Summing Paths for a Particle in a Box.

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(ricevuto il 2 Aprile 1979)

Considering the present wide-spread use of path integrals (1) in field theory, elementary-particle physics, and collective phenomena (2) it is surprising how many standard text book problems of quantum mechanics have not been solved within this framework. Recently, this gap was filled for the hydrogen atom (3). In this note we would like to exhibit the path integration for a particle in a box (infinite square well). While in Schrödinger theory this system has a trivial solution, a careful classification of paths is needed before Feynman's formula can be evaluated.

In the grated version in which the time-axis is divided into $N+1$ intervals via $t_l = \varepsilon l + t_a$, $l = 0, 1, \ldots, N+1$, the problem consists in performing the infinite product of integrals

$$\langle x_b, t_b | x_a, t_a\rangle = \lim_{N\to\infty} \frac{1}{\sqrt{2\pi i\varepsilon/m}} \prod_{i=1}^{N} \int_0^L \frac{\mathrm{d}x_i}{\sqrt{2\pi i\varepsilon/m}} \exp\left[i\sum_{i=1}^{N+1} \frac{m}{2\varepsilon}(x_i - x_{i-1})^2\right] \tag{1}$$

with the basis difficulty that the integral over the finite box $x \in (0, L)$, is not completely Gaussian but would render error functions if done in the brute-force way. In order to circumvent this we formally extend the range of integration to cover the infinite interval $x \in (-\infty, \infty)$. After this we develop a convenient procedure for subtracting all amplitudes running through the physically inaccessible domain $x > L$, $0 > x$.

In order to organize this program we construct an extended zone scheme by dividing the x, t space into infinitely many strips at $x = 0, \pm L, \pm 2L, \ldots$. Consider all paths running from a fixed initial point x_a to a final point x_b within the box. Let us compare these with two more sets of paths: those going to new final end points $x_b^{(n)}$ which are

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(1) V. N. POPOV: CERN preprint TH 2424 (1974); *Functional Integrals in Quantum Field Theory and Statistical Physics* (Moscow, 1976) (in Russian).
(2) H. KLEINERT: *Fortschr. Phys.*, **26**, 565 (1978); *Collective field theory of superliquid* ^{3}He, extended version of Erice Lecture Notes (1978).
(3) I. H. DURU and H. KLEINERT: FU Berlin preprint (February 1979).

displaced against x_b by n multiples of $2L$ ($n = \pm 1, \pm 2, \ldots$),

$$x_b^{(n)} = x_b + 2nL \tag{2}$$

(the point x_b itself may be considered as $x_b^{(0)}$), and those going to $\bar{x}_b^{(n)}$ defined by

$$\bar{x}_b^{(n)} \equiv -x_b + 2nL\,. \tag{3}$$

The point is now that at a fixed x_a, summing paths over all end points $x_b^{(n)}$ and subtracting them for all $\bar{x}_b^{(m)}$ eliminates all paths which do not run *completely within* the physically permitted potential well $x \in (0, L)$. In order to see this consider a path which touches the upper (lower) wall $x \equiv L$ ($x \equiv 0$) once at t_1 and is then reflected (see fig. 1). There

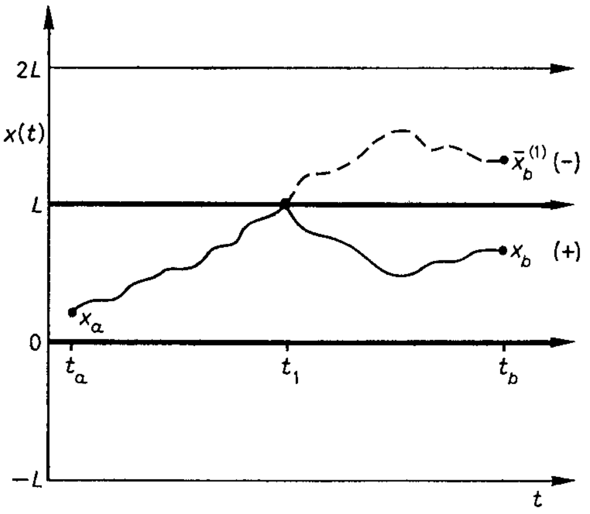

Fig. 1. – A curve with one reflection on the upper wall of the box. Its contribution is eliminated in the path integral by subtracting the path to $\bar{x}_b^{(1)}$ with the same action.

is a partner to this path in the extended-zone scheme arrives at $\bar{x}_b^{(1)}$ ($\bar{x}_b^{(0)}$) and has exactly the same action. By summing all paths to x_b and subtracting those to $\bar{x}_b^{(1)}$, ($\bar{x}_b^{(0)}$) the amplitude receives no contribution from single reflections on the upper (lower) wall.

