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The partition function of an interacting many body system

Beyond the perturbed static path approximation (PSPA)

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Abstract. Based on the path integral approach the partition function of a many body system with separable two body interaction is calculated in the sense of a semiclassical approximation. The commonly used Gaussian type of approximation, known as the perturbed static path approximation (PSPA), breaks down near a crossover temperature due to instabilities of the classical mean field solution. It is shown how the PSPA is systematically improved within the crossover region by taking into account large non-Gaussian fluctuations and an approximation applicable down to very low temperatures is carried out. These findings are tested against exact results for the archetypical cases of a particle moving in a one dimensional double well and the exactly solvable Lipkin-Meshkov-Glick model. The extensions should have applications in finite systems at low temperatures as in nuclear physics and mesoscopic systems, *e.g.* for gap fluctuations in nanoscale superconducting devices previously studied within a PSPA type of approximation.

PACS. 05.30.-d Quantum statistical mechanics – 24.60.-k Statistical theory and fluctuations – 74.25.Bt Thermodynamic properties – 21.10.Ma Level density

1 Introduction

Thermodynamic properties of interacting many body systems are of fundamental interest for all kinds of condensed matter. A particular challenge has been the temperature range where strong quantum effects render simple mean field theories insufficient. For finite systems with separable two-body interaction much can be gained by relying on approximate techniques to evaluate the partition function. Typical examples include certain mesoscopic systems, *e.g.* ultrasmall superconducting metallic grains [1] on which substantial research has focused recently.

A very elegant approach to approximate the partition function is provided by the path integral formalism. There, the usual trick [2,3] is to turn the two-body interaction *via* a Hubbard-Stratonovich transformation into terms containing only one-body operators and an auxiliary field. While the static part of this field determines the static mean field result, many body quantum fluctuations are encoded in its dynamical part. The latter one can systematically be accounted for in the sense of a semiclassical approximation. Accordingly, a static approximation has been developed originally in order to study finite size effects in small superconductors [4]. The static path approximation (SPA) has also been used in nuclear physics to calculate thermodynamic properties and level densities of hot nuclei [5]. Later it has been extended by the SPA+RPA [6], the perturbed static path approximation (PSPA, the name which we take over in the following) [7], or the correlated static path approximation (CSPA) [8,9]. These approaches account for small Gaussian fluctuations around the classical mean field and are thus applicable in a temperature range where quantum effects are no longer negligible. This way, from the approximate partition function a variety of thermodynamic quantities have been calculated in the literature: the free and internal energy, the specific heat and the level density of the system [6,7,10,11]. In addition thermal expection values of observables [7] and strength functions [7,9] have been deduced. While many of these calculations have been carried out in exactly solvable models [6–9] also reasonable agreement with experimental data was shown for the level density of finite nuclei [10,11]. Further, the formalism has been put forward in [11] to take into account the coupling to the continuum and in [12] an extension of the PSPA to describe dissipative decay out of metastable states has been developed in a self-consistent fashion. Very recently, the improvements of the SPA have been applied to small strongly correlated condensed matter systems. For example, using the CSPA odd-even effects in small superfluid systems [14] and motivated by new experiments on ultrasmall superconducting metallic grains [1] gap fluctuations and pairing effects in finite size superconductors have been examined [15].

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As noted above, these conventional improvements of the SPA take into account quantum effects on the RPA level only, *i.e.* Gaussian fluctuations, and thus, are plagued by the problem that they break down at a certain temperature T_0. Physically, at this temperature the classical mean field solution becomes unstable in functional space and large fluctuations render the Gaussian approximation insufficient. This has some features in common [13,12] with the change of stability at a crossover temperature occuring in the description of dissipative decay *e.g.* in Josephson junctions [16] but is different in detail. By thoroughly analysing the appearence of instabilities for the many body problem at lower temperatures, we go beyond the PSPA to achieve a smooth behavior around T_0. For temperatures sufficiently below T_0 the partition function is dominated by field configurations away from the classical mean field around which a Gaussian approximation is again valid. In this paper we lay out the general theory and discuss its validity in comparison to exactly solvable models before it can be applied to realistic systems.

We start with a brief outline of the main results of the conventional PSPA and introduce the notation used in the sequel (Sect. 2). The extension of the PSPA around the critical temperature T_0 is developed in Section 2.2 which in Section 2.3 allows for a treatment of the temperature range far below T_0. In Section 3 our results are first applied to a one-dimensional double well, before in Section 4 we turn to the thermodynamic properties of the Lipkin-Meshkov-Glick model [17].

2 Partition function of an interacting many body system

In this paper we want to approximate the partition function of a system described by a Hamiltonian of the following structure

$$\hat{\mathcal{H}} = \hat{H} + \frac{k}{2}\,\hat{F}\hat{F}\ . \tag{1}$$

Here $\hat{H}$ and $\hat{F}$ are hermitian one body operators and the product $\hat{F}\hat{F}$ mimics an effective separable two body interaction. In the sequel, for the general analysis we always assume $[\hat{H},\hat{F}] \neq 0$, the simplification to the case of commuting operators is straightforward. Further, the coupling constant $k = -|k|$ is taken to be negative (attractive interaction) [18] according *e.g.* to isoscalar modes. The effect of repulsive interaction has been studied in [19]. The ansatz (1) defines a minimal microscopic model for a system with one collective degree of freedom [18]. An extension of the methods proposed in this paper to systems with more (independent) collective degrees of freedom is then feasible, though it may be tedious in detail.

The partition function of the grand canonical ensemble reads

$$\mathcal{Z}(\beta) = \mathrm{Tr}\,\exp\left(-\beta(\hat{\mathcal{H}} - \mu\hat{A})\right) = \mathrm{Tr}\,\hat{U}\ , \tag{2}$$

where $\beta = 1/T$ is the inverse temperature (in units with $k_\mathrm{B} \equiv 1$) and the chemical potential μ keeps the particle number $\langle\hat{A}\rangle$ fixed on average. In principle, one should work with truly fixed particle numbers, *i.e.* within the canonical ensemble. However, as we are mainly interested in the dependence of system properties on excitation energy or temperature, it is more convenient to exploit (2). A very elegant way to do this is to represent $\mathcal{Z}(\beta)$ as a functional integral in imaginary time [2], which also allows to systematically include fluctuations around the mean field. Given the form of the Hamiltonian in (1) the mean field approximation starts with a Hubbard-Stratonovich transformation [20] of the imaginary time path integral corresponding to (2). Accordingly, the product $\hat{F}\hat{F}$ is split by introducing an auxiliary path $q(\tau)$ as a collective variable. Since this procedure is well-known (see *e.g.* [7,2,3]) we simply state here the basic results which will then serve as the starting point for our analysis[1].

After introducing the Fourier expansion

$$q(\tau) = q_0 + \sum_{r\neq 0} q_r\,\exp(\mathrm{i}\nu_r\tau)\ , \qquad q_{-r} = q_r^*\ , \tag{3}$$

with the Matsubara frequencies

$$\nu_r = \frac{2\pi}{\hbar\beta}\,r \equiv \frac{2\pi}{\hbar}\,rT\ \ , \qquad r = \pm 1,\ \pm 2,\ \pm 3\ \ldots, \tag{4}$$

the partition function may be written in a form containing a static, *i.e.* q_0 dependent, part and a dynamical factor, namely,

$$\mathcal{Z}(\beta) = \sqrt{\frac{\beta}{2\pi|k|}}\int_{-\infty}^{+\infty}\mathrm{d}q_0\ \exp[-\beta\mathcal{F}^{\mathrm{SPA}}(\beta,q_0)]\ C(\beta,q_0). \tag{5}$$

