

# Self-consistent quantal treatment of decay rates within the perturbed static path approximation

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The framework of the perturbed static path approximation is used to calculate the partition function of a finite Fermi system from a Hamiltonian with a separable two body interaction. Therein, the collective degree of freedom is introduced in self-consistent fashion through a Hubbard-Stratonovich transformation. In this way, all transport coefficients that dominate the decay of a metastable system are defined and calculated microscopically. Otherwise the same formalism is applied as in the Caldeira-Leggett model to deduce the decay rate from the free energy above the so called crossover temperature  $T_0$ .

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## I. INTRODUCTION

Commonly quantum versions of the decay rate of damped metastable systems are treated on the basis of the Caldeira-Leggett model [1]. For an exhaustive overview on this topic we may refer to the review papers by Hänggi *et al.* [2], Ingold [3], or Weiss [4]. Unfortunately, this model assumes some simplified coupling to a linear heat bath. Furthermore, it does not make any predictions about the input of such important quantities as the potential energy and the inertia, which need to be chosen on an entire phenomenological level. These features do not allow the model to be applied to self-bound Fermi systems. There, one would like to see the collective variables introduced in some self-consistent fashion, with a microscopic treatment of *all* transport coefficients alike.

One possible attempt to overcome these deficiencies is formulated in Ref. [5] (with references to earlier papers) in connection to nuclear physics. It is based on a quantal transport equation that is derived within a locally harmonic approximation exploiting linear response theory. It is this approximation that allows one to treat a more complicated coupling between the collective variable and the intrinsic degrees of freedom. A transport equation necessarily describes evolution in real time. Therefore, in barrier regions quantum effects can be accounted for only above a critical temperature  $T_c$ , which is larger than the so called crossover temperature  $T_0$ , which one encounters for imaginary time propagation [6]. As one knows, the same feature holds true also for the Caldeira-Leggett model [7,8]. Another disadvantage of the derivation of this transport equation mentioned is that it bases on the deformed shell model. Surely, it allows one to calculate all transport coefficients on the same footing. But as one does not start from a genuine two body interaction, self-consistency is handled on a semi-microscopic level only.

It is the aim of the present paper to do first steps to overcome these deficiencies. This is possible by adapting a previously developed formalism to evaluate the partition function for bound systems with separable two body interactions.

One starts from the so called static path approximation (SPA) functional integrals as an approximation to the classical or high-temperature limit [9–11]. Then small scale fluctuations around this static path are treated to second order, such that quantum effects come in through local random-phase approximation (RPA). In the literature this is referred to as RPA-SPA [12], the perturbed static path approximation (PSPA) in Ref. [13] (the name that we are taking over) or correlated static path approximation (CSPA) in Ref. [14].

## II. PARTITION FUNCTION OF A FINITE FERMION SYSTEM

Finally, we are interested in generalizing the formulas of dissipative tunneling to a system where the collective degrees of freedom are introduced self-consistently. The simplest Hamiltonian that may serve this purpose is of the following structure:

$$\hat{H} = \hat{H}_0 + \frac{k}{2} \hat{F} \hat{F}, \quad (1)$$

with (Hermitian) one body operators  $\hat{H}_0$  and  $\hat{F}$ . The product  $\hat{F} \hat{F}$  mimics an effective separable two body interaction. For isoscalar modes, the case we have in mind predominantly, the coupling constant  $k$  is negative [15]. As we shall see later,  $\hat{F}$  describes one collective degree of freedom. The ansatz (1) should be considered to define a microscopic model, for just this collective mode we want to address to Ref. [15]. Neglecting spin and isospin degrees of freedom, a general two body interaction may be written as a sum of separable terms

$$\hat{H} = \hat{H}_0 + \frac{1}{2} \sum_i k_i \hat{F}_i \hat{F}_i. \quad (2)$$

For instance, one might exploit an expansion into multipole operators. In case the latter are not Hermitian the product must be replaced by  $\hat{F}_i^\dagger \hat{F}_i$  (see, e.g., Sec. 4.4.7 of Ref. [16]).

### A. The general form of the partition function

The partition function of the grand canonical ensemble reads

$$Z(\beta) = \text{Tr} \exp[-\beta(\hat{H} - \mu \hat{A})] = \text{Tr} \hat{U}, \quad (3)$$

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where  $\beta = 1/T$  is the inverse temperature and  $\hat{H}$  is the Hamiltonian (1). The chemical potential  $\mu$  is needed in order to keep the particle number  $\langle \hat{A} \rangle$  fixed on average. It would be more appropriate to work with truly fixed particle number. But as we are mainly interested in the dependence of transport properties on excitation energy or temperature in this paper, this simplification should be accepted. An exact evaluation of (3) is prohibited by the presence of the two body interaction. Treating the latter in mean field approximation facilitates the calculation greatly. A convenient technical tool to incorporate this approximation is to use functional integrals (in imaginary time propagation) [17], with which fluctuations about the mean field may be treated as well. An elegant form of handling this problem is given through the Hubbard-Stratonovich transformation [18], by which the collective variable  $q(\tau)$  is introduced. To keep the present exposition as short as possible we save ourselves from repeating the derivations of [9–14] but simply state the basic results that will then serve as the starting point for our generalizations. Mind, however, that the notation has been adapted to that used in transport theory [19].

After introducing the Fourier expansion of the collective variable

$$q(\tau) = q_0 + \sum_{r \neq 0} q_r \exp(i\nu_r \tau), \quad (4)$$

where the so called Matsubara frequencies

$$\nu_r = \frac{2\pi}{\hbar\beta} r \equiv \frac{2\pi}{\hbar} rT \quad \text{with } r = \pm 1, \pm 2, \pm 3 \dots \quad (5)$$

(in units with  $k_B = 1$ ) have been used, the partition function may be written in the following form within the PSPA [see Eq. (21) of [13]]:

$$Z(\beta) = \sqrt{\frac{\beta}{-2\pi k}} \int_{-\infty}^{+\infty} dq_0 e^{i\beta/2k} q_0^2 z(\beta, q_0) \mathcal{C}(\beta, q_0). \quad (6)$$

