Damped collective motion of isolated many body systems within a variational approach to functional integrals

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Two improvements with respect to previous formulations are presented for the calculation of the partition function \( Z \) of small, isolated and interacting many body systems. By including anharmonicities and employing a variational approach quantum effects can be treated even at very low temperatures. A method is proposed of how to include collisional damping. Finally, our approach is applied to the calculation of the decay rate of metastable systems.

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Small many body systems like atomic nuclei and metal clusters may undergo self-sustained collective motion. In the former case this has long been established experimentally for situations where the nucleons may be assumed to move in a time-dependent state with no additional excitation energy. In the last few years one is also able to measure properties of single, isolated metallic grains. Although such systems consist of (many) particles of identical or similar nature collective motion only involves one or a few time dependent parameters. The latter must be introduced so that they obey certain basic relations for the intrinsic (particle) degrees of freedom. One, for instance, is to introduce collective degrees of freedom via a Hubbard-Stratonovich transform (HST). This is especially useful when the nature of the collective motion can be guessed and attributed to one generator \( \hat{\mathcal{F}} \), fol-

\[ \hat{H} = \hat{H}_0 + \frac{k}{2} \hat{\mathcal{F}} \hat{\mathcal{F}}, \tag{1} \]

in which the coupling constant \( k \) is negative for isoscalar modes. Of course, this might be understood as one prominent term in an expansion of a general two-body interaction \( \hat{V}^{(2)} \) into a complete series of separable terms like \( \hat{H} = \hat{T} + \hat{V}^{(2)} = \hat{H}_0 + \frac{1}{2} \sum_{\mu \nu} k_{\mu \nu} \hat{F}^\mu \hat{F}^\nu \). For the sake of simplicity we will restrict our discussion to the model case, but treatments of more terms are feasible and have already been undertaken for applications which are simpler than those we have in mind (see e.g. 3, 4). For zero thermal excitation the \( \hat{H}_0 \) might be assumed to simply represent the dynamics of independent particles. However, in case the constituents themselves are excited this may no longer be true as then incoherent, residual interactions \( \hat{V}^{(2)}_{\text{res}} \) may play a role, with an ever increasing role the larger the excitation. In the nuclear case it is known that single particle excitations acquire a finite width if they are away from the Fermi level by only 5 – 8 MeV. This effect is further enhanced if the system of particles is thermally excited. In the present Letter we want to show how these effects may be accounted for in the functional integral approach. Moreover, in contrast to previous formulations 3, 4, 5, we also demonstrate the usefulness of generalizing the variational formulation of 3, 6 to many body systems.

Our basic theoretical tool will be the partition function \( Z \) which at given temperature \( T = 1/(\hbar k_B \beta) \) may be expressed as

\[ Z(\beta) = \sqrt{\frac{\beta}{2\pi i |k|}} \int dq_0 \exp\left[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_0)\right] \zeta(\beta, q_0). \tag{2} \]

The \( \mathcal{F}^{\text{SPA}}(\beta, q_0) \) is a free energy which depends on the collective variable \( q_0 \), treated here in the static limit, which in this context in the literature is referred to as “Static Path Approximation” (SPA). It may be written as \( \mathcal{F}^{\text{SPA}}(\beta, q_0) = q_0^2/(2|k|) - T \ln z(\beta, q_0) \), where \( z(\beta, q_0) \) is the grand canonical partition function calculated for the static one body hamiltonian \( \hat{H}_0[q_0] = \hat{H}_0 + q_0 \hat{F} \). Actually, the collective variable is “time-dependent” and is introduced via the HST. Using this manipulation the two body interaction \( k \hat{F} \hat{F}/2 \) disappears. The dependence on the imaginary time \( \tau \) is treated through the Fourier series \( q(\tau) = q_0 + \sum_{\nu \neq 0} q_\nu \exp(i\nu\tau), \) with the Matsubara frequencies \( \nu_\tau = 2\pi\tau/(\hbar\beta) = 2\pi T/\hbar. \) Genuine quantum effects in collective motion are hidden in the factor

\[ \zeta(\beta, q_0) = \int D\nu \exp[-s\nu(\beta, q_0)/\hbar]. \tag{3} \]

The key stone for improvements over the SPA is given by the Euclidean action \( S_\text{E} \). In the so called “Perturbed SPA” (PSPA) – also known as “SPA+RPA” or “Correlated SPA” (CSPA) – this \( S_\text{E} \) is expanded to second order in the \( q_\nu \). In this way quantum effects are treated at the level of a local RPA, see e.g. 6, 7, 8. In an extension of this approximation we shall want to make use of terms up to fourth order and write the action as (see also 10, 11).
The interesting point is that the coefficients \( \lambda \) and \( \rho \) can be expressed by the one body Green functions associated with the Hamiltonian \( \mathcal{H}_{\text{HST}}[q_0] \), which at first may be assumed to represent simply independent particles for which the Green function is \( g_k^{(0)}(z) = (z - \epsilon_k)^{-1} \). In such a case the coefficient \( \sigma_{rstu} \) of fourth order consists of terms like \[ \lambda \]