Here

$$\mathcal{F}^{\mathrm{SPA}}(\beta,q_0) = \frac{1}{2|k|}\,q_0^2 - \frac{1}{\beta}\ln z(\beta,q_0) \tag{6}$$

plays the role of an effective static free energy. It is not the free energy $\mathcal{F}(\beta) = -T\ln\mathcal{Z}(\beta)$ of the total self-bound system, but the one of the constituents moving in a mean field that is kept fixed at the static collective variable q_0. For this reason we call $\mathcal{F}^{\mathrm{SPA}}(\beta,q_0)$ the "intrinsic free energy" from now on, where the index "SPA" already refers to the simplest "static path approximation" to (5) (see Sect. 2.1). In (6) there appears the grand canonical partition function

$$\begin{aligned} z(\beta,q_0) &= \mathrm{Tr}\,\exp\left(-\beta(\hat{h}_0(q_0) - \mu\hat{A})\right) \\ &= \prod_l\left(1+\exp\left(-\beta(\epsilon_l(q_0)-\mu)\right)\right) \end{aligned} \tag{7}$$

[1] We note that our notation has been adapted to the one used in [21,12] and relates to that of [7] in the following way: $\hat{H}_0 \leftrightarrow K$, $\hat{F} \leftrightarrow V$, $k<0 \leftrightarrow -\chi<0$, $q \leftrightarrow \chi\sigma$, $z \leftrightarrow \zeta_0$, $\mathcal{C} \leftrightarrow \zeta_0'$, $\hbar \leftrightarrow 1$.

belonging to the static part of the Hamiltonian (1) in mean field approximation

$$\hat{h}_0(q_0) = \hat{H} + q_0\,\hat{F}. \tag{8}$$

Obviously, $\hat{h}_0(q_0)$ is a sum of only one body operators with eigenenergies $\epsilon_l(q_0)$.

All contributions from the dynamical part of the auxiliary path $q(\tau)$ are contained in the factor $C(\beta, q_0)$ which can be formally written as [7]

$$C(\beta, q_0) = \int \mathcal{D}'q\ \exp\left(-\frac{\beta}{|k|}\sum_{r>0}|q_r|^2 + \ln\langle\hat{\mathcal{U}}_q\rangle_{q_0}\right) \tag{9}$$

with the measure

$$\mathcal{D}'q = \lim_{\substack{N\to\infty \\ N\varepsilon=\hbar\beta}} \prod_{r=1}^{(N-1)/2} \frac{\beta}{\pi|k|}\,\mathrm{dRe}(q_r)\,\mathrm{dIm}(q_r)\ . \tag{10}$$

Here, the thermal expectation value of the evolution operator $\hat{\mathcal{U}}_q$ has to be evaluated with respect to the static one-body Hamiltonian (8) and reads in terms of a time-ordered product

$$\langle\hat{\mathcal{U}}_q\rangle_{q_0} = \left\langle \hat{\mathcal{T}}\exp\left(-\frac{1}{\hbar}\int_0^{\hbar\beta}\mathrm{d}\tau\,\hat{h}_1(\tau, q_r)\right)\right\rangle_{q_0}\ . \tag{11}$$

The "dynamical" Hamiltonian

$$\hat{h}_1(\tau, q_r) = \hat{F}(\tau)\,\delta q(\tau) \tag{12}$$

with $\delta q(\tau) = q(\tau) - q_0$ may be understood as the time dependent correction to the static mean field Hamiltonian $\hat{h}_0(q_0)$ given in (8). Hence, it is convenient to work in an interaction picture based on $\hat{h}_0(q_0)$ and define time dependent operators as, *e.g.*

$$\hat{F}(\tau) = \mathrm{e}^{\hat{h}_0(q_0)\tau/\hbar}\ \hat{F}\ \mathrm{e}^{-\hat{h}_0(q_0)\tau/\hbar}\ . \tag{13}$$

The partition function (5) together with (6) and (9) is still exact, however, written in a way which allows for a systematic approximative evaluation. Namely, all quantum fluctuations, *i.e.* modes with Matsubara frequencies $\nu_r \neq 0$, are hidden in $\langle\hat{\mathcal{U}}_q\rangle_{q_0}$. Thus, the basic idea is to successively account for dynamical information in $\mathcal{Z}(\beta)$ by expanding the thermal expectation value $\langle\hat{\mathcal{U}}_q\rangle_{q_0}$ around its static value in terms of the deviations $\delta q(\tau)$. This way, generalizing equation (27) of [7] to fourth order in the q_r one finds:

$$\begin{aligned}
&\ln\langle\hat{\mathcal{U}}_q\rangle_{q_0}^{\mathrm{ePSPA}} \\
&= \frac{1}{2!\,\hbar^2}\sum\!\!\int\ q_r q_s\ \mathrm{e}^{\mathrm{i}\nu_r\tau_r}\mathrm{e}^{\mathrm{i}\nu_s\tau_s}\ \langle\hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\rangle_{q_0} \\
&+\frac{1}{3!\,\hbar^3}\sum\!\!\int\ q_r q_s q_t\ \mathrm{e}^{\mathrm{i}\nu_r\tau_r}\mathrm{e}^{\mathrm{i}\nu_s\tau_s}\mathrm{e}^{\mathrm{i}\nu_t\tau_t} \\
&\times\langle\hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\hat{F}(\tau_t)\rangle_{q_0} \\
&+\frac{1}{4!\,\hbar^4}\sum\!\!\int\ q_r q_s q_t q_u\ \mathrm{e}^{\mathrm{i}\nu_r\tau_r}\mathrm{e}^{\mathrm{i}\nu_s\tau_s}\mathrm{e}^{\mathrm{i}\nu_t\tau_t}\mathrm{e}^{\mathrm{i}\nu_u\tau_u} \\
&\times\langle\hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\hat{F}(\tau_t)\hat{F}(\tau_u)\rangle_{q_0} \\
&-\frac{1}{8\,\hbar^4}\sum\!\!\int\ q_r q_s q_t q_u\ \mathrm{e}^{\mathrm{i}\nu_r\tau_r}\mathrm{e}^{\mathrm{i}\nu_s\tau_s}\mathrm{e}^{\mathrm{i}\nu_t\tau_t}\mathrm{e}^{\mathrm{i}\nu_u\tau_u} \\
&\times\langle\hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\rangle_{q_0}\langle\hat{\mathcal{T}}\hat{F}(\tau_t)\hat{F}(\tau_u)\rangle_{q_0} \\
&+\mathcal{O}(q_r^5).
\end{aligned} \tag{14}$$

The symbol $\sum\!\!\int$ abbreviates summation over all involved r, s, $\ldots \neq 0$ and integration of all involved τ_r, τ_s, $\ldots$ from 0 to $\hbar\beta$. Because of the τ-integrations and the fact that $\langle\hat{F}(\tau)\rangle_{q_0}$ is τ-independent all terms involving such a factor – for instance terms linear in q_r – vanish immediately and are therefore omitted in (14).

2.1 Conventional PSPA – Expansion to second order

The simplest approximation to $\mathcal{Z}(\beta)$, coined the static path approximation (SPA), neglects all dynamical contributions, *i.e.* one puts $\hat{h}_1(\tau, q_r) \equiv 0$. As a result $\mathcal{C}^{\mathrm{SPA}}(\beta, q_0) \equiv 1$. The SPA is the classical limit where all many body quantum fluctuations are absent. For lower temperatures when quantum properties tend to become important, fluctuations around the classical limit can be incorporated within the conventional version of the perturbed static path approximation (PSPA). There, the expansion (14) is truncated after the second order terms in the q_r [6–12,14,15], which effectively means to describe quantum effects on the RPA level. Within the PSPA the dynamical factor $C(\beta, q_0)$ is approximated by [12]

$$C^{\mathrm{PSPA}}(\beta, q_0) = \int \mathcal{D}'q\ \exp\left(-\frac{\beta}{|k|}\sum_{r>0}\left(1 + k\chi(q_0, \mathrm{i}\nu_r)\right) q_r q_{-r}\right). \tag{15}$$

Here, the FF-response function $\chi(q_0, \omega)$ defined by

$$\delta\langle\hat{F}\rangle_{q_0}(\omega) = -\chi(q_0, \omega)\ \delta q(\omega) \tag{16}$$

has to be evaluated at the Matsubara frequencies $\mathrm{i}\nu_r$ along the imaginary axis. Because of $q_{-r} = q_r^*$ all integrals in (15) are of Gaussian type, and cause no problem as long as

$$\lambda_r(\beta, q_0) \equiv 1 + k\chi(q_0, \mathrm{i}\nu_r) > 0 \quad \text{for all} \quad r > 0\ . \tag{17}$$