Here  $k < 0$  and

$$\begin{aligned} z(\beta, q_0) &= \text{Tr} \exp\{-\beta[\hat{h}_0(q_0) - \mu\hat{A}]\} \\ &= \prod_l (1 + \exp\{-\beta[\epsilon_l(q_0) - \mu]\}), \end{aligned} \quad (7)$$

is the grand canonical partition function belonging to the static part of the Hamiltonian in mean field approximation

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

which is simply a sum over one body operators. The corresponding one body Schrödinger equation at some given  $q_0$  reads

$$\hat{h}_0(q_0)|l(q_0)\rangle = \epsilon_l(q_0)|l(q_0)\rangle. \quad (9)$$

The appearance of the  $q_0$  reflects the static version of the self-consistency relation for the mean field

$$q = k\langle \hat{F} \rangle, \quad (10)$$

which relates the collective variable  $q$  to the expectation value of the operator  $\hat{F}$ . The exponent in the first factor of the integrand of Eq. (6) is easily understood as to represent the static part of the correction  $-k\langle \hat{F} \rangle^2/2$ , which the energy  $\langle \hat{h}_0 \rangle$  in the independent particle picture gets from the two body interaction. Neglecting the factor  $\mathcal{C}$  one obtains the partition function in SPA [9–11]

$$\begin{aligned} Z^{\text{SPA}}(\beta) &= \sqrt{\frac{\beta}{-2\pi k}} \int_{-\infty}^{+\infty} dq_0 e^{i\beta/2k} q_0^2 z(\beta, q_0) \\ &\equiv \sqrt{\frac{\beta}{-2\pi k}} \int_{-\infty}^{+\infty} dq_0 \exp[-\beta\mathcal{F}^{\text{SPA}}(\beta, q_0)]. \end{aligned} \quad (11)$$

In the second line of Eq. (11) the symbol  $\mathcal{F}^{\text{SPA}}(\beta, q_0)$  has been introduced to represent the free energy. It is not the one of the total system (or total nucleus) which would be given by the relation

$$Z(\beta) = \exp[-\beta\mathcal{F}(\beta)], \quad (12)$$

when the partition function is identified as  $Z(\beta) = Z^{\text{SPA}}(\beta)$ . Rather, the  $\mathcal{F}^{\text{SPA}}(\beta, q_0)$  represents the free energy of the system of nucleons whose mean field is kept fixed at the  $q_0$ . In a common language of transport theory one would call it the free energy of the intrinsic degrees of freedom.

So far, any contribution from the dynamics in the collective variable  $q(\tau)$  has been neglected. Formally this may be accounted for by writing the correction factor as the following path integral [13]:

$$\mathcal{C}(\beta, q_0) = \int \mathcal{D}'q \exp\left(\frac{\beta}{k} \sum_{r>0} |q_r|^2 + \ln\langle \hat{U}_q \rangle_{q_0}\right), \quad (13)$$

with the measure

$$\mathcal{D}'q = \lim_{\substack{N \rightarrow \infty \\ N\epsilon = \hbar\beta}} \prod_{r=1}^{(N-1)/2} \frac{\beta}{-\pi k} d\text{Re}(q_r) d\text{Im}(q_r). \quad (14)$$

In Eq. (13) there appears the thermal expectation value of an evolution operator  $\hat{U}_q$ , which can be expressed by the following (imaginary) time-ordered product:

$$\begin{aligned} \langle \hat{U}_q \rangle_{q_0} &= \frac{1}{z(\beta, q_0)} \text{Tr} \left( \exp[-\beta\hat{h}_0(q_0)] \right. \\ &\quad \left. \times \widehat{\mathcal{T}} \exp \left[ -\frac{1}{\hbar} \int_0^{\hbar\beta} d\tau \hat{h}_1(\tau, q_r) \right] \right). \end{aligned} \quad (15)$$

The Hamiltonian

$$\hat{h}_1(\tau, q_r) = \hat{F}(\tau) \delta q(\tau), \quad (16)$$

may be understood as the time dependent correction to the static mean field given in Eq. (8). Here, the time dependence of the operator part is defined as

$$\hat{F}(\tau) = e^{\hat{h}_0(q_0)\tau/\hbar} \hat{F} e^{-\hat{h}_0(q_0)\tau/\hbar}, \quad (17)$$

which means through the interaction picture based on the Hamiltonian  $\hat{h}_0(q_0)$  of Eq. (8) and thus depends on the static  $q_0$ . The fluctuation of the collective variable  $\delta q(\tau) = q(\tau) - q_0$  in Eq. (16) is related to the fluctuating mean field through Eq. (10). It may be noted that the  $\tau$  dependence of the  $c$  number  $q$  is meant to be the correct one, not that of any interaction picture.

The partition function (6) may finally be written in the following compact form:

$$Z(\beta) = \sqrt{\frac{\beta}{-2\pi k}} \int_{-\infty}^{+\infty} dq_0 \exp[-\beta \mathcal{F}(\beta, q_0)], \quad (18)$$

if again one uses the concept of the ‘‘intrinsic free energy,’’ which now is given by

$$\mathcal{F}(\beta, q_0) = -\frac{1}{2k} q_0^2 - \frac{1}{\beta} \ln z(\beta, q_0) - \frac{1}{\beta} \ln \mathcal{C}(\beta, q_0). \quad (19)$$

### B. The perturbed static path approximation (PSPA)

We are now going to evaluate the general formula (13) within the so called PSPA. It is defined as that approximation in which the exponent appearing in Eq. (15) is expanded to second order in the  $q_r$ . This leads to the common Gaussian approximation that is known to be related to the semiclassical limit. Following Ref. [13] one may write

$$\begin{aligned} \ln \langle \hat{\mathcal{U}}_q \rangle_{q_0}^{\text{PSPA}} &= \frac{1}{2\hbar^2} \sum_{r,s \neq 0} q_r q_s \int_0^{\hbar\beta} d\tau \int_0^{\hbar\beta} d\sigma \\ &\times e^{i\nu_r \tau} e^{i\nu_s \sigma} \langle \hat{\mathcal{T}}\hat{F}(\tau)\hat{F}(\sigma) \rangle_{q_0}, \end{aligned} \quad (20)$$

with the  $\tau$  dependence of the operators as defined in Eq. (17). Likewise, according to Eq. (15), the expectation value is to be calculated with the density operator corresponding to the same unperturbed Hamiltonian  $\hat{h}_0(q_0)$ . It is this feature that will allow us to introduce and work with response functions. As we shall see below, this is of advantage for at least two reasons, which in a sense are related to each other. The final result, say for the decay rate of metastable states, has much in common with the linear response formulation of transport theory within a locally harmonic approximation [5]. From this approach one knows how the response functions have to be modified in order to introduce dissipation.

