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Asymptotic behaviour of a particle in a uniformly expanding potential well

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Abstract. Behaviours of classical and quantum particles in an infinitely deep flat well with uniformly growing width are compared and examined for infinitely large instants of time. In particular, the correspondence between certain classes of classical and quantum states is pointed out and asymptotic effects of 'squeezing' of the momentum probability densities are derived.

1. Introduction

The dynamics of a classical and a quantum particle in a potential well of infinite depth and time-dependent width has become a subject of some interest since the pioneering papers of Fermi and Ulam [1]. In their model, a particle bounces between two impenetrable rigid walls one of which moves according to a given function of time, say $L(t)$. Much work had been carried out on the model [2–5] when $L(t)$ was periodic and a chaotic behaviour of a classical particle appeared. The quantized version of this classically chaotic model has been the subject of efforts in the last few years [6–12] as well as its semiclassical limit [8, 12].

Of the problems related to the Fermi–Ulam model, the question for what functions $L(t)$ the corresponding Schrödinger equation can be solved exactly has also attracted much attention [13–19]. Exact wavefunctions obeying suitable Dirichlet boundary conditions were first found by Doescher and Rice [13] for the case of a uniformly expanding or contracting potential well. All of the following studies [14–19] proved in many ways that other exactly solvable cases are restricted to just a few motions of the well's wall obeying $L^3\ddot{L} = a$, where $a =$ constant. This easily solvable second-order equation, as a special case ($a = 0$), contains the case solved in [13].

The simplicity of the model, with $L(t)$ being a linear function of time, allowed us to consider a number of interesting problems. Among them we should mention: an analysis of the properties of Berry's phase in a moving boundary problem [11, 20], the prediction of possible non-local effects appearing in such a situation [21–23] and the construction of exact and semiclassical propagators [17, 24–27].

The purpose of the present paper is to give further support to properties of systems with moving boundaries. To our knowledge, the question raised in the title of our paper has not been fully discussed in the existing literature. Some detailed results on the subject are scattered in a few works [10, 14, 28, 29] and have occasionally been obtained in other studies.

What we are about to present first are both classical and quantum formulae necessary for the discussion of asymptotic positions, momenta and their probability distributions. Next, we will contrast the classical behaviour of these quantities with their quantum counterparts. All our formulae are exact and as such are our final conclusions.

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2. Basic formulae

Let us consider a particle of mass m, with position x which belongs to the interval $[0, L(t)]$ with $L \equiv L_0 + ut$. The velocity u of the expansion is constant. Apart from the reaction of this constraint no other forces act on the particle.

It is known [15] that by the appropriate transformation of x and t the width of the interval of admissible positions can be made time-independent and no forces appear in the transformed equations of motion. In fact, when

$$y = \frac{L_0 x}{L(t)}$$

and

$$\tau(t) = \int_0^t \frac{L_0^2}{L^2(t)}\,\mathrm{d}t = \frac{L_0 t}{L(t)} \tag{1}$$

then:

(i) the classical equation of motion

$$\begin{aligned} &m\ddot{x} = 0 \qquad x \in (0, L(t)) \\ &\text{with} \quad \dot{x} \to -\dot{x} + 2u \quad \text{when} \quad x = L(t) \\ &\text{and} \quad \dot{x} \to -\dot{x} \quad \text{when} \quad x = 0 \end{aligned} \tag{2}$$

is transformed to the equation

$$my'' = 0 \quad \text{where} \quad y \in (0, L_0) \quad \text{and at the boundaries} \quad y' \to -y'. \tag{3}$$

Here the dots mean derivatives with respect to the time t, while the apostrophes denote the derivatives with respect to the new time τ. The momentum transforms in the following way:

$$p = \frac{L_0 \tilde{p}}{L(t)} + um\frac{y}{L_0} \tag{4}$$

where $p = m\dot{x}$ and $\tilde{p} = my'$. A solution of equation (3) can be found and it is of the form $((\mathrm{d}y/\mathrm{d}\tau)_{\tau=0} \equiv y_0' \neq 0)$:

$$y(\tau) = \tfrac{1}{2}L_0\left[1 + (-1)^{\alpha(\tau)}\operatorname{sgn}(y_0')\right] - (-1)^{\alpha(\tau)} y_0'(\tau - \tau_1)_{\mathrm{mod}\,\Delta\tau} \tag{5}$$

