ФИЗИКА ЭЛЕМЕНТАРНЫХ ЧАСТИЦ И АТОМНОГО ЯДРА
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WHEN PHYSICS HELPS MATHEMATICS: CALCULATION OF THE SOPHISTICATED MULTIPLE INTEGRAL

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WHEN PHYSICS HELPS MATHEMATICS: CALCULATION OF THE SOPHISTICATED MULTIPLE INTEGRAL

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There exists a remarkable connection between the quantum mechanical Landau–Zener problem and purely classical-mechanical problem of a ball rolling on a Cornu spiral. This correspondence allows us to calculate a complicated multiple integral, a kind of multidimensional generalization of Fresnel integrals. A direct method of calculation is also considered but found to be successful only in some low-dimensional cases. As a byproduct of this direct method, an interesting new integral representation for $\zeta(2)$ is obtained.

Имеется замечательное соответствие между квантово-механической задачей Ландау–Зенера и задачей классической механики о шаре, вращающемся по спирали Корню. Это соответствие позволяет вычислить сложный многомерный интеграл, являющийся многомерным обобщением интеграла Френеля. Также рассмотрено прямое вычисление интеграла, однако такой способ успешен только в некоторых случаях для небольших размерностей. Как приложение прямого метода получено новое интересное представление для $\zeta(2)$.

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INTRODUCTION

According to Vladimir Arnold [1], mathematics can be considered as some branch of physics. In writing this note we have no intention to advocate such a point of view. Nevertheless, in our opinion the following calculus problem is a hard nut to crack if only mathematical considerations are being used. The problem lies in exactly calculating the multiple integral of the type

$$I_n = \int\limits_{-\infty}^{\infty} ds_1 \int\limits_{-\infty}^{s_1} ds_2 \cdots \int\limits_{-\infty}^{s_{2n-1}} ds_{2n}\ \cos\left(s_1^2 - s_2^2\right)\ \cdots \cos\left(s_{2n-1}^2 - s_{2n}^2\right). \qquad (1)$$

Because of the $s_1 \leftrightarrow s_2$ symmetry, the $n = 1$ case is simple

$$I_1 = \frac{1}{2!} \int\limits_{-\infty}^{\infty} ds_1 \int\limits_{-\infty}^{\infty} ds_2\ \left(\cos s_1^2\, \cos s_2^2 + \sin s_1^2\, \sin s_2^2\right) = \frac{\pi}{2}, \qquad (2)$$

since its calculation involves known Fresnel integrals

$$\int_{-\infty}^{\infty} ds\ \cos s^2 = \int_{-\infty}^{\infty} ds\ \sin s^2 = \sqrt{\frac{\pi}{2}}.$$

However, already for $n \geqslant 2$ the above symmetry is lost and things quickly become messy. The $n = 2$ and $n = 3$ cases lie at the borderline. They can be done with some efforts even though the calculations become noticeably more involved. Unfortunately, they do not admit an apparent generalization by using the induction method. Already for $n = 4$, the attempt to use the same methods meets difficulties. Nevertheless, we found a way to calculate such a type of integrals by invoking some physical arguments.

1. «IF YOU CANNOT SOLVE A PROBLEM, THEN THERE COULD BE AN EASIER PROBLEM YOU CAN SOLVE»

Trying to follow George Pólya's advice, let us consider the following system of ordinary differential equations:

$$\frac{d}{ds}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \frac{1}{R}\begin{pmatrix} 0 & 0 & -\sin\dfrac{as^2}{2} \\ 0 & 0 & \cos\dfrac{as^2}{2} \\ \sin\dfrac{as^2}{2} & -\cos\dfrac{as^2}{2} & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}. \tag{3}$$

Such a system of equations emerges naturally when one tries to describe a motion of a sphere S^2 rolling on the flat surface $\mathbf{R}^2$ without slippage. More accurately, it describes the rolling of a sphere of radius R along the Cornu spiral on $\mathbf{R}^2$ whose curvature $\kappa = as$ is proportional to the arc-length s [3,4]. But what is the relation of this problem to our integral (1)?

