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# On the boundary conditions in Feynman's approach to the finite-temperature polaron problem

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**Abstract.** A complete analysis of the polaron problem allows us to determine the correct boundary conditions to be applied to the paths for the evaluation of the density matrix at the endpoints of the temperature range $1/kT\varepsilon(0, \beta)$. Thus the trace is properly defined when calculating the partition function for a dynamical system of a particle interacting with a boson field and the role of spatial translational invariance, when present, is elucidated.

## 1. Introduction

One of the first thorough applications of the path integral method to physical systems has been the polaron problem. Since the original paper by Feynman [1, 2] all the approximations and the different routes for overcoming the various difficulties have met a common problem: how must the endpoint values be chosen for the particle trajectories on which the path integral is performed?

In the case of zero temperature ($\beta \to \infty$) however, the choice of the endpoints $\boldsymbol{r}(0)$ and $\boldsymbol{r}(\beta)$ is purely a matter of convenience. This is because the energy of the ground state $\boldsymbol{E}_0$ for the interacting system is obtained by looking at the exponential decay rate of the density matrix $\hat{\rho}$ as a function of $\beta$. Thus, projection of the density matrix on the ground state of the free oscillators does not influence this dependence and gives rise to a reduced density matrix $\rho_{00}(\boldsymbol{r}, \boldsymbol{r}')$ for the particle, which gives

$$\lim_{\beta \to \infty} \frac{1}{\beta} \log \rho_{00}(\boldsymbol{r}, \boldsymbol{r}') = -E_0. \tag{1}$$

Here the limit of (1) is independent of the choice of any $\boldsymbol{r}, \boldsymbol{r}'$. The usual procedure in Feynman's approach to the polaron problem is thus justified: the variables $\boldsymbol{r}$ and $\boldsymbol{r}'$ appearing in (1) are taken equal to zero and in the course of the calculation any contribution, which arises from terms that are very small when $\beta$ is large, is disregarded.

On the contrary, in the case of finite temperature, correct handling of the boundary conditions is crucial. The full partition function $Z$ is now requested. This implies that the traces have to be performed on the full density matrix. Our starting point is the expression for $Z$ as the trace of a path integral on closed trajectories for the particle, after the oscillator's coordinates have been integrated out exactly:

$$\begin{aligned} Z &= Z_{\mathrm{ph}} \operatorname{Tr} \oint \mathscr{D}\boldsymbol{r}(\tau) \exp\left(\frac{1}{\hbar} S[\boldsymbol{r}]\right) \\ Z_{\mathrm{ph}} &= (2 \sinh \beta\hbar\omega/2)^{-N} \end{aligned} \tag{2}$$

is the partition function of the $N$ free longitudinal optical phonons of frequency $\omega$ (units $\hbar = m = \omega = 1$ will be chosen in the following) and $S$ is the reduced action as a functional of the particle trajectory:

$$S = -\tfrac{1}{2}\int_0^\beta \dot{\boldsymbol{r}}^2\, \mathrm{d}\tau + \frac{\alpha}{\sqrt{8}}\oint_0^\beta \mathrm{d}\tau\, \mathrm{d}\sigma\, D_{\omega=1}(|\tau-\sigma|)|\boldsymbol{r}_\tau - \boldsymbol{r}_\sigma|^{-1} \tag{3}$$

written in terms of the phonon propagator in imaginary time:

$$D_\omega(u) \equiv \frac{\cosh \omega(u-\beta/2)}{\sinh(\beta\omega/2)} \underset{\beta\to\infty}{\sim} \exp(-\omega u). \tag{4}$$

This kernel reduces to Feynman's in the limit $\beta \to \infty$. Equation (3) accounts for a retarded interaction of the particle with itself at previous times, so that $S$ can be viewed as somehow describing a two-particle system. The symbol Tr stands here for taking the extremum of the loop $\boldsymbol{r}(0) \equiv \boldsymbol{r}(\beta) \equiv \boldsymbol{r}_1$ as a variable and integrating on it. As (2) factorises in equal contributions arising from the three cartesian coordinates, from now on we consider only one of them, $x(t)$.

