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Effective descriptions of complex quantum systems: path integrals and operator ordering problems

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Dedicated to Bernhard Mühlschlegel on the occasion of his 80th birthday

We study certain aspects of the effective, occasionally called collective, description of complex quantum systems within the framework of the path integral formalism, in which the environment is integrated out. Generalising the standard Feynman-Vernon Caldeira-Leggett model to include a non-linear coupling between "particle" and environment, and considering a particular spectral density of the coupling, a coordinate-dependent mass (or velocity-dependent potential) is obtained. The related effective quantum theory, which depends on the proper discretisation of the path integral, is derived and discussed. As a result, we find that in general a simple effective low-energy Hamiltonian, in which only the coordinate-dependent mass enters, cannot be formulated. The quantum theory of weakly coupled superconductors and the quantum dynamics of vortices in Josephson junction arrays are physical examples where these considerations, in principle, are of relevance.

1 Introduction

Since the seminal contributions by Richard Feynman in 1948, it is clear that the description of quantum and quantum statistical systems can be based either on wave-functions and the Schrödinger equation, or on the path integral prescription for computing the propagator and/or the partition function. Both descriptions are equivalent: Given a certain Schrödinger equation, the corresponding path integral can be formulated, and, alternatively, a path integral expression can be used to define a quantum theory. In particular, the latter route appears to have advantages in complex many-body systems and for field theories. These topics are, of course, well documented in several textbooks, for example, by Feynman and Hibbs [1], Schulman [2], Sakita [3], and Kleinert [4]. In order to set the stage, consider e. g. the partition function of a simple quantum system,

$$Z = \int \mathcal{D}x \exp(-S_E/\hbar) \ , \tag{1}$$

where S_E is the Euclidean action,

$$S_E[x(\tau)] = \int_0^\beta d\tau \left[\frac{m}{2}\dot{x}^2 + V(x)\right] \ . \tag{2}$$

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As usual, m is the mass of the particle, $V(x)$ the potential, and $\dot{x} \equiv \partial x/\partial\tau$. The symbol $\mathcal{D}x$ is a short-hand notation for a multi-dimensional integral, defined through a discretisation of the interval $0 \ldots \beta$, by putting $\tau_j = j\epsilon$, $j = 0, 1, 2, \ldots, N$ ($\beta = N\epsilon$), and $x(\tau_j) = x_j$, in the limit $N \to \infty$, $\epsilon \to 0$ so that $\beta = \hbar/k_B T$ (where T is the temperature) remains finite. With an appropriate deformation of the time-integration contour, and adding appropriate source fields, Eq. (1) can be generalised to a generating functional for real-time correlation functions, e. g., in analogy to the diagrammatic technique due to Keldysh [5]. Note that, when evaluating the multi-dimensional integral in Eq. (1), the correct integration measure is essential – and that appropriate paths have to be taken into account: for the propagator, x_0 and x_N are to be kept fixed, while for the partition function, $x_0 = x_N$ with an additional integration with respect to this variable (since Z is a trace).

In a more general situation, say, in which the potential is velocity dependent (as for a charged particle) it is essential to choose the correct discrete representation, which is known as the mid-point prescription, i. e.

$$\int d\tau \dot{x} a(x) \to \epsilon \sum_j \frac{(x_j - x_{j-1})}{\epsilon} a\left(\frac{x_j + x_{j-1}}{2}\right) . \tag{3}$$

This prescription ensures that the corresponding Hamiltonian operator contains the symmetric form $\hat{p}a(\hat{x}) + a(\hat{x})\hat{p}$, and hence its hermiticity. (The physically relevant case for this example is, of course, in three dimensions.) A closely related problem appears in the theory of Brownian motion, in particular, for the Ornstein-Uhlenbeck process, defined by the Langevin equation

$$\eta\dot{x} = -kx + \xi(t) , \tag{4}$$

where $\xi(t)$ represents Gaussian white noise (with zero average). Considering the generalisation where $-kx$ is replaced by some function $f(x)$, and starting from the Gaussian probability density for the noise, it is straightforward to derive the probability density for the random process $x(t)$, $W(\{x\})$, with the help of Eq. (4):

$$W(\{x\})\mathcal{D}x = W(\{\xi\})\mathcal{D}\xi . \tag{5}$$

The result is unique, as is the corresponding Fokker-Planck equation; the intermediate steps, however, depend on the discretisation procedure, the two cases discussed in this context being connected with the names Itô (forward rule) and Stratonovich (mid-point rule) [6]. In the former, the Jacobian of the transformation is a mere constant, but the integral of $\dot{x}f(x)$ has a non-trivial contribution; in the latter, the integral of $\dot{x}f(x)$ depends only on the end-points – but care is needed to evaluate the Jacobian. Physically, this difficulty is related to the irregularity of the Brownian motion, and hence can be cured, for example, by introducing a finite mass term $m\ddot{x}$ into Eq. (4). A concise discussion of the question of operator ordering and functional formulations in both quantum and stochastic dynamics[1] can be found in [8]; the arguments given above, to the best of our knowledge, were first formulated by Schmid [9] (see also [10]).

Until now, we implicitly assumed that the Hamilton operator of the system in question is given – and we will make the same assumption in the following sections, as we have in mind applications to condensed matter physics. We would mention, however, that a more general question is (still) studied intensively in mathematical physics: Given a classical Hamiltonian function, what is the "correct" quantum theory? For an introduction to related topics, see, for example, [11]; in this connection, the concept of Weyl ordering ([3], chap. VI, and [11]; see also below) is useful: as is well known, a Weyl ordered Hamiltonian corresponds to a path integral defined by the mid-point rule. In complex many-body systems, a related question shows up

[1] An "elementary" treatment of the "path integral associated with the Fokker-Planck equation" was given by Bernhard Mühlschlegel in [7], with emphasis "on the structure of the equation of motion and its relation to a self-adjoint problem". The coordinate-dependent mass considered here corresponds to a coordinate-dependent diffusion "constant" in the Fokker-Planck language.

in a natural way when formulating an effective quantum theory by integrating out a subset of the variables – and this is the focus of the present paper.