As the matrices

$$M(s) = \begin{pmatrix} 0 & 0 & -\sin\dfrac{as^2}{2} \\ 0 & 0 & \cos\dfrac{as^2}{2} \\ \sin\dfrac{as^2}{2} & -\cos\dfrac{as^2}{2} & 0 \end{pmatrix}$$

do not commute for different values of s, the solution of (3) is given by the time ordered exponential

$$U(s,s_0)=T\exp\left(\int\limits_{s_0}^{s}M(s_1)\,ds_1\right)=1+\int\limits_{s_0}^{s}M(s_1)\,ds_1+$$
$$+\int\limits_{s_0}^{s}ds_1\int\limits_{s_0}^{s_1}ds_2M(s_1)M(s_2)+\int\limits_{s_0}^{s}ds_1\int\limits_{s_0}^{s_1}ds_2\int\limits_{s_0}^{s_2}ds_3\,M(s_1)M(s_2)M(s_3)+\ldots \tag{4}$$

so that

$$\left(\begin{array}{c} x(s)\\ y(s)\\ z(s)\end{array}\right)=U(s,s_0)\left(\begin{array}{c} x(s_0)\\ y(s_0)\\ z(s_0)\end{array}\right). \tag{5}$$

Let us take a closer look at the individual terms of the above infinite series (4). Writing the matrix $M(s_i)$ in the block-form

$$M_i\equiv M(s_i)=\left(\begin{array}{cc} 0 & \chi_i\\ -\chi_i^T & 0\end{array}\right),$$

where

$$\chi_i=\frac{1}{R}\left(\begin{array}{c} -\sin\dfrac{as_i^2}{2}\\ \cos\dfrac{as_i^2}{2}\end{array}\right),$$

it is easy to prove by induction that

$$M_1M_2\cdots M_{2n+1}=$$
$$=\left(\begin{array}{cc} 0 & (-1)^n\chi_1\chi_2^T\cdots\chi_{2n-1}\chi_{2n}^T\chi_{2n+1}\\ (-1)^{n+1}\chi_1^T\chi_2\cdots\chi_{2n-1}^T\chi_{2n}\chi_{2n+1}^T & 0\end{array}\right),$$

and

$$M_1M_2\cdots M_{2n}=\left(\begin{array}{cc} (-1)^n\chi_1\chi_2^T\cdots\chi_{2n-1}\chi_{2n}^T & 0\\ 0 & (-1)^n\chi_1^T\chi_2\cdots\chi_{2n-1}^T\chi_{2n}\end{array}\right).$$

But

$$\chi_i^T\chi_{i+1}=\frac{1}{R^2}\,\cos\frac{a}{2}(s_i^2-s_{i+1}^2).$$

Besides, then our calculation is supplemented by the following initial and boundary conditions:

$$s_0=-\infty,\quad s=\infty,\quad x(-\infty)=y(-\infty)=0,\quad z(-\infty)=1, \tag{6}$$

in view of these relations and taking into account (5) and (4), we finally obtain

$$z(\infty) = 1 + \sum_{n=1}^{\infty} \frac{(-1)^n}{R^{2n}} \int_{-\infty}^{\infty} ds_1 \int_{-\infty}^{s_1} ds_2 \cdots \int_{-\infty}^{s_{2n-1}} ds_{2n}\, f_n(s_1, s_2, \ldots, s_{2n}), \quad (7)$$

where

$$f_n(s_1, s_2, \ldots, s_{2n}) = \cos\frac{a}{2}(s_1^2 - s_2^2)\, \cos\frac{a}{2}(s_3^2 - s_4^2) \cdots \cos\frac{a}{2}(s_{2n-1}^2 - s_{2n}^2).$$

After rescaling

$$s_i \to \sqrt{\frac{2}{a}}\, s_i, \quad (8)$$

our original integral (1) indeed shows up in the series (7):

$$z(\infty) = 1 + \sum_{n=1}^{\infty} (-1)^n \left(\frac{2}{aR^2}\right)^n I_n. \quad (9)$$

Thus, if we can find $z(\infty)$, we can find I_n as well! But how can we find $z(\infty)$?