For systems with q_0-regions where the local RPA frequencies $\omega_\nu(\beta, q_0)$ obtained by the condition $1 + k\chi(q_0, \omega_\nu) = 0$

are purely imaginary equation (17) defines a condition for that temperature below which the conventional version of the PSPA breaks down due to a vanishing $\lambda_1(\beta, q_0)$. This breakdown temperature T_0 where $\lambda_1(1/T_0, q_0) = 0$ for the first time is known from the theory of dissipative tunneling [22] as the "crossover temperature" (for many body systems see [12])

$$T_0 = \max_{q_0} \frac{\hbar\,|\omega_\nu^{\rm inst}(q_0)|}{2\pi} \tag{18}$$

with $\omega_\nu^{\rm inst}(q_0)$ as imaginary local RPA frequencies. Now, the condition (17) is guaranteed for all $T > T_0$ and we obtain for the partition function within conventional PSPA [7,12] the integral (5) with the dynamical factor $C(\beta, q_0)$ providing improvement over pure SPA taken as

$$C^{\rm PSPA}(\beta, q_0) = \prod_{r>0} \frac{1}{\lambda_r(\beta, q_0)}\,. \tag{19}$$

2.2 Extended PSPA – Expansion to fourth order

The instabilities that lead to the breakdown of the conventional PSPA at T_0 are due to the fact that all fluctuations q_r are treated only up to second order. Since the Gaussians in q_r have a typical width (see (15))

$$\Delta_r = \sqrt{\frac{|k|}{2\beta\lambda_r(\beta, q_0)}} = \sqrt{\frac{|k|T}{2\lambda_r(\beta, q_0)}}\quad, \tag{20}$$

first Δ_1 grows as temperature approaches T_0 from above, *i.e.* $\lambda_1(\beta, q_0) \to 0$. Correspondingly, fluctuations in q_1-direction increase which in turn renders the Gaussian approximation for the q_1-mode insufficient. In contrast, the other amplitudes q_2, q_3, ... remain still sufficiently small for a harmonic approximation to be valid. Therefore in the expansion (14) terms higher than second order must be taken into account *only* for the q_1 and q_{-1} mode. This is very similar to the procedure used in the framework of dissipative tunneling in order to overcome the irregularity of the decay rate at T_0 [22]. Working along these lines a consistent approximation to the partition function (5) is obtained for temperatures near T_0 by taking for $C(\beta, q_0)$

$$C^{\rm ePSPA}(\beta, q_0) = \int \mathcal{D}'q\ \exp\left(-\frac{\beta}{|k|}\,A(\beta, q_0, q_r)\right). \tag{21}$$

The relevant effective multidimensional fluctuation potential turns out to be

$$\begin{aligned} A(\beta, q_0, q_r) = &\sum_{r>0} \lambda_r(\beta, q_0)\, q_r q_{-r} + 3c_3^+(\beta, q_0)\, q_1^2 q_{-2} \\ &+ 3c_3^-(\beta, q_0)\, q_{-1}^2 q_2 + 6c_4(\beta, q_0)\, q_1^2 q_{-1}^2. \end{aligned} \tag{22}$$

Here, other terms *e.g.* of the type $q_1 q_s q_{-s-1}$ or $q_1 q_{-1} q_s q_{-s}$ ($s > 1$) are negligible in the sense of a semiclassical approximation as they contribute only in lower order [22].

The relevant coefficients containing third and fourth order $\hat{F}$ correlations read:

$$c_3^+(\beta, q_0) = \tag{23}$$
$$\frac{-|k|/\beta}{3!\,\hbar^3} \int \mathrm{e}^{\mathrm{i}\nu_{+1}\tau_r} \mathrm{e}^{\mathrm{i}\nu_{+1}\tau_s} \mathrm{e}^{\mathrm{i}\nu_{-2}\tau_t}\ \langle \hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\hat{F}(\tau_t)\rangle_{q_0}$$
$$c_3^-(\beta, q_0) = \tag{24}$$
$$\frac{-|k|/\beta}{3!\,\hbar^3} \int \mathrm{e}^{\mathrm{i}\nu_{-1}\tau_r} \mathrm{e}^{\mathrm{i}\nu_{-1}\tau_s} \mathrm{e}^{\mathrm{i}\nu_{+2}\tau_t}\ \langle \hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\hat{F}(\tau_t)\rangle_{q_0}$$
$$\begin{aligned} c_4(\beta, q_0) = &\frac{-|k|/\beta}{4!\,\hbar^4} \int \mathrm{e}^{\mathrm{i}\nu_{+1}\tau_r} \mathrm{e}^{\mathrm{i}\nu_{+1}\tau_s} \mathrm{e}^{\mathrm{i}\nu_{-1}\tau_t} \mathrm{e}^{\mathrm{i}\nu_{-1}\tau_u} \\ &\times \Big(\langle \hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\hat{F}(\tau_t)\hat{F}(\tau_u)\rangle_{q_0} \\ &- 3\langle \hat{\mathcal{T}}\hat{F}(\tau_r)\hat{F}(\tau_s)\rangle_{q_0} \langle \hat{\mathcal{T}}\hat{F}(\tau_t)\hat{F}(\tau_u)\rangle_{q_0} \Big)\,. \end{aligned} \tag{25}$$

The integrals symbolize integrations over all involved τ from 0 to $\hbar\beta$. Mind that only Matsubara frequencies with indices $r, s, t, u = \pm 1, \pm 2$ enter these formulas. The explicit evaluation of these coefficients is a crucial step in order to apply the ePSPA to many body systems as we will demonstrate in detail in Section 4.1. In particular, we will prove in Section 4.1 (see (46)) that the τ integrations of (14) imply the sum rule $r+s+t+\ldots = 0$ for the indices involved which considerably simplifies the calculation.

Let us now turn to the q_r integrals in (21). Integrals with $|r| > 1$ are still of Gaussian type and can easily be carried out as long as $\lambda_2(\beta, q_0) > 0$ is sufficiently large. While all integrations for $|r| > 2$ just provide factors $1/\lambda_r$ like in conventional PSPA, the integrals over q_2 and $q_{-2} = q_2^*$ require special care. To this end the variables q_2 and q_{-2} are transformed to variables $q_2' = \mathrm{Re}\, q_2$ and $q_2'' = \mathrm{Im}\, q_2$ which cast the relevant part of (22) in the form

$$\begin{aligned} a(\beta, q_0, q_2', q_2'') = &\lambda_2(\beta, q_0)\,(q_2')^2 \\ &+3\left(c_3^-(\beta, q_0)\, q_{-1}^2 + c_3^+(\beta, q_0)\, q_1^2\right)\ q_2' \\ &+\lambda_2(\beta, q_0)\,(q_2'')^2 \\ &+3\mathrm{i}\left(c_3^-(\beta, q_0)\, q_{-1}^2 - c_3^+(\beta, q_0)\, q_1^2\right)\ q_2''. \end{aligned} \tag{26}$$

The corresponding two Gaussian integrals can be easily solved:

$$\begin{aligned} &\frac{\beta}{\pi|k|} \int \mathrm{d}q_2' \mathrm{d}q_2''\ \exp\left(-\frac{\beta}{|k|}\ a(\beta, q_0, q_2', q_2'')\right) \\ &\qquad = \frac{1}{\lambda_2(\beta, q_0)}\ \exp\left(\frac{\beta}{|k|}\ \frac{9c_3^-(\beta, q_0)c_3^+(\beta, q_0)}{\lambda_2(\beta, q_0)}\ q_1^2 q_{-1}^2\right). \end{aligned} \tag{27}$$