The same procedure eliminates at the same time all paths with two or more successive reflections at the upper (lower) wall (see fig. 2).

Consider now a path reflected once at the upper wall for t_1 and at the lower wall for $\bar{t}_1$ (see fig. 3). This path has three partners of equal action in the extended zone scheme, namely those going to $x_b^{(1)}, \bar{x}_b^{(0)}, \bar{x}_b^{(1)}$. Adding the paths to x_b, $x_b^{(1)}$, and subtracting those to $\bar{x}_b^{(0)}, \bar{x}_b^{(1)}$ eliminates all paths reflected once at the upper and afterwards at the lower wall.

The same statement is true for multiple successive reflections first on the upper and then on the lower wall for the same reason as before.

In order to generalize this procedure we classify all paths in the following way: We count how often the path is reflected on the upper wall and on the lower wall in alternative order. If the number n of the reflections is even, and the first reflection is at the upper wall, we have to sum paths to $x_b^{(1-n/2)}, x_b^{(2-n/2)}, \ldots, x_b^{(n/2)}$ and subtract those to $\bar{x}_b^{(1-n/2)}, \bar{x}_b^{(2-n/2)}, \ldots, \bar{x}_b^{(n/2)}$ (for the lower wall the end points are $x_b^{(-n/2)}, \ldots, x_b^{(n/2-1)}$ and $\bar{x}_b^{(-n/2+1)}, \ldots, \bar{x}_b^{(n/2)}$). If the number of reflections is odd and first at the upper wall the

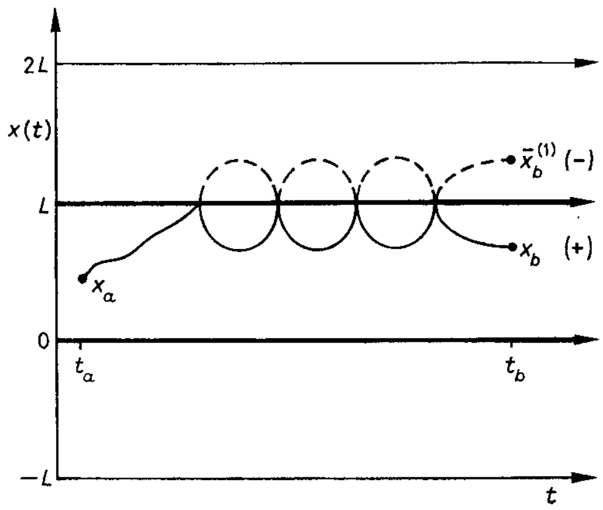

Fig. 2. – A path which reflects successively on the upper wall is eliminated by the same subtraction procedure as in fig. 1.