2. SPINORIZATION AND THE HOPF MAP

Now we shall follow the advice of Jacques Hadamard: «*The shortest path between two islands of truths in the real domain passes through the complex plane*». By adopting his suggestion to our case it is convenient at this point to use two complex variables a and b instead of three real variables x, y, and z through relations [5]

$$x = ab^* + ba^*, \quad y = i(ab^* - ba^*), \quad z = aa^* - bb^*. \quad (10)$$

Notice: introduction of two complex variables is equivalent to looking at solution for our problem in $\mathbf{C}^2$! Furthermore, in view of the initial conditions and Eq. (3), the variables x, y, and z are constrained to unit sphere S^2. This causes the variables a and b to be constrained to S^3, that is to obey the equation $|a|^2 + |b|^2 = 1$. See [5] for more details. Interestingly enough, under these conditions Eq. (10) describes the Hopf map $S^3 \to S^2$ [6]. From [5] it can be seen that the complex variables a and b must satisfy the following system of differential equations:

$$i\frac{d}{ds}\begin{pmatrix} a \\ b \end{pmatrix} = -\frac{1}{2R}\begin{pmatrix} 0 & \mathrm{e}^{-ias^2/2} \\ \mathrm{e}^{ias^2/2} & 0 \end{pmatrix}\begin{pmatrix} a \\ b \end{pmatrix}, \quad (11)$$

if the real variables x, y, and z satisfy (3). Now we can again formally solve (11) by using the time-ordered exponential series. This time, however, the solution is known and it was obtained by Rojo in [2]. We just shortly repeat it to ensure the continuity of our exposition. The solution is formally given by

$$\begin{pmatrix} a(s) \\ b(s) \end{pmatrix} = U(s, s_0) \begin{pmatrix} a(s_0) \\ b(s_0) \end{pmatrix}, \tag{12}$$

where

$$U(s, s_0) = 1 - i \int\limits_{s_0}^{s} H(s_1) ds_1 + (-i)^2 \int\limits_{s_0}^{s} ds_1 \int\limits_{s_0}^{s_1} ds_2\, H(s_1)\, H(s_2) + \ldots, \tag{13}$$

with

$$H(s) = -\frac{1}{2R} \begin{pmatrix} 0 & \mathrm{e}^{-ias^2/2} \\ \mathrm{e}^{ias^2/2} & 0 \end{pmatrix}.$$

The imposed initial conditions (6) are now translated into

$$a(-\infty) = 1, \quad b(-\infty) = 0. \tag{14}$$

Since the unitary evolution (12) conserves the norm $aa^* + bb^*$, from (14) we obtain back the equation for 3-sphere, that is $aa^* + bb^* = 1$, valid for any «time» s. This result implies that

$$z(\infty) = |a(\infty)|^2 - |b(\infty)|^2 = 2|a(\infty)|^2 - 1. \tag{15}$$

Evidently, we need only to calculate $a(\infty)$ to obtain $z(\infty)$.

By examining the product of $H(s_i)$ matrices, we observe that for the odd number of multipliers the matrix product does not have nonzero diagonal terms and, hence, does not contribute to $a(\infty)$ thanks to the initial conditions (14). The remaining terms with even number of multipliers have easily calculable nonzero diagonal elements so that we get

$$a(\infty) = 1 + \left(\frac{i}{2R}\right)^2 \int\limits_{-\infty}^{\infty} ds_1\, \mathrm{e}^{-ias_1^2/2} \int\limits_{-\infty}^{s_1} ds_2\, \mathrm{e}^{ias_2^2/2} + \ldots$$

After rescaling (8), this expression acquires the form

$$a(\infty) = 1 + \sum_{n=1}^{\infty} (-1)^n \left(\frac{1}{2aR^2}\right)^n J_n, \tag{16}$$

where

$$J_n = \int\limits_{-\infty}^{\infty} ds_1\, \mathrm{e}^{-is_1^2} \int\limits_{-\infty}^{s_1} ds_2\, \mathrm{e}^{is_2^2} \int\limits_{-\infty}^{s_2} ds_3\, \mathrm{e}^{-is_3^2} \cdots \int\limits_{-\infty}^{s_{2n-1}} ds_{2n}\, \mathrm{e}^{is_{2n}^2}. \tag{17}$$

