Time-dependent entropy of simple quantum model systems

Jörn Dunkel* and Sergey A. Trigger
Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin, Germany
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Information-theoretic entropy measures are useful tools for quantifying the spreading of quantum states in phase space. In the present paper, we compare the time evolution of the joint entropy for three simple quantum systems: (i) a free Gaussian wave packet, (ii) a wave packet in a monochromatic electromagnetic field, and (iii) a wave packet tunneling through a δ barrier. As initial condition maximal classical states are used, which minimize the Heisenberg uncertainty and the entropy. It is found that, in all three cases, the joint entropy increases in time.

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I. INTRODUCTION

The transition between quantum and classical behavior of physical systems has been in the center of intensive research during the past decades (for reviews, see [1–4]). New theoretical insights were complemented by modern experiments, which have impressively confirmed quantum phenomena such as the superposition of states [5,6] or the existence of Schrödinger cat states [7,8]. Thus, considerable progress has been achieved in the conceptual understanding of measurement processes [9–11] and decoherence phenomena (see, e.g., Zurek *et al.* [12–14]).

In order to characterize the intrinsic evolution of quantum states, different information-theoretic entropy measures have been discussed in the literature for both open and closed quantum systems [1,3,15–21]. Among the best known examples are the von Neumann entropy, the Wehrl entropy, and the joint entropy, introduced by Leipnik [16]. As discussed by Anastopoulos and Halliwell [19], the von Neumann entropy is particularly useful for studying environmentally induced effects in open quantum systems, because it is constant for unitary evolutions of pure states as typical of closed systems. In contrast, Wehrl entropy [19,20] and joint entropy [16,21] can also be used to quantify the loss of information, associated with temporally evolving pure quantum states [22].

The objective of this paper is to explicitly illustrate this fact by calculating the joint entropy for analytically tractable quantum models. More precisely, we will compare the joint entropy for the following three examples: (i) the simplest free Gaussian wave packet case [22], (ii) the evolution of Gaussian wave packets in the presence of oscillating external fields, and (iii) the tunneling of a Gaussian wave packet through a δ barrier.

Before discussing these examples in Sec. III, we shall briefly review essential definitions and entropy concepts in the next part.

II. BASIC DEFINITIONS

Consider a classical (nonquantum) system with $d=DN$ degrees of freedom, where N is the particle number and D the number of spatial dimensions. Further, let $f(t,x,p) = f(t,x_1,\ldots,x_d,p_1,\ldots,p_d)$ denote the non-negative, time-dependent phase-space density function of this system. Assuming that f has been normalized to unity,

$$\int \mathrm{d}x\, \mathrm{d}p f(t,x,p) = 1,$$

the related (dimensionless) Gibbs-Shannon entropy is defined by

$$S(t) = -\frac{1}{N!}\int \mathrm{d}x\, \mathrm{d}p f \ln(h^d f), \tag{1}$$

where $h=2\pi\hbar$ is the Planck constant. (If boundaries are not specified, then it is assumed throughout that integrals range from $-\infty$ to $+\infty$.)

If one is interested in generalizing the classical entropy definition (1) to quantum systems, then the main problem consists in finding an appropriate quantum counterpart for the classical phase-space density f. Different approaches to this problem, which have become widely accepted nowadays, go back to alternative proposals made by von Neumann, Wehrl, and Leipnik [16], respectively. To briefly illustrate the underlying ideas, let us consider a mixed quantum system described by the normalized density matrix (in position-space representation)

$$\rho(t,x,x') = \sum_\alpha w_\alpha \psi_\alpha(t,x)\psi_\alpha^*(t,x'), \quad \sum_\alpha w_\alpha = 1.$$

For example, in the case of the canonical equilibrium ensemble with temperature T, one usually assumes classical probabilities

$$w_\alpha = \frac{\exp(-\epsilon_\alpha/k_BT)}{\sum_\alpha \exp(-\epsilon_\alpha/k_BT)}, \tag{2}$$

where k_B is the Boltzmann constant and ϵ_α denotes the energy eigenvalues with normalized eigenfunctions ψ_α. In general, according to von Neumann's definition, the quantum analog of Eq. (1) reads

*Electronic address: dunkel@physik.hu-berlin.de

$$S_N(t) = -\,\mathrm{Sp}(\rho \ln \rho). \tag{3}$$

A peculiar feature, which follows directly from definition (3), is that, in the case of isolated systems, the von Neumann entropy $S_N(t)$ is time independent for arbitrary nonequilibrium initial conditions—similar to the Gibbs entropy of classical isolated systems [23].

In particular, for pure quantum states with $w_\alpha = 0$ for all but one α, the von Neumann entropy vanishes identically—i.e., $S_N(t) \equiv 0$ for all times t. Consequently, the von Neumann entropy is useful, if one aims to quantify the specific gain and loss of information associated with environmental effects (change of the $\dot{w}_\alpha$'s), but at the same time, $S_N(t)$ does *not* capture the additional *intrinsic* variation of information, as it already appears for temporally evolving pure quantum states (see examples discussed in Sec. III). For instance, one possibility to obtain a time-dependent quantum entropy is to consider a coarse-grained version of the density matrix ρ [23].

An alternative description of the evolution of quantum systems, leading to another quantum entropy definition, is based on Wigner functions [24,25]. Given the matrix elements $\rho(t,x,x')$ of the statistical operator, the corresponding Wigner function is defined by

$$f_W(t,x,p) = \int \frac{\mathrm{d}y\, e^{ipy/\hbar}}{(2\pi\hbar)^d}\, \rho\left(t, x - \frac{y}{2}, x + \frac{y}{2}\right). \tag{4}$$

In analogy to the classical distribution function f, the Wigner function f_W can be used to calculate quantum corrections for classical thermodynamical quantities (in the high-temperature limit). In the limit case $h \to 0$, the Wigner function converges to the classical distribution function. For pure states with $\rho = \psi\psi^*$, the Wigner function can be represented through the wave function in the form

$$f_W(t,x,p) = \int \frac{\mathrm{d}y\, e^{ipy/\hbar}}{(2\pi\hbar)^d}\, \psi\left(t, x - \frac{y}{2}\right) \psi^*\left(t, x + \frac{y}{2}\right).$$

By integrating f_W over x or p, respectively, the quantum probability densities are regained. Moreover, one can reconstruct the pure quantum state ψ from f_W; i.e., the quantum system is completely described by its Wigner function [8,26].