What is left are the q_1-integrals. These are integrals over an exponential with an exponent given by

$$\lambda_1(\beta, q_0)\, q_1 q_{-1} + B(\beta, q_0)\, q_1^2 q_{-1}^2\ , \tag{28}$$

where the coefficient $B(\beta, q_0)$ is defined as

$$B(\beta, q_0) = 6c_4(\beta, q_0) - \frac{9c_3^-(\beta, q_0)c_3^+(\beta, q_0)}{\lambda_2(\beta, q_0)}\,. \tag{29}$$

To proceed further it is convenient to introduce polar coordinates ρ and ϕ instead of q_1 and $q_{-1} = q_1^*$, such that the phase integral can be done. After an additional substitution $z = \rho^2$ the q_1 integrals reduce to

$$\frac{\beta}{\pi|k|}\int_0^{2\pi}\mathrm{d}\phi\int_0^{\infty}\mathrm{d}\rho\ \rho\ \exp\left(-\frac{\beta}{|k|}\left(\lambda_1\,\rho^2+B\,\rho^4\right)\right)$$
$$=\frac{\beta}{|k|}\int_0^{\infty}\mathrm{d}z\ \exp\left(-\frac{\beta}{|k|}\left(\lambda_1(\beta,q_0)\,z+B(\beta,q_0)\,z^2\right)\right). \tag{30}$$

Eventually, together with the contributions from (27) and (30) the expression (21) for the new dynamical factor reads in "extended PSPA"

$$C^{\mathrm{ePSPA}}(\beta,q_0)=\prod_{r>1}\frac{1}{\lambda_r(\beta,q_0)}$$
$$\times\frac{\beta}{|k|}\int_0^{\infty}\mathrm{d}z\,\exp\left(-\frac{\beta}{|k|}\left(\lambda_1(\beta,q_0)z+B(\beta,q_0)z^2\right)\right). \tag{31}$$

In case that q_1 fluctuations are small so that third and fourth order terms in q_1 and q_{-1} are negligible – $B(\beta,q_0)\ll\lambda_1(\beta,q_0)$ – the factor $C^{\mathrm{ePSPA}}(\beta,q_0)$ reduces to $C^{\mathrm{PSPA}}(\beta,q_0)$ (see (19)). For temperatures $T<T_0$ and q_0 for which $\lambda_1<0$ but $|\lambda_1|$ again sufficiently large, the integral in (31) can be evaluated in stationary phase approximation. The result is

$$C^{\mathrm{ePSPA}}(\beta,q_0)=\prod_{r>1}\frac{1}{\lambda_r(\beta,q_0)}$$
$$\times\sqrt{\frac{2\pi\beta}{|k|\,B(\beta,q_0)}}\ \exp\left(\frac{\beta}{|k|}\frac{\lambda_1^2(\beta,q_0)}{4B(\beta,q_0)}\right). \tag{32}$$

Here, the exponential reveals the change of stability at $T=T_0$ as now the contribution to $\mathcal{Z}(\beta)$ of those q_0 where $\lambda_1<0$ is enhanced compared to their static value $\exp[-\beta\mathcal{F}^{\mathrm{SPA}}(\beta,q_0)]$.

The ePSPA smoothly connects the temperature range above T_0 with that below T_0. Its precise lower bound of validity is determined by two conditions: $B(\beta,q_0)$ defined in (29) and $\lambda_2(\beta,q_0)$ (see (17)) must both be positive and sufficiently large *for all* q_0. Even if $B>0$ also for $T<T_0$ the ePSPA definitely fails at $T=T_0/2$ where λ_2 vanishes. Physically, the instability of the PSPA at $T=T_0$ corresponds to an instability in q_1 direction in functional space of that classical mean field solution $q_0=q_0^c$ for which $\lambda_1(1/T_0,q_0^c)=0$. At the temperature where the ePSPA breaks down, *i.e.* where $\lambda_2=0$, the classical field at q_0^c becomes unstable in q_2 direction in functional space. This scenario proceeds with decreasing temperature.

2.3 Treatment of low temperatures $T \ll T_0$

In the last section we have proposed an extension of the conventional PSPA that is applicable down to temperatures not too far below T_0. As already mentioned, this approximation breaks down near $\lambda_2=0$ where the q_2-mode amplitude becomes large. Naively, one could think to "regularize" the q_2-mode divergency in the same way as for the q_1-mode around T_0. However, if both q_1 *and* q_2 are large even higher order coupling terms to q_r modes ($|r|>2$) in the expansion must be taken into account (compare our remark after Eq. (22)). This proceeds to the divergencies at $\lambda_3=0$ and so on. Hence, practically an analytical treatment analogous to the T_0 case is no longer possible for temperatures $T\ll T_0$. In particular, for $T\to 0$ *all* modes q_r must be assumed to be large so that in the worst case any kind of semiclassical approximation to $\mathcal{Z}(\beta)$ fails.

On the other hand, for $T\ll T_0$, but still $T>0$, we expect that integrals of the type (5) are dominated by the contributions around the minima $q_{0,i}^{min}, i=1,\ldots,M$ of the intrinsic free energy (6) provided $\beta\mathcal{F}^{\mathrm{SPA}}(\beta,q_0^c)$ exceeds $\beta\mathcal{F}^{\mathrm{SPA}}(\beta,q_{0,i}^{min})$ by terms sufficiently larger than of order 1. Under the additional condition that the correction factor $C^{\mathrm{ePSPA}}(\beta,q_0)$ is a smooth function of q_0 compared to the exponential we can apply a saddle point approximation to evaluate (5) together with (31):

$$\mathcal{Z}^{\mathrm{ePSPA}}(\beta)\approx\sum_{i=1}^{M}\frac{1}{\sqrt{|k|\,d^2\mathcal{F}^{\mathrm{SPA}}/dq_0^2|_{q_{0,i}^{\min}}}} \tag{33}$$
$$\times\exp\left[-\beta\mathcal{F}^{\mathrm{SPA}}(\beta,q_{0,i}^{\min})\right]\ C^{\mathrm{ePSPA}}(\beta,q_{0,i}^{\min}).$$

The *assumption* that $C^{\mathrm{ePSPA}}(\beta,q_0)$ is smooth compared to $\exp[-\beta\mathcal{F}^{\mathrm{SPA}}(\beta,q_0)]$ – variations of the dynamical factor are negligible on the scale on which the exponential varies – bases on the fact that all approximations of SPA type are semiclassical approximations. This condition is certainly not fulfilled in regions where the dynamical factor diverges. The divergencies, occuring whenever $\lambda_r(\beta,q_0)=0$ ($r>1$) only appear in those q_0-regions where the RPA frequencies are imaginary and of sufficiently large amount, thus, corresponding to saddle points of the full free energy. Therefore we may assume that they need not be considered for low temperatures (but still sufficiently above $T=0$). Accordingly, the following interpolation between the ePSPA and the saddle point approximation (33) seems to be natural: For $T\ll T_0$ we restrict the q_0 integration in (5) with (31) to those regions where $\lambda_1>0$ meaning that *all* $\lambda_r>0$, *i.e.*,

$$C^{\mathrm{LTA}}(\beta,q_0)=\theta[\lambda_1(\beta,q_0)]\ C^{\mathrm{ePSPA}}(\beta,q_0) \tag{34}$$

where $\theta(\cdot)$ denotes the step function. This interpolation is called "low temperature approximation" (LTA) henceforth. It requires to solve $\lambda_1(\beta,q_0^c)=0$ for given $\beta>\beta_0=1/T_0$ to determine $q_0^c(\beta)$. As a continuous function of β starting at $q_0^c(\beta_0)$, $q_0^c(\beta)$ describes the broadening of the instability region around $q_0^c(\beta_0)$ where $\lambda_1<0$ [23]. The ePSPA extends to temperatures somewhat below T_0, while the LTA is valid if with decreasing temperature $T<T_0$ the contribution of the instability region around $q_0^c(\beta_0)$ to the q_0 integral becomes negligible. Therefore both approximations match in a narrow temperature range below T_0. Further, by formally extending the LTA to $T>T_0$ one

recovers the ePSPA since then $\lambda_1 > 0$ for all q_0, while for $T \ll T_0$ the saddle point result (33) is regained. As already mentioned, in general there is a lower bound for the LTA. Contributions of mean fields around q_0^c can only be neglected as long as the exponential enhancement in (32) due to the dynamical instability is still compensated for by the difference between $\mathcal{F}^{\rm SPA}(\beta, q_0^c)$ and $\mathcal{F}^{\rm SPA}(\beta, q_{0,i}^{min})$. For very low temperatures this can no longer be taken for granted.