In contrast to I_n, the multiple integral J_n is doable. It can be calculated as follows [2]. First, we write

$$J_n = \int_{-\infty}^{\infty} ds_1 \cdots \int_{-\infty}^{\infty} ds_{2n}\, \theta(s_1 - s_2) \cdots \theta(s_{2n-1} - s_{2n})\, e_n(s_1^2, \ldots, s_{2n}^2),$$

with

$$e_n(s_1^2, \ldots, s_{2n}^2) = \exp\{-i(s_1^2 - s_2^2 + s_3^2 - s_4^2 + \ldots + s_{2n-1}^2 - s_{2n}^2)\}.$$

Then, we use the integral representation for the Heaviside step function

$$\theta(s) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} d\omega\, \frac{\mathrm{e}^{i\omega s}}{\omega - i\epsilon} = \begin{cases} 1, & \text{if } s > 0, \\ 1/2, & \text{if } s = 0, \\ 0, & \text{if } s < 0. \end{cases} \tag{18}$$

Using the result, we can perform the integrals over ds_i. For this purpose we sequentially complete the squares, e.g.,

$$i\left[s_2(\omega_2 - \omega_1) + s_2^2\right] = i\left[\left(s_2 + \frac{\omega_2 - \omega_1}{2}\right)^2 - \frac{(\omega_2 - \omega_1)^2}{4}\right],$$

and then evaluate the Gaussian integrals

$$\int_{-\infty}^{\infty} \mathrm{e}^{\pm i s^2}\, ds = \int_{-\infty}^{\infty} (\cos s^2 \pm i \sin s^2)\, ds = \sqrt{\frac{\pi}{2}}\,(1 \pm i).$$

As a result, we finally obtain

$$J_n = \pi^n \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i} \cdots \int_{-\infty}^{\infty} \frac{d\omega_{2n-1}}{2\pi i} \times \\ \times \frac{\exp\left\{\dfrac{i}{2}\left[\omega_2(\omega_1 - \omega_3) + \omega_4(\omega_3 - \omega_5) + \ldots + \omega_{2n-2}(\omega_{2n-3} - \omega_{2n-1})\right]\right\}}{(\omega_1 - i\epsilon)(\omega_2 - i\epsilon) \cdots (\omega_{2n-1} - i\epsilon)}. \tag{19}$$

As can be seen, the terms quadratic in ω_i are all canceled thanks to the alternating signs in exponents in (17). It is this feature that distinguishes, as we shall demonstrate in the next section, the calculation of J_n from the calculation of I_n and makes the integral J_n solvable. For this purpose we rescale even-index variables $\omega_{2i} \to 2\omega_{2i}$ in (19) and perform integrals in these variables taking into account (18). The result is:

$$J_n = \pi^n \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i} \int\limits_{-\infty}^{\infty} \frac{d\omega_3}{2\pi i} \cdots$$
$$\cdots \int\limits_{-\infty}^{\infty} \frac{d\omega_{2n-1}}{2\pi i} \frac{\theta(\omega_1-\omega_3)\theta(\omega_3-\omega_5)\cdots\theta(\omega_{2n-3}-\omega_{2n-1})}{(\omega_1-i\epsilon)(\omega_3-i\epsilon)\cdots(\omega_{2n-1}-i\epsilon)},$$

or

$$J_n = \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i} \int\limits_{-\infty}^{\omega_1} \frac{d\omega_3}{2\pi i} \cdots \int\limits_{-\infty}^{\omega_{2n-3}} \frac{d\omega_{2n-1}}{2\pi i} \frac{\pi^n}{(\omega_1-i\epsilon)(\omega_3-i\epsilon)\cdots(\omega_{2n-1}-i\epsilon)}. \tag{20}$$

It is the symmetry of the integrand in (20) that makes the calculation of (20) as easy as the calculation of I_1 from which our story had begun. In the present case we obtain

$$J_n = \pi^n \frac{1}{n!}\left[\int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i} \frac{1}{\omega_1 - i\epsilon}\right]^n = \frac{\pi^n}{n!}\left[\theta(0)\right]^n = \frac{1}{n!}\left(\frac{\pi}{2}\right)^n. \tag{21}$$

Then (16) shows that

$$a(\infty) = \exp\left(-\frac{\pi}{4aR^2}\right), \tag{22}$$

and from (15) we get

$$z(\infty) = 2\exp\left(-\frac{\pi}{2aR^2}\right) - 1 = 1 + \sum_{n=1}^{\infty}(-1)^n \frac{2}{n!}\left(\frac{\pi}{2aR^2}\right)^n.$$

Comparing with (9), we finally obtain the desired expression for the integral I_n:

$$I_n = \frac{2}{n!}\left(\frac{\pi}{4}\right)^n. \tag{23}$$

3. DIRECT CALCULATION OF I_2

If you are still unhappy by our use of indirect methods of calculation of deceptively simply looking integral (1), here we discuss some features of the direct method. Unfortunately, as far as we can see, it works well only for small values of n.