However, as well known, due the noncommutativity of coordinates and momenta in quantum theory, the function f_W in general takes negative values. In order to obtain a non-negative function, Husimi proposed to convolute f_W with the Gaussian kernel

$$G(x,p;x',p') = \frac{1}{(2\pi\sigma_p\sigma_x)^d} \exp\left[-\frac{(x-x')^2}{2\sigma_x^2} - \frac{(p-p')^2}{2\sigma_p^2}\right].$$

If the uncertainty relation $\sigma_p\sigma_x \geqslant \hbar/2$ is fulfilled, then the resulting convoluted Husimi function

$$f_H(t,x,p) = \int \mathrm{d}x'\, \mathrm{d}p'\, G(x,p;x',p')\, f_W(t,x',p') \tag{5}$$

is non-negative [27]. Choosing σ_p and σ_x such that $\sigma_p\sigma_x = \hbar/2$ holds and replacing the classical distribution function f in Eq. (1) by the Husimi function f_H, one obtains the so-called Wehrl entropy $S_W(t)$. The properties of $S_W(t)$ have been extensively studied by Anastopoulos and Halliwell in the context of quantum Brownian motion [19,20]. Nevertheless, one should emphasize that, by construction, the Wehrl entropy contains an additional free parameter (σ_x or σ_p). This implies that $S_W(t)$ cannot represent a "fundamental" entropy definition for quantum systems.

As already pointed out in the Introduction, the objective of the present paper is to focus on the loss of information, associated with the quantum evolution of pure states. According to the above discussion, neither the von Neumann entropy S_N (which is constant for pure states) nor the Wehrl entropy S_W (which contains an additional arbitrary parameter) provides satisfactory information-theoretic measures for this purpose. Therefore, we shall pursue below another approach, which goes back to Leipnik [16] and can be described as follows: Consider a normalized quantum state $\psi(t,x)$ governed by the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi, \quad \hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + U(t,x). \tag{6}$$

According to the Born interpretation [28], the functions $|\psi(t,x)|^2$ and $|\tilde{\psi}(t,p)|^2$, where

$$\tilde{\psi}(t,p) = \int \frac{\mathrm{d}x\, e^{-ipx/\hbar}}{(2\pi\hbar)^{d/2}}\, \psi(t,x), \tag{7}$$

give the quantum probability densities for position and momentum coordinates, respectively. Leipnik proposed to consider the product function (joint distribution for pure states)

$$f_J(t,x,p) = |\psi(t,x)|^2 |\tilde{\psi}(t,p)|^2 \geqslant 0. \tag{8}$$

Similar to the Wigner function f_W, also the function f_J characterizes the evolution of quantum states in phase space, even though it contains less information than f_W. Inserting Eq. (8) into Eq. (1) yields the joint entropy $S_J(t)$ for the pure state $\psi(t,x)$, which can equivalently be rewritten in the form

$$S_J(t) = -\int \mathrm{d}x |\psi(t,x)|^2 \ln|\psi(t,x)|^2 - \int \mathrm{d}p |\tilde{\psi}(t,p)|^2 \ln|\tilde{\psi}(t,p)|^2 - \ln h^d. \tag{9}$$

In the next section, the quantity $S_J(t)$ is studied for three simple model systems.

III. JOINT ENTROPY FOR ONE-DIMENSIONAL MODEL SYSTEMS

As recently discussed in [22], the joint entropy $S_J(t)$ provides a useful time-dependent measure for the intrinsic information loss of temporally evolving, pure quantum states (e.g., for the simplest case of free d-dimensional Gaussian wave packets it was shown that $S_J(t)$ grows monotonously for $t > 0$). Furthermore, it was proposed in [22] that this "quantum trend," driven by Heisenberg's uncertainty principle, could be a rather universal property of pure quantum systems. Here we shall pursue this idea further by also considering the influence of external potentials on the evolution of initially maximal classical states (MACS's).

In Sec. III A we briefly review some essential results discussed in [22], restricting ourselves to the case $d=1$. Subsequently, the investigation will be extended to Schrödinger problems with nonvanishing external potentials (Secs. III B and III C).

A. Free motion

For $U\equiv 0$ and $d=1$ the Schrödinger equation (6) has the normalized Gaussian wave packet solution (see, e.g., [29,30])

$$\psi_f(t,x) = \left(\frac{\alpha}{2\pi}\right)^{1/4} \frac{e^{i(k_0 x-\beta k_0^2 t)}}{\sqrt{\alpha + i\beta t}} \exp\left[-\frac{(x-v_0 t)^2}{4(\alpha+i\beta t)}\right], \quad (10)$$

where $\beta=\hbar/(2m)$ and $\sqrt{\alpha}$ is the initial width of the wave packet. The solution (10) yields

$$\langle p(t)\rangle = p_0 = \hbar k_0, \quad \Delta p(t) = \hbar/(2\sqrt{\alpha}),$$

$$\langle x(t)\rangle = v_0 t = p_0 t/m, \quad \Delta x(t) = \sqrt{\alpha + \beta^2 t^2/\alpha}. \quad (11)$$

[Here, as usual, the standard deviation of an observable A is defined by $\Delta A(t)=\sqrt{\langle A^2(t)\rangle - \langle A(t)\rangle^2}$, where $\langle\cdot\rangle$ denotes the expectation with respect to ψ.] From Eqs. (11) one finds immediately the time- dependent uncertainty relation [29]

$$\Delta x(t)\Delta p(t) = \frac{\hbar}{2}\sqrt{1+\frac{\beta^2 t^2}{\alpha^2}} \geqslant \frac{\hbar}{2}. \quad (12)$$

This implies that at time $t=0$ the solution (10) is a MACS, since only then does the left-hand side (LHS) equal the RHS in Eq. (12). Using Eqs. (10), (7), and (9), a straightforward calculation of the joint entropy gives [22]

$$S_J^f(t;d=1) = \ln\left[\frac{e}{2}\sqrt{1+\frac{\beta^2 t^2}{\alpha^2}}\right], \quad (13)$$

where $e=2.7182\ldots$ is the Euler number. For completeness, we mention that for a D-dimensional free wave packet one finds, correspondingly,

$$S_J^f(t;d=D) = D\, S_J^f(t;d=1).$$

It is worthwhile to note that Eq. (13) is in agreement with the following general inequality for the joint entropy:

$$S_J(t) \geqslant \ln\left(\frac{e}{2}\right), \quad (14)$$

originally derived by Leipnik [16] for *arbitrary* one-dimensional one-particle wave functions. Another important feature of the result (13) is the monotonous increase of joint entropy in time. In [22] it was suggested that this is a general property of quantum systems. Below we will demonstrate that, at least asymptotically, this property also holds for more complicated quantum systems.

