 \tag{12} \]
\begin{table}
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|}
\hline
$g_{m=0}^{(2)}$ & $g_{m=0}^{(4)}$ & $g_{m=0}^{(6)}$ & $g_{m=0}^{(8)}$ & $g_{m=0}^{(10)}$ & $E_{RG}$ \\
\hline
1.5140 & 2.4 & 0 & 0 & 0 & 0.56134 \\
1.4522 & 1.5343 & 0 & 0 & 0 & 0.55807 \\
1.4643 & 1.7706 & 3.9484 & 0 & 0 & 0.55855 \\
1.4617 & 1.7110 & 2.8109 & $-16.662$ & 0 & 0.55847 \\
1.4662 & 1.7236 & 3.0112 & $-16.794$ & $-237.46$ & 0.55848 \\
\hline
\end{tabular}
\caption{Table 1: comparison of the ground state energy $E_{GR}$ of the anharmonic oscillator for $M = \Omega = 1$, $\lambda = 2.4$ and different truncations of the potential. The exact value is $E_{exact} = 0.55915$}
\end{table}

The numerical solution of the flow equations \cite{10,11} shows a good convergence for $N = 10^8$ and $\beta = 10^5$. There are no significant improvement for larger values of $N$ or $\beta$. At first, we have tried different truncations of the polynomial potential and found the best values by keeping only the couplings $g^{(4)}$ and $g^{(6)}$ as is shown in table 1 where we can also read the different values of the couplings at the end of the flow when $m = 0$. Adding more coupling does not improve the result, on the contrary. In fact in order to get better results we can not truncate the effective potential because in quantum mechanics each coupling constant is relevant. Even when the couplings $g^{(8)}$ and $g^{(10)}$ take large negative values they do not influence very much the flows of the other couplings. Then, it seems that around its minimum the potential is well fitted by a polynomial interaction of order six.

A detailed comparison of the truncation at $x^6$ with Kleinert’s variational method is given in table 2. All the couplings are relevant because they grow as we iterate the RG equation. Surprisingly, the truncation of the potential at the six order gives always better results than those of the variational method. The advantage of the latter lies on the fact that one can improve it systematically with a perturbation expansion which is convergent (see \cite{1}). In our case the only way to improve it is to consider the potential as a whole. This requires a numerical study which is difficult to achieve due to the very slow convergence of the iterations in the zero temperature case.
Table 2: comparison of the exact ground state energy $E_{\text{exact}}$ with the variational energy $E_{\text{var}}$ and the energy $E_{RG}$ obtained from the flow of our truncated potential.
\[
\begin{array}{|c|c|c|c|c|}
\hline
\lambda & E_{RG} & g_{m=0}^{(2)} & g_{m=0}^{(4)} & g_{m=0}^{(6)} \\
\hline
4.8 & 0.073 & 0.366 & 0.821 & 4.288 \\
7.2 & 0.189 & 0.681 & 1.955 & 13.02 \\
9.6 & 0.266 & 0.960 & 3.111 & 23.34 \\
\hline
\end{array}
\]

Table 3: Ground state energy and flow of the coupling constants for the double well potential.

### 4.1 The double well potential

In this part we consider the case of the double potential with a frequency \( \Omega = -1 \). The results for some values of the coupling \( \lambda \) (see Table 3) show that \( g_{m=0}^{(2)} > 0 \). It means that the quantum fluctuations smear out completely the double well as it must be, because the effective potential is a convex quantity at \( T = 0 \). For \( \lambda = 2.4 \) our truncation is not accurate enough to get a positive term in the logarithm of equation (8). For all larger couplings our approximation is enough to show the spreading of the double potential by the quantum fluctuations.

### 5 The Feynman Kleinert method

In this section, we give some comments concerning the FK method improved by the renormalization group. In the FK method, one tries to find a quadratic potential at each point \( x_0 \) fitting at best the effective potential. One improves this procedure by looking for a quadratic potential \( M\Omega_m x^2 \) fitting the potential \( V_m(x_0) \) at each step of the renormalization group flow. Then by improving in such manner the FK method one will take into account some contributions of the Kleinert’s variational perturbation expansion \([1]\). To achieve this, we follow Kleinert’s method and insert in the right hand side of (5) the trial frequency \( \Omega_m^2(x_0) \) (see \([1]\)).

\[
\exp \left( -\frac{T}{\hbar} V_{m-1}(x_0) \right) = \int \frac{dx_m dx_{\bar{m}}}{2\pi \hbar} \exp \left( -\frac{\epsilon}{\hbar} M \left( \omega_m^2 + \Omega_m^2(x_0) \right) |x_m|^2 \right)
\]
\[ \exp \left( -\frac{\varepsilon}{\hbar} \left( \sum_{n=0}^{N+1} V_m \left( x_0 + \frac{\exp(i\omega_m t_n) x_m}{\sqrt{N+1}} + H.C. \right) - M\Omega_m^2(x_0)|x_m|^2 \right) \right) \]