In the usual variational theory the particle trajectory $x'(t)$ is needed, which minimises the approximate quadratic action inclusive of a driving term $f$:

$$S_f = -\tfrac{1}{2}\int_0^\beta \dot{x}^2\, \mathrm{d}t - \frac{C}{2}\oint_0^\beta \mathrm{d}t\, \mathrm{d}s\, D_W(|t-s|)(x_t - x_s)^2 + \int_0^\beta f_t x_t\, \mathrm{d}t \tag{5}$$

where

$$f_t = \mathrm{i}k_x[\delta(t-\tau) - \delta(t-\sigma)]. \tag{5$'$}$$

The approximate quadratic action $S_0$ is obtained from $S_f$ by putting $f = 0$. It is questionable whether the equation of motion for $x(t)$ can be solved in closed form with arbitrary periodic boundary conditions so that the evaluation of the trace appears as an ill-defined task. Nevertheless we will show that the crucial requirement of translational invariance for actions $S$ and $S_0$ is a sufficient condition for achieving the full result. Moreover it is possible to give a non-ambiguous procedure in the case when the translational invariance is not fulfilled, decoupling the variables of an equivalent system. In this way the problem of the influence of the boundary conditions on $x(t)$ is settled once and for all.

It is customary in the literature to introduce a model Lagrangian for a two-particle system from the very outset, claiming that it might help in avoiding mathematical difficulties connected with the asymptotic behaviour and the boundary conditions [2, 3]. The polaron at finite temperature has been discussed by Osaka [4] long ago assuming the normal coordinates of this model as independent variables and taking the traces with respect to both of them. Actually, previous path integral results for the harmonic oscillator [5] obtained from the first-order Lagrangian equation of motion needed auxiliary degrees of freedom to be introduced, on which integration is eventually performed.

In the polaron problem the equation of motion to be solved for $x(t)$ is integro-differential and can be solved by introducing an auxiliary variable $y(t)$, so that $x(t)$ and $y(t)$ satisfy a system of second-order ordinary differential equations. The boundary conditions for $x(t)$ are given by

$$x(0) = x(\beta) = x_1. \tag{6}$$

On the contrary those to be imposed on $y(t)$ are not self-evident. In analogy to (6) the following conditions are assumed:

$$y(0)=y(\beta)=y_1 \tag{7}$$

and an extra integration on the variable $y_1$ is needed.

The model Lagrangian is invoked to make this step legitimate but, to our knowledge, no further investigation has been done on the actual equivalence between the model dynamical system and the original equation of motion. On the contrary, with an appropriate choice of boundary conditions on $y(t)$, which follow directly from its definition, we can show that the equivalence is well stated.

Besides, the translational invariance, if present, allows for drastic simplifications in the evaluation of the trace, so that one can get rid of the model altogether. In this way our discussion of the finite- and zero-temperature polaron problem is possible, which accounts for all approximations in the $\beta\to\infty$ limit.

We believe that, although it might appear a minor point as far as the polaron theory is concerned, it turns out to be very relevant when non-translationally invariant systems are considered. Similarly, some care has to be taken in this context, when holomorphic representation of Hamiltonians is used [6], in evaluating time-ordered Green functions via a path integral method [7].

## 2. Polaron variational calculation

To give an estimate of (2) in the case of the polaron problem the variational method based on the approximate quadratic action $S$ is reduced to the evaluation of the following average value:

$$\left\langle \exp\left(\int_0^\beta f_t x_t \,\mathrm{d}t\right)\right\rangle_{S_0} \equiv \frac{\mathrm{Tr}\oint \mathscr{D}x\, \mathrm{e}^{S_f}}{\mathrm{Tr}\oint \mathscr{D}x\, \mathrm{e}^{S_0}} = \frac{\mathrm{Tr}\exp(S_f[x'_t])}{\mathrm{Tr}\exp(S_0[x''_t])}. \tag{8}$$

The expression of $S_f$ is given by (5) while $S_0$ is obtained by dropping the driving force term. The last equality follows from the fact that the driven action $S_f$ is quadratic. Here $x'_t(x''_t)$ is the solution of the Euler equation that stems from searching for the minimum of the action $S_f(S_0)$:

$$\ddot{x}_t = 2C\int_0^\beta \mathrm{d}s\, D_W(|t-s|)(x_t-x_s)-f_t \tag{9}$$

with periodic boundary conditions

$$x(0)=x_1 \qquad x(\beta)=x_1. \tag{9'}$$

If $x^0(t)$ is the solution of (9) with $x_1=0$, then the translational invariance of $S_0$ ensures that

$$x'(t)=x^0(t)+x_1. \tag{10}$$

That is, the minimising loop based at $x_1$ is obtained from the one based at the origin through a translation of amplitude $x_1$. On the other hand