Furthermore, according to Eqs. (12) and (13), the MACS property is not conserved in time; the logarithmic divergence of the joint entropy reflects a permanent loss of information, representing an intrinsic property of the evolving quantum system. Since Eqs. (12) and (13) are equivalent for free Gaussian wave packets, the joint entropy contains the same amount of information as the uncertainty relation; for more complicated problems, this will not be the case anymore, because in general for $t>0$ the wave functions will essentially deviate from the initial Gaussian shape.

Although the above free wave packet example is rather simple, it is helpful to elucidate some general properties of the joint entropy. For more complicated problems with nonvanishing potentials $U(t,x)$, an exact calculation of the joint entropy becomes more difficult or in most cases—especially in two or three spatial dimensions—even impossible. Therefore, when including external fields in the remainder, we continue to concentrate on analytically tractable problems with $d=1$. The results will be compared with those just discussed for one-dimensional free wave packet.

B. Oscillating external fields

As slightly more complicated examples, which are still exactly solvable, we next consider the time-periodic potentials

$$U^s(t,x) = qE_0 x\sin(\Omega t), \quad (15a)$$

$$U^c(t,x) = qE_0 x\cos(\Omega t). \quad (15b)$$

These potentials describe, in the dipole approximation [31], the interaction between a quantum particle with electric charge q and an oscillating, monochromatic electric field with amplitude E_0 and frequency Ω. Analytic solutions of the corresponding relativistic quantum wave equations were first discussed by Gordon [32] and Volkov [33] about 70 years ago. Recently, however, this problem has reattracted considerable theoretical interest [34–38]. Here we will use results for the corresponding Schrödinger equation (6), as derived by Rau and Unnikrishnan [34].

Before discussing the solutions, it is useful to transform to rescaled dimensionless quantities

$$x' = x\left(\frac{m\Omega}{\hbar}\right)^{1/2}, \quad p' = \frac{p}{(M\Omega\hbar)^{1/2}}, \quad t' = \Omega t,$$

$$E_0' = \frac{qE_0}{(M\Omega^3\hbar)^{1/2}}, \quad \psi'(t',x') = \left(\frac{m\Omega}{\hbar}\right)^{-1/4}\psi(t,x).$$

Formally, this corresponds to fixing characteristic units such that $\hbar=m=\Omega=q=1$. Dropping for convenience the primes again, the rescaled Schrödinger equation (6) takes the simplified form

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi + U^{s/c}(t,x)\psi, \quad (16)$$

where the rescaled potentials read

$$U^s(t,x) = E_0 x\sin t, \quad (17a)$$

$$U^c(t,x) = E_0 x\cos t. \quad (17b)$$

First, let us consider U^s from Eq. (17a). According to formula (19) of Ref. [34], the time-dependent fundamental solution of Eq. (16) is given by

$$\phi_p^s(t,x) = \exp\left[-iE_0^2\left(\frac{1}{8}\sin 2t - \sin t + \frac{3}{4}t\right)\right]\exp[-iE_0x(1 - \cos t) - iE_0p(\sin t - t)]\exp\left[i\left(px - \frac{p^2}{2}t\right)\right]. \quad (18)$$

From this solution, one can construct special solutions via superpositioning. As in the previous example, we would like to consider solutions which are MAC states at initial time $t = 0$. This can be achieved by setting

$$\psi^s(t,x) = \left(\frac{\alpha}{2\pi^3}\right)^{1/4}\int \mathrm{d}p\, e^{-\alpha(p-p_0)^2}\phi_p^s(t,x), \quad (19)$$

where the parameter p_0 determines the initial momentum. The integral (19) can be calculated analytically, yielding

$$\psi^s(t,x) = \left(\frac{\alpha}{2\pi}\right)^{1/4}\frac{e^{-\alpha p_0^2 - iE_0x(1-\cos t)}}{\sqrt{\alpha + it/2}} \times \exp\left\{-\frac{[x + E_0(t - \sin t) - 2i\alpha p_0]^2}{4(\alpha + it/2)}\right\} \times \exp\left\{-iE_0^2\left[\frac{3}{4}t + \left(\frac{1}{4}\cos t - 1\right)\sin t\right]\right\}. \quad (20)$$

From this solution one finds the two normalized quantum probability densities

$$|\psi^s(t,x)|^2 = \left[\frac{2\alpha}{\pi(4\alpha^2 + t^2)}\right]^{1/2} \times \exp\left\{-\frac{2\alpha[x - p_0t + E_0(t - \sin t)]^2}{4\alpha^2 + t^2}\right\},$$

$$|\tilde{\psi}^s(t,p)|^2 = \left(\frac{2\alpha}{\pi}\right)^{1/2}\exp\{-2\alpha[p - p_0 + E_0(1 - \cos t)]^2\}. \quad (21)$$

Obviously, each of the two densities in Eq. (21) corresponds to a Gaussian with oscillating mean value. More precisely, we find

$$\langle x(t)\rangle = (p_0 - E_0)t + E_0\sin t,$$

$$\langle p(t)\rangle = (p_0 - E_0) + E_0\cos t, \quad (22a)$$

and, furthermore,

$$\Delta x(t) = \frac{1}{2}\left(4\alpha + \frac{t^2}{\alpha}\right)^{1/2}, \quad \Delta p(t) = \frac{1}{2\sqrt{\alpha}}. \quad (22b)$$

Thus, after reinstating quantities $\hbar$, m, Ω, and q one arrives at exactly the same uncertainty relation as found earlier for the free particle; see Eq. (12). Moreover, by explicitly calculating the joint entropy on the basis of Eq. (21), one can show that $S_J^{s/c}(t)$ coincides with the free-particle result (13).