We want to remark that for specific systems further approximations may exist in the region $T \ll T_0$, possibly better adapted to the problem in question. This may be particularly true for very low temperatures $T \to 0$ if new phenomena, sometimes associated with the appearance of new symmetries like in the case of Goldstone modes, require special care (*cf.* the cases of a one-dimensional double well and the Lipkin-Meshkov-Glick model below in Sects. 3 and 4). As long as one is interested in approximation schemes applicable to general situations without referring to individual system properties, however, the LTA presented above seems to us the only consistent one.

3 Application I: One dimensional potential

In order to illustrate the utility of the the above approximations we turn to exactly solvable models and first apply the formalism to the one-dimensional case.

Consider a particle of mass M in a one dimensional potential $V(q)$. The imaginary time path integral representation is given by

$$\mathcal{Z}(\beta) = \int \mathrm{d}q' \oint_{q'} \mathcal{D}q(\tau)\ \exp\left(-S^{\rm E}[q(\tau), \dot{q}(\tau)]/\hbar\right) \quad (35)$$

with the Euclidean action

$$S^{\rm E}[q(\tau), \dot{q}(\tau)] = \int_0^{\hbar\beta} \mathrm{d}\tau \left(\frac{M}{2}\,\dot{q}^2(\tau) + V(q(\tau))\right). \quad (36)$$

In (35) we first have to sum over all paths $q(\tau)$ starting and ending at a given end-point $q(0) = q(\hbar\beta) = q'$ and second sum up contributions from all these end-points q'.

In order to be able to apply the ideas of Section 2.2, the potential must be expanded up to fourth order in the Fourier coefficients q_r ($|r| > 0$) introduced in (3). After carrying out the τ integration we obtain for the exponent:

$$\begin{aligned} -S^{\rm E}[q_r]/\hbar = &-\beta V(q_0) - \beta \sum_{r>0} \left(M\nu_r^2 + V''(q_0)\right) |q_r|^2 \\ &- \frac{\beta V^{(3)}(q_0)}{3!} \sum_{r,s,t\neq 0} \delta_{r+s+t,0}\ q_r q_s q_t \\ &- \frac{\beta V^{(4)}(q_0)}{4!} \sum_{r,s,t,u\neq 0} \delta_{r+s+t+u,0}\ q_r q_s q_t q_u\,. \end{aligned} \quad (37)$$

For the case of one dimensional potentials the sum rule $r+s+t+u = 0$ simply stems from this τ integration. Here $V(q_0)$ plays the same role as $\mathcal{F}^{\rm SPA}(\beta, q_0)$ in (5). As before the coefficients q_1 and q_{-1} become large at the crossover temperature

$$T_0 = \max_{q_0}\ \frac{\hbar}{2\pi}\sqrt{\frac{-V''(q_0)}{M}} \quad (38)$$

and therefore have to be taken into account up to fourth order. Then, with $\lambda_r(\beta, q_0) \equiv M\nu_r^2 + V''(q_0)$, $c_3^+(\beta, q_0) = c_3^-(\beta, q_0) \equiv V^{(3)}(q_0)/3!$, and $c_4(\beta, q_0) \equiv V^{(4)}(q_0)/4!$ we gain

$$\mathcal{Z}(\beta) = \sqrt{\frac{M}{2\pi\hbar^2\beta}} \int \mathrm{d}q_0\ \exp\left[-\beta V(q_0)\right]\ C(\beta, q_0). \quad (39)$$

In case of the pure SPA we have $C^{\rm SPA}(\beta, q_0) \equiv 1$, in case of the conventional PSPA

$$C^{\rm PSPA}(\beta, q_0) = \prod_{r>0} \frac{M\nu_r^2}{M\nu_r^2 + V''(q_0)}\,, \quad (40)$$

and for the extended PSPA

$$\begin{aligned} C^{\rm ePSPA}(\beta, q_0) = &\prod_{r>1} \frac{M\nu_r^2}{M\nu_r^2 + V''(q_0)} \\ &\times \int_0^\infty \mathrm{d}z\ \exp\left\{ -\beta\left[\left(M\nu_1^2 + V''(q_0)\right) z \right.\right. \\ &\left.\left. + \frac{1}{4}\left(V^{(4)}(q_0) - \frac{(V^{(3)}(q_0))^2}{M\nu_2^2 + V''(q_0)}\right) z^2 \right] \right\}. \end{aligned} \quad (41)$$

Let us now turn to the specific case of a particle of mass $M = 1/2$ ($\hbar = 1$) moving in the quartic potential

$$V(q) = -\Lambda\, q^2 + (1-\Lambda)\, q^4 + \frac{\Lambda^2}{4(1-\Lambda)} \quad \text{with} \quad 0 \le \Lambda < 1. \quad (42)$$

This potential coincides with a quartic oscillator for $\Lambda = 0$ and develops a barrier of height $V(0) = \Lambda^2/(4(1-\Lambda))$ for positive Λ. Potentials of the form (42) have often been used to qualitatively understand characteristic properties of high dimensional systems as *e.g.* phase transitions. Here we find that the shape of $V(q)$ describes the main features encoded in the intrinsic free energy of the Lipkin-Meshkov-Glick model which we will consider in detail below (see Sect. 4.2). There, the appearance of a phase transition is equivalent to the development of a barrier for $\Lambda > 0$ in $V(q)$. Further, from (38) and (42) the inverse crossover temperature can simply be derived as $\beta_0 = 1/T_0 = 2\pi/\hbar \cdot \sqrt{M/(2\Lambda)} = \pi/(\hbar\sqrt{\Lambda})$. In Figure 1 the free energy

$$\mathcal{F}(\beta) = -\frac{1}{\beta}\,\ln \mathcal{Z}(\beta) \quad (43)$$

is depicted within various approximations for $\Lambda = 0.9$.

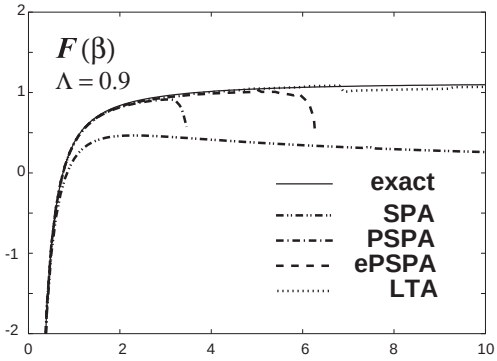

Fig. 1. $\mathcal{F}(\beta)$ of the double well (42) computed for various approximations and $\Lambda = 0.9$.

4 Application II: The Lipkin-Meshkov-Glick model

The approximations derived in the preceding sections are designed to describe low temperature thermodynamic properties of interacting many body systems. In contrast to simple one-dimensional cases, here, an additional challenge arises through the calculation of the expansion coefficients in (14) and (23–25).