\[
\frac{[k]}{4!} \sum_{i,k,m,o} F_{i\omega} F_{k\omega} F_{m\omega} F_{o\omega} \times
\left\{ n(\epsilon_i) g_{iv}^{(0)}(\omega_i + i\nu_r) g_{ik}^{(0)}(\omega_i - i\nu_s) g_{im}^{(0)}(\omega_i - i\nu_{st}) + n(\epsilon_o) g_{io}^{(0)}(\omega_o - i\nu_r) g_{ik}^{(0)}(\omega_o - i\nu_{rs}) g_{im}^{(0)}(\omega_o - i\nu_{st})
\right. 
\left. + n(\epsilon_s) g_{i}^{(0)}(\omega_k + i\nu_r) g_{s}^{(0)}(\omega_k + i\nu_{rs}) g_{m}^{(0)}(\omega_k - i\nu_l) + n(\epsilon_m) g_{i}^{(0)}(\omega_m + i\nu_{st}) g_{o}^{(0)}(\omega_m + i\nu_{rs}) g_{k}^{(0)}(\omega_m + i\nu_l) \right\}
\]

(4)

to give just one example of what these quantities look like.

At the level of PSPA it is useful to connect the coefficient \( \lambda \) to the response function \( \chi(\omega) \) defined through \( \delta(F) = -\chi(\omega) \delta(\omega) \). We get \( \lambda_r = \frac{1}{2}(1 + k\chi(\nu_r)) \delta_{r,-r} = \frac{1}{2} \lambda_r \delta_{r,-r} \). (6)

The \( \lambda_r \) serves as the stiffness in \( q_r \)-direction:

\[
s_{\text{PSPA}} = \frac{\hbar \beta}{|k|} \sum_{r>0} \lambda_r |q_r|^2 = \frac{\hbar \beta}{|k|} \sum_{r>0} \frac{\prod_{l<k}(\nu_r^2 + \omega_{kl}^2)}{\prod_{l<k}(\nu_r^2 + \omega_{kl}^2)} |q_r|^2
\]

(7)

The unperturbed intrinsic excitations \( \hbar \omega_{kl} = \epsilon_k - \epsilon_l \) are to be calculated from the eigenvalues of \( \mathcal{H}_{\text{HST}}[q_0] \). The \( \nu_{kl} \), on the other hand, are to be found from the secular equation \( 1 + k \chi(\nu_{kl}) = 0 \) and represent the local RPA frequencies. For an unstable collective mode \( \mu \) the \( \omega_{\mu}^2 \) is negative such that \( \lambda_{\mu} \) may become negative as well. This happens for temperatures below the so called crossover temperature \( T_0 \). There the dynamical fluctuations in \( q_{\mu} \)-direction become too large for the harmonic approximation to be justified. Formally, this shows up when \( \chi(\omega) \) Gaussian integrals become divergent \( \iint \). The name crossover temperature is borrowed from work in \[ \iint \] the latter has been developed for the system of a particle moving in a one dimensional potential. It allows one to evaluate the quantum \( Z \) at arbitrary temperatures. Using the formalism of coherent states, these ideas have been applied to many body systems in \[ \iint \]. Here we want to make use of the expansion \[ \iint \]. Details of this novel method will be given in a forthcoming paper. The main idea consists in rewriting \( \iint \) as

\[
\zeta(\beta, q_0) = \int \mathcal{D}[q] \exp[-s_{\Omega}^{(0)}]/\hbar \exp[-(s_{E} - s_{\Omega}^{(0)})/\hbar] = \zeta_{\Omega}^{(0)} \exp[-(s_{E} - s_{\Omega}^{(0)})/\hbar]/\hbar
\]

(8)

The reference action \( s_{\Omega}^{(0)} \) is introduced to specify an averaging procedure for which one may exploit the inequality

\[
\exp[-(s_{E} - s_{\Omega}^{(0)})/\hbar]/\hbar \geq \exp[-\langle s_{E} - s_{\Omega}^{(0)} \rangle_{\Omega}/\hbar]
\]

(9)

for an optimization of the expression on the right hand side, which is easier to evaluate than the average in \( \iint \). The reference action should be chosen such that the normalization factor \( \zeta_{\Omega}^{(0)} = \int \mathcal{D}[q] \exp[-s_{\Omega}^{(0)}]/\hbar \) in \( \iint \) can be evaluated exactly. A reasonable choice can be constructed from the PSPA action \( \iint \) by replacing the RPA frequencies \( \omega_{kl} \) by variational parameters \( \Omega_{\mu} \): \[ \iint \]

\[
s_{\Omega}^{(0)} = \frac{\hbar \beta}{[k]} \sum_{\mu>0} \frac{\prod_{l<k}(\nu_r^2 + \Omega_{\mu}^2)}{\prod_{l<k}(\nu_r^2 + \omega_{kl}^2)} |q_r|^2
\]

(10)