In the next section, Sect. 2, we briefly recapitulate the essence of the Feynman-Vernon [12] Caldeira-Leggett [13] model, which is based on the assumption that, in a complex many-body system, a suitable coordinate ("particle") can be identified; and that this particle is weakly coupled to the remaining degrees of freedom ("bath"). The choice of the coupling and the bath, the latter typically assumed to be a set of harmonic oscillators, depends on the problem under consideration: in particular, the choice which corresponds to an effective dissipation has attracted considerable attention (see [14] and [15] for reviews). The following Sect. 3 is devoted to weakly coupled superconductors where, as shown from microscopic theory [16–18], the coupling between particle (i.e. the order parameter phase) and environment (i.e. the electronic degrees of freedom) can be considered as non-linear, reflecting the 2π-periodicity of the phase variable [19]. As a result, a phase-dependent mass (i.e. capacitance in this case) is found in the effective action [17, 18]; see also [20, 21]. In the central Sect. 4, we investigate in detail one of the simplest models corresponding – in the classical limit and for low frequencies – to a coordinate-dependent mass in the effective action. We briefly review some classical aspects, and discuss the relation between operator ordering and path integral formulation. Using the (discrete) path integral formulation as well as perturbation theory and a variational approach, we then discuss the question whether, in general, an effective low-energy quantum description exists which can be expressed in terms of the coordinate-dependent mass. The conclusions are summarised in Sect. 5.

2 The paradigmatic model

The Feynman-Vernon Caldeira-Leggett [12, 13] (FV-CL) model is defined through the following Hamilton operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) + \sum_{\mu} \left[\frac{\hat{p}_\mu^2}{2} + \frac{\omega_\mu^2}{2} \Big(\hat{x}_\mu - \frac{C_\mu}{\omega_\mu^2} \hat{x} \Big)^2 \right] \tag{6}$$

where $\hat{p}$, $\hat{x}$ and $\hat{p}_\mu$, $\hat{x}_\mu$ denote the momentum and position operators of the particle and the environment, respectively, the latter being labelled by μ. The masses of the oscillators, without loss of generality, have been put equal to unity, and the $\{C_\mu\}$ are the particle-environment coupling constants. We have chosen the form of the coupling above so that certain counter terms are avoided. For the next step, it is important that the coupling, $\hat{x} \sum_\mu C_\mu \hat{x}_\mu$, is linear in the bath variables $\{\hat{x}_\mu\}$, in order to allow them to be integrated out easily. (We could, of course, have chosen a coupling to the momenta $\{\hat{p}_\mu\}$ as well.) Performing the integration, one finds an effective action which contains the particle variable only; the properties of the bath and the particle-bath coupling are absorbed in a certain correlation function. The result is

$$S_E^{(\mathrm{eff})} = S_E^{(0)} + S_E^{(1)} \,, \tag{7}$$

where $S_E^{(0)}$ is given by Eq. (2), and

$$S_E^{(1)} = \frac{1}{2} \int_0^\beta d\tau \int_0^\beta d\tau' \alpha(\tau - \tau') \Big[x(\tau) - x(\tau') \Big]^2 \,. \tag{8}$$

Here the function $\alpha(\tau)$, which is an even function of time, is given by

$$\alpha(\tau) = (2\beta)^{-1} \sum_\omega \mathrm{e}^{-i\omega\tau} \sum_\mu \frac{C_\mu^2}{\omega^2 + \omega_\mu^2} \tag{9}$$

and has the alternative representation

$$\alpha(\tau) = \int_{-\infty}^{+\infty} \frac{d\nu}{2\pi} J(\nu) [-b(-\nu)] \mathrm{e}^{-\nu|\tau|} \tag{10}$$

where $J(\nu)$ is given by

$$J(\nu) = \frac{\pi}{2} \sum_{\mu} \frac{C_\mu^2}{\omega_\mu} \Big[\delta(\nu - \omega_\mu) - \delta(\nu + \omega_\mu) \Big] \ . \tag{11}$$

Above, $\omega = 2\pi n/\beta$ are the Matsubara frequencies, and $b(\cdot)$ is the Bose function. The dissipative case is realised by choosing an infinite set of bath oscillators with a dense frequency distribution, so that $J(\nu) = \eta\nu$ for small ν, which corresponds to $\alpha(\omega) = \alpha(0) - (\eta/2)|\omega|$ and, in the zero-temperature limit ($\beta \to \infty$), to $\alpha(\tau) = (\eta/2\pi)\tau^{-2}$. The parameter η is the viscosity, entering the classical (real-time) equation of motion in the form $m\ddot{x} + \eta\dot{x} = \ldots$; for further details, see, for example, [13] and [22]. Note the close correspondence of $J(\nu)$ to the function $\alpha^2 F(\nu)$, well-known from the theory of superconductivity [23].

In contrast, consider a situation where there is a gap in the spectrum of the bath oscillators, so that $J(\nu) = 0$ for $|\nu| < \Delta$. Then $\alpha(\omega) = \alpha(0) - (m/2)\lambda\omega^2$ for small frequencies, thereby defining the parameter λ (> 0). This implies a mass enhancement according to $m \to m(1 + \lambda)$, well-known from the polaron problem; compare [1], Chap. 11-4, or [2], Chap. 21. Explicit results are easily obtained for the simplest case of a *single* bath oscillator.

