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Diffraction in time with dissipation

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Abstract

The more usual problems discussed in classical mechanics in elementary textbooks are the non-dissipative ones in which there is a Hamiltonian representing the energy as a constant of motion. The translation of this type of problem to quantum mechanics is very well known. Conversely, there are very simple classical mechanical problems that involve dissipation, but whose translation to quantum mechanics on the basis of a corresponding Hamiltonian is sometimes misinterpreted, since the underlying classical formalism involves non-canonical transformations that lead to non-unitary transformations of the quantum mechanical wavefunctions. In this paper we shall discuss the problem of a beam of particles of given momentum incident from the left on a shutter that is opened at time $t = 0$. The solution has the well known properties of diffraction in time, but we will analyse it quantum mechanically both when dissipation is and is not present. The objective is to get a better understanding of the effect of dissipation in the quantum mechanical picture and to estimate the influence of the above mentioned non-unitary transformations on this particular problem.

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1. Introduction

When starting a course in classical mechanics one usually considers first problems in which there is no dissipation, where the force is independent of time and the gradient of a potential. The energy is then an integral of motion and using the Hamiltonian formalism we can derive the equation of motion from which we can obtain the coordinates and momenta as functions of time.

A trivial case is the one in which we just have one dimension where

$$E = \frac{1}{2}p^2 + V(x) \tag{1}$$

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with E being the energy and x, p, the coordinate and momentum and where in the following we use units in which the mass $m = 1$. Later we also impose this requirement on the Planck constant $\hbar = 1$.

From Hamilton's equations, with $E = H$,

$$\frac{\mathrm{d}x}{\mathrm{d}t} = p \qquad \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial V}{\partial x} \tag{2}$$

and taking into account the conservation of E in (1) we have

$$\int_{x_0}^{x} \frac{\mathrm{d}x}{\sqrt{2[E - V(x)]}} = t \tag{3}$$

and so the problem is solved by a quadrature.

While the type of problem mentioned above is interesting, in most physical situations we also have dissipation of energy due to friction or other causes, and many of these problems are frequently just as easy to solve. For example if the dissipation is just a linear function of the momentum or, in our units, of the velocity, the equation of motion becomes

$$\ddot{x} + \gamma\dot{x} + \frac{\partial V}{\partial x} = 0 \tag{4}$$

where γ is some positive real constant and a dot indicates a derivative with respect to time.

Considering for the moment the case when there is no potential, i.e. $V(x) = 0$ the solution of (4) is

$$p = p_0\mathrm{e}^{-\gamma t} \qquad x = \frac{p_0}{\gamma}(1 - \mathrm{e}^{-\gamma t}) + x_0 \tag{5}$$

where x_0, p_0 are the initial values of (x, p). Note that when $t \to \infty$ then $x \to (p_0/\gamma) + x_0$ which is a constant, and so it does not become ∞ as would happen in the case of no dissipation. This result will be relevant in the later discussion.

While many problems with dissipation are almost as easy to solve in classical mechanics as those that do not have this characteristic, the situation is quite different in quantum mechanics. For non-dissipative problems we have a Hamiltonian, and for the one-dimensional case such as that of (1), it is identical to the energy and by replacing p by $-\mathrm{i}\partial/\partial x$ it transforms into the time-dependent Schrödinger equation

$$-\frac{1}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = \mathrm{i}\frac{\partial\Psi(x,t)}{\partial t} \tag{6}$$

where, as the left-hand side is independent of time, we can assume $\Psi(x,t) = \psi(x)\exp(-\mathrm{i}Et)$ and equation (6) for $\psi(x)$ becomes the stationary Schrödinger equation where the right-hand side is replaced by $E\psi(x)$.

For dissipative problems, even for those as simple as that of equation (4), the situation is much more complex. We could reduce them to non-dissipative problems if we added an external system with which they could interact, but this implies including many, in some cases an infinite, number of extra degrees of freedom. There is a way of introducing a Hamiltonian for problems of type (4) but it presents some paradoxes that have been discussed by many people [1] including one of the authors (DS) [2]. We shall discuss these paradoxes in section 4.