$$S_f[x'_t]=S_f[x^0_t]+x_1\int_0^\beta f(t)\,\mathrm{d}t \tag{11}$$

but, in turn, the true action $S$ is also translationally invariant. Then

$$\int_0^\beta f(t)\,\mathrm{d}t = 0 \tag{12}$$

so that the important result follows:

$$S_f[x_t'] = S_f[x_t^0] = \tfrac{1}{2}\int_0^\beta \mathrm{d}t\, f(t)x^0(t) \tag{13}$$

i.e. the driven action is translationally invariant when evaluated along the loops that minimise it. It is worthwhile remarking that only two of the three conditions for the validity of Noether's theorem [8] are fulfilled, as the integrand of $S_f$ is not itself translationally invariant, due to the presence of the driving term $f(t)x(t)$. Thus, strictly speaking, no constant of motion is associated with the group of translation defined by (10). It turns out, however, that the time average of the mass centre velocity is zero.

Thanks to (13) which is valid also when $f_t$ is taken to be zero, we are able to calculate immediately the traces that appear in (8), thus giving

$$\left\langle \exp\left(\int_0^\beta f_t x_t\,\mathrm{d}t\right)\right\rangle = \exp(S_f[x_t^0]). \tag{14}$$

This equation is similar in form to Feynman's equation (28) in [1], but we stress that it is true in full generality at finite temperature, while Feynman's equation is obtained in the zero-temperature limit $\beta \to \infty$.

The problem is now reduced to the explicit calculation of $x(t)$. Following Feynman we define an auxiliary variable

$$y(t) = \frac{W}{2}\int_0^\beta \mathrm{d}s\, D_W(|t-s|)x(s) \tag{15}$$

in terms of which the Euler equation (9) transforms into the system of coupled equations:

$$\begin{aligned} \ddot{y} &= W^2(y-x) \\ \ddot{x} &= (4C/W)(x-y) - f_t \end{aligned} \tag{16}$$

with boundary conditions (9′) together with

$$y(0) = y(\beta). \tag{16'}$$

Condition (16′) follows from the definition of $y(t)$ at once. Essentially the method by Osaka† is to solve (16) with the conditions (9′) and (16′) introducing a model Euclidean Lagrangian $L(x, y)$ that generates (16) and diagonalising it. Its eigenfrequencies are 0 and $V^2 = W^2 + 4C/W$ corresponding to the normal coordinates $\eta$ and $\xi$ respectively, which are

$$\begin{aligned} \eta &= (W^2/V^2)(4Cy/W^3 + x) \\ \xi &= (W^2/V^2)(y-x). \end{aligned} \tag{17}$$

The Lagrangian then separates as

$$L_f(\eta, \xi) = -\tfrac{1}{2}(V^2/W^2)\dot{\eta}^2 + f_t\eta - \tfrac{1}{2}M(\dot{\xi}^2 + V^2\xi^2) + \gamma_t\xi. \tag{18}$$

† Contrary to [4] our whole exposition is in imaginary time.

Here $\eta$ describes the centre of mass of the particles $x, y$ subjected to the action of the driving force $f_t$, while the relative coordinate $\xi$ describes an harmonic oscillator of mass $M = 4CV^2/W^5$ and frequency $V$, driven by the force $\gamma_t = -4Cf_t/W^3$. The decoupled equations of motion are then

$$\ddot{\eta} = -(W^2/V^2)f_t$$
$$\ddot{\xi} = V^2\xi + (W^2/V^2)f_t. \tag{19}$$

It is apparent here that the property of invariance (13) is reflected on the variable $\eta(t)$, which plays the role that $x'(t)$ had in the original problem (9). We note that the transformation (17), when applied directly to system (16), leads to (19) straightforwardly with no need to resort to any model Lagrangian as we have done here.

In Osaka's paper the traces appearing in (8) are integrations on the values of $\eta_1$ and $\xi_1$. While the integration on $\eta_1$ is automatically taken into account, the integration on $\xi_1$ has to be performed. This implies that variables $\eta$ and $\xi$ are on the same foot and assumes that the boundary conditions for the two are both periodic. Equation (16′) is thus forced to be split into

$$y(0) = y_1 \qquad y(\beta) = y_1 \tag{20}$$

which determines the origin $\xi_1$ of the loop $\xi(t)$ that has to be integrated out. However, an arbitrary value of the endpoint $y_1$ could not be compatible with the definition of $y(t)$ given by (15), so that the equivalence of system (16) with the Euler equation (9) is not assured.

