Effective Hamiltonian with holomorphic variables

Alessandro Cuccoli and Valerio Tognetti
Dipartimento di Fisica dell’Università di Firenze and Istituto Nazionale di Fisica della Materia (INFN), Largo E. Fermi 2, I-50125 Firenze, Italy

Riccardo Giachetti
Dipartimento di Fisica dell’Università di Firenze and Istituto Nazionale di Fisica Nucleare (INFN), Largo E. Fermi 2, I-50125 Firenze, Italy

Riccardo Macciocchi
Dipartimento di Fisica dell’Università di Firenze, Istituto Nazionale di Fisica della Materia (INFN), and Istituto Nazionale di Fisica Nucleare (INFN), Largo E. Fermi 2, I-50125 Firenze, Italy

Ruggero Vaia
Istituto di Elettronica Quantistica del Consiglio Nazionale delle Ricerche, via Panciatichi 56/30, I-50127 Firenze, Italy, and Istituto Nazionale di Fisica della Materia (INFN)

The pure-quantum self-consistent harmonic approximation (PQSCHA) permits to study a quantum system by means of an effective classical Hamiltonian. In this work the PQSCHA is reformulated in terms of the holomorphic variables connected to a set of bosonic operators. The holomorphic formulation, based on the holomorphic path integral for the Weyl symbol of the density matrix, makes it possible to directly approach general Hamiltonians given in terms of bosonic creation and annihilation operators.

The concept of effective potential in quantum statistical mechanics was introduced by Feynman \cite{1} by means of a variational method for the imaginary time path integral. The method was improved by Giachetti and Tognetti \cite{2} and Feynman and Kleinert \cite{3} using the Lagrangian path integral. Several applications to condensed matter have demonstrated its usefulness. \cite{4} The generalization to Hamiltonian path integrals was performed for treating nonstandard Hamiltonians, where there is no separation between a quadratic kinetic energy and a configurational potential, and for which the Feynman-Jensen inequality does not hold in general. An effective Hamiltonian for systems with nonstandard Hamiltonians, where there is no separation between a quadratic kinetic energy and a configurational potential, and which the Feynman-Jensen inequality does not hold in general, is made possible by means of the pure-quantum self-consistent harmonic approximation (PQSCHA). \cite{5} Nevertheless, this generalization can not be applied in a natural way to field-theory models which are described in terms of creation and destruction operators: the natural classical-like counterpart of this models requires, in the Bose case, holomorphic variables. We present here the derivation of the effective Hamiltonian in the framework of PQSCHA for Bose systems by using an holomorphic path integral for the Weyl symbol of the density matrix $\hat{\rho} = \exp(-\beta\mathcal{H})$.

Consider a system of $N$ bosons and let $\hat{a} = \{\hat{a}_\mu\}_{\mu=1,...,N}$, $\hat{a}^\dagger = \{\hat{a}_\mu^\dagger\}_{\mu=1,...,N}$ be the creation and annihilation operators. The quantum statistical average of an operator $\hat{O}(\hat{a}^\dagger, \hat{a})$ has a natural expression in terms of the Weyl symbols of $\hat{O}$ and $\hat{\rho}$, respectively $\hat{O}(\hat{a}^\dagger, \hat{a}) = \int dz_1 dz_2 \cdots dz_N \rho(z_1, z_2, \cdots, z_N) \hat{O}(\hat{a}(z_1, z_2, \cdots, z_N), \hat{a}^\dagger(z_1, z_2, \cdots, z_N))$, where $\rho(z_1, z_2, \cdots, z_N)$ is a probability distribution.