It comes as no surprise that an analogous result is obtained, if one considers U^c from Eq. (17b). According to formulas (22) and (23) in [34], for Eq. (17b) one must use the fundamental solution

$$\phi_p^c(t,x) = \exp\left[-iE_0^2\left(-\frac{1}{8}\sin 2t + \frac{1}{4}t\right)\right]\exp[-iE_0x\sin t - iE_0p(\cos t - 1)]\exp\left[i\left(px - \frac{p^2}{2}t\right)\right] \quad (23)$$

instead of Eq. (18). Substituting indices s by c in Eq. (19), one then obtains

$$\psi^c(t,x) = \left(\frac{\alpha}{2\pi}\right)^{1/4}\frac{e^{-\alpha p_0^2 - iE_0x\sin t}}{\sqrt{\alpha + it/2}} \times \exp\left\{-\frac{[x + E_0(t - \cos t) - 2i\alpha p_0]^2}{4(\alpha + it/2)}\right\} \times \exp\left[-\frac{i}{4}E_0^2(t - \cos t\sin t)\right]. \quad (24)$$

This gives the densities

$$|\psi^c(t,x)|^2 = \left[\frac{2\alpha}{\pi(4\alpha^2 + t^2)}\right]^{1/2}\exp\left\{-\frac{2\alpha[x - p_0t + E_0(1 - \cos t)]^2}{4\alpha^2 + t^2}\right\},$$

$$|\tilde{\psi}^c(t,p)|^2 = \left(\frac{2\alpha}{\pi}\right)^{1/2}\exp[-2\alpha(p - p_0 + E_0\sin t)^2], \quad (25)$$

yielding

$$\langle x(t)\rangle = p_0t - E_0 + E_0\cos t,$$

$$\langle p(t)\rangle = p_0 - E_0\sin t, \quad (26)$$

while, for the standard deviations, Eqs. (22b) are regained.

In summary, if identical MACS initial conditions are considered, then—compared with the free wave packet case—the presence of the monochromatic oscillating fields is neither reflected by the uncertainty relation nor by the joint entropy (in spite of the fact that the joint probability functions $f_J^{c/s}$ and f_J^f are different).

C. Tunneling through a δ-peak potential

As third example, consider the Schrödinger equation (6) with $d = 1$ and time-independent potential

$$U(x) = U_0\delta(x), \quad U_0 > 0, \quad (27)$$

corresponding to an infinitely high and infinitely thin barrier at $x = 0$. Similar to before, we take as initial condition a Gaussian MACS

$$\psi(0,x) = \left(\frac{1}{2\pi\alpha}\right)^{1/4}\exp\left[ik_0x - \frac{(x - x_0)^2}{4\alpha^2}\right], \quad (28)$$

where it is further assumed that

$$\langle x(0)\rangle = x_0 < 0,$$

$$\langle p(0)\rangle = \hbar k_0 > 0, \quad (29a)$$

and

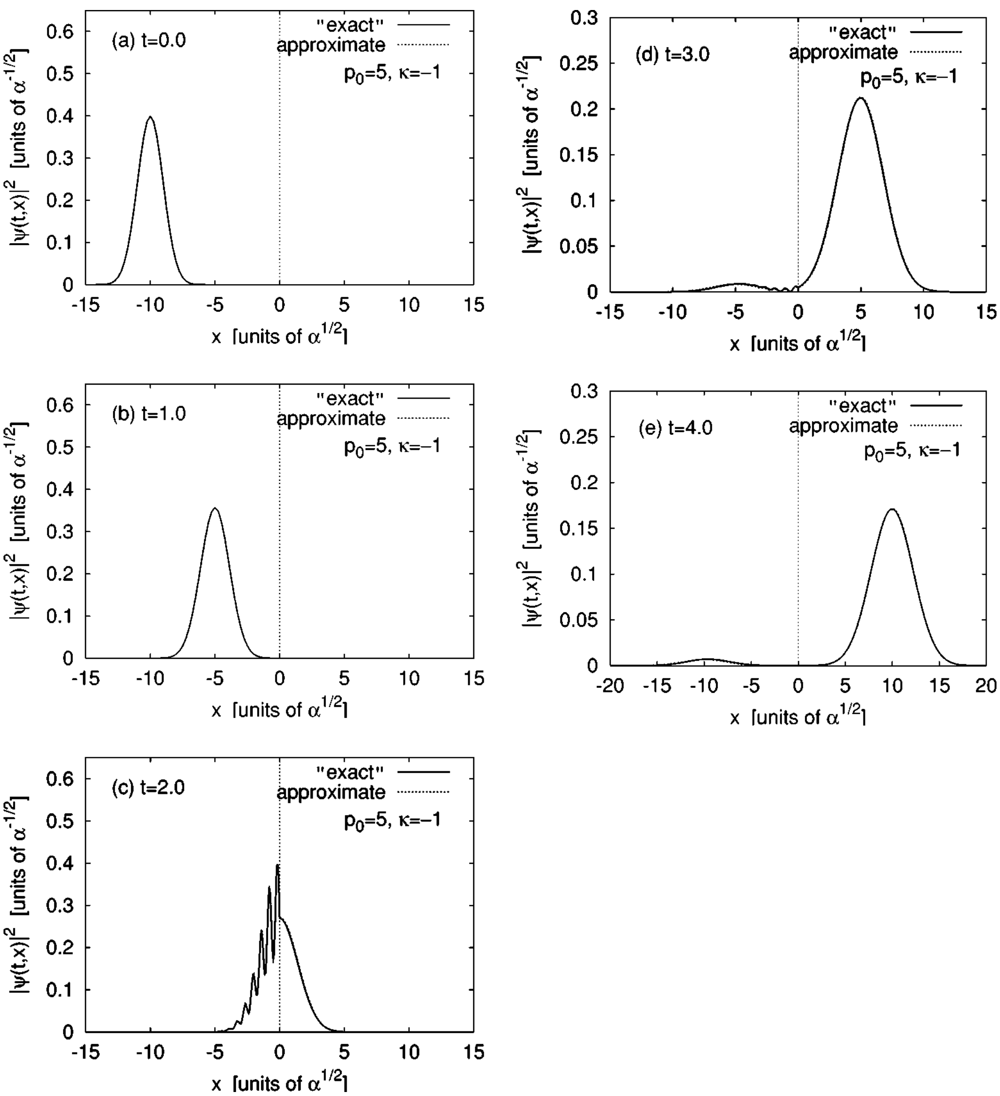

FIG. 1. Tunneling of a MAC state through the potential barrier $U(x)=U_0\delta(x)$: Evolution of the spatial probability density $|\psi(t,x)|^2$ for "large" initial momentum p_0. Solid lines correspond to the "exact" solution (31) and dashed lines to the approximate result (32). Time t is measured in units $\tau=m\alpha/\hbar$ and x in units $\sqrt{\alpha}$, where $\sqrt{\alpha}$ determines the initial width of the wave packet. The remaining parameter values are $x_0=-10$, $k_0=p_0/\hbar=5$, and $U_0=1$ with units given by $[x_0]=\sqrt{\alpha}$, $[k_0]=1/\sqrt{\alpha}$, and $[U_0]=\hbar\sqrt{\alpha}/\tau$.