Generalisations can be obtained by considering a non-linear coupling between particle and environment, i. e. by replacing $\hat{x}$ by a non-linear function $g(\hat{x})$ in the last term of Eq. (6). Furthermore, several environments can be introduced, for convenience chosen to be independent of each other, so that

$$\{\hat{p}_\mu, \hat{x}_\mu\} \to \{\hat{p}_\mu^{(m)}, \hat{x}_\mu^{(m)}\} \ , \quad g(\hat{x}) \to g^{(m)}(\hat{x}) \ . \tag{12}$$

As a result, Eq. (8) generalises to the following expression:

$$S_E^{(1)} = \frac{1}{2} \sum_{m} \int_0^\beta d\tau \int_0^\beta d\tau' \alpha^{(m)}(\tau - \tau') \Big[g^{(m)}(x(\tau)) - g^{(m)}(x(\tau')) \Big]^2 \ . \tag{13}$$

It is clear that in general an equivalent Hamiltonian description does not exist; we return to this question in Sect. 4.

3 Weakly coupled superconductors

In this section, we briefly review the steps which lead to an effective quantum description of weakly coupled superconductors, i. e. Josephson junctions [16–18], and recall how the effective action also can be derived within the generalisation of the FV-CL model as given by Eq. (13). The starting point is the BCS model of superconductivity, i. e. electrons which weakly attract each other. Two of these BCS superconductors are weakly coupled by the tunneling Hamiltonian [24], which allows for electron transfer from one superconductor to the other. In the first step, within the path integral formulation, complex order parameter fields are introduced to decouple the attractive interaction. Similarly, the Coulomb interaction between charges near the junction surfaces, which becomes an effective capacitive interaction, is described by a voltage field. In an intermediate step, we obtain a form which is bilinear in the four-dimensional (left/right, spin-up/spin-down) space of the fermionic (Grassmann) variables. In the second step, the fermionic fields are integrated out. In addition, it is advantageous to perform a gauge transformation which makes the particle-hole off-diagonal elements real and reveals the role of the order parameter phases. In a third step, the action is expanded (up to second order) in the tunnel matrix elements. Based on a detailed analysis of the different contributions one can show that the effective low-frequency action, which is a functional of the phase difference ϕ across the junction, is given by

$$S_E^{(\mathrm{JJ})} = S_E^{(\mathrm{C})} + S_E^{(\mathrm{T})} \tag{14}$$

where

$$S_E^{(\mathrm{C})} = \int_0^\beta d\tau \left[\frac{\hbar^2 C}{8e^2} \dot{\phi}^2 - \frac{\hbar I}{2e} \phi \right] \tag{15}$$

contains the capacitive energy (capacitance: C) as well as the contribution from the external current (I), and

$$S_E^{(\mathrm{T})} = \hbar \int_0^\beta d\tau \int_0^\beta d\tau' \left[-\alpha(\tau - \tau') \cos \frac{\phi(\tau) - \phi(\tau')}{2} + \beta(\tau - \tau') \cos \frac{\phi(\tau) + \phi(\tau')}{2} \right] . \tag{16}$$

Here we use the same notation as in [16]. The kernels $\alpha(\cdot)$ and $\beta(\cdot)$ are related to the diagonal and off-diagonal (equilibrium) Green's functions of the superconductors, and hence can be expressed through the functions $I_n(\nu)$ and $I_c(\nu)$ which characterise the quasiparticle current and the supercurrent across the junction [25] (see also [19]). Considering zero temperature and slow variations (compared to the inverse gap frequency) in time, we may use the expansions $\alpha(\omega) = \alpha_0 - \alpha_2\omega^2/2$ and $\beta(\omega) = -\beta_0 + \beta_2\omega^2/2$ (where α_2, β_0, β_2 are all positive; α_0 is irrelevant) to show that the β_0-term leads to the usual cosine potential, $-E_J \cos\phi$, where $E_J = \pi\hbar\Delta/4e^2R_N$ is the Josephson coupling energy; and that the α_2- and β_2-contributions change the capacitance (i. e. the "mass") according to

$$C \to C(\phi) = C + C_{\mathrm{qp}} \left(1 - \frac{1}{3} \cos\phi \right) \tag{17}$$

where $C_{\mathrm{qp}} = 3\pi\hbar/(32\Delta R_N)$; Δ is the superconducting gap, assuming the two superconductors to be equal, and R_N the normal-state resistance of the junction.

The above model, often – for simplicity – considered in the limit $C_{\mathrm{qp}} \ll C$, is also a good starting point for discussing the quantum properties of an array of Josephson junctions, for example the quantum dynamics of a vortex [26]: in this case, a position-dependent mass arises due to the lattice structure of the underlying array of superconducting grains.[2]

Considering again Eq. (13), it is apparent that the effective action of a Josephson junction, Eq. (16), can be "derived" from the generalisation of the FV-CL model by an appropriate choice of $g^{(m)}(\cdot)$ and $\alpha^{(m)}(\cdot)$, in particular, using $g^{(1)}(\phi) = \sin(\phi/2)$, and $g^{(2)}(\phi) = \cos(\phi/2)$; see [19] for details.