Indeed, let us write

$$I_2 = \int\limits_{-\infty}^{\infty} ds_1 \int\limits_{-\infty}^{\infty} ds_2 \int\limits_{-\infty}^{\infty} ds_3 \times$$
$$\times \int\limits_{-\infty}^{\infty} ds_4\, \theta_4(s_1, s_2, s_3, s_4)\, \cos\left(s_1^2 - s_2^2\right)\, \cos\left(s_3^2 - s_4^2\right), \quad (24)$$

where

$$\theta_4(s_1, s_2, s_3, s_4) = \theta(s_1 - s_2)\, \theta(s_2 - s_3)\, \theta(s_3 - s_4). \quad (25)$$

Then, as in the previous section, we use the integral representation for the step function and notice that

$$\int\limits_{-\infty}^{\infty} ds_1 \int\limits_{-\infty}^{\infty} ds_2\, \mathrm{e}^{i\omega_1 s_1}\, \mathrm{e}^{-is_2(\omega_1-\omega_2)}\, \cos\left(s_1^2 - s_2^2\right) = \frac{1}{2} \int\limits_{-\infty}^{\infty} ds_1 \int\limits_{-\infty}^{\infty} ds_2 \times$$
$$\times \left[\exp\left(-i\frac{\omega_1^2}{4} + i\left(s_1 + \frac{\omega_1}{2}\right)^2 + i\frac{(\omega_1-\omega_2)^2}{4} - i\left(s_2 + \frac{\omega_1-\omega_2}{2}\right)^2\right) + \right.$$
$$\left. + \exp\left(i\frac{\omega_1^2}{4} - i\left(s_1 - \frac{\omega_1}{2}\right)^2 - i\frac{(\omega_1-\omega_2)^2}{4} + i\left(s_2 - \frac{\omega_1-\omega_2}{2}\right)^2\right)\right] =$$
$$= \pi \cos\left[\frac{1}{4}\omega_2(2\omega_1 - \omega_2)\right]. \quad (26)$$

Similar calculations are done for integrals over ds_3 and ds_4. As a result, after rescaling $\omega_2 \to 2\omega_2$, we end up with the result:

$$I_2 = \pi^2 \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i} \int\limits_{-\infty}^{\infty} \frac{d\omega_2}{2\pi i} \int\limits_{-\infty}^{\infty} \frac{d\omega_3}{2\pi i}\, \frac{\cos\left[\omega_2(\omega_1 - \omega_2)\right]\, \cos\left[\omega_2(\omega_3 - \omega_2)\right]}{(\omega_1 - i\epsilon)(\omega_2 - i\epsilon)(\omega_3 - i\epsilon)}. \quad (27)$$

The integrals over $d\omega_1$ and $d\omega_3$ can be easily calculated. Indeed,

$$\int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i}\, \frac{\cos\left(\omega_1\omega_2 - \omega_2^2\right)}{\omega_1 - i\epsilon} = \frac{1}{2} \int\limits_{-\infty}^{\infty} \frac{d\omega_1}{2\pi i} \left[\frac{\mathrm{e}^{i\omega_1\omega_2}}{\omega_1 - i\epsilon}\, \mathrm{e}^{-i\omega_2^2} + \frac{\mathrm{e}^{-i\omega_1\omega_2}}{\omega_1 - i\epsilon}\, \mathrm{e}^{i\omega_2^2}\right] =$$
$$= \frac{1}{2}\left[\theta(\omega_2)\, \mathrm{e}^{-i\omega_2^2} + \theta(-\omega_2)\, \mathrm{e}^{i\omega_2^2}\right].$$

