

Extended Feynman Formula for Harmonic Oscillator

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A slight modification of Feynman's original method leads to the Maslov correction in the path integral formula of a harmonic oscillator. Caustics are treated in a direct geometric way.

1. INTRODUCTION

As pointed out by Souriau (1976), Feynman's formula for a harmonic oscillator (Feynman and Hibbs, 1965, p. 63)

$$K(x_2, t_2 | x_1, t_1) = \left(\frac{m\omega}{2\pi i \hbar \sin \omega(t_2 - t_1)} \right)^{1/2} \times \exp \left\{ \frac{im\omega}{2\hbar \sin \omega(t_2 - t_1)} \times [(x_1^2 + x_2^2) \cos \omega(t_2 - t_1) - 2x_1x_2] \right\} \quad (1.1)$$

is valid only for $|t_2 - t_1| < \pi/2$, a half-period. The general expression is obtained (Souriau, 1976) by introducing the Maslov correction (Souriau, 1976; Arnold, 1967; Guillemin and Sternberg, 1977) and given as

$$K(x_2, t_2 | x_1, t_1) = \left(\frac{m\omega}{2\pi \hbar |\sin \omega(t_2 - t_1)|} \right)^{1/2} \exp \left\{ -\frac{i\pi}{2} \left[\frac{1}{2} + Ent \frac{\omega(t_2 - t_1)}{\pi} \right] \right\} \times \exp \left\{ \frac{im\omega}{2\hbar \sin \omega(t_2 - t_1)} \times [(x_1^2 + x_2^2) \cos \omega(t_2 - t_1) - 2x_1x_2] \right\} \quad (1.2)$$

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for $t_2 \neq t_1 + k(\tau/2)$, where k is an integer, and

$$K(x_2, t_2 | x_1, t_1) = \exp \left\{ -\frac{i\pi}{2} k \right\} \delta(x_1 - (-1)^k x_2) \quad (1.3)$$

for $t_2 = t_1 + k(\tau/2)$, where k is an integer (caustics).

The effect of the correction factor

$$\exp \left\{ -\frac{i\pi}{2} Ent \frac{\omega(t_2 - t_1)}{\pi} \right\}$$

is a jump in phase at every half-period, observed by Gouy (1890) in classical optics and having the consequence of reversing the interference pattern (see Guillemin and Sternberg, 1977, for details). A similar phenomenon is observed in electron optics (Schulmann, 1975) as well as in molecular (Miller, 1970; Marcus, 1971) and nuclear (Levit et al., 1974) scattering. Equation (2) is more or less well known (Combe et al., 1978; Levit et al., 1974); it is generally derived by Morse's theory (Milnor, 1963). At caustics, i.e., for $t_2 = t_1 + k(\tau/2)$, k integer, most of the authors have observed that (1.2) diverges; they study then the corrections due to higher-order perturbation. Souriau (1976) derives (1.3) by an indirect way, noting the relation to metaplectic representation.

The aim of this paper is to show how the above results may be obtained by slightly modifying Feynman's original method.

2. FEYNMAN'S METHOD

First, we resume briefly Feynman's original method (Feynman and Hibbs, 1965, pp. 58–73) in computing the quantum mechanical kernel for a harmonic oscillator.

Suppose $|t_2 - t_1| < \tau/2$, the half-period (assumed implicitly by Feynman). Then, for any pair of points $x_1, x_2 \in \mathbb{R}$ there is a unique classical path $\bar{\gamma}: t \rightarrow \bar{\gamma}(t) \in \mathbb{R}$ between (x_1, t_1) and (x_2, t_2) . It is useful to write then any path γ in the form $\gamma = \bar{\gamma} + \eta$, where the "varied curves" η vanish at the end points: $\eta(t_1) = \eta(t_2) = 0$.