$$\left|\frac{x_0}{\Delta x(0)}\right| = \left|\frac{x_0}{\sqrt{\alpha}}\right| \gg 1 \tag{29b}$$

hold. The conditions (29a) mean that the maximum of wave packet approaches the barrier from the left, while Eq. (29b) states that, at time $t=0$, the particle is (almost) surely localized on the left-hand side of the barrier. For fixed initial position $x_0<0$ and initial momentum $p_0=\hbar k_0>0$, the time of the collision with the barrier can be defined as

$$t_c = \frac{|x_0|}{p_0/m} = \frac{m|x_0|}{\hbar k_0}. \tag{30}$$

As we shall see below, the quantity t_c can be used to identify peculiarities in the entropy curves $S_J(t)$.

1. Evolution of the spatial density

If the condition (29b) is satisfied, then one finds the following integral representation for the related time-dependent solution (see the Appendix for details of the calculation):

$$\psi(t,x) \simeq \left(\frac{\alpha}{2\pi^3}\right)^{1/4} \int_{-\infty}^{\infty} \mathrm{d}\, k e^{-\alpha(k_0-k)^2} e^{i(k_0-k)x_0 - i\beta k^2 t} \times \left[\frac{k}{k-i\kappa}\exp(ikx) + \Theta(-x)\frac{2\kappa}{k-i\kappa}\sin(kx)\right]. \tag{31}$$

Here $\Theta(x)$ denotes the unit-step function, defined in Eq. (A28), and the parameter

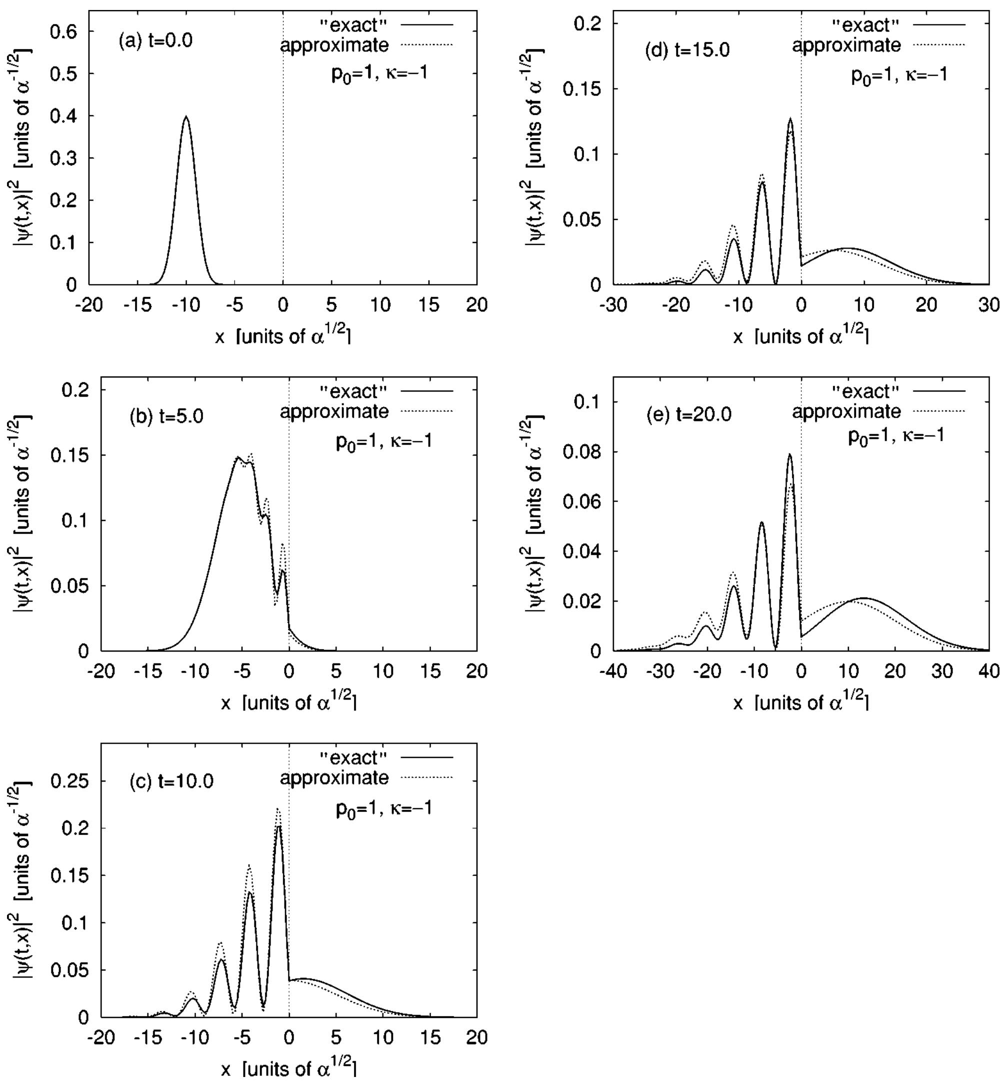

FIG. 2. Tunneling through the δ barrier for "moderate" initial momentum $p_0=1$ (units and all other parameters are chosen as in Fig. 1). Here the transmission (tunneling) probability approximately equals the reflection probability. As a consequence, for $t>t_c$ the joint entropy is much larger than in the case of "large" and "small" initial momenta; compare Fig. 4.