Our main interest, though, is to find some simple time-dependent quantum mechanical problems which can have either dissipative or non-dissipative characteristics, so as to compare their behaviour as function of time. The example we shall choose is that of diffraction in time, a problem one of us (MM) discussed in [3] and, from another standpoint, more recently [4]. It consists of the time evolution of a beam of particles of definite momentum restricted to the range $-\infty \leqslant x \leqslant 0$ by a shutter at $x = 0$. At time $t = 0$ the shutter is removed and the behaviour of the wavefunction $\Psi(x,t)$ is analysed in the interval $0 \leqslant x \leqslant \infty$. This problem, which has no dissipation, will be reviewed in sections 2 and 3. We shall analyse a similar problem in which dissipation is present. In section 4 we compare the results for the two cases and also indicate how to solve some of the paradoxes present in the dissipative case.

2. Diffraction in time

The problem with diffraction in time, mentioned in the previous section, corresponds to finding a wavefunction $\Psi(x,t)$ satisfying, in our units, the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial\Psi(x,t)}{\partial t} = -\frac{1}{2}\frac{\partial^2\Psi(x,t)}{\partial x^2} \tag{7}$$

with the initial value

$$\Psi(x,0) = \exp(\mathrm{i}kx)\theta(-x) \tag{8}$$

where k will now denote the value of the momentum of the particles behind the shutter and $\theta(x)$ is the step function:

$$\theta(x) = \begin{cases} 1 & \text{if} \quad x > 0 \\ 0 & \text{if} \quad x < 0. \end{cases} \tag{9}$$

The determination of the time-dependent wavefunction, which from now on we shall denote by $M(x,k,t)$, can be done in many ways either by making it fulfil an ordinary differential equation as in [3] or using the Green function of the one-dimensional time-dependent Schrödinger equation [5]. We then arrive at the result

$$\begin{aligned} M(x,k,t) &= \tfrac{1}{2}\exp[\mathrm{i}(kx - \tfrac{1}{2}k^2 t)]\,\mathrm{erfc}\,(\mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\omega) \\ &= \mathrm{e}^{-\mathrm{i}\frac{\pi}{4}}\exp\left[\mathrm{i}\left(kx - \frac{1}{2}k^2 t\right)\right]\frac{1}{\sqrt{2}}\left\{\left[\frac{1}{2} + C(\omega)\right] + \mathrm{i}\left[\frac{1}{2} + S(\omega)\right]\right\} \end{aligned} \tag{10}$$

where

$$\omega = \frac{kt - x}{\sqrt{2t}} \tag{11}$$

and the error integral is

$$\mathrm{erfc}(z) = \frac{2}{\sqrt{\pi}}\int_z^\infty \mathrm{e}^{-y^2}\,\mathrm{d}y \tag{12}$$

while the Fresnel integrals are defined by

$$C(\omega) = \sqrt{\frac{2}{\pi}}\int_0^\omega \cos y^2\,\mathrm{d}y \tag{13}$$

$$S(\omega) = \sqrt{\frac{2}{\pi}}\int_0^\omega \sin y^2\,\mathrm{d}y. \tag{14}$$

The expression $|M(x,k,t)|^2$ gives the probability density of finding the particle at point x, at time t, when initially it was on the left-hand side of the shutter, i.e. with $x \leqslant 0$, and had a momentum k. From equation (10) we see that

$$|M(x,k,t)|^2 = \tfrac{1}{2}\left\{\left[\tfrac{1}{2} + C(\omega)\right]^2 + \left[\tfrac{1}{2} + S(\omega)\right]^2\right\} \tag{15}$$

which is identical to the expression of the intensity of light in Fresnel diffraction by a straight edge.

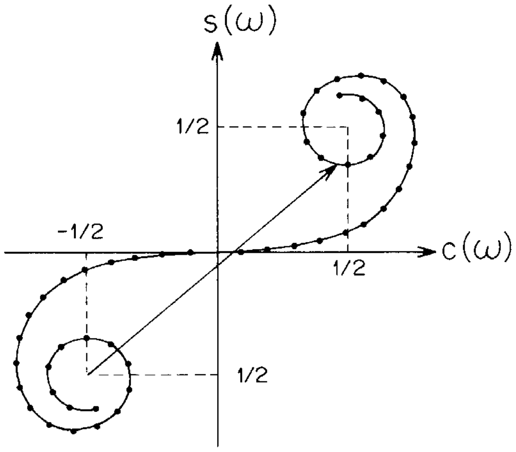

Figure 1. Cornu spiral. The value of ω is marked along the curve while the values of the Fresnel integrals $C(\omega)$ and $S(\omega)$ are given, respectively, by the abscissa and ordinate. One-half of the square of the magnitude of the vector from the point $(-1/2, -1/2)$ to a point on the curve with given ω gives the probability density for that value of ω.