4.1 Expansion coefficients for many body systems

For the Hamiltonian (1) the coefficients $c_3^{\pm}$ and c_4 are calculated by evaluating the τ-integrals in (23–25). The calculation is performed completely parallel to the one presented in [7]. Hence, we restrict ourselves here to *one* contribution to the fourth order coefficient to exemplify the general strategy. We also will prove the sum rule $r+s+t+u=0$ exploited in (22–25) here. To this end we consider general indices r, s, t, $u \neq 0$ at first. One has to rewrite the operators $\hat{F}(\tau)$ in terms of creation and annihilation operators $\hat{F}(\tau) = \sum_{kj} F_{kj} \hat{a}_k^\dagger(\tau)\hat{a}_j(\tau)$ and then calculate the time ordered averages using the finite temperature Wick theorem [2]. Evaluating all possible contractions the unperturbed temperature Green functions enter, *i.e.*

$$-\langle \hat{\mathcal{T}} \hat{a}_j(\tau_r)\hat{a}_k^\dagger(\tau_s)\rangle_{q_0} = \delta_{jk}\, g_k^{(0)}(\tau_r-\tau_s) = \delta_{jk}\,\frac{1}{\beta}\sum_{K=-\infty}^{\infty}\frac{\mathrm{e}^{-\mathrm{i}\omega_K(\tau_r-\tau_s)}}{\mathrm{i}\hbar\omega_K - e_k(q_0)}, \tag{44}$$

where $\omega_K = (2K+1)\pi/\hbar\beta$ [2] and $e_k(q_0)$ corresponds to the eigenenergies of (8) *via* $e_k(q_0) = \epsilon_k(q_0) - \mu$. The integrands of all multiple τ integrals therefore turn into factors like *e.g.*

$$\exp\left(\mathrm{i}\,\frac{2\pi}{\hbar\beta}\,(r+I-O)\,\tau_r\right). \tag{45}$$

[2] Mind that our ω_K correspond to the ν_k of [7] and our ν_r are equivalent to the ω_r of [7].

After carrying out all τ integrals we obtain the conditions $r+I-O=0$, $s-I+K=0$, $t-K+M=0$ and $u+O-M=0$. Putting these conditions together we easily obtain the requirement

$$r+s+t+u=0. \tag{46}$$

Moreover, we have only one summation index $I = -\infty\ldots\infty$ left besides r, s, $t \neq 0$ which will actually be further restricted by the requirement r, s, t, $u = \pm 1, \pm 2$ in (23) – (25). One can show after some straightforward but lengthy algebra that *one* typical contribution to the fourth order coefficient $c_4(\beta, q_0)$ reads:

$$\frac{-|k|/\beta}{4!}\sum_{i,k,m,o} F_{io}(q_0)F_{ki}(q_0)F_{mk}(q_0)F_{om}(q_0) \times \sum_{I=-\infty}^{\infty}\frac{1}{\mathrm{i}\hbar\omega_I - e_i(q_0)}\,\frac{1}{\mathrm{i}\hbar(\omega_I+\nu_r)-e_o(q_0)} \frac{1}{\mathrm{i}\hbar(\omega_I-\nu_s)-e_k(q_0)}\,\frac{1}{\mathrm{i}\hbar(\omega_I-\nu_{s+t})-e_m(q_0)}. \tag{47}$$

The infinite sum over I is calculated by exploiting the frequency summation technique [24]. One uses the replacement $\mathrm{i}\omega_I \to z$ and the residue theorem for contour integration in the complex z-plane together with the observation that the function $-\hbar\beta/(\exp(\hbar\beta z)+1)$ has poles at $\mathrm{i}\omega_I$ with residues 1. After a deformation of the integration contour such that it encycles the poles of (47) we obtain the following final form:

$$\begin{aligned}&\frac{|k|}{4!}\sum_{i,k,m,o} F_{io}(q_0)F_{ki}(q_0)F_{mk}(q_0)F_{om}(q_0) \\ &\times\Bigg\{ n(\epsilon_i)\,\frac{1}{\epsilon_{io}+\mathrm{i}\hbar\nu_r}\,\frac{1}{\epsilon_{ik}-\mathrm{i}\hbar\nu_s}\,\frac{1}{\epsilon_{im}-\mathrm{i}\hbar\nu_{s+t}} \\ &+\, n(\epsilon_o)\,\frac{1}{\epsilon_{oi}-\mathrm{i}\hbar\nu_r}\,\frac{1}{\epsilon_{ok}-\mathrm{i}\hbar\nu_{r+s}}\,\frac{1}{\epsilon_{om}-\mathrm{i}\hbar\nu_{r+s+t}} \\ &+\, n(\epsilon_k)\,\frac{1}{\epsilon_{ki}+\mathrm{i}\hbar\nu_s}\,\frac{1}{\epsilon_{ko}+\mathrm{i}\hbar\nu_{r+s}}\,\frac{1}{\epsilon_{km}-\mathrm{i}\hbar\nu_t} \\ &+\, n(\epsilon_m)\,\frac{1}{\epsilon_{mi}+\mathrm{i}\hbar\nu_{s+t}}\,\frac{1}{\epsilon_{mo}+\mathrm{i}\hbar\nu_{r+s+t}}\,\frac{1}{\epsilon_{mk}+\mathrm{i}\hbar\nu_t}\Bigg\}.\end{aligned} \tag{48}$$

Here $n(\epsilon) = (1+\exp(\beta(\epsilon-\mu)))^{-1}$ are the Fermi occupation numbers and $\epsilon_{ik}(q_0)$ are the energy differences between the states $|i(q_0)\rangle$ and $|k(q_0)\rangle$ of the static Hamiltonian $\hat{h}_0(q_0)$. This way, by solving the static one body Schrödinger equation belonging to (8) and evaluating sums as in (48) all needed coefficients are known and the corresponding approximations to $\mathcal{Z}(\beta)$ can be applied.

We note that the factor in brackets in (48) also appears in [7] where strength functions are calculated in the conventional PSPA formalism. There, time ordered expectation values of products of one body operators $\hat{D} = \sum_{kj} D_{kj}\hat{a}_k^\dagger\hat{a}_j$ like $\langle\hat{\mathcal{T}}\hat{\mathcal{U}}_q\hat{D}^\dagger(\tau)\hat{D}(0)\rangle_{q_0}$ are evaluated. To this end $\hat{\mathcal{U}}_q$ [see (11) and (14)] has to be expanded up to second order in the q_r. As a consequence, fourth order terms in $\hat{a}_k^\dagger(\tau)\hat{a}_j(\tau)$ come into play even though the approximation to $\hat{\mathcal{U}}_q$ is still of Gaussian type.

4.2 The model

There are only few many body systems which allow for an exact evaluation. One is the Lipkin-Meshkov-Glick model [17] which has been used to test the results of conventional PSPA for years (see *e.g.* [6,7,9]). In the last part of the paper we want to apply the approximations derived in Section 2 to this model. The Lipkin-Meshkov-Glick Hamiltonian reads

$$\hat{\mathcal{H}} = 2\epsilon \hat{J}_z + 2k\hat{J}_x^2 \ , \tag{49}$$

and has the structure of a Hamiltonian with two body interaction with $\hat{H} = 2\epsilon\hat{J}_z$ and $\hat{F} = 2\hat{J}_x$. In (49) the operators $\hat{J}_x$ and $\hat{J}_z$ obey angular momentum commutation relations and $k = -|k|$ is a negative coupling constant describing an attractive interaction.

Let us briefly recall [6,7,9] the most important features of the PSPA applied to the Hamiltonian (49). The static part (8) of the one body Hamiltonian is given by

$$\hat{h}_0(q_0) = 2\epsilon\hat{J}_z + 2q_0\hat{J}_x \tag{50}$$

and its eigenvalues are g-fold degenerated

$$\bar{\epsilon}^2(q_0) = \epsilon^2 + q_0^2 \ . \tag{51}$$

Energy differences $\epsilon_{ik}(q_0)$ can therefore only have the three different values $0, \pm 2\bar{\epsilon}(q_0)$. For the grand canonical partition function belonging to (50) one easily obtains at a given collective coordinate q_0 [see (7)]

$$z(\beta, q_0) = \left(2\cosh\left(\frac{\beta\bar{\epsilon}(q_0)}{2}\right)\right)^{2g} \ . \tag{52}$$

The PSPA correction factor (19) can be written as

$$C^{\mathrm{PSPA}}(\beta, q_0) = \frac{\sinh(\beta\bar{\epsilon}(q_0))}{\beta\bar{\epsilon}(q_0)} \ \frac{\hbar\beta\varpi(\beta, q_0)/2}{\sinh(\hbar\beta\varpi(\beta, q_0)/2)} \tag{53}$$

where the RPA frequencies read

$$\left(\frac{\hbar\varpi(\beta, q_0)}{2}\right)^2 = \bar{\epsilon}^2(q_0) - \kappa\,\frac{\epsilon^3}{\bar{\epsilon}(q_0)}\,\tanh\left(\frac{\beta\bar{\epsilon}(q_0)}{2}\right), \tag{54}$$

with the dimensionless coupling parameter([3])

$$\kappa = \frac{|k|g}{\epsilon} > 0. \tag{55}$$

For $\kappa > 1$ the equilibrium value of q_0 undergoes a phase transition at a critical temperature T_c which is determined from the condition that one can find a q_0 with zero RPA frequency from (54). This phase transition manifests itself in the development of a barrier in the intrinsic free energy for $T < T_c$ corresponding to imaginary RPA frequencies. Thus, the crossover temperature T_0 where the factor (53) diverges is determined from the condition $(\hbar\beta\varpi(\beta, q_0)/2)^2 = -\pi^2$. We note that one always has $T_0 < T_c$. For $\kappa < 1$ no phase transition occurs and the RPA frequencies are always real.

