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APPENDIX

SELF-CONSISTENT APPROXIMATION

At this point we like to introduce an alternative approach to Feynman-Kleinert approximation. It is developed by a Legendre transform and cumulant expansion via self-consistent theory used to study the anharmonic crystals for long time ago[Choquard 1967, Samathiyakanit and Glyde 1973]. Let us consider the action of one particle in one-dimensional potential

$$S = \int_0^{\beta\hbar} d\tau\left[\frac{M}{2}\dot{x}^2 + V(x)\right]. \tag{1}$$

Now we try to expand in Taylor series the potential $V(x)$ about any point x_0, then

$$\begin{aligned} V(x) &= V(x_0) + (x - x_0)\,V'(x_0) + \frac{1}{2!}(x - x_0)^2\,V''(x_0) \\ &\quad + \frac{1}{3!}(x - x_0)^3\,V'''(x_0) + \ldots \quad . \end{aligned} \tag{2}$$

We can construct an exponential operator by using the fact that $e^x = 1 + x + x^2/2! + x^3/3! + \ldots$ in order to rewrite (2) in a new form as follow

$$V(x) = e^{(x - x_0)\nabla}\,V(x_0), \tag{3}$$

where $\nabla = \partial/\partial x$ and $e^{(x - x_0)\nabla}$ expressed as an exponential operator

$$\begin{aligned} e^{(x - x_0)\nabla} &= 1 + (x - x_0)\,\nabla + \frac{1}{2!}(x - x_0)^2\nabla^2 \\ &\quad + \frac{1}{3!}(x - x_0)^3\nabla^3 + \ldots \quad . \end{aligned} \tag{4}$$

For any distribution function, we have the expectation

$$\langle V(x) \rangle = \langle e^{(x-x_0)\nabla} \rangle V(x_0) . \quad (5)$$

Next we use a cumulant expansion of $\langle e^{x} \rangle$ [Kubo 1962], defined as

$$\langle e^{x} \rangle = \exp\Big\{ \langle x \rangle + \frac{1}{2}[\langle x^2 \rangle - \langle x \rangle^2] - \frac{1}{6}[\langle x^3 \rangle - 3\langle x \rangle^2 \langle x \rangle + 2\langle x \rangle^3] + \ldots \Big\}, \quad (6)$$

to expand $\langle e^{(x-x_0)\nabla} \rangle$ in the following

$$\langle e^{(x-x_0)\nabla} \rangle = \exp\Big\{ [\langle x - x_0 \rangle \nabla] + \frac{1}{2}\Big[\langle (x-x_0)^2 \rangle \nabla^2 - \langle (x-x_0)\nabla \rangle^2\Big] + \ldots \Big\}. \quad (7)$$

In case of Gaussian averaging, only the expectation value of $(x-x_0)^2$ is not zero[Kubo 1962], then we have

$$\langle e^{(x-x_0)\nabla} \rangle = \exp\Big\{ \frac{1}{2}\langle (x-x_0)^2 \rangle \nabla^2 \Big\} \quad (8)$$

Now we back to the action S in (1) to construct a trial or model action S_0, of course we should construct it in a harmonic form with a force constant $\emptyset$ or $M\Omega^2$. That is

$$S_0 = \int_0^{\beta\hbar} d\tau \Big[\frac{M}{2}\dot{x}^2 + \frac{1}{2}\emptyset (x-x_0)^2 \Big], \quad (9)$$

note that we shift the center to x_0. In the same manner with the other approach we can write that

$$Z = Z_0 \langle e^{-S_0/\hbar} \rangle_0 \quad (10)$$

where $\langle \ldots \rangle_0$ is the expectation calculated with the trail distribution $e^{-S_0/\hbar}$ and Z_0 is the trial partition function. By using the first cumulant expansion in (10) we obtain

$$
\begin{aligned}
Z &= Z_0 \exp\{ \langle -(S - S_0)/\hbar \rangle_0 \} \\
&= Z_0 \exp\left\{ -\frac{1}{\hbar}\int_0^{\beta\hbar} d\tau\left[\langle V(x)\rangle_0 - \frac{1}{2}\text{Ø}\left\langle (x - x_0)^2 \right\rangle_0 \right] \right\} \\
&= Z_0 \exp\left\{ -\beta\left[\langle V(x)\rangle_0 - \frac{1}{2}\text{Ø}\left\langle (x - x_0)^2 \right\rangle_0 \right] \right\}. \qquad (11)
\end{aligned}
$$