However the variable ω of (11) has a very different meaning from the optical problem as it is now a function of time. That is the reason that, in the original paper, it was given the name of 'diffraction in time'.

If we want to have snapshots of the probability density $|M(x, k, t)|^2$ at given instances of time we can make use of the Cornu spiral diagram [6] of figure 1. The values $C(\omega)$ and $S(\omega)$ are given along the abscissa and ordinate while ω is marked along the curve itself. The value of $|M(x, k, t)|^2$ is one-half of the square of the distance between the point $\left(-\frac{1}{2}, -\frac{1}{2}\right)$ in the plane of figure 1 to the given point on the curve corresponding to the value ω. For t fixed and x going from $-\infty$ to $+\infty$ we see from (11) that ω goes from $-\infty$ to $+\infty$ passing through $\omega = 0$ when $x = x_0 \equiv kt$. With the help of the Cornu spiral we then obtain that $|M(x, k, t)|^2$ has the form of the solid curve of figure 2. The classical distribution of particles at time t is indicated by the dashed plot in figure 2 terminating abruptly at $x_0 = kt$.

Having thus reviewed the non-dissipative case of removing a shutter from a beam of particles of momentum k which was restricted originally to $-\infty \leqslant x \leqslant 0$, we shall now discuss a similar problem in which dissipation is present.

3. Diffraction in time with dissipation

A classical problem involving dissipation is frequently formulated through a Newton equation in which an appropriate extra force is included as indicated, for example, in the term $\gamma\dot{x}$ in (4). This equation, in contrast with equation (1) for the Hamiltonian of a non-dissipative problem, gives no hint on how it can be translated to a quantum mechanical form.

We must then look into more phenomenologically motivated ways to obtain equation (4). In particular, we consider those that include some type of effective Hamiltonians, albeit ones that besides x, p might depend also explicitly on the time t, and thus do not correspond to a conserved energy as they are not invariant under time translation. The historically first, and most frequently used, time-dependent Hamiltonian $\bar{H}$ was proposed by Caldirola [7] and Kanai [8] in the form

$$\bar{H} = \tfrac{1}{2}\mathrm{e}^{-\gamma t}\bar{p}^2 + \mathrm{e}^{\gamma t}V(\bar{x}). \tag{16}$$

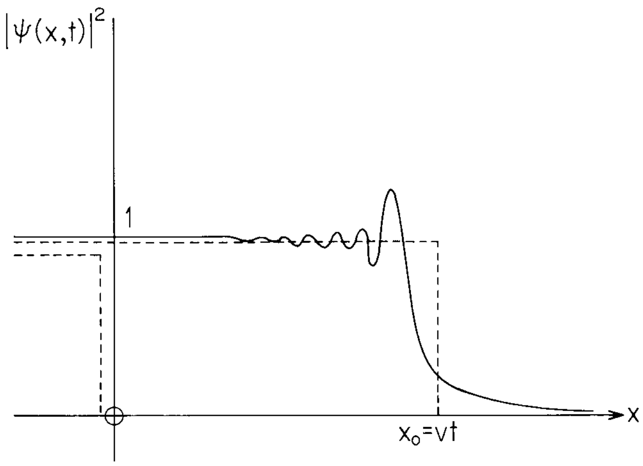

Figure 2. Probability density for observing a particle at a given time as a function of distance from the shutter. The dashed plot extending to $x = x_0$ represents the classical result at a time t after opening the shutter. In the units we use $x_0 = vt = kt$, where v is the initial velocity of the particle.

In this section we shall systematically use $\bar{x}$, $\bar{p}$ with a bar above and show later that they are related to x, p by a non-canonical transformation.