where

$$\tau_1 = \frac{1}{2y_0'}\{[1 + \operatorname{sgn}(y_0')]L_0 - 2y_0\} \tag{6}$$

$$\Delta\tau = \frac{L_0}{|y_0'|} \tag{7}$$

$$\alpha(\tau) = \mathrm{Int}\left(\frac{\tau(t) - \tau_1}{\Delta\tau}\right) \tag{8}$$

and here the symbol $\mathrm{Int}(x)$ is understood as the greatest integer not larger than x. Note that $y_0 = x_0$, $y_0' = \dot{x}_0 - ux_0/L_0$ and, when $y_0' = 0$, the solution of (3) is simply $y(\tau(t)) = y_0$.

(ii) The quantum equation of motion

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} \tag{9}$$

with $\psi(x, t) \equiv 0$ for $x \notin (0, L(t))$ transforms to

$$i\hbar\frac{\partial\Phi}{\partial\tau} = -\frac{\hbar^2}{2m}\frac{\partial^2\Phi}{\partial y^2} \tag{10}$$

with $\Phi(y,\tau) \equiv 0$ for $y \notin (0, L_0)$. Here $\Phi = \mathcal{O}\psi$, with

$$\mathcal{O} = \left(\frac{L(t)}{L_0}\right)^{1/2} \exp\left\{-\mathrm{i}\frac{muL(t)y^2}{2\hbar L_0^2}\right\}.$$

The momentum operator transforms as in (4) and now $p = -\mathrm{i}\hbar(\partial/\partial x)$ and $\tilde{p} = -\mathrm{i}\hbar(\partial/\partial y)$. The general solution of (10) which fulfils the desired boundary conditions reads:

$$\Phi = \sum_n a_n \Phi_n = \left(\frac{2}{L_0}\right)^{1/2} \sum_n a_n \sin\left(\frac{n\pi y}{L_0}\right) \exp\left\{-\frac{\mathrm{i}}{\hbar} E_n \tau(t)\right\} \tag{11}$$

with $E_n = \hbar^2\pi^2 n^2/2mL_0^2$ and $\sum_n |a_n|^2 = 1$. Mean values of the operators y, p, y^2 and p^2 in the state ψ, which is a general solution of (9), are as follows:

$$\begin{aligned}
\langle y\rangle &= \frac{L_0}{2} - \frac{2L_0}{\pi^2}\widetilde{\sum_{n\neq m}}\frac{S_{mn}}{m^2-n^2}\\
\langle p\rangle &= \frac{mu}{L_0}\langle y\rangle + \frac{\hbar}{\mathrm{i}L(t)}\widetilde{\sum_{m\neq n}} S_{mn}\\
\langle y^2\rangle &= \frac{L_0^2}{3} - \frac{L_0^2}{2\pi^2}\sum_n \frac{|a_n|^2}{n^2} + \frac{2L_0^2}{\pi^2}\sum_{m\neq n}\frac{(-1)^{m+n}S_{mn}}{m^2-n^2}\\
\langle p^2\rangle &= \left(\frac{mu}{L_0}\right)^2\langle y^2\rangle + \left(\frac{\hbar\pi}{L(t)}\right)^2\sum_n |a_n|^2 n^2 + \frac{\mathrm{i}\hbar mu}{L(t)}\sum_{m\neq n}(-1)^{m+n}S_{mn}
\end{aligned} \tag{12}$$

where $S_{mn} = a_m^* a_n (4mn/(m^2-n^2)) \exp(-\mathrm{i}(E_n - E_m)\tau(t)/\hbar)$ and the symbol $\widetilde{\sum}$ denotes a summation over odd values of $m+n$. It follows from (1) that in the y–τ plane the evolution stops at

$$\tau(\infty) = \frac{L_0}{u}. \tag{13}$$

This property considerably simplifies studies of asymptotic properties of both classical and quantum uniformly expanding wells.