4 Coordinate-dependent mass and effective Hamiltonian

In Sect. 2 we have shown that a coordinate-dependent mass can be considered as originating from a quite simple model, namely a particle coupled non-linearly to a harmonic oscillator of finite frequency.[3] Hence we will study in this section the following Hamilton operator in more detail:

$$H = \frac{\hat{p}^2}{2m} + V(\hat{x}) + \frac{1}{2}\left[\hat{p}_\mu^2 + \omega_\mu^2 \hat{x}_\mu^2\right] + g(\hat{x})\hat{x}_\mu + \frac{g^2(\hat{x})}{2\omega_\mu^2} . \tag{18}$$

The subscript "μ" is kept for easy distinction. As an alternative, we may perform a unitary transformation [31]: Defining $U = \exp[ig(\hat{x})\hat{p}_\mu/\hbar\omega_\mu^2]$, we obtain

$$\tilde{H} \equiv U^+ H U = \frac{1}{2m}\Big(\hat{p} + a(\hat{x}, \hat{p}_\mu)\Big)^2 + V(\hat{x}) + \frac{1}{2}\left[\hat{p}_\mu^2 + \omega_\mu^2 \hat{x}_\mu^2\right] \tag{19}$$

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[2] In the absence of additional shunt resistors, and for zero external current, it is important that the phase variable is defined on the interval $0 \ldots 2\pi$, with 0 and 2π to be identified, thus requiring a different interpretation of the path integral; see e. g. [2], Chap. 23.

[3] Some aspects of this model were discussed a while ago [27]. In particular, it was pointed out that it is legitimate to define an effective Hamiltonian by tracing over some of the system's variables.

where $a(\hat{x},\hat{p}_\mu) = g'(\hat{x})\hat{p}_\mu/\omega_\mu^2$. In $\tilde{H}$, the coupling is to the momentum of the oscillator, and involves directly the derivative of the coupling function, $g'(\hat{x})$ (which turns out to be useful). We also note that in the derivation of the effective action on the basis of the transformed Hamiltonian, it is convenient to consider the phase-space representation of the path integral, and to integrate first with respect to the particle momenta.

4.1 The polaronic toy model: classical aspects

In order to derive the classical low-frequency effective action of the model defined by Eq. (18) or Eq. (19), we concentrate on the zero-temperature limit where $\alpha(\tau) = (4\omega_\mu)^{-1}\exp(-\omega_\mu|\tau|)$, and consider slow variations in time (compared to ω_μ^{-1}) so that we may expand the effective action as

$$S_E^{(1)} = \frac{1}{2}\int d\tau \int d\tau' \alpha(\tau-\tau')\Big[g(x(\tau)) - g(x(\tau'))\Big]^2 \approx \frac{\alpha_2}{2}\int d\tau\,[g_1(x)]^2\,\dot{x}^2 \tag{20}$$

where $g_1(x) = dg(x)/dx$; the constant $\alpha_2 = -[\alpha''(\omega)]_{\omega\to 0}$ is given by ω_μ^{-4}. For $g_1(x) \equiv 1$, the mass enhancement is simply given by the factor $1+\alpha_2/m$, as discussed in Sect. 2. The last expression in (20) follows by noting that the integrand in the effective action is strongly peaked for $\tau \approx \tau'$, allowing for the approximations

$$x(\tau) \approx x\left(\frac{\tau+\tau'}{2}\right) + \frac{\Delta\tau}{2}\dot{x}\left(\frac{\tau+\tau'}{2}\right)\ ,\ x(\tau') \approx x\left(\frac{\tau+\tau'}{2}\right) - \frac{\Delta\tau}{2}\dot{x}\left(\frac{\tau+\tau'}{2}\right)\ , \tag{21}$$

where $\Delta\tau = \tau - \tau'$ denotes the difference time, and also expanding $g(x(\tau))$ and $g(x(\tau'))$.

Clearly, the effective action of this "polaronic toy model" corresponds to the classical Lagrangian and Hamiltonian

$$\mathcal{L} = \frac{1}{2}m(x)\dot{x}^2 - V(x) \quad\leftrightarrow\quad \mathcal{H} = \frac{p^2}{2m(x)} + V(x) \tag{22}$$

with $m(x) = m + \alpha_2[g_1(x)]^2)$ denoting the coordinate-dependent mass, and $\dot{x} = dx/dt$. The canonical momentum is $p = m(x)\dot{x}$, and the classical equation of motion reads

$$m(x)\ddot{x} + \frac{1}{2}m'(x)\dot{x}^2 = -V'(x)\ . \tag{23}$$

Of course, the energy, $E = m(x)\dot{x}^2/2 + V(x)$, is conserved. In the present – one-dimensional – case (see also [3] and [4], as well as [28] and [29] for related discussions of the general case) it is obvious that the above expressions can be "simplified" by the coordinate transformation $z = z(x)$, defined by $m(x)\dot{x}^2 = \bar{m}\dot{z}^2$ [21,26]. The equation of motion then reads $\bar{m}\ddot{z} = -dU(z)/dz$, where $U(z) \equiv V(x(z))$. Clearly, we have to assume $m(x) > 0$ in order to assure stability; and we will assume below that $m(x)$ is differentiable.

The example discussed in Sect. 3, i. e. weakly coupled superconductors, corresponds to $m(x) = m_0 + m_1\cos x$ with $m_0 = (\hbar^2/4e^2)(C + C_{\rm qp})$, $m_1 = -(\hbar^2/4e^2)C_{\rm qp}/3$, and the momentum to $\hbar/2e$ times the charge. In addition, $V(x) = -E_J\cos\phi - (\hbar I/2e)\phi$; in case the Josephson contact is embedded in a superconducting ring, instead of the term $\sim\phi$, a quadratic contribution $(\phi-\phi_{\rm ext})^2/2L$ arises [32] where $\phi_{\rm ext}$ and L are proportional to the external magnetic flux and the inductance of the ring, respectively.