#### 1. Exploiting Green and response functions

The time ordered average in Eq. (20) can be identified with the two body Matsubara function of the one body operator  $\hat{F}$  [20],

$$\tilde{\mathcal{G}}(q_0, \tau - \sigma) = -\frac{1}{\hbar} \langle \hat{\mathcal{T}}\hat{F}(\tau)\hat{F}(\sigma) \rangle_{q_0}. \quad (21)$$

On the other hand the retarded  $FF$ -response function is given by

$$\begin{aligned} \tilde{\chi}^R(q_0, t-s) &= \frac{i}{\hbar} \theta(t-s) \langle \hat{F}(t)\hat{F}^\dagger(s) - \hat{F}^\dagger(s)\hat{F}(t) \rangle_{q_0} \\ &= \tilde{\chi}(q_0, t-s). \end{aligned} \quad (22)$$

(Henceforth, we shall omit the upper index ‘‘R’’). It describes the response of the expectation value  $\langle \hat{F} \rangle$  to the variations of  $q$  in real time evolution

$$\langle \hat{F} \rangle_{q_0}(t) = - \int_{-\infty}^{\infty} ds \chi(q_0, t-s) [q(s) - q_0]. \quad (23)$$

The spectral representations  $\mathcal{G}(q_0, i\nu_r)$  of Eq. (21) and  $\chi(q_0, \omega)$  of Eq. (22) are obtained by Fourier series and Fourier transformations, respectively. As both have the same spectral density, one may prove [20] them to be connected by the analytic continuation  $i\nu_r \leftrightarrow \omega + i\epsilon$ :

$$\mathcal{G}(q_0, i\nu_r) \leftrightarrow -\chi^R(q_0, \omega). \quad (24)$$

The response function may be continued to the whole complex plane via Ref. [5]

$$X(q_0, z) = \int_{-\infty}^{\infty} \frac{d\Omega}{\pi} \frac{\chi''(q_0, \Omega)}{\Omega - z} \quad \text{for } \text{Im } z \neq 0, \quad (25)$$

with  $\chi''(q_0, \omega)$  being the imaginary (dissipative) part of  $\chi(q_0, \omega)$ . The form (25) defines two branches. The one that is analytic in the upper half plane coincides with the retarded function  $\chi^R(q_0, z)$  and the one analytic in the lower half plane defines the advanced function  $\chi^A(q_0, z)$ . Both branches may be continued analytically into the other half planes. Below we will make use only of the retarded response  $\chi^R(q_0, z) \equiv \chi(q_0, z)$ . On the imaginary axis ( $z = iw$  with  $w \in \mathbf{R}$ ) it has the following symmetry properties:

$$[\chi(q_0, iw)]^* = \chi[q_0, (iw)^*] = \chi(q_0, -iw) = \chi(q_0, iw). \quad (26)$$

This property, together with the relations (21) and (24) may be exploited to calculate the  $\tau$  integrals in Eq. (20) as

$$\ln \langle \hat{\mathcal{U}}_q \rangle_{q_0}^{\text{PSPA}} = \beta \sum_{r>0} |q_r|^2 \chi(q_0, i\nu_r). \quad (27)$$

Mind that because of the reality of the collective variable one has  $q_r^* = q_{-r}$ . The result (27) may be plugged into Eq. (13) to arrive at the following form:

$$\mathcal{C}^{\text{PSPA}}(\beta, q_0) = \int \mathcal{D}'q \exp\left(\frac{\beta}{k} \sum_{r>0} [1 + k\chi(q_0, i\nu_r)] |q_r|^2\right). \quad (28)$$

The remaining integrals hidden in  $\mathcal{D}'q$  are of Gaussian type. As we stick to the case  $k < 0$ , they cause no problem as long as

$$1 + k\chi(q_0, i\nu_r) > 0 \quad \text{for } r > 0. \quad (29)$$

As we shall see soon, this leads to a condition on the temperature below which the PSPA breaks down, as already noticed in Refs. [12,13]. Here, this condition only has been rewritten in terms of the response functions used in the linear response approach to nuclear transport (see, e.g., [5]). In this language the final result for  $\mathcal{C}^{\text{PSPA}}$  reads

$$\mathcal{C}^{\text{PSPA}}(\beta, q_0) = \prod_{r>0} [1 + k\chi(q_0, i\nu_r)]^{-1}, \quad (30)$$

and that for the partition function of the PSPA becomes

$$\begin{aligned} Z^{\text{PSPA}}(\beta) &= \sqrt{\frac{\beta}{-2\pi k}} \int_{-\infty}^{+\infty} dq_0 \\ &\quad \times \exp[-\beta\mathcal{F}^{\text{SPA}}(\beta, q_0)] \mathcal{C}^{\text{PSPA}}(\beta, q_0) \\ &= \sqrt{\frac{\beta}{-2\pi k}} \int_{-\infty}^{+\infty} dq_0 e^{l\beta/2k} q_0^2 z(\beta, q_0) \\ &\quad \times \prod_{r>0} [1 + k\chi(q_0, i\nu_r)]^{-1}. \end{aligned} \quad (31)$$

## 2. Response functions in the independent particle model

Before we discuss further the condition (29) in the next section, let us recall how the response function looks in the model of independent particles, as defined by the Hamiltonian  $\hat{h}_0$  of Eq. (8). It is not difficult to convince oneself of the following form for the dissipative part of the  $FF$ -response function

$$\chi''(q_0, \omega) = -\frac{\pi}{\hbar} \sum_{l,k} |F_{lk}(q_0)|^2 n_{lk}(q_0) \delta[\omega - \epsilon_{lk}(q_0)/\hbar], \quad (32)$$

where

$$\begin{aligned} F_{lk}(q_0) &= \langle l(q_0) | \hat{F} | k(q_0) \rangle, \\ \epsilon_{lk}(q_0) &= \epsilon_l(q_0) - \epsilon_k(q_0), \end{aligned} \quad (33)$$

$$n_{lk}(q_0) = n[\epsilon_l(q_0)] - n[\epsilon_k(q_0)],$$

and  $n(e)$  being the Fermi occupation numbers

$$n(e) = \frac{1}{1 + \exp[\beta(e - \mu)]}. \quad (34)$$

Within this model it can easily be seen, that the  $\chi(q_0, z)$  is given by

$$\chi(q_0, z) = -\frac{1}{\hbar} \sum_{l,k} |F_{lk}(q_0)|^2 \frac{n_{lk}(q_0)}{\epsilon_{lk}(q_0)/\hbar - z}. \quad (35)$$

Notice, please, that along the real axis the  $z$  must be chosen identical to  $\omega + i\epsilon$ . For details about these response functions we may refer to Ref. [5].