Using Hamilton's equations we get from $\bar{H}$ that

$$\dot{\bar{x}} = \frac{\partial \bar{H}}{\partial \bar{p}} = \mathrm{e}^{-\gamma t}\bar{p} \tag{17}$$

$$\dot{\bar{p}} = -\frac{\partial \bar{H}}{\partial \bar{x}} = -\mathrm{e}^{\gamma t}\frac{\partial V(\bar{x})}{\partial \bar{x}} \tag{18}$$

and thus from (17) we have

$$\bar{p} = \mathrm{e}^{\gamma t}\dot{\bar{x}} \qquad \dot{\bar{p}} = \gamma \mathrm{e}^{\gamma t}\dot{\bar{x}} + \mathrm{e}^{\gamma t}\ddot{\bar{x}}. \tag{19}$$

Subtracting (18) from the $\dot{\bar{p}}$ in (19) and cancelling the common factor $\mathrm{e}^{\gamma t}$ we then get the equation of motion

$$\ddot{\bar{x}} + \gamma\dot{\bar{x}} + \frac{\partial V}{\partial \bar{x}} = 0 \tag{20}$$

which is exactly the same as the one in (4) but in terms of the barred coordinates.

Note that in our units ($\hbar = m = 1$) we have in the non-dissipative case $p = \dot{x}$ while in (19) $\bar{p} = \mathrm{e}^{\gamma t}\dot{\bar{x}}$. This implies, if we assume $\bar{x} = x$, that $\bar{p} = \mathrm{e}^{\gamma t}$ which will be relevant for later analysis.

For the quantum mechanical form of the dissipative problem we can proceed as in going from (1) to (6) but now replacing, in (16), $\bar{p}$ by $-\mathrm{i}\partial/\partial\bar{x}$, $\bar{x}$ by $\bar{x}$ and $\bar{H}$ by $\mathrm{i}\partial/\partial t$ to get

$$\mathrm{i}\frac{\partial\bar{\Psi}}{\partial t} = \mathrm{e}^{-\gamma t}\left(-\frac{1}{2}\frac{\partial^2\bar{\Psi}}{\partial\bar{x}^2}\right) + \mathrm{e}^{\gamma t}V(\bar{x})\bar{\Psi}. \tag{21}$$

Again we put a bar on the wavefunction $\bar{\Psi}(\bar{x}, t)$ as it is related to the physical $\Psi(x, t)$ by a non-unitary connection which was derived in [2] and will be reviewed in the next section.

We now restrict ourselves to the case when $V(\bar{x}) = 0$ and consider again the shutter problem of the previous section in the presence of dissipation. This implies finding the $\bar{\Psi}(\bar{x}, t)$

solution of

$$\mathrm{i}\frac{\partial\bar{\Psi}}{\partial t} = \mathrm{e}^{-\gamma t}\left(-\frac{1}{2}\frac{\partial^2\bar{\Psi}}{\partial\bar{x}^2}\right) \tag{22}$$

$$\bar{\Psi}(\bar{x}, t = 0) = \exp(\mathrm{i}\bar{k}\bar{x})\theta(-\bar{x}). \tag{23}$$

If we multiply equation (22) by $\mathrm{e}^{\gamma t}$ we can replace in the left-hand side the time variable t by

$$\tau = \frac{1}{\gamma}\left(1 - \mathrm{e}^{-\gamma t}\right) \tag{24}$$

and as it has the property that for $t = 0$, $\tau = 0$, our problem reduces to finding the solution of

$$\mathrm{i}\frac{\partial\bar{\Psi}}{\partial\tau} = -\frac{1}{2}\frac{\partial^2\bar{\Psi}}{\partial\bar{x}^2} \qquad \bar{\Psi}(\bar{x}, \tau = 0) = \exp(\mathrm{i}\bar{k}\bar{x})\theta(-\bar{x}) \tag{25}$$

which is exactly the same problem as discussed in the previous section but in which we have to substitute t by τ, x by $\bar{x}$ and k by the constant $\bar{k}$.

Thus the solution of (25) is

$$\bar{\Psi}(\bar{x}, t) = M(\bar{x}, \bar{k}, \tau) \tag{26}$$

with ω of (11) replaced by

$$\bar{\omega} = \frac{\bar{k}\tau - \bar{x}}{\sqrt{2\tau}}. \tag{27}$$

We could discuss the dependence of $M(\bar{x}, \bar{k}, \tau)$ or $|M(\bar{x}, \bar{k}, \tau)|^2$ as we did in the last section for the non-dissipative problem, but we will defer this analysis until after establishing the relations between $\bar{x}$ and $\bar{\Psi}$ with x and Ψ.