Then, using the Jensen-Peierls inequality

\[ \int d\mu(x) \exp (-O(x)) \geq \exp \left( -\int d\mu(x)O(x) \right) \]

for any positive measure \( \mu \) normalized to one, and following the same steps as in Kleinert’s book [1], we obtain the following RG inequality for the potential

\[ V_{m-1}(x_0) \leq \frac{1}{\beta} \log \left( 1 + \frac{\Omega_m^2(x_0)}{\omega_m^2} \right) \frac{1}{\sqrt{2\pi a_m^2}} \int \exp \left( -(x-x_0)^2/2a_m^2(x_0) \right) \] \[ V_m(x) . \]

where

\[ a_m^2(x_0) = \frac{2}{\beta M} \frac{1}{\omega_m^2 + \Omega_m^2} . \]

Let us call \( V_{a_m^2} \), the integral on the right hand side of the inequality. Minimizing the right hand side in the variable \( \Omega_m^2 \) we obtain the best approximation for \( V_{m-1} \). The frequency

\[ \Omega_m^2(x_0) = \frac{2}{\beta M} \frac{\partial}{\partial a_m^2} V_{a_m^2}(x_0), \] (13)

gives the following equation, which can be solved recursively, starting from \( \Omega_m^2(x_0) = 0 \)

\[ \Omega_m^2(x_0) = \int \frac{dx}{\sqrt{2\pi}} \exp \left( -x^2/2 \right) \frac{1}{2\sqrt{a_m^2}} V_m^{(1)}(x_0 + \sqrt{a_m^2(x_0) x}). \] (14)

Keeping this value for \( \Omega_m^2 \), enables us to rewrite the approximation

\[ V_{m-1}(x_0) = \frac{1}{\beta} \log \left( 1 + \frac{\Omega_m^2(x_0)}{\omega_m^2} \right) \frac{1}{\sqrt{2\pi a_m^2}} \int \exp \left( -(x-x_0)^2/2a_m^2(x_0) \right) \] \[ V_{a_m^2}(x) \right) \] .

which is the variational RG equation. For finite \( \beta \), it is possible to solve (15), firstly by computing recursively \( \Omega_m^2(x_0) \), secondly by calculating \( V_{a_m^2} \) and inserting this result in the Renormalization group equation. We plan to use this equation in another paper. In the following section we check its validity in the limiting cases.

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5.1 Infinite temperature

Recall that for large $N$, $\omega_m^2$ is equivalent to $\left(\frac{2\pi m}{\beta}\right)^2$. Then for $\beta \to 0$, $\frac{\Omega_m^2(x_0)}{\omega_m^2}$ and $\frac{\Omega_m^2}{\Omega_m^2 + \omega_m^2}$ are of order $\beta^2$ and $a_m^2(x_0)$ is of order $\beta$. Inserting these results in the equation for $V_{a_m^2}$ gives $V_{a_m^2} = V_m(x_0)$. For $\beta \to 0$ we recover the usual invariance for the flow of the effective potential:

$$V_{m-1}(x_0) = V_m(x_0).$$

5.2 Zero temperature

In the limit $\beta \to \infty$, $a_m^2(x_0)$ is now of order $\frac{1}{\beta}$. To obtain $\Omega_m^2$ we expand the potential $V_m$ in a series of $a_m^2$. To lowest order we obtain: $\Omega_m^2(x_0) = \frac{V_m^{(2)}(x_0)}{M}$. In the same way, we get the lowest order: $V_{a_m^2}(x_0) = V_m(x_0)$. Then keeping only the relevant terms, the limit for $\beta \to 0$ gives again the Wegner Houghton equation:

$$V_{m-1}(x_0) = V_m(x_0) + \frac{1}{\beta} \log \left(1 + \frac{V_m^{(2)}(x_0)}{\omega_m^2 M}\right)$$

To understand why we recover the WH equation, one compares with the Kleinert’s variational perturbation expansion. In the RG equation for the potential at $T = 0$, the contributions of all the higher loops terms are included in the flow of the couplings. By choosing a variational frequency which flows in the RG equation we automatically take into account all the higher loops of the variational perturbation expansion and the result must be independent of the variational frequency. In other words, by integrating mode after mode we automatically resume the perturbation expansion and we cannot improve it. A possibility to resume partially the higher loops would be to integrate a lot of modes at each step, and to deduce the variational frequency for the resulting potential.

6 Conclusion

The RG equation for the potential of a quantum particle at finite temperature was derived. This equation does not allow us to compute non-perturbative quantities. Then we suggest to use the Feynman Kleinert’s
variational method improved by the RG. At zero temperature we recovered the Wegner Houghton equation which was used to compute the ground state energy of the anharmonic oscillator. It would be also interesting to compute the RG equation for the effective action. Our preliminary work show the generation of non local interactions. We also plan to apply the RG procedure for systems with many quantum particles in the discretized path integral representation.

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