## 3. The crossover temperature

Let us elaborate now on the convergence condition (29) for the  $q_r$  integrals in Eq. (28), finally to establish connection to an analogous condition that shows up while treating dissipative tunneling at finite temperature within the Caldeira-Leggett model [21,22]. To this end, the following identity is useful [13]:

$$1 + k\chi(q_0, i\nu_r) = \frac{\prod_{\nu} [\nu_r^2 + \omega_{\nu}^2(q_0)]}{\prod'_{k>l} \{\nu_r^2 + [\epsilon_{lk}(q_0)/\hbar]^2\}}, \quad (36)$$

which is valid for all  $r \neq 0$ . The frequencies  $\omega_{\nu}(q_0)$  appearing here are those of the local RPA associated to the local vibrations of the mean field around  $q_0$ . They satisfy a secular equation [13], which can easily be brought to the form

$$1 + k\chi(q_0, z) = 0, \quad (37)$$

by analytically continuing the function  $\mathcal{G}(q_0, i\nu_r)$  to complex  $z$  by way of Eqs. (24) and (25). As the denominator of the ratio on the right of Eq. (36) is real and positive the condition (29) can be reformulated as

$$\prod_{\nu} [\nu_r^2 + \omega_{\nu}^2(q_0)] > 0, \quad (38)$$

as already mentioned in Refs. [12,13]. In case that all local RPA modes are stable, and hence that all  $\omega_{\nu}(q_0)$  are real, the condition is fulfilled for any temperature, viz for  $T \geq T_0 \equiv 0$  [mind Eq. (5)]. For *unstable RPA modes*, on the other hand, *one* pair of corresponding frequencies  $\omega_{\nu}^{\text{inst}}(q_0)$  becomes purely imaginary, in which case Eq. (38) can be fulfilled only above a certain minimal temperature  $T_0(q_0)$ . The latter may vary with  $q_0$ , but it is possible, of course, to define a minimal global temperature  $T_0$  by

$$T_0 = \max \frac{\hbar |\omega_{\nu}^{\text{inst}}(q_0)|}{2\pi}, \quad (39)$$

such that Eq. (29) is fulfilled for all  $T > T_0$ . This temperature is identical [23] to the so called ‘‘crossover temperature’’ (here, of course, for an undamped system) that shows up in the Caldeira-Leggett model when dealing with unstable modes of dissipative quantum systems [22]. There, the notion ‘‘crossover’’ indicates a transition in the nature of the decay of a metastable system. Above  $T_0$  the process is dominated by thermally activated decay (‘‘thermal hopping’’) with the effects of genuine barrier penetration in the quantum sense to become dominant only below this  $T_0$  (called ‘‘dissipative tunneling’’ for damped quantum systems). Evidently, in a typical situation, the  $T_0$  of Eq. (39) would correspond to that  $q_0$  where the top of the barrier is located.

### III. THE PSPA FOR DISSIPATIVE PHENOMENA

To elaborate on the connection to the treatment of dissipative tunneling within the Caldeira-Leggett model we need to introduce dissipation. As mentioned previously, the most natural way is through the response function. This can best be seen at the secular equation (37). For real  $z = \omega = \omega^*$ , for which the response function splits into its real (reactive) and imaginary (dissipative) part,  $\chi(\omega) = \chi'(\omega) + i\chi''(\omega)$ , one gets

$$\begin{aligned} 1 + k\chi'(\omega) &= 0, \\ \chi''(\omega) &= 0. \end{aligned} \quad (40)$$

Whenever the function  $\chi''(\omega)$  is given by a discrete sum of  $\delta$  functions located at  $\epsilon_{lk}(q_0)/\hbar$ , as shown in Eq. (32), the second equation is automatically fulfilled at the solutions  $\omega_\nu$  of the first equation. These solutions are either real or purely imaginary without any sign of dissipation, reflecting the fact that the local RPA as discussed above corresponds to time reversible dynamics. This argument shows that irreversibility is intimately related to the functional form of the dissipative part  $\chi''(\omega)$  of the response function. A genuinely microscopic approach would require to consider explicitly couplings of the simple particle-hole configurations to more complicated states [17]. Definitely, this is beyond the scope of the functional integral method underlying the present model. In a more phenomenological approach one might argue to dress the single particle states with complex self-energies that itself may vary with temperature, for details see Ref. [5] or Ref. [24], where the inclusion of pairing is discussed. An even simpler way is to effectively perform the transition to a continuous spectrum, which directly corresponds to the procedure one employs in the Caldeira-Leggett model in typical solid state applications [1–4,22]. However, even for a finite nucleus such a transition is justified for not too small excitations. Indeed, as one knows from nuclear reaction theory [25], for not too small energies resonances do overlap, implying that the true compound states lie dense for excitations above about 10–20 MeV. On the level of the independent particle model one simply might employ energy averages, which in turn are related to finite observation times of the system; for details the reader may refer to Ref. [5].

