Variational Approach to the Level Density of Many Body Systems

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Based on the functional integral approach the partition function $\mathcal{Z}(\beta)$ at finite temperature $T = 1/\beta$ of a many body system with separable two body interaction can be calculated in the sense of a semiclassical approximation. The widely used Perturbed Static Path Approximation (PSPA) [1] breaks down near a crossover temperature T_0 as soon as the classical mean field solution becomes unstable. Improvements beyond the PSPA for $T \approx T_0$ and $T \ll T_0$ are desirable in order to get reasonable approximations for many body systems in the low temperature range where usual Monte Carlo techniques become unfeasible. Note please that often the critical temperature T_c of phase transitions is of the same order of magnitude as the crossover temperature T_0.

In [2] a systematic improvement within the crossover region has been undertaken by accounting for large non-Gaussian fluctuations. Here, we report on a more recent development [3] that takes over ideas of a variational principle [4] – so far formulated for one dimensional systems only – to many body systems. Starting from the functional integral for the partition function a correction factor that accounts for quantum fluctuations $q_{r\neq 0}$ around the mean value $q_0 = \langle q(\tau)\rangle$ of an imaginary time path can be written in the form

$$\begin{aligned}\zeta(\beta, q_0) &= \int \mathcal{D}'q \, \exp\left[-S_E(\beta, q_0)/\hbar\right] \\ &= \zeta_\Omega^{q_0} \, \langle \exp\left[-(S_E - S_\Omega^{q_0})/\hbar\right]\rangle_\Omega^{q_0} \, . \qquad (1)\end{aligned}$$

Using the fourth order expansion of the Euklidian action [2] one gets

$$\begin{aligned}S_E(\beta, q_0) &= \sum_{r,s\neq 0} \lambda_{rs}(\beta, q_0)\, q_r q_s + \sum_{r,s,t\neq 0} \rho_{rst}(\beta, q_0)\, q_r q_s q_t \\ &+ \sum_{r,s,t,u\neq 0} \sigma_{rstu}(\beta, q_0)\, q_r q_s q_t q_u + \mathcal{O}(q_r^5) \qquad (2)\end{aligned}$$

with $\mathcal{D}'q$ being that functional integral measure where the q_0 integration is excluded. The coefficients λ, ρ and σ have been calculated in [2]. In the second line of (1) a local reference action $S_\Omega^{q_0}$ has been introduced that is chosen such that it can be treated exactly. Using the Jensen Peierls inequality we get the following condition for the average:

$$\langle \exp\left[-(S_E - S_\Omega^{q_0})/\hbar\right]\rangle_\Omega^{q_0} \geq \exp\left[-\langle S_E - S_\Omega^{q_0}\rangle_\Omega^{q_0}/\hbar\right] \qquad (3)$$

For the reference action $S_\Omega^{q_0}$ the form of PSPA is used, i.e. (2) truncated after the second order, but with the local RPA frequencies $\varpi_\mu(\beta, q_0)$ replaced by *adjustable parameters* $\Omega_\mu(\beta, q_0)$. The variational principle consists in varying the $\Omega_\mu(\beta, q_0)$ such that the right hand side of (3) becomes maximal.

Our general formulas have been tested at the exactly solvable Lipkin-Meshkov-Glick model (LMG).

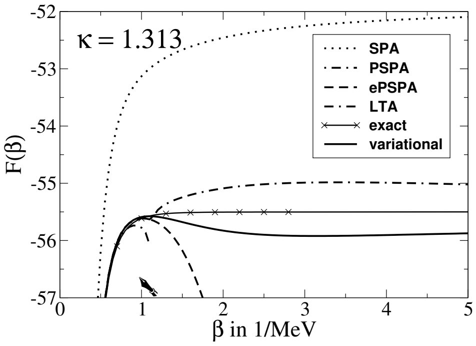

Fig. 1: Free energy of the LMG for coupling $\kappa = 1.313$ as a function of β. The phase transition where the barrier builds up occurs at $\beta_c = 0.4\,\mathrm{MeV}^{-1}$ and the inverse crossover temperature $\beta_0 = 1.1392\,\mathrm{MeV}^{-1}$ is marked by an arrow.

At the example of the free energy of the many body system one sees from Fig. 1 that using the variational principle the problem of the crossover temperature does not show up. The combination $(2\pi/\hbar\beta)^2 + \Omega^2(\beta, q_0)$ is *always positive*. Compared to the PSPA and the "extended PSPA" (ePSPA) of [2], which become extremely bad in the region of $\beta \lesssim \beta_0$ and $\beta \lesssim 2\beta_0$ respectively, the variational free energy is completely regular. Even at very low temperatures, viz large β it provides a reasonable approximation to the exact free energy. The only deficiency is that due to the neglect of fluctuations higher than fourth order in q_r the physical property of thermal stability is slightly violated for $\beta > 1.5\,\mathrm{MeV}^{-1} > \beta_0$.

The development of approximations like the SPA and its improvements [1] was motivated by the need for calculating nuclear level densities as a function of the excitation energy $\mathcal{E}^*$. Given the partition function this can be achieved by an inverse Laplace transform. Within a saddle point approximation (Darwin-Fowler method) one finds the behaviour for the level density of the LMG shown in Fig. 2:

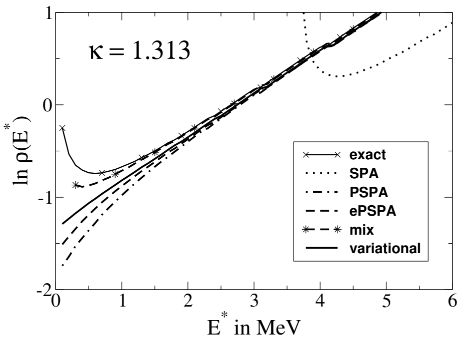

Fig. 2: Level density of the LMG for coupling $\kappa = 1.313$ as a function of the excitation energy $\mathcal{E}^*$.

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