First of all it follows from (5) that

$$y(\tau(\infty)) = \tfrac{1}{2}L_0\left[1 - (-1)^\beta\right] + (-1)^\beta \frac{L_0}{u}(|\dot{x}_0|)_{\mathrm{mod}\,u} \tag{14}$$

where $\beta = \mathrm{Int}(|\dot{x}_0|/u)$. As can be seen from (14) $y(\tau(\infty))$ *does not depend on* $y_0 = x_0$. Moreover, from (4) one has in the limit $t \to \infty$

$$p(t\to\infty) = mu\frac{y(\tau(\infty))}{L_0}. \tag{15}$$

Since $y/L_0 \in [0, 1]$ for $0 \leqslant t < \infty$ this result confirms the physical intuition that *asymptotic momenta must be positive and not larger than mu*.

From (14) and (15) it follows that

$$p(t\to\infty) \equiv p(p_0, u) = \tfrac{1}{2}\left[1 - (-1)^\beta\right]mu + (-1)^\beta(|p_0|)_{\mathrm{mod}(mu)} \tag{16}$$

and $p(t \to \infty)$ depends solely on p_0, while $y(t \to \infty)$ becomes via (15) a simple function of $p(t \to \infty)$. In figure 1 the relation between $p(t \to \infty)$ and p_0 given in (16) is presented. The above observation facilitates calculations of the asymptotic form of the (y, p)-probability density.

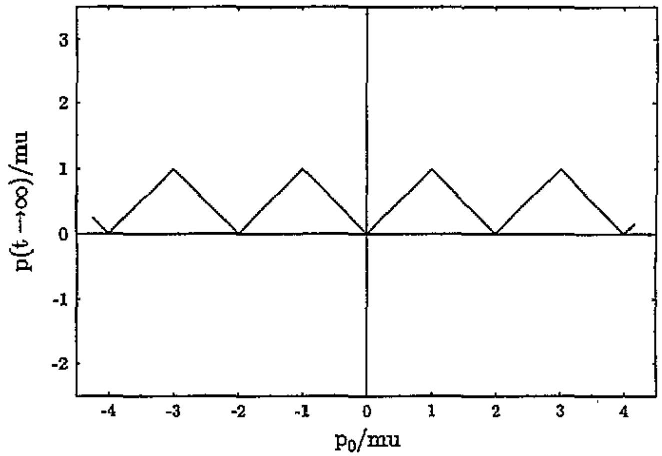

Figure 1. Asymptotic values of the momentum $p(t \to \infty)$ versus initial values of the momentum p_0.

If at $t = 0$ an ensemble of classical particles in an expanding well is described by the probability distribution function $f_0(y, p)$, $0 \leqslant y \leqslant L_0$, $-\infty < p < \infty$, then from (14) and (15) one gets

$$f_\infty(y, p) = \iint \mathrm{d}y_0\, \mathrm{d}p_0\, \delta\left(y - \frac{L_0 p}{mu}\right)\delta(p - p(p_0, u))\, f_0(y_0, p_0)$$

and finally

$$f_\infty(y, p) = \delta\left(y - \frac{L_0 p}{mu}\right) \sum_{k=-\infty}^{\infty} [P_{p,0}(2kmu - p) + P_{p,0}(2kmu + p)] \quad (17)$$

with $y \in [0, L_0]$, $p \in [0, mu]$, where $P_{p,0}(p) = \int_0^{L_0} f_0(y, p)\, \mathrm{d}y$. For $p \notin [0, mu]$ the probability distribution function $f_\infty(y, p) \equiv 0$. From (17) it readily follows that

$$P_{y,\infty}(y) = \frac{mu}{L_0} P_{p,\infty}\left(\frac{muy}{L_0}\right) \quad (18)$$

where $P_{y,\infty}(y) = \int_{-\infty}^{\infty} f_\infty(y, p)\, \mathrm{d}p$ and $P_{p,\infty}(p) = \int_0^{L_0} f_\infty(y, p)\, \mathrm{d}y$. Thus, *the memory of the initial position of the particles is lost in the asymptotic state.* It is seen that an *expanding well squeezes asymptotically the initial momentum distribution.* A very simple illustration may be as follows.

If $P_{p,0}(p) = (1 - |p|/2Nmu)/2Nmu$ for $p \in [2Nmu, -2Nmu]$, N integer and $P_{p,0}(p) = 0$ outside this interval (a 'tent-like distribution'), then from (17) one gets

$$P_{p,\infty}(p) = \begin{cases} \dfrac{1}{mu} & \text{for} \quad p \in [0, mu] \\ 0 & \text{otherwise}. \end{cases} \quad (19)$$

3. Comparison of the classical and quantum behaviour

It is interesting to compare with the above classical results the behaviour of quantum particles.