4.2 Coordinate-dependent mass: some remarks on quantisation

The above considerations suggest a straightforward route to quantise a system with coordinate-dependent mass [3,4,28], namely to consider the z-version $H_z = \hat{p}_z^2/2\bar{m} + U(\hat{z})$ with $[\hat{p}_z,\hat{z}] = \hbar/i$. Transforming

back to the x-representation, the change in the integration measure (consider, e. g., a scalar product) has to be taken into account, since $dx = [\bar{m}/m(x)]^{1/2} dz$. The result is

$$H_{\rm pct} = \frac{1}{2}\frac{1}{m^{1/4}}\hat{p}\frac{1}{m^{1/2}}\hat{p}\frac{1}{m^{1/4}} + V(\hat{x}) \tag{24}$$

where $[\hat{p}, \hat{x}] = \hbar/i$, and the subscript indicates "point canonical transformation". Of course, the point canonical transformation also can be considered within the path integral formulation [3]: Starting from the standard expression for the short-time propagator $\langle z_j | \exp(-\epsilon \hat{H}_z/\hbar) | z_{j-1}\rangle$, namely

$$K_z(z_j, \epsilon | z_{j-1}, 0) = \Big(\frac{\bar{m}}{2\pi\hbar\epsilon}\Big)^{1/2} \exp\Big\{ -\frac{\epsilon}{\hbar}\Big[\frac{\bar{m}}{2\epsilon^2}(z_j - z_{j-1})^2 + U(z_{j-1})\Big]\Big\} , \tag{25}$$

the short-time propagator in x-representation is given by

$$K_{\rm pct}(x_j, \epsilon | x_{j-1}, 0) = \Big[\frac{m(x_j)m(x_{j-1})}{\bar{m}^2}\Big]^{1/4} K_z(z(x_j), \epsilon | z(x_{j-1}), 0) \ . \tag{26}$$

Using the coordinate representation, and taking the limit $\epsilon \to 0$, it is straightforward to confirm the Hamiltonian (24).

Alternatively, the concept of Weyl ordering can be introduced: It is well-known that a Weyl ordered Hamilton operator corresponds to the mid-point description of the path integral [30]. Considering a polynomial expression $\hat{p}^n \hat{x}^m$, the Weyl ordered form $(\hat{p}^n \hat{x}^m)_W$ is obtained by summing over all possible orders, and dividing by their total number. In particular, this implies

$$\Big(\hat{p} f(\hat{x})\Big)_{\rm W} = \frac{1}{2}\Big(\hat{p} f(\hat{x}) + f(\hat{x})\hat{p}\Big) \tag{27}$$

and

$$\Big(\hat{p}^2 f(\hat{x})\Big)_{\rm W} = \frac{1}{4}\Big(\hat{p}^2 f(\hat{x}) + f(\hat{x})\hat{p}^2\Big) + \frac{1}{2}\Big(\hat{p} f(\hat{x})\hat{p}\Big) \ , \tag{28}$$

provided a meaningful power series expansion of $f(\hat{x})$ exists. This leads to

$$H_{\rm W} = \frac{1}{8m}\hat{p}^2 + \hat{p}\frac{1}{4m}\hat{p} + \hat{p}^2\frac{1}{8m} + V(\hat{x}) \ . \tag{29}$$

The pct-Hamiltonian differs from the Weyl Hamiltonian, with the result [3]

$$H_{\rm pct} - \hat{H}_{\rm W} = \frac{\hbar^2}{32}\frac{[m'(\hat{x})]^2}{m(\hat{x})^3} \equiv \mathcal{W}(\hat{x}) \sim \hbar^2 \ . \tag{30}$$

Note that the difference has a definite sign. It was suggested by Ambegaokar [18] that the Weyl ordered form (29) is the correct one for the quantum theory of a Josephson junction.

Defining the mid-point $\bar{x}_j = (x_j + x_{j-1})/2$, we conclude that the short-time (small ϵ) propagator corresponding to $\hat{H}_{\rm W}$ is given by

$$K_{\rm W}(x_j, \epsilon | x_{j-1}, 0) = \int \frac{dp}{2\pi\hbar}\, {\rm e}^{ip(x_j - x_{j-1})/\hbar}\, {\rm e}^{-\epsilon\mathcal{H}(p, \bar{x}_j)/\hbar} \tag{31}$$

with $\mathcal{H}$ defined in Eq. (22); clearly

$$K_{\rm pct}(x_j, \epsilon | x_{j-1}, 0) = K_{\rm W}(x_j, \epsilon | x_{j-1}, 0) \cdot \exp[-\epsilon\mathcal{W}(\bar{x}_j)/\hbar] \ . \tag{32}$$

Note that $\bar{x}_j$ can be replaced by x_j in the last exponential factor, as well as in the potential energy. After integration with respect to the momentum, a "non-trivial" prefactor $\sim [m(\bar{x}_j)]^{1/2}$ arises; this prefactor ensures that the propagators reduce to a δ-function in the limit $\epsilon \to 0$.

4.3 The polaronic toy model: discrete path integrals

In order to determine the correct quantum theory of the simplest model of a particle coupled to an environment, we study the toy model Eq. (18) in more detail. The notation has been introduced in Sect. 1, and everything is straightforward: We retain the discrete version of the path integral in the coordinate representation, and then "integrate out" the oscillator degrees of freedom, with the result

$$Z/Z_\mu = \lim_{N\to\infty} \Big(\frac{m}{2\pi\hbar\epsilon}\Big)^{N/2} \int dx_1 \ldots dx_N \exp\Big(-\frac{S_E^{(0)} + S_E^{(1)}}{\hbar}\Big) \tag{33}$$

where Z_μ is the partition function of the oscillator. It is understood that $x_0 = x_N$. Furthermore, $S_E^{(0)}$ is given by the standard expression, while

$$S_E^{(1)} = \frac{\epsilon^2}{2} \sum_{i,j=1}^{N} \alpha_\mu(\tau_i - \tau_j) \Big[g(x_{i-1}) - g(x_{j-1})\Big]^2 \,. \tag{34}$$

Here $\alpha_\mu(\tau_i - \tau_j)$ is given by an expression similar to Eq. (9), namely

$$\alpha_\mu(\tau) = (2\beta)^{-1} \sum_{\omega}^{\text{1st BZ}} \mathrm{e}^{-i\omega\tau} \frac{1}{[\omega^2]_\epsilon + \omega_\mu^2} \tag{35}$$

where $[\omega^2]_\epsilon \equiv 2[1-\cos(\omega\epsilon)]/\epsilon^2$; the summation is restricted to, say, the first Brillouin zone, i.e. $n = -N/2+1, \ldots, N/2$ (assuming N to be even).