On the other hand, inspection of (15) shows that the most appropriate condition to be added to (9′) and (16′) is

$$\dot{y}(0) = \dot{y}(\beta). \tag{21}$$

In fact, $D_W$ can play the role of the Green function for the first of equations (16). Using the definition (4) we have [11]

$$\left(\frac{\partial^2}{\partial t^2} - W^2\right) D_W(|t-s|) = -2W\delta(t-s)$$

$$D_W|_{t=0} = \frac{\cosh W(s-\beta/2)}{\sinh W\beta/2} = D_W|_{t=\beta}.$$

Then the Green lemma yields

$$y_s - \frac{W}{2}\int_0^\beta D_W(|t-s|)x_t\,\mathrm{d}t = -\frac{1}{2W}\left(y_t\frac{\partial}{\partial t}D_W - D_W\frac{\mathrm{d}}{\mathrm{d}t}y_t\right)_{t=0}^{\beta}$$

the right-hand side vanishes when (16′) and (21) are fulfilled because

$$\frac{\partial}{\partial t}D_W|_{t=0} = \frac{W\sinh W(\beta/2-s)}{\sinh W\beta/2} = \frac{\partial}{\partial t}D_W|_{t=\beta}.$$

Now the full equivalence of system (16) and the Euler equation (9) is achieved. Using boundary conditions of (9′), (16′) and (21) the explicit form of $\eta_t$ and $\xi_t$ in terms of the initial value $x_1$ is

$$\eta_t = \eta_1 + \mathrm{i}k_x\frac{W^2}{V^2}\left((t-\sigma)\vartheta(t-\sigma) - (t-\tau)\vartheta(t-\tau) - (\tau-\sigma)\frac{t}{\beta}\right)$$

$$\xi_t = \xi_1 \frac{\sinh Vt + \sinh V(\beta - t)}{\sinh V\beta} - ik_x \frac{W^2}{V^3}\bigg(\sinh V(t-\sigma)\vartheta(t-\sigma)$$
$$- \sinh V(t-\tau)\vartheta(t-\tau) + \frac{\sinh Vt}{\sinh V\beta}[\sinh V(\beta-\tau) - \sinh V(\beta-\sigma)]\bigg) \tag{22}$$

where

$$\eta_1 = x_1 + ik_x \frac{V^2 - W^2}{2V^3}(D_V(\sigma) - D_V(\tau)) \qquad \xi_1 = ik_x \frac{W^2}{2V^3}\Big(D_V(\sigma) - D_V(\tau)\Big) \tag{23}$$

and the explicit form of $f_t$ of (5′) has been used. Here $\vartheta$ is the usual step function.

Inverting the transformation (17), condition (21) determines the initial value of $y(t)$ itself:

$$y_0 = y_\beta = x_1 + \frac{ik_x}{2V}(D_V(\sigma) - D_V(\tau)). \tag{24}$$

The loops $y(t)$ are obtained one from another by the same translational group of (10). When $\beta$ goes to infinity and $x_1 = 0$ in (24), the RHS vanishes and the boundary conditions for $y(t)$ underlying Feynman's original result appear†. Finally, equations (22) allow us to calculate directly $S_f[x_t^0]$, yielding

$$S_f[k_t^0] = -\frac{k_x^2}{2V^2}\bigg\{W^2|\tau-\sigma|\bigg(1 - \frac{|\tau-\sigma|}{\beta}\bigg) + \frac{V^2 - W^2}{V}\bigg[1 - \exp(-V|\tau-\sigma|)$$
$$+ \bigg(1 - \coth\frac{V\beta}{2}\bigg)(\cosh V|\tau-\sigma| - 1)\bigg]\bigg\} \tag{25}$$

which is exactly Osaka's result.

A few comments are now in order. The expressions of $\eta$ and $\xi$ given by (22) with the aid of our extra condition (21) guarantee the equivalence of system (16) with the Euler integro-differential equation (9) when transformed back to $x$ and $y$.

The major consequence is that there is no need to introduce any model through a suitable Lagrangian. Besides, it is arduous to think of a physical model system which satisfies boundary conditions like those of (9′), (16′) and (21).

While translational invariance helps in the evaluation of the traces in (8), as discussed, it is by no means invoked in determining the condition (21). On the other hand, the dependence of the endpoints of $y(t)$ on $x_1$ follows from (21) when translational invariance is also lacking, although it will not necessarily be linear as in (24). The trace can then be performed unambiguously as an integration only on $x_1$, as soon as the solution of the Euler equation for $x(t)$ is exhibited explicitly.

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† See [9, ch 21] and particularly Schulman's comment to Feynman's papers (p 181).

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