The quantum particle (QP) in the state Φ_n defined in (11), and the classical particle (CP) which moves with $y_0' = 0$ have, for arbitrary integer k, time-independent values of $\langle\Phi_n|y^k|\Phi_n\rangle$ and y^k, respectively.

Since $y_0' = 0$ means that $u \geqslant \dot{x}_0 = ux_0/L_0 \geqslant 0$, a CP does not collide with boundaries of the well and therefore has constant momentum as well. A QP in the state Φ_n has time-independent $\langle\Phi_n|p|\Phi_n\rangle$, but $\langle\Phi_n|p^2|\Phi_n\rangle$ is already time-dependent. This is because a QP in the state Φ_n may be viewed as representing an ensemble of CPs with a spectrum of momenta lying outside the interval $[0, mu]$ and thus losing energy during collisions with the moving boundary (equation (3)). In a different context, this and related phenomena can be considered as a consequence of a non-local character of quantum mechanics [21–23].

Solutions Φ_n of (10) and $y_0' = 0$ of (3) are two special states, quantum and classical, which belong:

the first, to the family of quantum solutions $\varphi(y,t)$): $\varphi(y,0) = \varphi^*(y,t \to \infty)$, and thus $|\varphi(y,0)|^2 = |\varphi(y,t \to \infty)|^2$. This can be accomplished by putting $a_n = r_n \exp(\mathrm{i}E_n\tau(\infty)/2\hbar)$, $r_n = r_n^*$ in (11). When only one of the r_n's is different from zero in (11), then φ equals Φ_n up to a factor of modulo 1;

the second, to the first of two subfamilies of classical initial conditions: $y_0' = 2bu$ or $y_0' = 2bu - 2y_0u/L_0$ with $|b|$ being zero or an integer. $y_0' = 0$ is found in the first subfamily when $b = 0$. It follows from what was said so far, that in the state φ the equality $\langle y^k\rangle_{t=0} = \langle y^k\rangle_{t\to\infty}$ holds, while the classical motion which starts from the above given two subfamilies of initial conditions has the property: $y_0^k = y^k(t \to \infty)$.

Generally speaking, in the state ψ, which is a superposition of the Φ_n's, the mean values of y^k are time-dependent via the oscillating factors $\exp(-\mathrm{i}(E_n - E_m)\tau(t)/\hbar)$. Oscillations vanish in the limit $t \to \infty$, i.e. for $\tau = L_0/u$. Mean values of the powers of p depend additionally on time via powers of $1/L(t)$. The relation $\langle p^k\rangle = (mu/L_0)^k\langle y^k\rangle$ is asymptotically valid in analogy to the classical case.

In figures 2 and 3 the time dependence of the mean values of x and p together with the corresponding mean-square deviations $(\Delta x^2)^{1/2}$ and $(\Delta p^2)^{1/2}$ are presented for some arbitrary choice of the initial state ψ.

It is interesting to calculate for a QP the p probability density when $t \to \infty$ and to compare the result with (18). Obviously

$$P_{y,\infty}(y) = |\Phi(y, \tau(\infty))|^2 \tag{20}$$

while

$$P_{p,t}(p) = |C(p,t)|^2 \tag{21}$$

where

$$C(p,t) = (2\pi\hbar)^{-1/2}\int_0^{L(t)} \exp(-\mathrm{i}px/\hbar)\psi(x,t)\,\mathrm{d}x\,. \tag{22}$$

Taking $\psi = \mathcal{O}^{-1}\Phi$ one gets

$$C(p,t) = \left(\frac{L(t)}{2\pi\hbar L_0}\right)^{1/2} \exp\left[-\mathrm{i}\frac{p^2}{2\hbar muL(t)}\right] \times \int_0^{L_0} \exp\{\mathrm{i}muL(t)[y/L_0 - p/mu]^2/2\hbar\}\Phi(y,\tau(t))\,\mathrm{d}y\,. \tag{23}$$

For finite t the integral in (21) is expressible in terms of Fresnel integrals and therefore the limit $t \to \infty$ may be performed effectively.