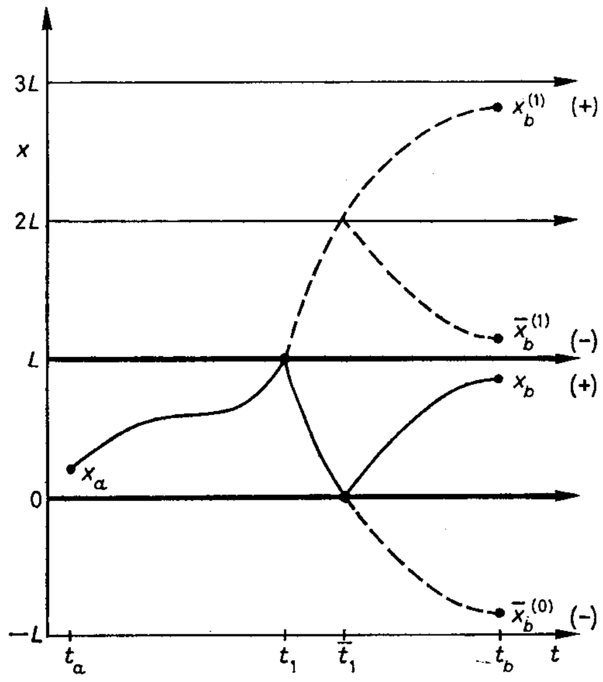

Fig. 3. – A path which reflects once on the upper and then on the lower wall is eliminated by summing over all paths to $x_b^{(1)}$ and subtracting all paths to $\bar{x}_b^{(0)}\,\bar{x}_b^{(1)}$.

end points are $x_b^{(-(n-1)/2)}, \ldots, x_b^{((n-1)/2)}$ and $\bar{x}_b^{(-(n-1)/2+1)}, \ldots, \bar{x}_b^{((n+1)/2)}$ (for the lower wall: $x_b^{(-(n-1)/2)}, \ldots, x_b^{((n-1)/2)}$ and $\bar{x}_b^{(-(n-1)/2)}, \ldots, \bar{x}_b^{((n-1)/2)}$).

In this classification successive reflections on the same wall can be contracted and counted as a single reflection, just as in the special case before.

The amplitude for a particle in a box can now be calculated by functionally integrating over the *whole* space and summing all paths going to $x_b^{(n)} \equiv x_b + 2nL$ while subtracting all those going to $\bar{x}_b^{(n)} \equiv -x_b + 2nL$

$$\langle x_b, t_b | x_a, t_a \rangle = \sum_{n=-\infty}^{\infty} \langle x_b + 2nL, t_b | x_a, t_a \rangle^0 - \sum_{n=-\infty}^{\infty} \langle -x_b + 2nL, t_b | x_a, t_a \rangle^0 , \tag{4}$$

where $\langle x_b, t_b | x_a, t_a \rangle^0$ denotes the amplitude for the free particle in the full space which is obtained by using $\int_{-\infty}^{\infty} dx_i$ in formula (1). Now the integral is Gaussian and can be integrated trivially to

$$\langle x_b, t_b | x_a, t_a \rangle = \frac{1}{\sqrt{2\pi i (t_b - t_a)/m}} \exp\left[i \frac{m}{t_b - t_a} (x_b - x_a)^2/2 \right] = \int_{-\infty}^{\infty} \frac{dp}{2\pi} \exp\left[ip(x_b - x_a) - i \frac{p^2}{2m} (t_b - t_a) \right]. \tag{5}$$

Performing the summation prescribed in eq. (4) gives

$$\begin{aligned} \langle x_b, t_b | x_a, t_a \rangle &= \sum_{n=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dp}{2\pi} [\exp[ip(x_b - x_a + 2nL)] - (x_b \to -x_b)] \cdot \\ &\cdot \exp\left[-i \frac{p^2}{2m} (t_b - t_a) \right] = \frac{\pi}{L} \sum_{\nu=-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{dp}{2\pi} \delta\left(p - \frac{\pi}{L} \nu \right) \cdot \\ &\cdot [\exp[ip(x_b - x_a)] - (x_b \to -x_b)] \exp\left[-i \frac{p^2}{2m} (t_b - t_a) \right] = \\ &= \frac{1}{L} \sum_{\nu=1}^{\infty} \left[\cos \frac{\pi}{L} \nu (x_b - x_a) - (x_b \to -x_b) \right] \exp\left[-i \frac{\pi^2}{L^2} \nu^2 \frac{1}{2m} (t_b - t_a) \right] = \\ &= \frac{2}{L} \sum_{\nu=1}^{\infty} \sin \frac{\pi}{L} \nu x_b \sin \frac{\pi}{L} \nu x_a \exp\left[-i \frac{\pi^2}{L^2} \nu^2 \frac{1}{2m} (t_b - t_a) \right]. \end{aligned} \tag{6}$$

This result displays the well-known normalized wave functions

$$\psi_\nu(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi}{L} \nu x , \qquad \nu = 1, 2, \ldots \tag{7}$$

of energy

$$E_\nu = \frac{\pi^2}{L^2} \nu^2 \frac{1}{2m} . \tag{8}$$