$$\kappa = -\frac{mU_0}{\hbar^2}$$

characterizes the height of the barrier. Unfortunately, because of the prefactors

$$c_1(k) = \frac{k}{k-i\kappa}, \quad c_2(k) = \frac{2\kappa}{k-i\kappa},$$

the integral (31) cannot be solved exactly. With regard to subsequent (numerical) calculations of the joint entropy, it turns out as useful to make an additional approximation by replacing in Eq. (31) the k-dependent functions $c_{1/2}(k)$ with the constants $c_{1/2}(k_0)$. These approximations are reasonable for sufficently large parameter values α in the Gaussian exponential of the integral (31), and one then obtains the approximate solution

$$\psi_0(t,x) \simeq \left(\frac{\alpha}{2\pi}\right)^{1/4}\left(\frac{1}{\alpha+i\beta t}\right)^{1/2}\frac{e^{ik_0x_0}}{k_0-i\kappa} \times \exp\left[-\frac{(x-x_0)^2+4i\alpha k_0^2\beta t}{4(\alpha+i\beta t)}\right]\Bigg\{k_0+i\Theta(-x) \times\kappa\left[\exp\left(-\frac{x_0x+2i\alpha k_0x}{\alpha+i\beta t}\right)-1\right]\Bigg\}. \qquad (32)$$

Figures 1–3 show the evolution of the spatial probability density $|\psi(t,x)|^2$ for three different choices of the quotient $k_0/|\kappa|$, characterizing the ratio between initial momentum and barrier height. In each diagram solid lines were numerically calculated using the "exact" solution (31), while dashed lines correspond to the approximate solution ψ_0 from Eq. (32). As one can deduce from these figures, ψ_0 provides indeed a useful approximation of the more exact solution (31). Moreover, one observes that the deviation between Eqs. (31) and (32) decreases for $k_0 \gg |\kappa|$; e.g., for $k_0/|\kappa|=5$ (see Fig. 1),

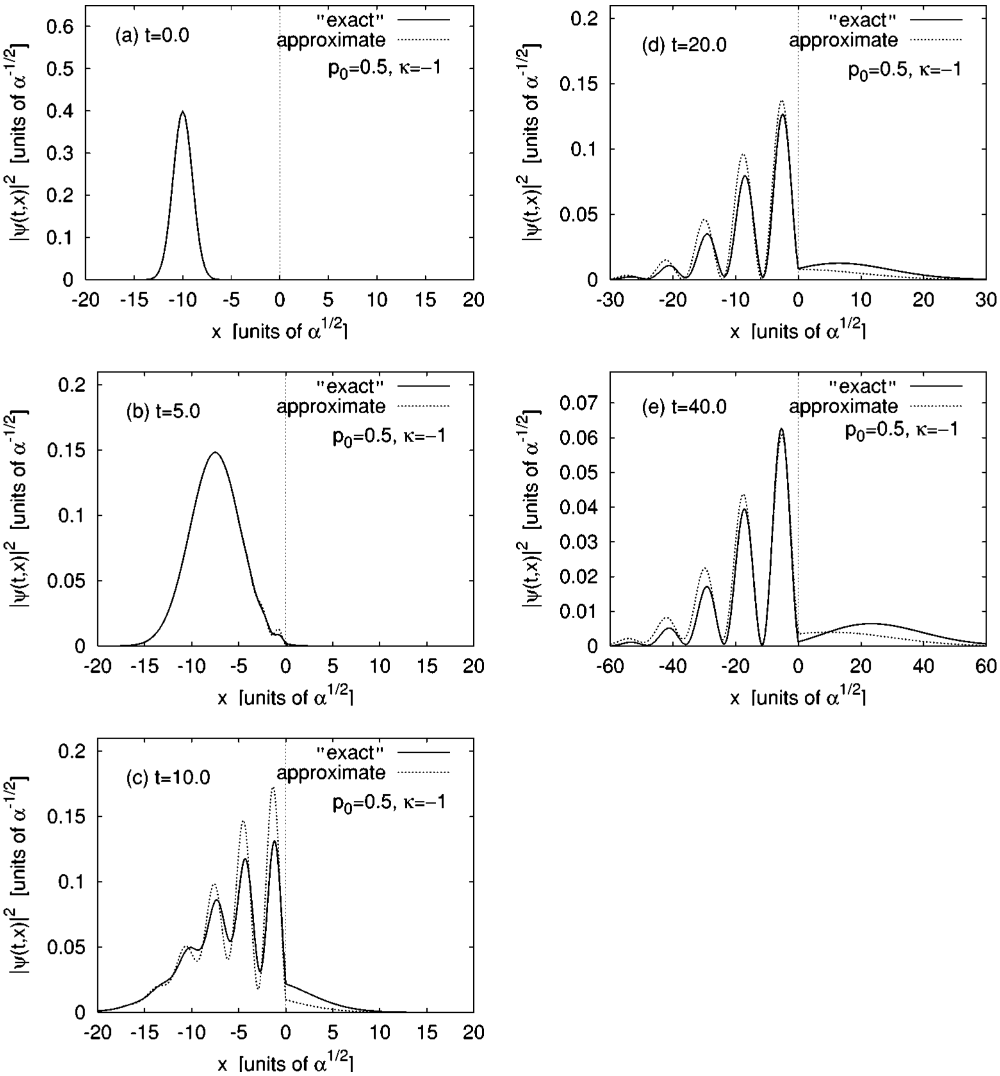

FIG. 3. Tunneling through the δ barrier for "small" initial momentum $p_0=0.5$ (units and all other parameters are chosen as in Figs. 1 and 2). Here the reflection probability is much larger than the tunneling probability. Moreover, one can see that the deviation of the approximate solution (32) from the "exact" solution (31) becomes more significant, if the initial momentum is small compared to the effective barrier height $|\kappa|$.

the dashed and solid lines are nearly indistinguishable.

2. Joint entropy

In order to calculate the joint entropy $S_J(t)$ via Eq. (9), one requires the Fourier-transformed wave function $\tilde{\psi}(t,p)$. For the wave $\psi(t,x)$ from Eq. (31) it is difficult to find an explicit formula for $\tilde{\psi}(t,p)$. Hence, it is also rather difficult to calculate $S_J(t)$ from the integral representation (31). However, as we have seen in the preceding section, the approximate solution ψ_0 from Eq. (31) provides a useful estimate of the true solution. Therefore, instead of Eq. (31), we will restrict ourselves below to considering the joint entropy for the approximate solution (32).