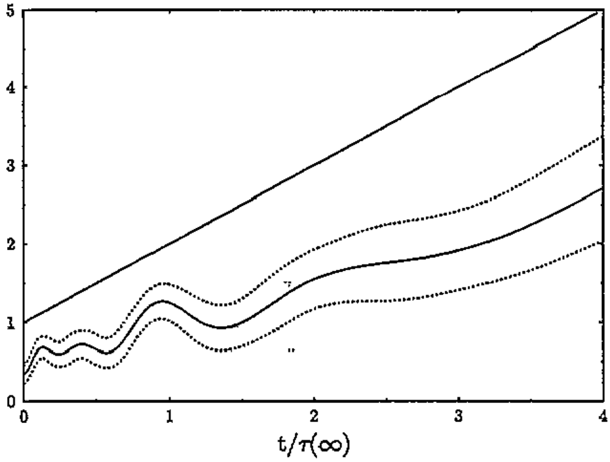

Figure 2. Mean values $\langle x\rangle$ (full curve) and $\langle x\rangle \pm \frac{1}{2}\langle x^2 - \langle x\rangle^2\rangle^{1/2}$ (dots) in units of L_0 as functions of time. Amplitudes a_n, which characterize the state ψ via (11), are real and equal to $a_n = N^{-1/2}\exp(-\gamma|n-n_0|)$, $\sum_n a_n^2 = 1$. The full line presents the expanding boundary: $L = L_0 + ut$, $L_0 = 3$, $u = 0.25$, $\hbar = 1$, $m = 1$, $n_0 = 2$ and $\gamma = 1.5$.

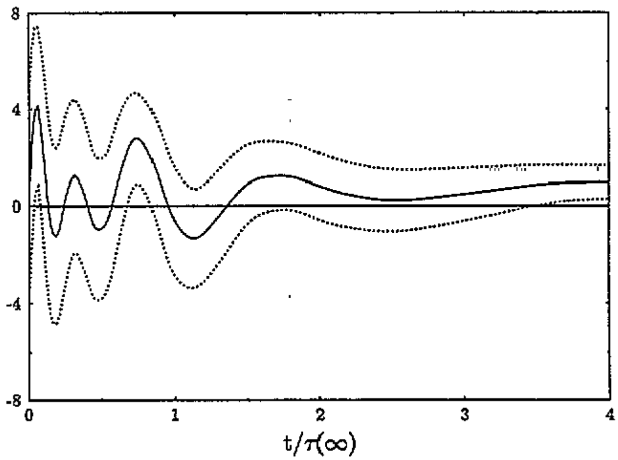

Figure 3. Mean values: $\langle p\rangle$ (full curve) and $\langle p\rangle \pm \frac{1}{2}\langle p^2 - \langle p\rangle^2\rangle^{1/2}$ (dots) in units of mu as functions of time. The state ψ and the values of parameters are the same as in figure 2.

Using the following representation of the Dirac δ-function:

$$\delta(z) = (\pi)^{-1/2}\,\mathrm{e}^{-\mathrm{i}\pi/4} \lim_{k\to\infty} k\,\mathrm{e}^{\mathrm{i}(kz)^2}$$

in the limit $t \to \infty$ equation (23) takes the form

$$C(p, t\to\infty) = \left(\frac{L_0}{mu}\right)^{1/2} \mathrm{e}^{\mathrm{i}\pi/4} \int_0^{L_0} \delta\left(y - \frac{pL_0}{mu}\right) \Phi(y, \tau(\infty))\,\mathrm{d}y\,.$$

Finally

$$P_{p,\infty}(p) = \frac{L_0}{mu} \left|\Phi\left(\frac{pL_0}{mu}, \tau(\infty)\right)\right|^2 \tag{24}$$