The idea is to decompose the path-integral expression for $\rho(z_1, z_2, \cdots, z_N)$ into a first sum over all paths with the same average point defined as $\frac{1}{Z} \int_0^\beta du (z^*(u), z(u))$, and a second sum over average points. For this we introduce in the path-integral a resolution of the identity that fixes the average point to $(\bar{z}, \bar{z})$ and we split the integration over the latter, defining the reduced density

$$\bar{\rho}(\bar{z}, z; \bar{z}, \bar{z}) = \int D[z^*(u), z(u)] \delta(\bar{z}, \bar{z}) \left[ 1 - \frac{1}{\beta} \int_0^\beta du (z^*(u), z(u)) \right] e^{S(z^*(u), z(u))},$$

where the Euclidean action $S(z^*(u), z(u))$ is given by

$$S(z^*(u), z(u)) = \int_0^\beta du \left[ \frac{1}{2} \left[ z^*(u)z(u) - z(z(u)) \right] - \mathcal{H}(z^*(u), z(u)) \right] - \frac{1}{2} \left[ \bar{z}^*(0)z(\beta) - \bar{z}(\beta)z(0) \right] - \left[ \bar{z}^*(0)(\mathcal{H}(\bar{z}(\beta) - \bar{z}(0)) \right] z - \bar{z}^*[\bar{z}(\beta) - \bar{z}(0)] \right] .$$

We take $\bar{\rho}(\bar{z}, z; \bar{z}, \bar{z})$ as an unnormalized probability distribution in the variables $(\bar{z}, \bar{z})$ and define its normalization constant as $\exp(-\beta\mathcal{H}_{eff}(\bar{z}, \bar{z}))$, so that
\[ \hat{\rho}(\hat{z}^*, \hat{z}; \hat{z}^*, \hat{z}) = e^{-\beta \mathcal{H}_{\text{eff}}(\hat{z}^*, \hat{z})} \mathcal{P}(\hat{z}^*, \hat{z}; \hat{z}^*, \hat{z}), \]  

and the average of \( \hat{O} \) can then be written

\[ \langle \hat{O} \rangle = \frac{1}{\mathcal{Z}} \int \frac{dz^*_\mu d\bar{z}^*_\mu}{2\pi i} \left[ \int d\mu(z^*, z) \langle \hat{O}(z^*, z) \mathcal{P}(z^*, z; \hat{z}^*, \hat{z}) \rangle e^{-\beta \mathcal{H}_{\text{eff}}(\hat{z}^*, \hat{z})}. \]  

It is natural to interpret \( \exp(-\beta \mathcal{H}_{\text{eff}}(\hat{z}^*, \hat{z})) \) as a classical-like effective density, whereas the probability distribution \( \mathcal{P}(z^*, z; \hat{z}^*, \hat{z}) \) describes the particle fluctuations around the point \((\hat{z}^*, \hat{z})\). In the classical limit it can be seen that \(\mathcal{P}(z^*, z; \hat{z}^*, \hat{z}) \to \delta((z^*, z) - (\hat{z}^*, \hat{z}))\) and \(\exp(-\beta \mathcal{H}_{\text{eff}}(\hat{z}^*, \hat{z}))\) tends to the classical Boltzmann factor; it follows that the probability \( \mathcal{P} \) describes the pure-quantum fluctuations of the particle thus providing a separation between classical-like and pure-quantum contribution to \( \langle \hat{O} \rangle \).

The evaluation of the reduced density \( \hat{\rho}(\hat{z}^*, z; \hat{z}^*, \hat{z}) \) will be done in a self-consistent approximation replacing \( \mathcal{H}(z^*(u), z(u)) \) in the action \(\mathcal{H}_{0} \) with a trial Hamiltonian quadratic in the displacements from the average point, namely

\[ \mathcal{H}_0(z^*, z; \hat{z}^*, \hat{z}) = \xi^* E(z^*, \hat{z}) \xi + \frac{1}{2} [\xi F(z^*, \hat{z}) \xi + \text{c.c.}] + w(z^*, \hat{z}). \]

where \((\xi^*, \xi) = (z^* - \bar{z}, z - \bar{z})\) and \(E = \{E_{\mu\nu}\}, F = \{F_{\mu\nu}\}\), and \(w\) are parameters depending on \((\hat{z}^*, \hat{z})\) that are to be optimized. The evaluation of \( \hat{\rho}(\hat{z}^*, z; \hat{z}^*, \hat{z}) \) is done by diagonalisation of the quadratic term,

\[ \sum_{\mu\nu} \left[ \xi^*_\mu E_{\mu\nu} \xi_{\nu} + \frac{1}{2} (\xi^*_\mu F_{\mu\nu} \xi_{\nu} + \text{c.c.}) \right] = \sum_k \omega_k \xi^*_k \xi_k, \]

with a canonical transformation \((\xi^*, \xi) \to (\tilde{\xi}^*, \tilde{\xi})\) that, thanks to the use of path integral with Weyl symbols, preserves at the same time the functional measure and the form of the action.