Therefore,

$$I_2 = \frac{\pi^2}{4} \int\limits_{-\infty}^{\infty} \frac{d\omega_2}{2\pi i}\, \frac{\left[\theta(\omega_2)\, \mathrm{e}^{-i\omega_2^2} + \theta(-\omega_2)\, \mathrm{e}^{i\omega_2^2}\right]^2}{\omega_2 - i\epsilon}. \quad (28)$$

Now we use the well-known result

$$\frac{1}{\omega - i\epsilon} = P\frac{1}{\omega} + i\pi\delta(\omega) \tag{29}$$

to split the integral (28) into the principal value and the δ-function parts:

$$I_2 = \frac{\pi^2}{4}(I_{2P} + I_{2\delta}).$$

Of course, the δ-function part is obtained instantly

$$I_{2\delta} = \frac{1}{2}.$$

As for the principal value part, we have

$$I_{2P} = \frac{1}{2\pi i}\lim_{\epsilon\to 0}\left[\int\limits_{\epsilon}^{\infty}\frac{\mathrm{e}^{-2i\omega_2^2}}{\omega_2}\,d\omega_2 + \int\limits_{-\infty}^{-\epsilon}\frac{\mathrm{e}^{2i\omega_2^2}}{\omega_2}\,d\omega_2\right] =$$

$$= \frac{1}{2\pi i}\lim_{\epsilon\to 0}\left[\int\limits_{\epsilon}^{\infty}\frac{\mathrm{e}^{-2i\omega_2^2}}{\omega_2}\,d\omega_2 - \int\limits_{\epsilon}^{\infty}\frac{\mathrm{e}^{2i\omega_2^2}}{\omega_2}\,d\omega_2\right] =$$

$$= -\frac{1}{\pi}\int\limits_{0}^{\infty}\frac{\sin(2\omega_2^2)}{\omega_2}\,d\omega_2 = -\frac{1}{2\pi}\int\limits_{0}^{\infty}\frac{\sin[(\sqrt{2}\omega_2)^2]}{(\sqrt{2}\omega_2)^2}\,d[(\sqrt{2}\omega_2)^2] = -\frac{1}{4}.$$

In making the last step we have used the Dirichlet integral

$$\int\limits_{0}^{\infty}\frac{\sin\omega}{\omega}\,d\omega = \frac{\pi}{2}.$$

Putting all terms together, we obtain finally

$$I_2 = \frac{\pi^2}{16}, \tag{30}$$

which is a special case of (23), as expected.

Can we think about the general case ($n > 2$) by acting in the manner just described? By repeating the above steps when $n > 2$, we obtain

$$I_n = \left(\frac{\pi}{2}\right)^n \int\limits_{-\infty}^{\infty}\frac{d\omega_2}{2\pi i}\int\limits_{-\infty}^{\infty}\frac{d\omega_4}{2\pi i}\cdots$$

$$\cdots\int\limits_{-\infty}^{\infty}\frac{d\omega_{2n-2}}{2\pi i}\frac{f_n(\omega_2,\omega_4,\ldots,\omega_{2n-2})}{(\omega_2 - i\epsilon)(\omega_4 - i\epsilon)\cdots(\omega_{2n-2} - i\epsilon)}, \tag{31}$$

where

$$f_n(\omega_2, \omega_4, \ldots, \omega_{2n-2}) = \\ = \phi(0, \omega_2)\, \phi(\omega_2, \omega_4) \cdots \phi(\omega_{2n-4}, \omega_{2n-2})\, \phi(\omega_{2n-2}, 0), \quad (32)$$

with

$$\phi(\omega_1, \omega_2) = \theta(\omega_1 - \omega_2)\, \mathrm{e}^{-i(\omega_1^2 - \omega_2^2)} + \theta(\omega_2 - \omega_1)\, \mathrm{e}^{-i(\omega_2^2 - \omega_1^2)}. \quad (33)$$

Evidently, for $n > 2$ things begin to look rather inconclusive and the above direct method needs some fresh input in order to be brought to completion.

