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COMMENT

On path integrals in spherical coordinates

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Abstract. An alternative derivation of the path integrals in spherical coordinates is presented for the purpose of discussing the nature of the quantum mechanical terms appearing in the action. It is shown that the Jacobian resulting from the transformation of the functional measure from cartesian coordinates changes the action by surface terms which then lead to the correct ordering contributions.

In cartesian coordinates the path integrals are formulated in terms of the classical action. However, it is a well known fact that, when one makes point canonical transformations or employs curvilinear coordinates, the action acquires some purely quantum mechanical terms, namely the ordering contributions. Hoping to achieve a better understanding of the nature of these terms, we present a new method for deriving the Hamiltonian path integral in spherical coordinates. Originally, the path integrals in polar coordinates were obtained by expressing the short time interval Green functions in terms of the polar coordinates by using some expansion recipies [1, 2]. The basic feature of the method introduced in this comment is that it demonstrates that the transformation of the functional measure from the cartesian coordinates adds surface terms to the action which then give rise to the correct ordering contributions. We expect that our procedure will also be applicable to problems that may arise in calculating the effective Hamiltonian resulting from the point transformations. In fact, similar techniques have already been employed succesfully in solving the path integrals for the Morse, the Wood-Saxon and some related potentials [3, 4].

We start with the phase space path integral for a particle m moving under the influence of a central potential $V(r)$ from the spacetime point $\boldsymbol{r}_a$, $t_a = 0$ to $\boldsymbol{r}_b$, $t_b = \tau$ in cartesian coordinates

$$K(\boldsymbol{r}_a, \boldsymbol{r}_b; \tau) = \int \mathscr{D}^3 r\, \mathscr{D}^3 p \exp\left(\mathrm{i} \int_0^\tau \mathrm{d}t (\boldsymbol{p}\cdot\dot{\boldsymbol{r}} - \boldsymbol{p}^2/2m - V(r))\right). \tag{1}$$

As usual this expression is understood as the limit of the time-graded formula:

$$K(\boldsymbol{r}_a, \boldsymbol{r}_b; \tau) = \lim_{\substack{n\to\infty \\ \varepsilon\to 0}} \int \prod_{j=1}^{n} \mathrm{d}^3 r_j \prod_{j=1}^{n+1} \frac{\mathrm{d}^3 p_j}{(2\pi)^3} \times \prod_{j=1}^{n+1} \exp\left[\mathrm{i}\left(\boldsymbol{p}_j \cdot (\boldsymbol{r}_j - \boldsymbol{r}_{j-1}) - \frac{\varepsilon p_j^2}{2m} - \varepsilon V(r_j)\right)\right] \tag{2}$$

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with

$$(n+1)\varepsilon=\tau \qquad \boldsymbol{r}=\boldsymbol{r}_a\,;\ \boldsymbol{r}_{n+1}=\boldsymbol{r}_b.$$

We pass to the spherical coordinates in two steps: First, we introduce the polar coordinates $\rho\in(0,\infty)$ and $\varphi\in(0,2\pi)$ in the xy plane

$$x=\rho\cos\varphi \qquad p_x=p_\rho\cos\varphi-\frac{\sin\varphi}{\rho}p_\varphi$$

$$y=\rho\sin\varphi \qquad p_y=p_\rho\sin\varphi+\frac{\cos\varphi}{\rho}p_\varphi. \tag{3}$$

Since there is no integration over the coordinate variables at point $\boldsymbol{r}_b$ in (2), we get a contribution ρ_b^{-1} to the Jacobian for $(\mathrm{d}p_x\,\mathrm{d}p_y)_{n+1}\rightarrow(\mathrm{d}p_\rho\,\mathrm{d}p_\varphi)_{n+1}$. Then (6) becomes

$$K(\boldsymbol{r}_a,\boldsymbol{r}_b\,;\tau)=\rho_b^{-1}\int\mathscr{D}(\rho,\varphi,z)\mathscr{D}(p_\rho,p_\varphi,p_z)$$
$$\times\exp\left\{\mathrm{i}\int_0^\tau\mathrm{d}t\left[p_\rho\dot\rho+p_\varphi\dot\varphi+p_z\dot z-\frac{1}{2m}\left(p_\rho^2+\frac{p_\varphi^2}{\rho^2}+p_z^2\right)-V(r)\right]\right\}. \tag{4}$$

To have a manifestly symmetric expression for the propagator with respect to points $\boldsymbol{r}_a$ and $\boldsymbol{r}_b$, we rewrite the factor ρ_b^{-1} as

$$\rho_b^{-1}=(\rho_a\rho_b)^{-1/2}\exp[\ln(\rho_b/\rho_a)^{-1/2}]$$
$$=(\rho_a\rho_b)^{-1/2}\exp\left(\mathrm{i}\int_0^\tau\mathrm{d}t\frac{\mathrm{i}\dot\rho}{2\rho}\right). \tag{5}$$

Introducing this formula into (4) and then translating p_ρ by $p_\rho\rightarrow p_\rho-\mathrm{i}/2\rho$ are obtain:

$$K(\boldsymbol{r}_a,\boldsymbol{r}_b\,;\tau)=(\rho_a\rho_b)^{-1/2}\int\mathscr{D}(\rho,\varphi,z)\mathscr{D}(p_\rho,p_\varphi,p_z)$$
$$\times\exp\left\{\mathrm{i}\int_0^\tau\mathrm{d}t\left[p_\rho\dot\rho+p_\varphi\dot\varphi+p_z\dot z-\frac{1}{2m}\left(p_\rho^2+\frac{p_\varphi^2-\frac14}{\rho^2}+p_z^2\right)+\frac{\mathrm{i}p_\rho}{2m\rho}-V(r)\right]\right\}. \tag{6}$$