[3] Our κ is defined as in [7] and should not be mixed up with the $\kappa = 1/k$ often used in nuclear physics [18].

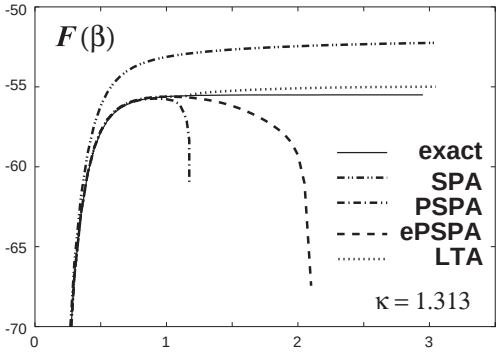

Fig. 2. $\mathcal{F}(\beta)$ of the Lipkin-Meshkov-Glick model (49) within various approximations for the parameters (56) and $\kappa = 1.313$. The phase transition occurs at $\beta_c = 0.4\,\mathrm{MeV}^{-1}$ and the inverse crossover temperature is $\beta_0 = 1.1392\,\mathrm{MeV}^{-1}$.

4.3 Free energy

For the Lipkin-Meshkov-Glick model the free energy has been calculated in [7] within the conventional PSPA. Here, we want to demonstrate the results of the extensions proposed above using the same set of parameters as in [6], namely,

$$\epsilon = 5\,\mathrm{MeV} \quad \text{and} \quad g = 10 \tag{56}$$

and various values for κ.

In Figures 2–3c we present plots of the free energy (43) as a function of the inverse temperature β. Figure 2 shows the global behavior for $\kappa = 1.313$ (the value used in [6]). Figures 3a–c illustrate a blow up of the region around T_0 for three different coupling strengths. The exact result can be obtained by a numerical diagonalization of the Hamiltonian (49) in a basis of eigenstates of $\hat{J}_z$ or $\hat{J}_x$ as explained in [6,7,9]. As expected, pure SPA deviates strongly from the exact results with decreasing temperature. For $\kappa < 1$ no phase transition occurs and the difference between conventional and extended PSPA is very small (see Fig. 3a). The inclusion of quantum effects on the RPA level in the conventional PSPA (19) improves the results a lot as long as β is not too close to the breakdown value $\beta_0 = 1/T_0$ (see Fig. 2). Here the conventional PSPA fails as the correction factor diverges for $\kappa > 1$. Instead, the extension (31) smoothly passes the crossover region and agrees very well with exact results even for inverse temperatures slightly above β_0. The ePSPA definitely breaks down near $\beta = 2\beta_0$ where $\lambda_2 = 0$. The LTA (see Sect. 2.3) smoothly matches with the ePSPA somewhat below β_0 and is able to cover even the range $\beta \gg \beta_0$ with astonishing accuracy.

One can also see in Figure 3b that the matching between ePSPA and LTA even though it appears to be continuous in temperature, may lead to discontinuities in first and higher order derivatives. The latter ones produce unphysical results for the internal energy and specific heat (see below) around the matching point close to T_0. This kind of behavior is typical for the matching between different semiclassical approximations each one designed for different ranges in parameter space. It can be overcome

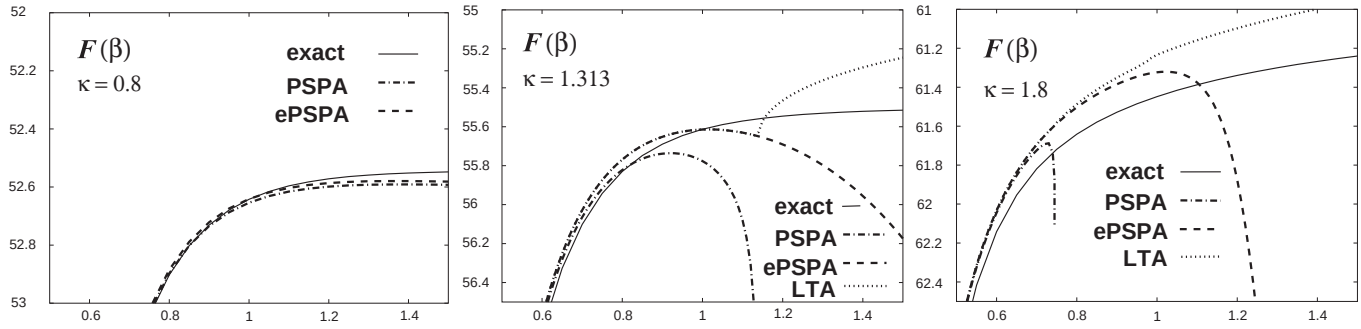

Fig. 3. Blow up of the crossover region for $\mathcal{F}(\beta)$ of the Lipkin-Meshkov-Glick model (49) within various approximations. Parameters are as in (56). For $\kappa = 0.8$ no phase transition occurs: $T_0 = 0$. For $\kappa = 1.313$ the inverse crossover temperature is $\beta_0 = 1.1392\,\mathrm{MeV}^{-1}$ whereas for $\kappa = 1.8$ the corresponding value is $\beta_0 = 0.7433\,\mathrm{MeV}^{-1}$.

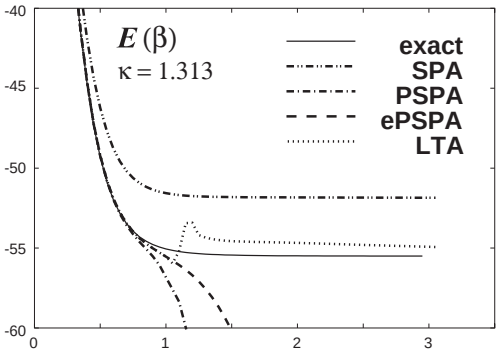

Fig. 4. $\mathcal{E}(\beta)$ of the Lipkin-Meshkov-Glick model (49) for the parameters of (56) and $\kappa = 1.313$. The phase transition occurs at $\beta_c = 0.4\,\mathrm{MeV}^{-1}$ and the inverse crossover temperature is $\beta_0 = 1.1392\,\mathrm{MeV}^{-1}$.

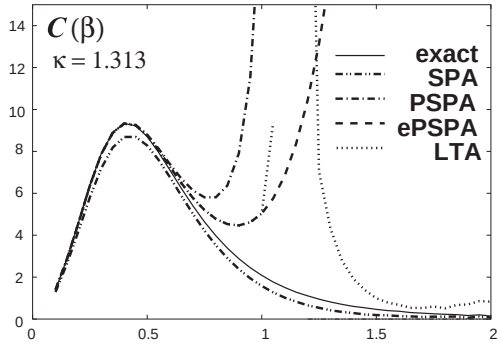

Fig. 5. $\mathcal{C}(\beta)$ of the Lipkin-Meshkov-Glick model (49) for the parameters of (56) and $\kappa = 1.313$. The phase transition occurs at $\beta_c = 0.4\,\mathrm{MeV}^{-1}$ and the inverse crossover temperature is $\beta_0 = 1.1392\,\mathrm{MeV}^{-1}$.

in principle by invoking uniform semiclassical approximations. Apart from that the ePSPA together with the LTA provide a practicable and very efficient way to evaluate the free energy over a broad temperature range.