4. DIRECT CALCULATION OF I_3

Now let us calculate

$$I_3 = \left(\frac{\pi}{2}\right)^3 I,$$

where

$$I = \int_{-\infty}^{\infty} \frac{dx}{2\pi i}\, \frac{\phi(0, x) f(x)}{x - i\epsilon}, \quad (34)$$

and

$$f(x) = \int_{-\infty}^{\infty} \frac{dy}{2\pi i}\, \frac{\phi(x, y)\, \phi(y, 0)}{y - i\epsilon}. \quad (35)$$

Using the relation (29) in (34), we get

$$I = \frac{1}{2}\phi(0, 0) f(0) + \lim_{\epsilon \to 0} \int_{\epsilon}^{\infty} \frac{dx}{2\pi i}\, \frac{\phi(0, x) f(x) - \phi(0, -x) f(-x)}{x}.$$

However, $\phi(0, 0) = 1$, while

$$f(0) = \int_{-\infty}^{\infty} \frac{dy}{2\pi i}\, \frac{\phi(0, y)\phi(y, 0)}{y - i\epsilon} = \frac{1}{2}\phi^2(0, 0) + \lim_{\epsilon \to 0} \int_{\epsilon}^{\infty} \frac{dy}{2\pi i}\, \frac{\phi^2(0, y) - \phi^2(0, -y)}{y},$$

and since

$$\phi^2(0, y) - \phi^2(0, -y) = \mathrm{e}^{-2iy^2} - \mathrm{e}^{2iy^2},$$

when $y \geqslant \epsilon > 0$, we get

$$f(0) = \frac{1}{2} - \frac{1}{\pi} \int_0^{\infty} \frac{\sin(2y^2)}{y}\, dy = \frac{1}{4},$$

and, therefore,

$$I = \frac{1}{8} + K, \tag{36}$$

where

$$K = \lim_{\epsilon \to 0} \int\limits_{\epsilon}^{\infty} \frac{dx}{2\pi i} \, \frac{\mathrm{e}^{-ix^2} f(x) - \mathrm{e}^{ix^2} f(-x)}{x}. \tag{37}$$

Now, using again (29), we have

$$f(x) = \frac{1}{2} \phi(x,0)\, \phi(0,0) + \lim_{\epsilon \to 0} \int\limits_{\epsilon}^{\infty} \frac{dy}{2\pi i} \, \frac{\phi(x,y)\, \phi(y,0) - \phi(x,-y)\, \phi(-y,0)}{y}$$

and since in (37) $x > 0$, we get

$$f(x) = \frac{1}{2} \, \mathrm{e}^{-ix^2} + \\ + \lim_{\epsilon \to 0} \int\limits_{\epsilon}^{\infty} \frac{dy}{2\pi i} \, \frac{\theta(x-y)\, \mathrm{e}^{-ix^2} + \theta(y-x)\, \mathrm{e}^{-i(2y^2 - x^2)} - \mathrm{e}^{-i(x^2 - 2y^2)}}{y}. \tag{38}$$

Analogously,

$$f(-x) = \frac{1}{2} \, \mathrm{e}^{ix^2} + \\ + \lim_{\epsilon \to 0} \int\limits_{\epsilon}^{\infty} \frac{dy}{2\pi i} \, \frac{\mathrm{e}^{-i(2y^2 - x^2)} - \theta(x-y)\, \mathrm{e}^{ix^2} - \theta(y-x)\, \mathrm{e}^{-i(x^2 - 2y^2)}}{y}. \tag{39}$$

In light of (37), (38), and (39),

$$K = K_1 + K_2,$$

where

$$K_1 = \frac{1}{2} \int\limits_{0}^{\infty} \frac{dx}{2\pi i} \, \frac{\mathrm{e}^{-2ix^2} - \mathrm{e}^{2ix^2}}{x} = -\frac{1}{2\pi} \int\limits_{0}^{\infty} \frac{\sin{(2x^2)}}{x} \, dx = -\frac{1}{8}$$

and

$$K_2 = -\int\limits_{0}^{\infty} \frac{dx}{x} \int\limits_{0}^{\infty} \frac{dy}{y} \, \frac{\theta(x-y)\, \cos{(2x^2)} + \theta(y-x)\, \cos{(2y^2)} - \cos 2(x^2 - y^2)}{2\pi^2}.$$