In this paper we would not like to penetrate any further into this discussion. Rather, in the sequel we would like to assume the  $\chi''(\omega)$  to be a continuous function of  $\omega$ . In this case the secular equation (37) may no longer be written as in Eq. (40) and its solutions become complex quantities. To be specific, instead of Eq. (32) we like to suggest and work with the following model function consisting of two Lorentzians of width  $\Gamma(q_0)$ :

$$\begin{aligned} \chi''(q_0, \omega) &= F^2(q_0) \left( \frac{\Gamma(q_0)/2}{[\omega - \mathcal{E}(q_0)]^2 + [\Gamma(q_0)/2]^2} \right. \\ &\quad \left. - (\mathcal{E} \leftrightarrow -\mathcal{E}) \right). \end{aligned} \quad (41)$$

It may be characterized as a generalization of the degenerate model often used in nuclear physics (see, e.g., Ref. [15]) to one where the nucleonic states are spread over a certain region determined by the width  $\Gamma(q_0)$ . The strength of these intrinsic excitations is parametrized by the quantity  $F^2(q_0)$ . A straightforward generalization could be seen in a summation of more than one term. In a sense the reduced form (41) corresponds to what has been called the “one pole approximation” (see, e.g., Ref. [5]). It is valid whenever the strength distribution is dominated by one peak, which then finally implies to have one prevailing collective mode. The parameters appearing in Eq. (41) could be calculated in various ways, as indicated within the linear response approach, for instance, but even the random matrix model (RMM) might be used (see, e.g., Ref. [5]).

Inserting the spectral density (41) into Eq. (25) the full response function can be calculated, which is needed both for the secular equation (37) as well as for the condition (29). The integral can be carried out with the help of the residue theorem noticing that the integrand has five poles altogether, situated at  $\Omega = z$  and  $\Omega = \pm \mathcal{E}(q_0) \pm i\Gamma(q_0)/2$ , and closing the loop in the appropriate half plane. The final result for the retarded response function reads

$$\chi(q_0, z) = F^2(q_0) \frac{\mathcal{E}(q_0)}{\mathcal{E}(q_0)^2 + [\Gamma(q_0)/2]^2 - i\Gamma(q_0)z - z^2}. \quad (42)$$

(The advanced response function would be obtained by changing  $-i$  into  $+i$ .) For the condition (29) one needs to know this function along the positive imaginary axis. There, the denominator is always positive implying that  $\chi(q_0, iw)$  is finite for real  $w$ . Furthermore, it is seen that  $\chi(q_0, iw)$  still is real for continuous spectra.

#### A. Transport coefficients of collective motion

We are now going to write the secular equation for collective motion in terms of transport coefficients, as it is known for the damped oscillator. This is achieved best by rewriting Eq. (42) in the form of the oscillator response function

$$\chi(q_0, z) = \frac{-1}{M(q_0)} \frac{1}{z^2 + i\Gamma(q_0)z - \Omega^2(q_0)} \equiv \chi_{\text{osc}}(q_0, z). \quad (43)$$

The parameters introduced here correspond to the *nucleonic* (or “intrinsic”) motion at any value of  $q_0$  and are *uniquely* derived from Eq. (42) as follows:

$$\begin{aligned} M(q_0) &= -\frac{1}{2} \left. \frac{\partial^2 \chi^{-1}(q_0, z)}{\partial z^2} \right|_{z=0} = \frac{1}{\mathcal{E}(q_0)F^2(q_0)}, \quad (44) \\ M(q_0)\Omega^2(q_0) &= \chi^{-1}(q_0, z=0) = \frac{\mathcal{E}(q_0)^2 + [\Gamma(q_0)/2]^2}{\mathcal{E}(q_0)F^2(q_0)}, \quad (45) \end{aligned}$$

$$M(q_0)\Gamma(q_0) = i \left. \frac{\partial \chi^{-1}(q_0, z)}{\partial z} \right|_{z=0} = \frac{\Gamma(q_0)}{\mathcal{E}(q_0)F^2(q_0)}. \quad (46)$$

These transport coefficients may be interpreted as the (local) coefficients of inertia, frequency, and friction for the nucleonic mode. Plugging Eq. (43) into Eq. (37) one obtains

$$0 = 1 + k \chi(q_0, z) = \frac{z^2 + i\Gamma(q_0)z - \Omega^2(q_0) - k/M(q_0)}{z^2 + i\Gamma(q_0)z - \Omega^2(q_0)}. \quad (47)$$

This equation may be fulfilled only for a vanishing numerator, which leads to the secular equation for the local frequencies  $z^\pm(q_0)$  of collective motion, namely,

$$(z^\pm)^2 + i\Gamma(q_0)z^\pm - \mathfrak{w}^2(q_0) = 0, \quad (48)$$

with the local *collective* frequency being defined as

$$\mathfrak{w}^2(q_0) = \Omega^2(q_0) + k/M(q_0) < \Omega^2(q_0). \quad (49)$$

The last inequality is given because we are dealing with isoscalar modes where  $k < 0$ . Notice that the collective frequency  $\mathfrak{w}$  may become purely imaginary, whereas the intrinsic one  $\Omega$  is always real [see Eq. (45)].

Now the frequencies  $z^\pm(q_0)$  are no longer real quantities. A convenient form is seen to be

$$z^\pm(q_0) = |\mathfrak{w}(q_0)| \left[ \pm \sqrt{\text{sgn } \mathfrak{w}^2(q_0) - \eta^2(q_0)} - i\eta(q_0) \right], \quad (50)$$

with

$$\eta(q_0) = \frac{\Gamma(q_0)}{2|\mathfrak{w}(q_0)|}. \quad (51)$$

The dimensionless parameter  $\eta(q_0)$  measures the degree of damping: It is smaller (larger) than 1 if the (local) collective motion is underdamped (overdamped). In the stable case  $\mathfrak{w}^2(q_0) > 0$  the frequencies  $z^\pm(q_0)$  of Eq. (50) are found in the lower complex half plane symmetrically to the imaginary axis for  $\eta(q_0) < 1$  and on the negative imaginary axis for  $\eta(q_0) > 1$ . In the unstable case  $\mathfrak{w}^2(q_0) < 0$  they always lie on the imaginary axis, but now the frequency  $z^+(q_0)$  is in the upper half plane.

It may be worthwhile to briefly compare Eq. (47) with the undamped case. It is easily recognized that for vanishing  $\Gamma$  the form (47) turns into Eq. (37) under the following conditions: (a) Eq. (36) is evaluated at  $z$  instead of  $i\nu_r$ , (b) simply one (pair of) local collective mode(s)  $\mathfrak{w}(q_0)$  is considered instead of all local RPA modes  $\omega_\nu(q_0)$ , (c) the intrinsic frequencies  $\epsilon_{lk}(q_0)/\hbar$  are replaced by  $\Omega(q_0)$ .