4.4 Internal energy and specific heat

The internal energy (comp. [6])

$$\mathcal{E}(\beta) = -\frac{\partial}{\partial\beta}\,\ln\mathcal{Z}(\beta) \tag{57}$$

is shown in Figure 4. In the crossover region $\beta \approx \beta_0$ the extended PSPA again is an improvement over conventional PSPA but tends to fail for larger β. The low temperature approximation of Section 2.3 delivers reasonable values for $\beta > \beta_0$. As already mentioned above, it shows unphysical discontinuities close to $\beta_0 = 1/T_0$.

The specific heat of the system (comp. [6])

$$\mathcal{C}(\beta) = \beta^2\,\frac{\partial^2}{\partial\beta^2}\,\ln\mathcal{Z}(\beta) \tag{58}$$

is seen in Figure 5. Pure SPA turns out to provide a reasonable *global* approximation of the specific heat over a broad range of temperatures, whereas the conventional and extended PSPA lead to very good results at higher temperatures, smaller β, but deviate already for $\beta < \beta_0$. The LTA of Section 2.3 again shows a discontinuity at $\beta = \beta_0$ and supplies a reasonable estimate for $\beta > \beta_0$.

4.5 Level densities

As already mentioned in the introduction the development of the conventional PSPA was motivated to some extent by the need to calculate 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 inverse thermal temperature β^* from $\mathcal{E}^* = \mathcal{E}(\beta^*) - \mathcal{E}_0$ and arrives at the following formula for the level density [25]:

$$\rho(\mathcal{E}^*) = \frac{1}{\sqrt{2\pi\,\mathcal{D}}}\;\exp[\mathcal{S}(\beta^*) - \beta^*\mathcal{E}_0]\,. \tag{59}$$

The entropy is given by $\mathcal{S}(\beta) = \beta\,[\mathcal{E}(\beta) - \mathcal{F}(\beta)]$ and

$$\mathcal{D} = \left|\left(\frac{\partial^2}{\partial\beta^2}\,\ln\mathcal{Z}(\beta)\right)_{\beta=\beta^*}\right| = \left|\frac{1}{(\beta^*)^2}\,\mathcal{C}(\beta^*)\right|\,. \tag{60}$$

Results are depicted in Figure 6. Here, high excitation

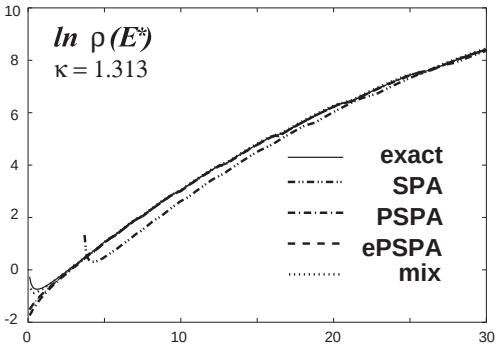

Fig. 6. $\ln \rho(\mathcal{E}^*)$ of the Lipkin-Meshkov-Glick model (49) for the parameters of (56) and $\kappa = 1.313$. $\mathcal{E}^*$ is measured in MeV.

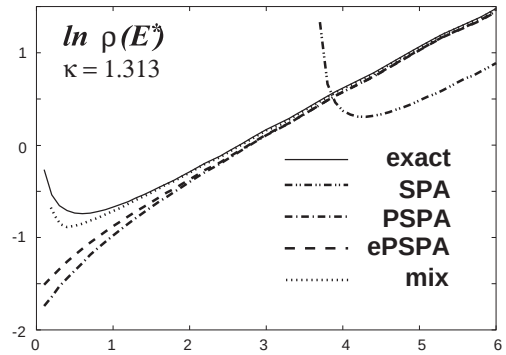

Fig. 7. Magnification of Figure 6 for small excitations.

energies correspond to high temperatures. For this reason approximations of SPA type are expected to be exact at large $\mathcal{E}^*$ as confirmed in Figure 6. For low excitations the situation is different. The pure SPA is not able to deliver results for $\mathcal{E}^* \lesssim 4\,\mathrm{MeV}$. The reason is simply that the SPA result for the internal energy is about 4 MeV larger than the exact result at small temperatures (see Fig. 4) and therefore the condition $\mathcal{E}(\beta^*) - \mathcal{E}_0 = \mathcal{E}^* \lesssim 4\,\mathrm{MeV}$ cannot be fulfilled within SPA. The conventional and extended PSPA results agree with the exact ones much better than those of pure SPA. Essential deviations only occur for $\mathcal{E}^* \lesssim 2\,\mathrm{MeV}$ and the extended version is a little better than the conventional one (see Fig. 7).

The main problem of the conventional and extended PSPA with respect to the level density can be traced back to the quantity $\mathcal{D}$ of (60) that is proportional to the specific heat $\mathcal{C}(\beta^*)$ and enters in the denominator of (59). Divergencies in the specific heat as seen for PSPA and ePSPA in Figure 5 therefore have a tremendous impact on the results for the level density. Therefore both types of PSPA deliver level densities that are too small which becomes significant at small excitations corresponding to $\beta \gtrsim \beta_0$. The following strategy seems to be reasonable: In order to calculate the level density using (59) we exploit an approximation for the specific heat that is *globally* reasonable and combine it with the best approximation at hand for the internal and free energy. That means to use *pure SPA* (see Fig. 5) for the specific heat and the ePSPA/LTA for the remaining quantities. As shown in Figure 7 this procedure improves the conventional and extended PSPA a great deal at low excitations. Remarkably, it even describes the bending up of the level density qualitatively correct.

5 Conclusion

We have applied the path integral approach to approximately evaluate the partition function of a finite interacting many body system in the low temperature regime. This requires to extend the conventional PSPA down to temperatures below the crossover temperature T_0. At these temperatures the simple mean field solution becomes unstable and large quantum fluctuations arise. The crucial step is to go beyond the Gaussian approximation on which the PSPA relies and take into account anharmonicities of certain critical vibrational modes. This procedure stabilizes the semiclassical type of approximation to the path integral of the partition function and holds true down to temperatures $T \approx T_0/2$. There, an instability in another direction in functional space shows up, which successively proceeds to occur at all $T_r = T_0/r$ $(r > 1)$. In order to treat the temperature range $T \ll T_0$, but still sufficiently above $T = 0$, we proposed an approximation where only mean fields with small quantum fluctuations around the minima of the static free energy are taken to contribute.

In this way, we could study thermodynamic properties of the archetypical Lipkin-Meshkov-Glick model even far below the crossover temperature. In particular, for the free and internal energies results were gained, that agree very well to the exact ones. Combining our extensions to the PSPA with pure SPA we obtained very accurate results for the level density even at low excitation energies.

Improvements beyond the PSPA for $T \approx T_0$ and $T \ll T_0$ are desirable in order to get reasonable approximate results for many body systems in the low temperature range where usual Monte Carlo techniques become very expensive. This is particularly true as often the critical temperature T_c where a phase transition takes place and the crossover temperature T_0 where the PSPA breaks down are of the same order of magnitude. For instance, for finite nuclei one finds for the nucleus ^{164}Er that $T_c \approx 0.45\,\mathrm{MeV}$, while PSPA is reliable only for $T > 0.25\,\mathrm{MeV}$ [14]. In [10] the range of applicability of PSPA is given by $T > 0.2\,\mathrm{MeV}$ for the nuclei ^{104}Pd and ^{114}Sn.

In general, for these or even lower temperatures (of the order of $10^{-1}\,\mathrm{MeV}$ and below for nuclei) the concept of temperature is at least doubtful for small isolated systems. This is different for systems on a mesoscopic scale. There the coupling to a macroscopic heat bath is always present such that temperature can be fixed from outside. Further, the number of constituents is typically much larger as *e.g.* for finite nuclei. Accordingly, as addressed above, the conventional PSPA has been applied to small superconducting and superfluid systems. For superconducting particles of nanometer scale one roughly finds $T_0 \approx T_c/2$ [15] so that an extension of the PSPA is clearly relevant. Work in this direction is in progress.

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