Note that we could discretise the path integral equally well by starting the time division of the momentum variable at $j=0$ and ending at $j=n$. Then we would get a contribution ρ_a^{-1} to the Jacobian for the $(\mathrm{d}p_x\mathrm{d}p_y)_0\rightarrow(\mathrm{d}p_\rho\mathrm{d}p_\varphi)_0$ transformation. Symmetrisation of this factor as

$$\rho_a^{-1}=(\rho_a\rho_b)^{-1/2}\exp\left(-\mathrm{i}\int_0^\tau\mathrm{d}t\frac{\mathrm{i}\dot\rho}{2\rho}\right)$$

would lead to the same equation as (6) with the sign of the imaginary term in the action reversed. However, the existence of such a term means a shift in the velocity $\dot\rho_j$

$$\rho_j-\rho_{j-1}\rightarrow\rho_j-\rho_{j-1}\pm\mathrm{i}\varepsilon/2m\rho_j$$

which disappears in the $\varepsilon\rightarrow0$ limit. The Green function of (6) then can be written as

$$K(\boldsymbol{r}_a,\boldsymbol{r}_b\,;\tau)=(\rho_a\rho_b)^{-1/2}\int\mathscr{D}(\rho,\varphi,z)\mathscr{D}(p_\rho,p_\varphi,p_z)$$
$$\times\exp\left\{\mathrm{i}\int_0^\tau\mathrm{d}t\left[p_\rho\dot\rho+p_\varphi\dot\varphi+p_z\dot z-\frac{1}{2m}\left(p_\rho^2+\frac{p_\varphi^2-\frac14}{\rho^2}+p_z^2\right)-V(r)\right]\right\}. \tag{7}$$

At this stage we would like to point out that, to perform the symmetrisation of the Jacobian in a rigorous way, we could first make an analytical continuation by $t \to it$ and $\boldsymbol{r} \to i\boldsymbol{r}$ in (1). This would save us from having an imaginary term in the action.

To complete the transformation to the spherical coordinates we now pass from ρ, z to $r \in (0, \infty)$ and $\theta \in (0, \pi)$ defined by

$$\rho = r \sin\theta \qquad z = r\cos\theta.$$

Introducing these coordinates into (7) and symmetrising the resulting Jacobian r_b^{-1} (or r_a^{-1}) in exactly the same fashion as before, we arrive at the correct form of the Hamiltonian path integral in spherical coordinates [2]:

$$K(\boldsymbol{r}_a, \boldsymbol{r}_b; \tau) = (r_a^2 r_b^2 \sin\theta_a \sin\theta_b)^{-1/2} \int \mathscr{D}(r, \theta, \varphi)\mathscr{D}(p_r, p_\theta, p_\varphi)$$
$$\times \exp\left\{ i \int_0^\tau dt \left[p_r\dot{r} + p_\theta\dot{\theta} + p_\varphi\dot{\varphi} - \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2 - \frac{1}{4}}{r^2} + \frac{p_\varphi^2 - \frac{1}{4}}{r^2\sin^2\theta} \right) - V(r) \right] \right\}. \tag{8}$$

At this point, for comparison, we briefly mention previous derivations of the above formula. For example in [2] this is achieved by expanding the configuration-space form of the short time interval amplitudes in terms of the Bessel functions. For that purpose the Lagrangian in the jth interval is written as

$$L_j = \frac{m}{2\varepsilon^2}(\boldsymbol{r}_j - \boldsymbol{r}_{j-1})^2 - V(r_j)$$
$$= \frac{m}{2\varepsilon^2}(r_j^2 - r_{j-1}^2) - \frac{m r_j r_{j-1}}{\varepsilon^2}\cos(\theta_j - \theta_{j-1})$$
$$- \frac{m r_j r_{j-1}}{\varepsilon^2} \sin\theta_j \sin\theta_{j-1}\cos(\varphi_j - \varphi_{j-1}) + \frac{m}{\varepsilon^2} r_j r_{j-1} \sin\theta_j \sin\theta_{j-1} - V(r_j). \tag{9}$$

Then the asymptotic form of the expansion formula for $\varepsilon \to 0$

$$\exp(z\cos\delta) = \sum_{\nu=-\infty}^{\infty} \exp(i\nu\delta) I_\nu(z) \tag{10}$$

is separately employed for the second and third terms of (9). These two separate expansions correspond to the two steps of our symmetrisation procedure.

In conclusion, the Jacobian resulting from the non-invariance of the path integral measure under coordinate transformations is the source of the ordering contributions in the action. This Jacobian depends only on the endpoint coordinates, and thus changes the action by surface terms. In other words, it modifies the Lagrangian by a total derivative which does not affect the classical equations of motion, but may give rise to quantum mechanical effects. The situation is similar to the appearance of the quantum mechanical symmetry-breaking phenomena in field theories [5]. To see this analogy we can recall the derivation of the chiral anomaly from the non-invariance of the path integral measure for gauge theories with fermions under the chiral transformations [6].

Finally we emphasise that if the endpoint Jacobian is constant, the effective action coincides with the classical one. That is why we do not have any ordering problem when we map the H atom path integral to the four-dimensional harmonic-oscillator Green function [7].

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