### B. The crossover temperature for damped motion

There is no change in the condition (29) for convergence of the integrals in Eq. (28). It is only that Eq. (29) takes on a different form in terms of the transport coefficients. More-

over, the  $\chi(q_0, i\nu_r)$  may be expressed by the transport coefficients by making use of Eq. (47). In this way Eq. (29) turns into

$$\nu_r^2 + \Gamma(q_0)\nu_r + \mathfrak{w}^2(q_0) > 0, \quad (52)$$

as a natural generalization of Eq. (38). Still, for a real collective frequency this condition is always fulfilled. For a purely imaginary one, on the other hand, Eq. (52) can be fulfilled only if the  $\nu_r$  is larger than

$$\nu_r^+ = |\mathfrak{w}(q_0)| \left[ -\eta(q_0) + \sqrt{\eta^2(q_0) - \text{sgn } \mathfrak{w}^2(q_0)} \right]. \quad (53)$$

Hence,  $T$  has to be larger than the local crossover temperature

$$T_0(q_0) = \frac{\hbar |\mathfrak{w}(q_0)|}{2\pi} \left[ \sqrt{1 + \eta^2(q_0)} - \eta(q_0) \right]. \quad (54)$$

Evidently, the  $T_0(q_0)$  is decreasing with growing damping strength  $\eta(q_0)$ . For  $\eta(q_0) \gg 1$  one has  $T_0(q_0) \sim 1/2\eta(q_0)$ . The global crossover temperature, finally, has to be defined as

$$T_0 = \max T_0(q_0). \quad (55)$$

For vanishing damping we recover Eq. (39) with  $\mathfrak{w}(q_0)$  being identical to  $\omega_\nu(q_0)$ .

## IV. THE FISSION RATE WITHIN THE PSPA

Imagine that we are given a heavy nucleus that may decay by fission, a process that is to be understood as collective motion across a barrier. It is known that at smaller temperatures this barrier may have substructure due to shell effects. Such details shall be neglected here. Rather we shall assume the process to be dominated by just one potential minimum and one pronounced barrier. Likewise, we shall discard any evaporation of light particles and  $\gamma$ 's. Moreover, the transfer of energy from the collective degree of freedom to the nucleonic ones will be supposed not to change much the latter's temperature. Under such circumstances the previously discussed path integral formulation may be applied, with a fixed temperature. As noted earlier, for the PSPA we expect great similarities to processes that are described on the basis of the Caldeira-Leggett Hamiltonian.

There, the decay rate  $R$  of unstable systems at not too small temperatures is traced back to the imaginary part of the free energy. As can be seen in the literature, see, e.g., [4], [3]: or [2], for  $T > T_0$  the following formula is in wide use:

$$R = -\frac{2}{\hbar} \frac{T_0}{T} \text{Im } \mathcal{F}(\beta). \quad (56)$$

It has originally been postulated in Refs. [26,27] and, in strict sense, still lacks a general proof from first principles. However, it can be said that it is capable of reproducing correctly certain limits. For instance, one recovers correctly Kramers' high-temperature limit, and in the quantum limit one gets the same functional form as obtained with real-time path integrals [7] or in a quantum transport theory [6].

To evaluate the imaginary part of the free energy one still uses the relation  $\mathcal{F}(\beta) = -T \ln Z(\beta)$  to the partition function. For an unstable system the latter attains an (exponentially small) imaginary part. Following Langer [26] this may be shown by applying the saddle point approximation and distorting the integration contour into the complex plane at the barrier. Expanding the logarithm to first order in the exponentially small quantity  $\text{Im} Z(\beta)/\text{Re} Z(\beta)$  the imaginary part of the free energy becomes

$$\text{Im} \mathcal{F}(\beta) \approx -T \frac{\text{Im} Z(\beta)}{\text{Re} Z(\beta)}. \quad (57)$$

Plugging Eq. (57) into Eq. (56) we obtain

$$R = \frac{2T_0}{\hbar} \frac{\text{Im} Z(\beta)}{\text{Re} Z(\beta)}. \quad (58)$$

The partition functions appearing here may be evaluated within the PSPA extending formula (31) to a dissipative system as outlined in Sec. III. Applying the saddle point approximation to the  $q_0$  integral in Eq. (31) we obtain

$$\begin{aligned} Z^{\text{PSPA}}(\beta)|_{q_a} &= \frac{1}{\sqrt{-k C_{\mathcal{F}}(q_a)}} \\ &\times \exp[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_a)] C^{\text{PSPA}}(\beta, q_a), \end{aligned} \quad (59)$$

as the contribution from the minimum and the purely imaginary expression

$$\begin{aligned} Z^{\text{PSPA}}(\beta)|_{q_b} &= \frac{i}{2\sqrt{-k |C_{\mathcal{F}}(q_b)|}} \\ &\times \exp[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_b)] C^{\text{PSPA}}(\beta, q_b), \end{aligned} \quad (60)$$

as the contribution from the barrier. Here, the stiffnesses

$$\partial^2 \mathcal{F}^{\text{SPA}}(\beta, q_0) / \partial q_0^2 = C_{\mathcal{F}}(q_0), \quad (61)$$

of the SPA free energy at fixed temperature appear, as it was assumed that the integrand is dominated by the exponential and that the correction factor  $C^{\text{PSPA}}(\beta, q_0)$  varies smoothly with  $q_0$ . The stationary points are thus defined by this free energy through  $\partial \mathcal{F}^{\text{SPA}} / \partial q_0 = 0$ . Evaluating the intrinsic free energy in SPA from Eq. (19) with  $C \equiv 1$  it is easy to convince oneself that the extremal points fulfill the relation

$$q_{a/b} = k \langle \hat{F} \rangle_{q_{a/b}}. \quad (62)$$

The derivatives of the eigenvalues  $\epsilon_l(q_0)$  with respect to  $q_0$  needed here may be obtained from time-independent perturbation theory. In Eq. (62) the indices  $a$  and  $b$  stand for the minimum and the maximum (or barrier) of  $\mathcal{F}^{\text{SPA}}(q_0)$ , respectively. The relations (62) are nothing else but the self-consistency condition (10) applied to the two stationary points of the system. Whereas Eq. (59) was obtained through

the common Gaussian integrals of the saddle point approximation, for Eq. (60) the integration contour had to be deformed such that it runs parallel to the positive imaginary axis. This is the reason for the additional factor 2 in the denominator of Eq. (60), see Refs. [26–28].