For $\psi_0(t,x)$ from Eq. (32) the related momentum wave function $\tilde{\psi}_0(t,p)$ can be easily calculated from Eq. (7), and one finds

$$\begin{aligned}\tilde{\psi}_0(t,p) = {} & \left(\frac{\alpha}{2^3\pi\hbar^2}\right)^{1/4}\frac{e^{i(p_0-p)x_0/\hbar}}{p_0-i\hbar\kappa}\\ & \times \exp\left[-\frac{\alpha(p-p_0)^2+ip^2\beta t}{\hbar^2}\right]\\ & \times \Bigg\{2p_0+i\hbar\kappa[\mathrm{Erf}(\gamma_-)-1]\\ & + i\hbar\kappa\exp\left(\frac{2ipx_0}{\hbar}-\frac{4\alpha pp_0}{\hbar^2}\right)[\mathrm{Erf}(\gamma_+)+1]\Bigg\},\end{aligned} \tag{33}$$

where $\mathrm{Erf}(x)$ denotes the error function, defined in Eq. (A17), and the abbreviations

$$\gamma_-(t,p) = \frac{\hbar x_0 + 2p\beta t + 2i\alpha(p_0-p)}{2\hbar\sqrt{\alpha+i\beta t}},$$

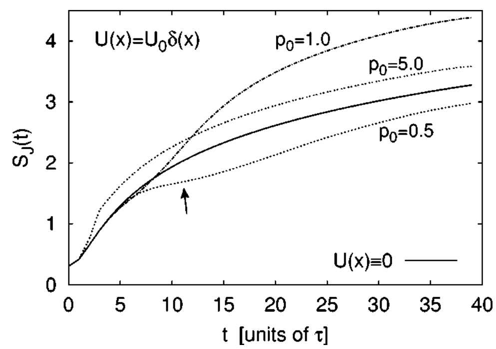

FIG. 4. MACS tunneling through the barrier $U_0\delta(x)$: time-dependent joint entropy for different initial momenta $p_0=\hbar k_0$, where $[k_0]=1/\sqrt{\alpha}$. The curves were obtained by numerical integration of Eq. (9) for the approximate solution (32). Parameter values and units were chosen as in Figs. 1–3; i.e., we have set $x_0=-10$ and $U_0=1$, where $[x_0]=\sqrt{\alpha}$, $[U_0]=\hbar\sqrt{\alpha}/\tau$ and $\tau=m\alpha/\hbar$. For comparison, we also plotted the joint entropy (13) for the spreading of free wave packet (solid line). The three nonsolid curves exhibit locally maximal slopes in the vicinity of the collision time $t_c=|x_0|/p_0$. Also note the appearance of the plateaulike region (arrow) for small initial momenta.

$$\gamma_+(t,p) = \frac{\hbar x_0 - 2p\beta t + 2i\alpha(p_0+p)}{2\hbar\sqrt{\alpha + i\beta t}}$$

have been introduced. On the basis of formulas (32) and (33), it is now straightforward to numerically calculate the related joint entropy $S_J(t)$ from Eq. (9). In Fig. 4, one can see examples of entropy curves, based on the same parameter values as used in Figs. 1–3. Analogous to preceding diagrams, the representation in Fig. 4 refers to the characteristic unit system defined by $m=\hbar=\sqrt{\alpha}=1$, where $\sqrt{\alpha}$ is the initial width of the wave packet. For example, we simply have $\beta=1/2$, $\kappa=-U_0$, etc., in these units. Furthermore, the related unit time reads $\tau=m\alpha/\hbar$ and the collision time t_c, defined in Eq. (30), reduces to $t_c=|x_0|/p_0$.

The joint entropy curves $S_J(t)$ in Fig. 4 were obtained by numerically integrating Eq. (9) with the computer software Mathematica [39]. The three nonsolid lines refer to the tunneling through the δ barrier. For comparison, we also the plotted the joint entropy (13) for the spreading of free wave packet (solid line). The main observations in Fig. 4 are the following

(i) For $t\to 0$, all four curves converge to the value $S_J(0)=\ln(e/2)=0.306\ldots$; compare Eq. (13). This reflects the fact that we have chosen special initial conditions, corresponding to MAC states.

(ii) For $t<t_c$ all three nonsolid curves in Fig. 4 run below the solid (free wave packet) entropy curve $S_L^f(t)$. This reflects the fact that, at the early stages of the tunneling process, the δ barrier hinders the spreading of the wave packet. In particular, for small initial momenta a plateaulike region appears, indicated by the arrow [but it should also be kept in mind that for $k_0\ll|\kappa|$ the approximate solution (32) becomes less reliable; see Fig. 3].

(iii) At $t\approx t_c$ the slope of the joint entropy exhibits a local maximum for the three non-solid curves in Fig. 4—i.e.,

$$\left.\frac{d^2S_J}{dt^2}\right|_{t\approx t_c}=0, \qquad \left.\frac{d^3S_J}{dt^3}\right|_{t\approx t_c}<0.$$

(iv) For $t>t_c$ the curve for "$p_0=1$," corresponding to a moderate initial momentum value, clearly dominates the other curves. Roughly speaking, this can be explained by the fact that for moderate initial momenta the tunneling probability approximately equals the reflection probability (compare Fig. 2), thus leading to maximum uncertainty.

(v) Each of the shown curves increases monotonously in time. However, the appearance of the plateaulike region (arrow) at low initial momenta seems to indicate that confinement effects due to interactions or external potentials might also lead to a temporary decrease of the joint entropy on short time scales. Of course, in such a scenario, Leipnik's inequality (14) constitutes a lower bound for $S_J(t)$.

IV. SUMMARY

We have studied the joint entropy for explicit time-dependent solutions of three simple one-dimensional Schrödinger problems: (i) the spreading of a free Gaussian wave packet, (ii) the motion of a wave packet in a monochromatic electromagnetic field, and (iii) the tunneling of a wave packet through a δ barrier. The second example can be considered as an open quantum system, because in this case the Hamiltonian is explicitely time dependent. In contrast, examples (i) and (iii) correspond to closed systems. As initial conditions maximal classical states have been used. MACS's minimize the Heisenberg uncertainty as well as the joint entropy. A quantum system that has been in a MACS at time $t=0$ inevitably evolves into a non-MACS at times $t>0$. This intrinsic property of quantum systems is, e.g., reflected by a monotonous increase of the joint entropy. Most likely, this quantum trend also manifests itself for other type of initial wave packets and external potentials, as well as in many-particle systems.