Evidently, when calculating the integrals for \( s_{E} - s_{\Omega}^{(0)} \) all terms disappear which are odd in \( q_r \). Hence, in the truncated expansion \( \iint \) only terms of second and fourth
order survive. Using the abbreviation \( \Pi_r = \prod_\mu (\nu_r^2 + \Omega_\mu^2) \),

\[
\langle \delta E \rangle^{\text{PSPA}}_{\Omega_0} = \frac{\hbar}{\beta} \sum_{r>0} \frac{\Pi_r}{\prod_\mu (\nu_r^2 + \Omega_\mu^2)} 
\]

\[
\langle \delta^{(4)} E \rangle^{\Omega_0}_{\Omega_0} = \frac{\hbar |k|}{\beta} \sum_{r,s>0} \sigma_{rs-rs} \frac{\prod_{\mu} (\nu_r^2 + \Omega_\mu^2)}{\prod_\mu (\nu_r^2 + \Omega_\mu^2)} .
\]

Collecting all contributions the dynamical corrections read

\[
\ln \zeta = \ln \zeta^{(0)}_{\Omega_0} - \frac{1}{\hbar} \langle \delta E \rangle^{\text{PSPA}}_{\Omega_0} - \frac{1}{\hbar} \langle \delta^{(4)} E \rangle^{\Omega_0}_{\Omega_0} ,
\]

which cannot be larger than \( \ln \zeta \). The advantage of this novel method over the SPA and the ePSPA is that it can be applied at any \( T \). The reason is that in contrast to the case of the PSA the factors \( \nu_r^2 + \Omega_\mu^2 \), which contribute to the stiffness in \( q_r \)-direction in \( \text{SPA} \), stay positive for all \( \Omega_\mu \). Consequently all Gaussian integrals in \( \ln \zeta \) converge.

To test the results we apply the exactly solvable Lipkin-Meshkov-Glick model (LMGM) [15], as used before in [16] for the SPA and the PSA. In Fig. 1 the free energy \( F = -T \ln Z \) associated to the total Hamiltonian \( H \) is compared with the approximations mentioned before. For the calculation the same set of parameters has been taken as in Fig. 1. The classical SPA gives reasonable results only at small \( \beta \) (high \( T \)). Inclusion of quantum effects at the level of local RPA within the PSPA delivers considerable improvement at not too large \( \beta \). However, even before its breakdown at \( \beta = \beta_0 \) it becomes unreliable. The ePSPA behaves completely smoothly in the crossover region but breaks down at \( \beta = 2\beta_0 \). Compared to these results, the improvement found for the variational approach is very striking. Notice please that it is free of discontinuities and the relative error is only of the order of 1%, even at very large \( \beta \).

So far the one body Green’s functions \( g^{(0)}_k(z) \) have been calculated within the picture of independent particle motion. As mentioned before, within this model the residual two body interaction \( V^{(2)}_{\text{res}} \) is neglected. This interaction describes the incoherent scattering of particles and holes and couples 1p1h states to more complicated ones. This mechanism may be understood as the origin of the damping of collective motion, see e.g. [16]. In the following we will account for such couplings by dressing the one body Green functions with self-energies \( \Sigma = \Sigma' - i\Gamma/2 \) meaning that \( g^{(0)}_k(z) \) is replaced by

\[
g^{(\Gamma)}_k(z) = (z - \epsilon_k - \Sigma_k(z) + i\Gamma_k(z))/2^{-1} \]

The dependence of the width \( \Gamma_k(\omega) \) on frequency and its variation with temperature is parameterized by the form

\[
\Gamma_k(\omega) = \frac{1}{\Gamma_0} \left[ \frac{1}{1 + \frac{1}{\pi} \left( \frac{\omega - \mu}{\Gamma_0} \right)^2 + \frac{\pi^2 T^2}{\mu^2}} \right] \]

suggested in [17]. For zero temperature it is in good agreement with empirical data for the widths of proton and neutron states [4]. Finally, some comments are in order concerning our approximation in handling the impact of \( V^{(2)}_{\text{res}} \). What is definitely implied in evaluating many-body Green functions is the application of a factorization approximation. However, it should be noticed that this is done for excitations of the intrinsic dynamics and not for the collective modes. One may therefore argue that coherent effects are small, in particular at larger thermal excitations. After all the SPA is meant to represent the high temperature limit.

Having established the connection between the PSPA and the theory of linear response one may take over the method developed there (see [16]) to extract transport coefficients for collective dynamics. For slow collective motion, as given for nuclear fission, it suffices to concentrate on the lowest mode of the collective response function. In that frequency regime, the latter may then be approximated by the response function of a damped
at the minimum
to the evaluation of the quantum decay rate we take the
dynamical factor

classical rate formula of the SPA can be calculated from the
of

quantum corrections

body problems will be given in a forthcoming paper. The
will take this procedure over to the case of the interact-
the CLM makes extensive use of this feature [12]. We
related to the imaginary part of the free energy. Indeed,
plification: Only

plastic action, see (5). With respect to the variational
rate for a particle in a one-dimensional cubic potential with
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