4. The non-unitary connections between Ψ and $\bar{\Psi}$

We derived the classical equation (20) for our dissipative problem from the $\bar{H}$ of (16) using the Hamiltonian equations. We could also have proceeded to do this through the Hamilton–Jacobi equation

$$\frac{\partial\bar{S}}{\partial t} + \bar{H}\left(\bar{x}, \frac{\partial\bar{S}}{\partial\bar{x}}, t\right) = 0 \tag{28}$$

where $\bar{S}$ is the action of our dissipative problem.

For the non-dissipative case the equation will be

$$\frac{\partial S}{\partial t} + H\left(x, \frac{\partial S}{\partial x}\right) = 0 \tag{29}$$

and the momenta for both cases are given by

$$\bar{p} = \frac{\partial\bar{S}}{\partial\bar{x}} \qquad p = \frac{\partial S}{\partial x}. \tag{30}$$

As we showed in the paragraph following equation (20) we have $\bar{x} = x$, $\bar{p} = p\mathrm{e}^{\gamma t}$ and we get the Poisson bracket relation in the space of canonical variables

$$\{\bar{x}, \bar{p}\}_{\bar{x},\bar{p}} = \frac{\partial\bar{x}}{\partial\bar{x}}\frac{\partial\bar{p}}{\partial\bar{p}} - \frac{\partial\bar{x}}{\partial\bar{p}}\frac{\partial\bar{p}}{\partial\bar{x}} = 1 \tag{31}$$

while for the physical variables x, p we obtain in this canonical space

$$\{x, p\}_{\bar{x},\bar{p}} = \frac{\partial x}{\partial\bar{x}}\frac{\partial p}{\partial\bar{p}} - \frac{\partial x}{\partial\bar{p}}\frac{\partial p}{\partial\bar{x}} = \mathrm{e}^{-\gamma t} \tag{32}$$

which indicates that $\bar{x}$, $\bar{p}$ and x, p are connected by a non-canonical relation, as the right-hand side of (32) is not one. Furthermore, as $\exp(-\gamma t) < 1$, except when $t = 0$, we see that Heisenberg's uncertainty relation is violated in the quantum version where the Poisson brackets are replaced by a commutator.

Since measurements are given in physical space, while our calculations in section 3 gave us the wavefunction $\bar{\Psi}(\bar{x}, \tau)$ in the canonical space, we have to transform this function to obtain the corresponding one for the physical variables.

For this purpose we use the relation between the action function $\bar{S}$ in the canonical space and S in the physical space that can be obtained from (30) as

$$\bar{S} = S\mathrm{e}^{\gamma t}. \tag{33}$$

Following Schrödinger's original analysis [9] we can write the action S in terms of the wavefunction Ψ i.e.

$$S = -\mathrm{i} \ln \Psi. \tag{34}$$

Applying the same definition for equation (33) we get

$$\bar{S} = -\mathrm{i} \ln \bar{\Psi} = \mathrm{e}^{\gamma t} S \tag{35}$$

which immediately leads to the desired relation between Ψ and $\bar{\Psi}$

$$\ln \bar{\Psi} = \mathrm{e}^{\gamma t} \ln \Psi \tag{36}$$

or

$$\Psi = \bar{\Psi}^{\mathrm{e}^{-\gamma t}}. \tag{37}$$

This allows us now to express the results of section 3 in the space of the physical variables, where Heisenberg's relation between these variables is not violated. In particular $\bar{\Psi}(\bar{x}, \tau)$ can now be transformed by the non-unitary connection into $\Psi(x, t)$.

Thus, as we have already determined $\bar{\Psi}$ in the previous section for the dissipative shutter problem, we can obtain the wavefunction $\Psi(x, t)$ relevant to the physical quantities x and p that corresponds to $\bar{\Psi}(\bar{x}, t)$ for the canonical variables $\bar{x} = x$ and $\bar{p}$ through relation (37). The next section illustrates the implications of this relation for the diffraction in time problem with dissipation.

5. Conclusion

From equations (24), (26) and (37) we conclude that the probability density for finding a particle at a point $x > 0$ at time $t > 0$ for the shutter problem with dissipation is

$$|\Psi(x, t)|^2 = |M[x, k, \gamma^{-1}(1 - \mathrm{e}^{-\gamma t})]|^{2\mathrm{e}^{-\gamma t}} \tag{38}$$

where now, for the purpose of comparison, we take the constant momentum $\bar{k}$ as equal to the one without dissipation, i.e. $\bar{k} = k$. For the original shutter problem this probability density is given by (15). We now discuss the two results.