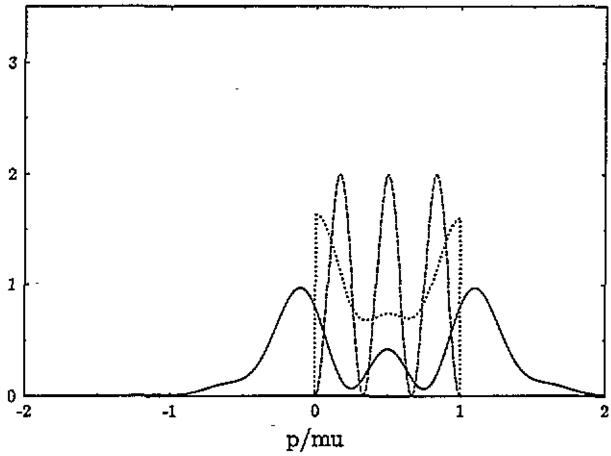

Figure 4. Initial momentum probability density $P_{p,0}^{(3)}(p)$ for $\psi(x, t = 0) = \psi_{n=3}(x, t = 0)$ (full curve) and resulting asymptotic quantum momentum probability density $P_{p,\infty}^{(3)}(p)$ (broken curve). The dotted curve represents asymptotic classical momenta probability density when at $t = 0$ a classical ensemble of particles had momenta probability density equal to $P_{p,0}^{(3)}(p)$ ($L_0 = 15, u = 1, m = 1, \hbar = 1$).

when $p \in [0, mu]$ and $P_{p,\infty}(p) \equiv 0$ for p from outside this interval.

For a QP the relation given in (18) follows from (20) and (24). *Squeezing of the momentum probability takes place in quantum dynamics as well.* For a QP one always has $P_{p,\infty}(0) = P_{p,\infty}(mu) = 0$ and this is the purely quantum effect.

Let us compare initial and final momentum probability distributions for two special cases.

(i) It follows from (21) and (24) that when at $t = 0$ the particle is in one of the ψ_n states ($\psi_n = \mathcal{O}^{-1}\Phi_n$), then

$$P_{p,\infty}^{(n)}(p) = \frac{2}{mu} \sin^2\left(\frac{n\pi p}{mu}\right). \tag{25}$$

We calculated $P_{p,0}^{(n)}(p)$ by performing numerically the integration in (22). In figure 4 both initial and final (asymptotic) quantum momentum probability densities are presented. Both curves are evidently invariant with respect to the transformation of variable p: $p \to mu - p$. For $P_{p,\infty}^{(n)}(p)$ this property is immediately visible in (25) while, for any finite t, the relation

$$C^{(n)}(p, t) = (-1)^{n+1} C^{(n)}(mu - p, t)\, \mathrm{e}^{[\mathrm{i}L(t)(-p+mu/2)/\hbar]} \tag{26}$$

which can be derived from the definition given in (22) explains the symmetry $P_{p,t}^{(n)}(p) = P_{p,t}^{(n)}(mu - p)$.

(ii) in the second example we assume that at $t = 0$ the particle is in the state Φ_n (see equation (11)). In this case we have from (21) and (22)

$$P_{p,0}^{(n)}(p) = \frac{2}{\pi\hbar L_0} \left(\frac{n\pi}{L_0}\right)^2 \frac{1 - (-1)^n \cos(pL_0/\hbar)}{\left[(p/\hbar)^2 - (n\pi/L_0)^2\right]^2}. \tag{27}$$

Now, the knowledge of $P_{p,\infty}^{(n)}(p)$ requires calculations of

$$a_m^{(n)} = \int_0^{L_0} \psi_m^*(x, t = 0)\Phi_n(x, t = 0)\, \mathrm{d}x.$$

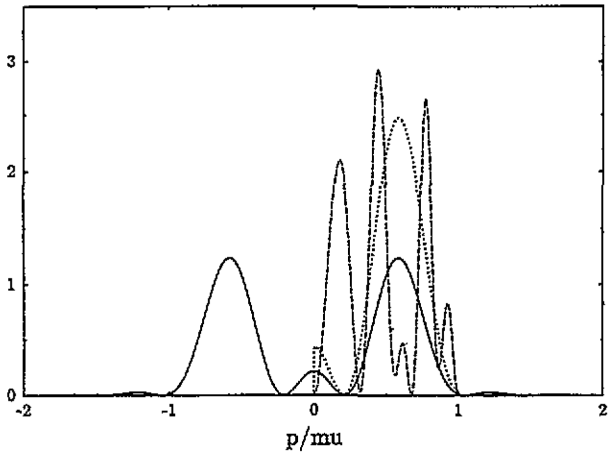

Figure 5. The same as in figure 4, but $\psi(x, t=0) = \Phi_{n=3}(x, t=0)$.