The quantum mechanical kernel, being expressed in terms of a Gaussian integral, is a product of two factors (Feynman and Hibbs, 1965):

$$K(x_2, t_2 | x_1, t_1) = \exp \left\{ \frac{i}{\hbar} S(\bar{\gamma}) \right\} F(t_2 - t_1) \quad (2.1)$$

$S(\bar{\gamma})$ is here the Hamiltonian action along the classical path $\bar{\gamma}$. For a harmonic oscillator

$$S(\bar{\gamma}) = \frac{m\omega}{2 \sin \omega(t_2 - t_1)} [(x_1^2 + x_2^2) \cos \omega(t_2 - t_1) - 2x_1 x_2] \quad (2.2)$$

The second factor in (2.1) depends only on $t_2 - t_1$ and is a result of integration over all paths η vanishing at the end points:

$$F(t_2 - t_1) = \int \exp \left\{ \frac{i}{\hbar} \int_{t_1}^{t_2} \frac{m}{2} [(\dot{\eta}(t))^2 - \omega^2 \eta^2(t)] dt \right\} \mathcal{D}\eta \quad (2.3)$$

In order to assign a precise mathematical meaning and compute (2.3), Feynman expands the η 's in Fourier series:

$$\eta(t) = \sum_{j=1}^{\infty} a_j \sin \frac{j\pi}{t_2 - t_1} (t - t_1) \quad (2.4)$$

and, instead of integrating over the η 's, integrates over the space of Fourier coefficients (a_1, a_2, \dots) :

$$F(t_2 - t_1) = \lim_{n \rightarrow \infty} \mathcal{J} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \exp \left\{ \sum_{j=1}^n \frac{im}{\hbar} \left[\left(\frac{\pi j}{t_2 - t_1} \right)^2 - \omega^2 \right] a_j^2 \right\} \times \frac{da_1}{A} \cdots \frac{da_n}{A} \quad (2.5)$$

The difficulty introduced by the infinite-valued Jacobian \mathcal{J} is removed by a suitable choice of the normalizing factors A , which symbolize the measure of integration in the space of Fourier coefficients.

Carrying out the integration and fitting the results to the case $\omega = 0$, a free particle, Feynman gets (1.1). The ambiguity caused by $i^{1/2}$ in (1.1) is physically unimportant, for it gives only an overall phase factor.

3. BEYOND CAUSTICS

Note that beyond caustics, i.e., for $|t_2 - t_1| > \tau/2$, but $|t_2 - t_1| \neq k(\tau/2)$ we have again a well-defined classical path between (x_1, t_1) and (x_2, t_1) and our formulas (2.1)–(2.4) are valid. A change to integration over Fourier coefficients is again possible. As to the factors \mathcal{J} , A , and integration order, note that they are *essentially the same*, as in (2.5): they depend only on the transformation $\eta \rightarrow (a_1, a_2, \dots)$ and are *completely independent* of “physics”, i.e., of the function to be integrated. Thus (2.5) will be perfectly meaningful as soon as we arrive to remove the ambiguity due to the

$$k = Ent \frac{\omega(t_2 - t_1)}{\pi} = Ent \frac{t_2 - t_1}{\tau/2} \quad (3.1)$$

number of negative terms in the sum of (2.5). This is achieved by an analytic

extension of the classical Fresnel integral, possible for $\text{Im } \lambda \geq 0$, $\lambda \neq 0$ (Souriau, 1978²; Guillemin and Sternberg, 1977)

$$F(\lambda) = \int_{-\infty}^{\infty} \exp\left(i \frac{\lambda}{2} x^2\right) dx = \begin{cases} \left(\frac{2\pi}{\lambda}\right)^{1/2} e^{i(\pi/4)}, & \text{for } \lambda > 0 \\ \left(\frac{2\pi}{-\lambda}\right)^{1/2} e^{-i(\pi/4)}, & \text{for } \lambda < 0 \end{cases} \quad (3.2)$$

Thus Feynman's formula has to be modified only by taking absolute value in $|\sin \omega(t_2 - t_1)|$ and multiplying by

$$\exp\left(-\frac{i\pi}{2} k\right) = \exp\left(-\frac{i\pi}{2} Ent \frac{\omega(t_2 - t_1)}{\pi}\right) \quad (3.3)$$

in accordance with (1.2).