An alternative version of $S_E^{(1)}$ can be obtained directly from the transformed Hamiltonian (19), with the following result:

$$\begin{aligned} \tilde{S}_E^{(1)} = {} & \frac{\epsilon}{2\omega_\mu^4} \sum_{i=1}^{N} g_1^2(\bar{x}_i) \Big(\frac{x_i - x_{i-1}}{\epsilon}\Big)^2 \\ & - \frac{\epsilon^2}{\omega_\mu^4} \sum_{i,j=1}^{N} \gamma_\mu(\tau_i - \tau_j) g_1(\bar{x}_i) g_1(\bar{x}_j) \frac{x_i - x_{i-1}}{\epsilon} \frac{x_j - x_{j-1}}{\epsilon} \,. \end{aligned} \tag{36}$$

In this form, the coordinate-dependent mass correction, $m_1(\bar{x}_i) = g_1^2(\bar{x}_i)/\omega_\mu^4$, is immediately identified; compare Eq. (20). The appearance of the mid-points in this expression is related to the approximation $g(x_j) - g(x_{j-1}) \approx g_1(\bar{x}_j) \cdot (x_j - x_{j-1})$ in an intermediate step.

The kernel $\gamma_\mu(\tau_i - \tau_j)$ can be related to $\alpha_\mu(\tau_i - \tau_j)$ by noting the relations

$$\alpha_\mu(0) = \frac{1}{2\omega_\mu^2} \;;\; \alpha_\mu(\omega) - \alpha_\mu(0) = -\frac{[\omega^2]_\epsilon \alpha_\mu(\omega)}{\omega_\mu^2} \;;\; \gamma_\mu(\omega) = [\omega^2]_\epsilon \alpha_\mu(\omega) \,, \tag{37}$$

which imply

$$\gamma_\mu(\tau_i - \tau_j) = \delta_{ij}/2\epsilon - \omega_\mu^2 \alpha_\mu(\tau_i - \tau_j) \,. \tag{38}$$

Using (37) and (38), the correspondence between $S_E^{(1)}$ and $\tilde{S}_E^{(1)}$ can be established directly. A more compact form also follows easily:

$$\tilde{S}_E^{(1)} = \omega_\mu^{-2} \sum_{i,j=1}^{N} \alpha_\mu(\tau_i - \tau_j) \left[g(x_i) - g(x_{i-1})\right] \left[g(x_j) - g(x_{j-1})\right] \,. \tag{39}$$

For zero temperature, $\alpha_\mu(\tau_i - \tau_j)$ can be found by an elementary integration.

4.4 Linearly coupled harmonic oscillators

In order to illustrate some aspects of the above results, we consider the special case of a linear coupling (i. e. x-independent mass renormalisation: $g(x) = g_1 \cdot x, m_1 = g_1^2/\omega_\mu^4$). In this case, the Fourier representation of the action is useful:

$$\tilde{S}_E^{(1)} = \omega_\mu^{-2} g_1^2 \, \beta^{-1} \sum_\omega \, [\omega^2]_\epsilon \, \alpha_\mu(\omega) \, |x(\omega)|^2 \; . \tag{40}$$

In addition, we assume that the "particle" is a harmonic oscillator of frequency ω_0. Then the following (standard) result is easily confirmed ($\epsilon \to 0$):

$$Z = Z_0 \cdot Z_\mu \cdot \prod_\omega \left[\frac{(\omega^2 + \omega_0^2)(\omega^2 + \omega_\mu^2)}{(\omega^2 + \omega_a^2)(\omega^2 + \omega_b^2)} \right]^{1/2} \; . \tag{41}$$

Here Z_0 and Z_μ are the partition function of the oscillator "0" and "μ", respectively. In addition, ω_a and ω_b denote the eigen-frequencies of the coupled two-oscillator system, which obey the relations

$$\omega_a^2 \cdot \omega_b^2 = \omega_0^2 \cdot \omega_\mu^2 \; , \quad \omega_a^2 + \omega_b^2 = \omega_0^2 + \omega_\mu^2 + (m_1/m)\omega_\mu^2 \; . \tag{42}$$

In particular, considering m_1/m fixed and $\omega_\mu \to \infty$, we find ω_a and ω_b to be given by $\omega_0(1 + m_1/m)^{-1/2}$ and $\omega_\mu(1 + m_1/m)^{1/2}$, respectively. Naturally, as long as $\omega_0 \ll \omega_\mu$, the low-temperature ($k_B T \ll \hbar\omega_\mu$) thermodynamics is determined by the low-frequency oscillator, implying an enhancement of the specific heat due to the coupling. Accordingly, the low-frequency response,[4] which is easily deduced from the above results, contains the inverse of $[(-i\omega+0)^2(1+m_1/m)+\omega_0^2]$, and hence also displays the mass enhancement $m \to m(1 + m_1/m)$.