The generalization of the PSPA correction factor (30) to damped quantum systems may be performed by replacing the response function (35) of the independent particle model by its continuous version (42). Furthermore, we may make use of the transport coefficients introduced in Sec. III A. In this way one gets

$$C^{\text{PSPA}}(\beta, q_0) = \prod_{r>0} \frac{\nu_r^2 + \Gamma(q_0)\nu_r + \Omega^2(q_0)}{\nu_r^2 + \Gamma(q_0)\nu_r + \varpi^2(q_0)}. \quad (63)$$

As mentioned earlier, in comparison to Eq. (36) there is only one (pair of) mode(s). The relation between the local nucleonic frequency  $\Omega(q_0)$  and the local collective frequency  $\varpi(q_0)$  is given by Eq. (49). It is worth stressing that the infinite product (63) is convergent. To guarantee this important feature, it suffices to have the same coefficients for local inertia and damping in the numerator and the denominator [29].

Plugging Eqs. (54), (59), and (60) into Eq. (58) we obtain the following expression for the PSPA decay rate of the system under consideration:

$$\begin{aligned} R^{\text{PSPA}} &= \frac{|\varpi_b|}{2\pi} (\sqrt{1 + \eta_b^2} - \eta_b) \\ &\times \sqrt{\frac{C_{\mathcal{F}}(q_a)}{|C_{\mathcal{F}}(q_b)|} \frac{\exp[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_b)]}{\exp[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_a)]}} \\ &\times \frac{C^{\text{PSPA}}(\beta, q_b)}{C^{\text{PSPA}}(\beta, q_a)}. \end{aligned} \quad (64)$$

Like in the sequel we have partly used indices “ $b$ ” instead of an argument  $q_b$  to keep our notation short. The two first factors, which in a sense represent dynamics, have come in through the crossover temperature  $T_0(q_0)$  discussed in Sec. III B, mind Eq. (54) in particular. Like in the Caldeira-Leggett model the decay rate factorizes into a classical part  $R_{\text{class}}^{\text{PSPA}}$  and a quantum correction factor  $f_{\text{qm}}^{\text{PSPA}}$ ,

$$R^{\text{PSPA}} = R_{\text{class}}^{\text{PSPA}} \times f_{\text{qm}}^{\text{PSPA}}, \quad (65)$$

with

$$\begin{aligned} R_{\text{class}}^{\text{PSPA}} &= \frac{|\varpi_b|}{2\pi} \sqrt{\frac{C_{\mathcal{F}}(q_a)}{|C_{\mathcal{F}}(q_b)|} \frac{\exp[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_b)]}{\exp[-\beta \mathcal{F}^{\text{SPA}}(\beta, q_a)]}} \\ &\times (\sqrt{1 + \eta_b^2} - \eta_b), \end{aligned} \quad (66)$$

and

$$f_{\text{qm}}^{\text{PSPA}} = \frac{C^{\text{PSPA}}(\beta, q_b)}{C^{\text{PSPA}}(\beta, q_a)}, \quad (67)$$

respectively.

Let us discuss first the factor  $R_{\text{class}}^{\text{PSPA}}$  that survives the classical limit, as no  $\hbar$  is involved. Evidently, it contains the common Arrhenius factor

$$\exp(-\beta E_b) = \exp\{-\beta[\mathcal{F}^{\text{SPA}}(\beta, q_b) - \mathcal{F}^{\text{SPA}}(\beta, q_a)]\}, \quad (68)$$

defined here by the difference  $E_b$  of the free energy between barrier and potential minimum. The influence of damping is given by the correction factor found first by Kramers [30], namely,

$$f_K = \sqrt{1 + \eta_b^2} - \eta_b. \quad (69)$$

It decreases monotonically with increasing  $\eta_b$  and for  $\eta_b \gg 1$  behaves like  $1/2 \eta_b$ . The remaining factor can be made to become proportional to the attempt frequency  $\varpi_a$  at the minimum by writing

$$\frac{|\varpi_b|}{2\pi} \sqrt{\frac{C_{\mathcal{F}}(q_a)}{|C_{\mathcal{F}}(q_b)|}} = \frac{\varpi_a}{2\pi} \sqrt{\frac{M_a}{M_b}} \sqrt{\frac{|C^{\text{coll}}(q_b)|}{C^{\text{coll}}(q_a)}} \sqrt{\frac{C_{\mathcal{F}}(q_a)}{|C_{\mathcal{F}}(q_b)|}}. \quad (70)$$

Here, use has been made of the relation between the frequency and inertia of the local mode and the associated stiffness,

$$C^{\text{coll}}(q_0) = M(q_0) \varpi^2(q_0). \quad (71)$$

Putting all factors together the classical rate may be written as

$$R_{\text{class}}^{\text{PSPA}} = R_K f_{\text{class}}^{\text{PSPA}}. \quad (72)$$

It contains Kramers' original form

$$R_K = \frac{\varpi_a}{2\pi} e^{-\beta E_b} (\sqrt{1 + \eta_b^2} - \eta_b), \quad (73)$$

as the first factor. In addition there is a another correction factor

$$f_{\text{class}}^{\text{PSPA}} = \sqrt{\frac{M_a}{M_b}} \sqrt{\frac{|C^{\text{coll}}(q_b)|}{C^{\text{coll}}(q_a)}} \sqrt{\frac{C_{\mathcal{F}}(q_a)}{|C_{\mathcal{F}}(q_b)|}}, \quad (74)$$

not present in the derivations based on the Caldeira-Leggett model. The reasons for that are obvious. First of all, in this model the inertia in the collective mode is simply put equal to a constant that renders the first factor on the right of Eq. (74) equal to unity. Second, the dynamical stiffness (71) is forced to be identical to the one of the phenomenologically introduced collective potential,  $\partial^2 V(q)/\partial q^2$  in Refs. [1,3,4]. This is achieved by working with a Hamiltonian in which from the beginning the collective part is renormalized by the term  $\chi(0)q^2/2$ , which in the linear response approach is induced by the static influence of the coupling. In this way only the dynamical part of the induced force appears, which in the end may lead to Ohmic friction. In our approach, where *all transport properties* of the collective dynamics are generated from the two body interaction, such manipulations

are not meaningful. In certain limits it is possible, however, to simplify the  $f_{\text{class}}^{\text{PSPA}}$  of Eq. (74). For slow collective motion, sometimes referred to as the zero frequency limit, the local stiffness (71) of collective motion may be shown to be represented by that of the free energy (61) (see, e.g., Ref. [5]) such that one simply has

$$f_{\text{class}}^{\text{PSPA}} \approx \sqrt{\frac{M_a}{M_b}}. \quad (75)$$

For a derivation of this factor based on a generalized version of Kramers' equation and picture of the decay we like to refer to Eq. [31].