The explicit result for \( \mathcal{P}_0 \) and \( \mathcal{H}_{\text{eff}} \) is:

\[ \mathcal{P}_0(z^*, z; \hat{z}^*, \hat{z}) = \prod_k \left( \frac{2}{L(f_k)} e^{-\frac{\tilde{\xi}^*_k \tilde{\xi}_k}{L(f_k)}} \right), \quad \mathcal{H}_{\text{eff}}(z^*, \hat{z}) = w(z^*, \hat{z}) + \frac{1}{\beta} \sum_k \ln \frac{\sinh f_k}{f_k}, \]

where \( f_k(\tilde{z}^*, \hat{z}) = \beta \omega_k(\tilde{z}^*, \hat{z})/2 \) and \( L(f_k) = \coth f_k - f_k^{-1} \) is the Langvin function. We will denote the \( \mathcal{P}_0 \)-averages by double brackets \( \langle \cdot \rangle \); of course \( \mathcal{P}_0 \) turns out to be a Gaussian centered in \((\hat{z}^*, \hat{z})\), so it is fully determined through its second moments \( \langle \tilde{\xi}^*_k \tilde{\xi}_{\kappa} \rangle = \delta_{kk'} \langle f_k \rangle /2, \langle \tilde{\xi}^*_k \tilde{\xi}_{\kappa} \rangle = \langle \tilde{\xi}^*_k \tilde{\xi}_{\kappa} \rangle = 0 \). The linear canonical transformation made can be used to express in a simple way the moments for the original variables, \((\xi^*_k, \xi_k)\).

In order to determine the parameters of \( \mathcal{H}_0 \) in a self-consistent way we require that the original and the trial Hamiltonian, and their second derivatives, have the same \( \mathcal{P}_0 \)-averages:

\[ \langle \mathcal{H}(z^* + \xi^*, \hat{z} + \xi) \rangle = \langle \mathcal{H}_0(z^* + \xi^*, \hat{z} + \xi; z^*, \hat{z}) \rangle = \sum_k \omega_k(z^*, \hat{z}) \frac{L(f_k(z^*, \hat{z}))}{2} + w(z^*, \hat{z}), \]

where \( \langle \cdot \rangle \) stands for the Gaussian average given by \( \mathcal{P}_0 \).

Finally we observe that a solution of the general problem for arbitrary values of \((\hat{z}^*, \hat{z})\) is rather difficult to determine for many degrees of freedom: a further simplification is in order. This is the low-coupling approximation \(\text{LCA}\) (LCA) and its main purpose is to make the averages \( \langle \cdot \rangle \) independent of the phase-space point \((\hat{z}^*, \hat{z})\), so that the above self-consistent equations are to be solved only once. The simplest way, consists in expanding the matrices \( E(z^*, \hat{z}), F(z^*, \hat{z}) \) around a self-consistent minimum of \( \mathcal{H}_{\text{eff}} \). The effective Hamiltonian and the expressions found for thermal averages are parallel to those shown in Ref. \[\text{[3]}\].

In perspective, one can think of translating this formalism to the fermionic case, getting “classical” expressions in terms of Grassman variables.

[1] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (Mc Graw Hill, New York, 1965).
[2] R. Giachetti and V. Tognetti, Phys. Rev. Lett. 55, 912 (1985).
[3] R. P. Feynman and H. Kleinert, Phys. Rev. A 34, 5080 (1986).
[4] A. Cuccoli et al., J. Phys.: Condens. Matter 7, 7891 (1995).
[5] A. Cuccoli, V. Tognetti, P. Verrucchi, and R. Vaia, Phys. Rev. A 45, 8418 (1992).
[6] F. A. Berezin, Sov. Phys. Usp. 23, 763 (1980).