4.5 Perturbation theory: quantum mechanics

A direct approach to the questions under discussion is given by quantum-mechanical perturbation theory, provided the coupling between particle and oscillator is small; this approach was also used in [20] for weakly coupled superconductors. We write $\tilde{H} = H_0 + H_1$, see Eq. (19), where H_0 is the Hamiltonian of the particle plus the oscillator; the coupling is given by

$$H_1 = \frac{1}{2m\omega_\mu^2} \Big(\hat{p} g_1(\hat{x}) + g_1(\hat{x}) \hat{p} \Big) \hat{p}_\mu + \frac{1}{2m\omega_\mu^4} \, [g_1(\hat{x})]^2 \hat{p}_\mu^2 \; . \tag{43}$$

The eigen-energies and -functions of H_0 are assumed to be given,

$$E_{n,\ell}^{(0)} = \varepsilon_n + \hbar\omega_\mu(\ell + 1/2) \; , \tag{44}$$

and we consider the $\{\varepsilon_n\}$ to be non-degenerate. Furthermore, we will assume that the level spacing of the particle is small compared to $\hbar\omega_\mu$. The eigen-functions are product states, $|n, \ell\rangle = |n\rangle \otimes |\ell\rangle$, where $|\ell\rangle$ refers to the harmonic oscillator functions. Using standard perturbation theory, we find in first order

$$\Delta E_{n,\ell}^{(1)} = \hbar\omega_\mu(\ell + 1/2) \cdot \langle n|m_1(\hat{x})|n\rangle/2m \; , \quad m_1(\hat{x}) = [g_1(\hat{x})]^2/\omega_\mu^4 \; , \tag{45}$$

which corresponds to an x-dependent frequency enhancement of the oscillator (as discussed in the previous subsection for a constant frequency enhancement). In second order, we encounter the energy denominator $\hbar\omega_\mu\Delta\ell + \varepsilon_n - \varepsilon_k$ with (i) $\Delta\ell = 0$, (ii) $\Delta\ell = \pm 1$, and (iii) $\Delta\ell = \pm 2$. The contribution (i) corresponds to the

[4] A detailed (perturbative) study of the mobility of "polaronic objects" is given in Appendix C of [26], including the "large" polaron. As can be seen from the polaron case, the self-energy-mass and transport-mass enhancement is generally not the same.

frequency enhancement mentioned above in second order perturbation theory in the particle subspace, and is of no interest here. Considering (ii) and (iii), we concentrate on the low-lying energies so that $\varepsilon_n \ll \hbar\omega_\mu$, $|\varepsilon_n - \varepsilon_k| \ll \hbar\omega_\mu$. Hence we neglect $\varepsilon_n - \varepsilon_k$ in the denominator and assume that the *restricted* sum $\sum_k |k\rangle\langle k|$ is a good approximation to the unity operator in the particle subspace; this assumes that there is a sufficient number of particle-energies in the relevant energy range. The contribution (iii) is also related to the x-dependent frequency correction of the oscillator, in second order and hence $\sim m_1^2$, and will be neglected as well. Finally, the dominant contribution (ii), $\sim m_1$, is given by

$$\Delta E^{(2),(\mathrm{ii})}_{n,\ell} = -\frac{1}{8m^2\omega_\mu^4}\,\langle n|\Big(\hat{p}g_1(\hat{x}) + g_1(\hat{x})\hat{p}\Big)^2|n\rangle\ . \tag{46}$$

Clearly, Eqs. (45) and (46) are consistent with the results discussed in the previous subsection. We conclude that the effective correction to the particle Hamiltonian, in this order, is given by

$$\begin{aligned} H_1^{\mathrm{eff}} &= \frac{\hbar\omega_\mu}{4m}\,m_1(\hat{x}) - \frac{1}{8m^2\omega_\mu^4}\Big(\hat{p}g_1(\hat{x}) + g_1(\hat{x})\hat{p}\Big)^2 \\ &= \frac{\hbar\omega_\mu}{4m}\,m_1(\hat{x}) - \frac{m_1}{2m^2}\hat{p}^2 + \frac{i\hbar m_1'}{2m^2}\hat{p} + \frac{\hbar^2 m_1''}{8m^2} - \frac{\hbar^2(g_1')^2}{8m^2\omega_\mu^4}\ . \end{aligned} \tag{47}$$

On the other hand, consider the pct- and Weyl-Hamiltonian, (24) and (29), with $m(\hat{x}) = m + m_1(\hat{x})$, in the limit of small m_1. In linear order in m_1, H_{pct} and H_{W} agree, with the result

$$H_{\mathrm{pct,W}} \simeq H_0 - \frac{m_1}{2m^2}\hat{p}^2 + \frac{i\hbar m_1'}{2m^2}\hat{p} + \frac{\hbar^2 m_1''}{8m^2}\ ; \tag{48}$$

here $H_0 = \hat{p}^2/2m + V(\hat{x})$. Obviously, Eqs. (47) and (48) are not consistent; only the terms proportional to $\hat{p}^2$ and $\hat{p}$ agree. Most notable is the large contribution due to the frequency renormalisation of the oscillator, compare (45), which is larger than the term (46) by a factor of the order of $\hbar\omega_\mu/\langle n|\hat{p}^2/m|n\rangle$.