In figure 5 initial and asymptotic p distributions are presented for this case.

In both examples it was also assumed that initial p distributions describe ensembles of CPs. Using (17), classical asymptotic p distributions were calculated and they are shown in figures 4 and 5 as well. *Quantum interferences led to the 'hole burning effects' in classical distributions.*

The classical asymptotic p distribution $P_{p,\infty}(p)$ which has the form (see equation (17))

$$P_{p,\infty}(p) = \sum_{k=-\infty}^{\infty} [P_{p,0}(2kmu - p) + P_{p,0}(2kmu + p)] \tag{28}$$

also has the symmetry mentioned in the example (i) if $P_{p,0}(p)$ does have this symmetry. This fact can be deduced from (28) and is clearly seen in figure 4.

One may ask now whether and when the classical time evolution of the $P_{p,t}^{(n)}(p)$, which starts from $P_{p,0}^{(n)}(p)$ given in example (i), conserves (as quantum evolution in this case does) the symmetry: $P_{p,t}^{(n)}(p) = P_{p,t}^{(n)}(mu - p)$.

It is not difficult to find out that, if in an ensemble of classical particles there are at $t = 0$ only pairs of particles having positions and momenta related in the following way: $x_{i1,0} + x_{i2,0} = L_0$ and $p_{i1,0} + p_{i2,0} = mu$ (1 and 2 labels particles in the ith pair), then the above-mentioned symmetry of $P_{p,t}^{(n)}(p)$ is conserved (particles from a pair collide with boundaries simultaneously). Our assumption on positions and momenta of particles in a pair means on the other hand, however, that the classical ensemble at $t = 0$ is characterized by the probability distribution function $f_0(x, p)$ which is invariant with respect to two simultaneous transformations: $x \to L_0 - x$ and $p \to mu - p$. Such a property has the Wigner distribution function derived from the state ψ_n of example (i).

In this case we have

$$P_{w,0}^{(n)}(x, p) = \frac{1}{\pi\hbar} \int \exp\left(\frac{-2\mathrm{i}pz}{\hbar}\right) \psi_n(x+z)\psi_n^*(x-z)\,\mathrm{d}z \tag{29}$$

where the integration is in the range $[-x, x]$ when $x < L_0/2$ and $[x - L_0, L_0 - x]$ when $x \geqslant L_0/2$. For $\psi_n(x, 0) = \exp(\mathrm{i}mux^2/2\hbar L_0)\Phi_n(x, 0)$, $\Phi_n(x, 0) = (2/L_0)^{1/2}\sin(n\pi x/L_0)$, equation (29) has the desired property $P_{w,0}(x, p) = P_{w,0}(L_0 - x, mu - p)$. We may assume, if we like, that the classical ensemble is at $t = 0$ in a Wigner state and the analogy between classical and quantum cases is still more pronounced.

Unlike the case of a classical well, in the asymptotic states of a quantum well information on the initial distribution of y (or x) and p is obviously still present via the function Φ. This is also the quantum effect and, needless to say, it stems from the fact that a QP *cannot be seen as just an ensemble of CPs, but is what is called a 'coherent ensemble'*.

4. Concluding remarks

In this paper we have derived exact classical and quantum-mechanical formulae for several quantities characterizing motion of a particle in an expanding potential well. In both approaches the problem was reduced by means of a generalized canonical transformation to a simpler one with a non-moving boundary. Contrary to the original Fermi–Ulam model its simplest version used here allowed us to get exact predictions as to the behaviour of classical and quantum states of the particle for any instant of time, even at infinity.

Some of our conclusions are distinguished in the text with italics. Among them one can find few intuitively obvious statements. In order to prove them formally one needs, however, exact formulae given in this work. Our other results relate the behaviour of the particle in the expanding well to some effects known in other areas of physics. Thus, though our study completes known facts about one of the variants of the Fermi–Ulam model, the conclusions derived in this paper are valid in a much wider context.

Finally, we should mention that some aspects of the case of the contracting well and the validity of the sudden or adiabatic approximations for the model could have been discussed within the scope of our formalism. These questions, however, have already been considered in a different way [27, 28].

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