Next, we turn to the *quantum corrections* to the classical rate (66), which in this approach is given by the ratio of the PSPA corrections  $C^{\text{PSPA}}(\beta, q_0)$  of Eq. (63) evaluated at the barrier and the minimum. With the help of the local nucleonic and collective frequencies  $\Omega(q_0)$  and  $\varpi(q_0)$  it writes

$$f_{\text{qm}}^{\text{PSPA}} = \prod_{r>0} \frac{\nu_r^2 + \Gamma_b \nu_r + \Omega_b^2}{\nu_r^2 + \Gamma_b \nu_r + \varpi_b^2} : \prod_{r>0} \frac{\nu_r^2 + \Gamma_a \nu_r + \Omega_a}{\nu_r^2 + \Gamma_a \nu_r + \varpi_a^2}. \quad (76)$$

The nice feature about this structure is that it converges for *all* conceivable values of the transport coefficients as long as  $T > T_0$ . The reason simply is that it is the ratio of two convergent products of type (63). As the alert reader may guess a simple generalization of the quantum correction factor of the Caldeira-Leggett model (see, e.g., Refs. [3,4]) to coordinate-dependent coefficients such as

$$f_{\text{qm}}^{\text{LC}} \rightarrow \prod_{r>0} \frac{\nu_r^2 + \Gamma_a \nu_r + \varpi_a^2}{\nu_r^2 + \Gamma_b \nu_r + \varpi_b^2} \quad (77)$$

(see, e.g., [32]) may (for Ohmic damping where  $\Gamma$  does not fall off for large frequencies) lead to problems of convergence. Indeed, for  $\Gamma_a \neq \Gamma_b$  the infinite product either converges to zero or diverges depending which one of the  $\Gamma$ 's is larger [29]. In Ref. [6] the form (77) has been derived on the basis of a quantum transport equation. In Ref. [33] this factor has been evaluated for microscopically calculated transport coefficients. To circumvent the convergence problem in Eq. (77) the individual  $\Gamma$ 's had been replaced by the arithmetic mean value  $2\bar{\Gamma} = \Gamma_a + \Gamma_b$ .

The local frequency of the collective motion  $\varpi$  is real at the minimum and purely imaginary at the barrier, whereas the frequency of the nucleonic motion  $\Omega$  is real everywhere. The denominator of the first term in Eq. (76) vanishes as  $T$  approaches  $T_0$ , corresponding to the definition of the crossover temperature in Sec. III B [see Eq. (52)], but all other factors are strictly positive. For this reason, at  $T_0$  the quantum correction factor  $f_{\text{qm}}^{\text{PSPA}}$  diverges to plus infinity, a feature well known from the Caldeira-Leggett model [22].

In the limit of very high temperatures  $T \gg \hbar \Omega$ , where  $\hbar \Omega$  represents the typical nucleonic excitation,  $f_{\text{qm}}^{\text{PSPA}}$  strictly converges to unity. For nuclear fission, collective motion is expected to be slow in the sense [31] of having



$$1 \text{ MeV} \approx \hbar \varpi \ll \hbar \Omega \approx \frac{41 \text{ MeV}}{A^{1/3}} \approx 6 \text{ MeV}. \quad (78)$$

One may expect quantum effects in collective motion to disappear already for  $T \gg \hbar \varpi$ . Indeed, the quantum correction factor will be close to unity already for  $T/\hbar \Omega = O(1)$ . At least this can be shown for the two factors of Eq. (76). Divide all numerators and denominators by  $\nu_r^2$  and neglect  $(\varpi/\nu_r)^2 \ll 1$  in the resulting denominators. This is justified simply because the condition  $T/\hbar \Omega \approx O(1)$  implies  $\Omega/\nu_r \approx 1/(2\pi r)$  [mind Eq. (5)]. Remain the terms which involve  $\Gamma/\nu_r$ . They can be neglected if  $T \gg (1/2\pi)\hbar\Gamma$  or  $T/\hbar\varpi \gg \eta/\pi$ . Microscopic computations of the transport coefficients show this condition to be fulfilled, although  $\eta$  itself increases with  $T$ ; see Fig. 3 of [31] or Fig. 5.2.10 of Ref. [5].

## V. CONCLUSION

We have been able to demonstrate how the PSPA can be extended to treat the decay of damped metastable systems. In this first step a simple schematic two body interaction has been taken and the nucleonic excitations have been assumed to be concentrated in one Lorentzian peak around a certain mean value. Generalizations to more general systems should not cause too many problems. So far we have concentrated on the quantum corrections to thermal hopping that take place above the critical temperature  $T_0$  [6,22]. At this temperature the common semi-classical treatment of functional

integrals breaks down, simply because for unstable modes the Gaussian integrals diverge for smaller temperatures. So far, this latter feature also limited the applications of the PSPA to bound systems [11–13]. There is hope that this deficiency can be overcome in very much the same way as it was possible for dissipative tunneling [22,34]. Work in this direction is under way [35].

There are several advantages of the method presented here, both over the usual approach to dissipative tunneling within the Caldeira-Leggett model [3,4], as well as with respect to the locally harmonic approximation (LHA) [5] to quantum transport. Different from the Caldeira-Leggett model, all transport properties derive from the two body interaction of the many body system. No phenomenological assumptions have to be made for any transport coefficient. The effects of the two body interaction are treated on a fully self-consistent level, largely because the collective variables can be introduced globally by way of the Hubbard-Stratonovich transformation. For the LHA, on the other hand, and on a quantum level this is possible only locally [5]. This method, however, is more flexible with respect to the thermal properties. There, one need not rely on the concept of a fixed temperature, an assumption that is questionable for isolated systems.

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