4.6 Perturbation theory: path integral

Within the path integral formalism, the first-order correction to the free energy is given by

$$\Delta F^{(1)} = \beta^{-1}\langle \tilde{S}_E^{(1)}\rangle_0 \tag{49}$$

where the average is with respect to the particle action alone. In order to evaluate this expression, we need the correlation function

$$\chi_{gg}(\tau - \tau') \equiv \langle g(x(\tau))g(x(\tau')\rangle_0 \quad\to\quad \langle \mathcal{T}_\tau\Big[g(\hat{x}(\tau))g(\hat{x}(\tau')\Big]\rangle_0\ , \tag{50}$$

where $\mathcal{T}_\tau$ is the time ordering operator. We express this correlation function with the help of the eigen-energies and -states, ε_n and $|n\rangle$, introduced above, with the result

$$\chi_{gg}(\tau - \tau') = Z_0^{-1}\sum_{n,k} \mathrm{e}^{-\beta\varepsilon_n/\hbar}\,|\langle n|g(\hat{x})|k\rangle|^2\,\mathrm{e}^{|\tau-\tau'|(\varepsilon_n-\varepsilon_k)/\hbar} \tag{51}$$

where $Z_0 = \sum_n \exp(-\beta\varepsilon_n/\hbar)$. Thus we find in the limit $\epsilon \to 0$ (compare Eq. (39)):

$$\begin{aligned} \Delta F^{(1)} &= \beta^{-1}\omega_\mu^{-2}\int_0^\beta d\tau \int_0^\beta d\tau'\ \alpha_\mu(\tau-\tau')\ \frac{\partial^2}{\partial\tau\partial\tau'}\chi_{gg}(\tau-\tau') \\ &= \beta^{-1}\omega_\mu^{-2}\sum_\omega \omega^2\,\alpha_\mu(\omega)\,\chi_{gg}(\omega)\ . \end{aligned} \tag{52}$$

The frequency sum is evaluated using standard techniques; we consider the limit $\beta\omega_\mu \gg 1$, and assume as above that the relevant energy differences $(\varepsilon_n - \varepsilon_k)^2$ are small compared to $(\hbar\omega_\mu)^2$. The result has the expected form,

$$\Delta F^{(1)} = Z_0^{-1} \sum_n \mathrm{e}^{-\beta\varepsilon_n/\hbar} \Delta E_n \ , \tag{53}$$

where $\Delta E_n = \langle n|H_1^{\mathrm{eff}}|n\rangle$ in agreement with Eqs. (45) and (46); see also (47).

To summarise briefly the results of Sects. 4.5 and 4.6, perturbation theory thus shows that there is an effective potential contribution $\sim m_1$ which can be interpreted as an x-dependent modulation of the ground state energy of the oscillator. Furthermore, the second term in H_1^{eff} is *not* consistent with the prediction based on the pct- or Weyl-Hamiltonian.

4.7 Variational approach

For several decades projector methods have been known to be a useful tool for deriving an effective description for a complex quantum system; recall e. g. Feshbach's approach [33] to nuclear reactions, and the Mori-Zwanzig formalism [34] in statistical physics. For the present case, we wish to derive an effective Hamiltonian defined as projection onto the ground state of the oscillator, eliminating its excited states. In close analogy to Feshbach's method, we use the following ansatz for the wave-function of the system, i. e. particle plus oscillator:

$$|\Psi\rangle = \sum_{\ell=0}^{L} |\psi_\ell\rangle \otimes |\ell\rangle \ . \tag{54}$$

Employing the variational principle of quantum mechanics, we obtain

$$\sum_{\ell'=0}^{L} (H)_{\ell,\ell'} \, |\psi_{\ell'}\rangle = E \, |\psi_\ell\rangle \tag{55}$$

and, after eliminating $|\psi_\ell\rangle$ with $\ell = 1, 2, \ldots, L$ from this set of equations, an effective E-dependent Hamiltonian can be defined by

$$H_{\mathrm{eff}}^{(\mathrm{L})}(E) \, |\psi_0\rangle = E \, |\psi_0\rangle \ . \tag{56}$$

Applying this procedure to the Hamiltonian given in Eq. (19), and taking $L = 1$ for simplicity, we find

$$\begin{aligned} H_{\mathrm{eff}}^{(1)}(E) = H_{00} &+ \frac{1}{2}\hbar\omega_\mu \Big(1 + \frac{m_1(\hat{x})}{2m}\Big) \\ &- \frac{\hbar}{8m^2\omega_\mu^3} \Big(\hat{p} g_1(\hat{x}) + g_1(\hat{x})\hat{p}\Big) X_3^{-1} \Big(\hat{p} g_1(\hat{x}) + g_1(\hat{x})\hat{p}\Big) \end{aligned} \tag{57}$$

where $H_{00} = \hat{p}^2/2m + V(\hat{x})$, and

$$X_3 = H_{00} + \frac{3}{2}\hbar\omega_\mu \Big(1 + \frac{m_1(\hat{x})}{2m}\Big) - E \ . \tag{58}$$

From these expressions, the perturbative results of the previous subsection follow easily, using the approximation $E \simeq \hbar\omega_\mu/2$, hence $X_3 \simeq \hbar\omega_\mu$, which is valid under the same conditions as discussed above. At present, it is unclear whether Eq. (57) would give meaningful results beyond this limit. Furthermore, a preliminary study of $H_{\mathrm{eff}}^{(2)}(E)$ indicates that it is not straightforward to derive concise conclusions within this method, for the most relevant case $m_1 \sim m$.

5 Conclusion

In this article we have studied several aspects of effective quantum theories, arising when a system is coupled to an environment and the latter is integrated out. We considered, in particular, the situation where the coupling between system and environment is non-linear: for the model case of a particle coupled to a single[5] high-frequency oscillator, this non-linear coupling effectively leads to a coordinate-dependent mass of the particle, on the classical level and for low frequencies.

However, on the quantum level, we have not been able to confirm the assertion that an effective low-energy theory can be formulated in which the coupling to the environment and the properties of the environment are expressed through the coordinate-dependent mass alone. This becomes apparent when considering the (discrete) path integral formulation, since high-frequency contributions to the effective action cannot simply be discarded. Consistently, it is easily seen in perturbation theory that due to the non-linearity, significant and model-dependent contributions arise which reflect the back-action of the particle on the environment.

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