To obtain the general condition for choosing the self-consistent force constant Ø, we consider the free energy $F \equiv -1/\beta \ln Z$. From (10) and (11) this may be written as a sum of harmonic and anharmonic parts

$$
\begin{aligned}
F &\equiv -\frac{1}{\beta}\ln Z_0 - \frac{1}{\beta}\ln \exp\left\{ -\frac{1}{\hbar}\langle S - S_0\rangle \right\} \\
&= -\frac{1}{\beta}\ln Z_0 + \left(\langle V(x)\rangle_0 - \frac{1}{2}\text{Ø}\left\langle (x - x_0)^2 \right\rangle_0 \right) \\
&= F_0[\text{Ø}] + \Delta F[\text{Ø}, B\,]. \qquad (12)
\end{aligned}
$$

Here F_0 is a function of Ø only and ΔF is a function of Ø and the correlation function

$$
B = \left\langle (x - x_0)^2 \right\rangle_0 . \qquad (13)
$$

The variation of Ø and B gives

$$
\delta F = \frac{\delta F_0}{\delta \text{Ø}}\,\delta\text{Ø} + \frac{\delta F_0}{\delta B}\,\delta B + \left(\frac{\delta \Delta F}{\delta \text{Ø}}\,\delta\text{Ø} + \frac{\delta \Delta F}{\delta B}\,\delta B \right) \qquad (14)
$$

Consider the derivative

$$
\frac{\delta F_0}{\delta B} = 0
$$

$$
\frac{\delta F_0}{\delta \text{Ø}} = \frac{1}{\beta\hbar Z_0}\int \mathcal{D}x\, e^{-S_0/\hbar}\,\frac{\delta S_0}{\delta \text{Ø}}
$$

$$= \frac{1}{2}\langle (x - x_0)^2 \rangle$$

$$= \frac{1}{2}B \tag{15}$$

so that

$$\delta F = \frac{1}{2}B\delta\varnothing + \left(\frac{\delta\Delta F}{\delta\varnothing}\delta\varnothing + \frac{\delta\Delta F}{\delta B}\delta B \right) \tag{16}$$

On introducing the function $R \equiv F - \frac{1}{2}B\varnothing$, which amounts to a Legendre transformation, (13) gives

$$\delta R = \delta F - \frac{1}{2}\varnothing\delta B - \frac{1}{2}B\delta\varnothing$$

$$= -\frac{1}{2}\varnothing\delta B + \left(\frac{\delta\Delta F}{\delta\varnothing}\delta\varnothing + \frac{\delta\Delta F}{\delta B}\delta B \right) \tag{17}$$

so that

$$\left(\frac{\delta R}{\delta B}\right)_{\varnothing} = -\frac{1}{2}\varnothing + \left(\frac{\delta\Delta F}{\delta B}\right)_{\varnothing}. \tag{18}$$

We now choose $\varnothing$ by including the anharmonic contribution to the free energy ΔF and requiring that the contribution from it to the force constant vanishes, that is from (18) that

$$\left(\frac{\delta\Delta F}{\delta B}\right)_{\varnothing} = 0 \tag{19}$$

This mean that $\varnothing$ is chosen so that the anharmonic contribution to the force constants is already include in the effective harmonic approximation. For the first cumulant approximation, ΔF is defined as, see (12)

$$\Delta F = \langle V(x)\rangle_0 - \frac{1}{2}\varnothing\langle (x - x_0)^2 \rangle_0 . \tag{20}$$

Then we have

$$\left(\frac{\delta \Delta F}{\delta B}\right)_{\emptyset} = \frac{\delta}{\delta B}\langle V(x)\rangle_0 - \frac{1}{2}\emptyset\,, \tag{21}$$

the condition (19) and the expression (5) give us

$$\frac{\delta}{\delta B}\exp\left\{\frac{1}{2}B\nabla^2\right\}V(x_0) = \frac{1}{2}\emptyset \tag{22}$$

so that

$$\emptyset = \nabla^2\langle V(x)\rangle_0. \tag{23}$$

This final result satisfy the condition for choosing Ω in Feynman-Kleinert method as described before, see Eq. (5.60) and note that $\emptyset = M\Omega^2$.

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