We first note from figure 1 of the Cornu spiral that $|M(x, k, t)|^2$ in figure 2 oscillates around one until x reaches a value close to $x = x_0 \equiv kt$, where it starts dropping to zero as indicated by the solid curve in figure 2.

We then remark that

$$1 - \mathrm{e}^{-\gamma t} < \gamma t \qquad \text{for} \quad t > 0 \tag{39}$$

and thus the time-dependent term in the right-hand side of (38) also oscillates around one until x reaches a value close to

$$x = x_0' \equiv k\tau = \frac{k}{\gamma}\left(1 - \mathrm{e}^{-\gamma t}\right) \tag{40}$$

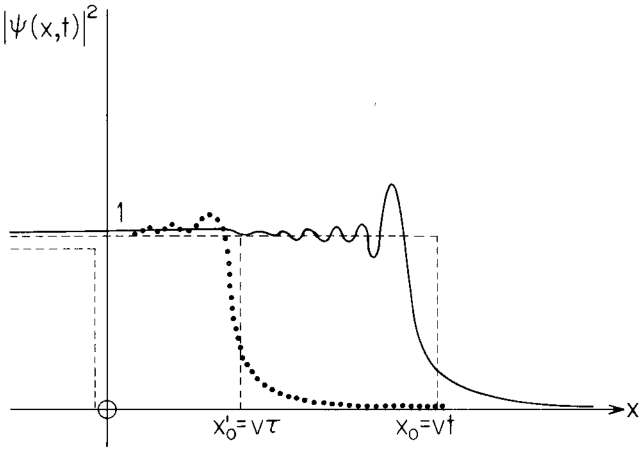

Figure 3. Probability density of observing a particle at a given time as a function of the distance from the shutter. The solid curve corresponds to the case without dissipation while the curve with points is the one with dissipation. The classical results are given by dashed plots that indicate the points $x_0 = vt = kt$ and $x'_0 = v\tau = k\tau$, without and with dissipation.

where it starts dropping to zero. From (39) we see that $x'_0 < x_0$ and thus, in the dissipative shutter problem, the particle remains closer to the origin than in the non-dissipative case. The exponent $e^{-\gamma t}$ in (38) is always smaller than one, and thus, when the probability density is close to one in the dissipative case, it diminishes (increases) the non-dissipative value when it is larger (smaller) than one. Thus the oscillations around one are damped when there is dissipation. We also see from the Cornu spiral of figure 1 that, in the dissipative case, at the points around $x = x'_0 \equiv k\tau$, the probability density descends from values close to one to those close to zero. In figure 3 we indicate the behaviour of $|\Psi(x,t)|^2$ as a function of x at a given time t, both when there is no dissipation (the solid curve) and when there is (the curve with points). These results agree with the classical expressions without dissipation, as after opening the shutter at time zero, the particle at time t reaches the value $x_0 = kt$, while with dissipation it only comes to the point $x'_0 = k\tau = (k/\gamma)(1 - e^{\gamma t})$.

Both of these facts are indicated by the dashed plots in figure 3. As the maximum value of x'_0 is (k/γ), as indicated in the discussion following equation (5), we also have that quantum mechanically, in the dissipative case, the particle has close to zero probability of being found at a distance from the origin $x = 0$ larger than (k/γ), independent of the time value.

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References

[1] Hasse R W 1975 *J. Math. Phys.* **16** 2005
Brittin W E 1950 *Phys. Rev.* **77** 396
Ray J R 1979 *Lett. Nuovo. Cimento* **25** 47
Greenberger D M 1979 *J. Math. Phys.* **20** 762

[2] Schuch D 1997 *Phys. Rev.* A **55** 935
Schuch D 1999 *Int. J. Quantum Chem.* **72** 537
[3] Moshinsky M 1952 *Phys. Rev.* **88** 625
[4] Man'ko V, Moshinsky M and Sharma A 1991 *Phys. Rev.* A **59** 1809
[5] Moshinsky M 1976 *Am. J. Phys.* **44** 1037
[6] Jahnke E and Emde F 1945 *Tables of Functions* 4th edn (New York: Dover) p 36
[7] Caldirola P 1941 *Nuovo Cimento* **18** 393
[8] Kanai E 1948 *Prog. Theor. Phys.* **3** 440
[9] Schrödinger E 1926 *Ann. Phys., Lpz.* **79** 361