4. AT CAUSTICS

For $t_2 = t_1 + k(\tau/2)$, k integer, the situation is radically changed: *all* classical paths starting from x_1 coalesce to $(-1)^k x_1$. Thus for any arbitrary pair of points x_1, x_2 , we have either no classical path at all or an infinity of classical paths between them. Feynman's method breaks down even in this latter case, because the coefficient of a_k^2 in (2.5) vanishes and the Fresnel integral diverges. In terms of "infinite-dimensional manifolds" (DeWitt-Morette, 1976; Horváthy and Úry, 1977; Milnor, 1963), (2.1) is valid if the Hamiltonian action, considered as a function defined on the set of all paths between x_1 and x_2 , has only one "critical point," i.e., classical path. At caustics this condition is not satisfied and one has to evaluate the Feynman integral by other means.

The easiest way is to work with operators, rather than with kernels merely. Remember that the time evolution of a system is given as

$$\psi_{t_2}(x_2) = [U_{t_2-t_1} \psi_{t_1}](x_2) = \int_{\mathbb{R}} K(x_2, t_2 | x_1, t_1) \psi_{t_1}(x_1) dx_1 \quad (4.1)$$

By the multiplication law one has

$$U_{k(\tau/2)} = [U_{\tau/4}]^{2k} \quad (4.2)$$

By (1.1) and (4.1)

$$[U_{\tau/4} \psi_{t_1}](x_2) = \int_{\mathbb{R}} \left(\frac{m\omega}{2\pi\hbar}\right)^{1/2} e^{-i\pi/4} e^{-(im\omega/\hbar)x_1 x_2} \psi_{t_1}(x_1) dx_1 \quad (4.3)$$

² He also conjectures that the fact that $F(\lambda)$ has an analytic extension only for $\text{Im } \lambda \geq 0$ seems to be related to the nonexistence of negative temperature for a thermodynamical system composed of harmonic oscillators.

essentially a *Fourier transform* and thus, noting that if the Fourier transform of a function is once more Fourier transformed, then one obtains the original function reflected with respect to $x = 0$, one gets

$$\psi_{t_2}(x_2) = e^{-(i\pi/2)k} \psi_{t_1}((-1)^k x_1) \tag{4.4}$$

which is just (1.3).

Note that (4.2) could be interpreted as

$$K(x_2, t_2|x_1, t_1) = \int K^\alpha(x_2, t_2|x_1, t_1) d\alpha \tag{4.5}$$

where α is a continuous parameter characterizing the “critical points” (i.e., classical paths) of S . The partial amplitudes K^α are composed of the contributions of the corresponding classical path $\bar{\gamma}^\alpha$ multiplied by the correction factor due to paths “oscillating around $\bar{\gamma}^\alpha$.” These “oscillating paths” are exactly those which pass through $\bar{\gamma}^\alpha(t_1 + \tau/4)$, $\bar{\gamma}^\alpha(t_1 + 3\tau/4)$, \dots , $\bar{\gamma}^\alpha[t_1 + (2k - 1)\tau/4]$:

$$K^\alpha(x_2, t_2|x_1, t_1) = \exp \frac{i}{\hbar} S(\bar{\gamma}^\alpha) F^\alpha(t_2 - t_1) \tag{4.6}$$

It is easy to see that the dividing points could be substituted by any ordered set $t^{(1)}, t^{(3)}, \dots, t^{(2k-1)}$ satisfying

$$t_1 < t^{(1)} < t_1 + \frac{\tau}{2} < \dots < t_1 + (k - 1) \frac{\tau}{2} < t^{(2k-1)} < t_1 + k \frac{\tau}{2} \tag{4.7}$$

(4.5) and (4.6) comprise the substitute to (2.1) valid for coalescing paths.

5. CONCLUDING REMARKS

In describing the propagator near caustics, one studies generally (DeWitt-Morette, 1976; Schulmann, 1975; Miller, 1970; Marcus, 1971; Levit et al., 1974; Massman and Rasmussen, 1975) the effect of higher-order corrections due to anharmonicity, which change our δ to a more realistic function. We conjecture, however, that the *phase* of the wavefunction will be determined essentially by the pure quadratic part, which we have studied. This would be observable in interference experiments, assuming we have a kind of *structural stability* (Souriau, 1977) in phase. This problem will be studied elsewhere.

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