After rescaling

$$x \to \frac{x}{\sqrt{2}}, \quad y \to \frac{y}{\sqrt{2}},$$

and using

$$\frac{dx}{x} = \frac{1}{2}\,\frac{d(x^2)}{x^2}, \quad \theta(x-y) = \theta(x^2-y^2), \;\text{ if }\; x>0 \;\text{ and }\; y>0,$$

as well as

$$\cos(x-y) = [\theta(x-y)+\theta(y-x)]\,\cos(x-y),$$

we end up with the result

$$I = K_2 = \frac{1}{4\pi^2}\int\limits_0^\infty \frac{dx}{x}\int\limits_0^x \frac{dy}{y}\,[\cos(x-y)-\cos x]. \tag{40}$$

To calculate the integral

$$\tilde{I} = \int\limits_0^\infty \frac{dx}{x}\int\limits_0^x \frac{dy}{y}\,[\cos(x-y)-\cos x],$$

we introduce a parametric integral related to it:

$$\tilde{I}(\alpha) = \int\limits_0^\infty \frac{dx}{x}\int\limits_0^x \frac{dy}{y}\,[\cos(x-\alpha y)-\cos x].$$

Note that $\tilde{I}(0)=0$ and $\tilde{I}(1)=\tilde{I}$, so that

$$\tilde{I} = \int\limits_0^1 \frac{d\tilde{I}(\alpha)}{d\alpha}\,d\alpha.$$

However,

$$\frac{d\tilde{I}(\alpha)}{d\alpha} = \int\limits_0^\infty \frac{dx}{x}\int\limits_0^x dy\,\sin(x-\alpha y) = \frac{1}{\alpha}\lim_{\epsilon\to 0}\int\limits_\epsilon^\infty \frac{dx}{x}\,[\cos(1-\alpha)x-\cos x]\,,$$

which is the same as

$$\frac{d\tilde{I}(\alpha)}{d\alpha} = \frac{1}{\alpha}\lim_{\epsilon\to 0}\left[\int\limits_{\epsilon(1-\alpha)}^\infty \frac{dx}{x}\,\cos x - \int\limits_\epsilon^\infty \frac{dx}{x}\,\cos x\right] = \lim_{\epsilon\to 0}\frac{Ci(\epsilon)-Ci(\epsilon(1-\alpha))}{\alpha},$$

where

$$Ci(x) = -\int_x^\infty \frac{dx}{x} \cos x$$

stands for the integral cosine function. Using the well-known series representation for this function

$$Ci(x) = \gamma + \ln x + \sum_{k=1}^{\infty} \frac{(-x^2)^k}{2k(2k)!},$$

$\gamma \approx 0.5772$ being the Euler constant, we get

$$\frac{d\tilde{I}(\alpha)}{d\alpha} = \frac{1}{\alpha} \lim_{\epsilon \to 0} [\ln \epsilon - \ln (1-\alpha)\epsilon] = -\frac{\ln (1-\alpha)}{\alpha},$$

and, therefore,

$$\tilde{I} = -\int_0^1 \frac{\ln (1-\alpha)}{\alpha} \, d\alpha = \zeta(2) = \frac{\pi^2}{6}.$$

We have just proved an interesting identity which seems to be a new integral representation for $\zeta(2)$:

$$\zeta(2) = \int_0^\infty \frac{dx}{x} \int_0^x \frac{dy}{y} \, [\cos (x-y) - \cos x]. \tag{41}$$

Collecting all pieces together, we get finally $I = 1/24$ and

$$I_3 = \frac{\pi^3}{8} \, \frac{1}{24} = \frac{2}{3!} \left(\frac{\pi}{4}\right)^3,$$

in agreement with (23).

5. CONCLUDING REMARKS

This problem had originally aroused in the context of a remarkable correspondence between the quantum mechanical Landau–Zener problem (known in the context of molecular scattering) and purely classical problem of a ball (that is 2-sphere) rolling on a Cornu spiral (that is on the curve in $\mathbf{R}^2$, known as Cornu spiral) recently established by Bloch and Rojo in [3, 4]. In fact, the main ingredient of this connection — the application of the Hopf map — goes back to Feynman, Vernon, and Hellwarth [5] who showed that the quantum evolution of any two-level system is determined by the classical evolution (precession) of the magnetic dipole moment of unit strength in an effective external magnetic field.

It is remarkable that physics helps to calculate a complicated integral (1). However, we suspect that there should be a direct method of calculation. For low values of n, we have provided some examples of the direct method. It is after the readers to tackle the case of general n.

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