In order to be able to calculate the joint entropy for the tunneling process through a δ peak potential [example (iii)], an approximate analytic solution of the corresponding time-dependent Schrödinger problem was derived (Appendix). By means of this solution, it could be shown that the slope of the corresponding joint entropy exhibits a local maximum in the vicinity of the collision time. Based on this observation one may conclude that, on many occasions, interactions tend to speed-up the joint entropy increase (i.e., the loss of phase-space information) in quantum systems. With respect to many-particle systems, an interesting question to be answered in the future is whether or not such quantum trends are important for the relaxation to thermodynamic equilibrium.

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APPENDIX: SOLVING SCHRÖDINGER's EQUATION FOR THE δ BARRIER

1. The problem

We wish to find the time-dependent solution $\psi(t,x)$ for the one-dimensional Schrödinger problem

$$i\hbar\frac{\partial}{\partial t}\psi = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + U_0\delta(x)\right]\psi \equiv \hat{H}\psi, \qquad (A1)$$

where $U_0 > 0$ and the initial condition is fixed as

$$\psi(0,x) = \left(\frac{1}{\sqrt{\pi}\lambda}\right)^{1/2}\exp\left[ik_0x - \frac{(x-x_0)^2}{2\lambda^2}\right]. \qquad (A2)$$

This corresponds to the initial Gaussian probability density

$$|\psi(0,x)|^2 = \frac{1}{\sqrt{\pi}\lambda}\exp\left[-\frac{(x-x_0)^2}{\lambda^2}\right], \qquad (A3)$$

which is normalized to unity:

$$1 = \int_{-\infty}^{\infty} \mathrm{d}x\, \psi^*(0,x)\psi(0,x). \qquad (A4)$$

Furthermore, we have at initial time $t=0$

$$\langle x(0)\rangle \equiv \int_{-\infty}^{\infty}\mathrm{d}x\, \psi^*(0,x)x\psi(0,x) = x_0, \qquad (A5a)$$

$$\langle p(0)\rangle \equiv -i\hbar\int_{-\infty}^{\infty}\mathrm{d}x\, \psi^*(0,x)\frac{\partial\psi}{\partial x}(0,x) = \hbar k_0, \qquad (A5b)$$

and the initial width of the wave packet reads

$$\Delta x(0) \equiv \sqrt{\langle x^2(0)\rangle - \langle x(0)\rangle^2} = \frac{\lambda}{\sqrt{2}}. \qquad (A5c)$$

The constant energy of the wave packet is given by

$$\langle\hat{H}(t)\rangle = \frac{\hbar^2k_0^2}{2m} + \frac{\hbar^2}{4m\lambda^2} + \frac{U_0}{\sqrt{\pi}\lambda}\exp\left(-\frac{x_0^2}{\lambda^2}\right). \qquad (A6)$$

2. Superposition of eigenfunctions

The eigenfunctions of the related stationary Schrödinger eigenvalue problem

$$\hat{H}\phi(x) = E\phi(x) \qquad (A7)$$

read (see, e.g., p. 147 in Ref. [29])

$$\phi_k^+(x) = \frac{1}{\sqrt{\pi}}\cos[k|x| + \eta(k)], \qquad (A8a)$$

$$\phi_k^-(x) = \frac{1}{\sqrt{\pi}}\sin(kx), \qquad (A8b)$$

with eigenvalues given by

$$E(k) = \frac{\hbar^2k^2}{2m} > 0. \qquad (A8c)$$

Note that symmetric and antisymmetric solutions are labeled by "+" and "−," respectively. From the matching condition

$$\phi_k'(0^+) - \phi_k'(0^-) = \frac{2mU_0}{\hbar^2}\phi_k(0), \qquad (A9)$$

one finds that for the phase of the symmetric solutions

$$\eta(k) = \arctan\left(\frac{\kappa}{k}\right), \quad \kappa = -\frac{mU_0}{\hbar^2}. \qquad (A10)$$

For $k,k' > 0$ the solutions $\{\phi_k^\pm\}$ satisfy the orthonormality relations

$$\int_{-\infty}^{\infty}\mathrm{d}x\, \phi_k^+(x)\phi_{k'}^+(x) = \delta(k-k'), \qquad (A11a)$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\, \phi_k^-(x)\phi_{k'}^-(x) = \delta(k-k'), \qquad (A11b)$$

$$\int_{-\infty}^{\infty}\mathrm{d}x\, \phi_k^+(x)\phi_{k'}^-(x) = 0. \qquad (A11c)$$

Hence, one can expand the solutions of the time-dependent Schrödinger problem (A1) in the form

$$\psi(t,x) = \int_0^{\infty}\mathrm{d}k[a_+(k)\phi_k^+(x) + a_-(k)\phi_k^-(x)]e^{-iE(k)t/\hbar}. \qquad (A12)$$

The restriction to non-negative k values suffices here, because $\phi_k^\pm(x) = \pm\phi_{-k}^\pm(x)$ holds. Furthermore, at time $t=0$ the condition

$$\psi(0,x) = \int_0^{\infty}\mathrm{d}k[a_+(k)\phi_k^+(x) + a_-(k)\phi_k^-(x)] \qquad (A13)$$

must be satisfied. Consequently, the coefficients $a_\pm(k)$ are determined by projection onto the initial condition:

$$a_\pm(k) = \int_{-\infty}^{\infty}\mathrm{d}x\, \phi_k^\pm(x)\psi(x,0). \qquad (A14)$$

This follows from the orthonormality relations (A11). Using the special initial condition (A2), one finds

$$a_+(k) = b_+(k) - b_+(-k), \qquad (A15a)$$

$$a_-(k) = b_-(k) - b_-(-k), \qquad (A15b)$$

where

$$b_+(k) \equiv \left[\frac{\lambda}{2\sqrt{\pi}(k^2+\kappa^2)}\right]^{1/2}\exp\left[i(k_0-k)x_0 - \frac{\lambda^2}{2}(k_0-k)^2\right] \times\left(k - i\kappa\,\mathrm{Erf}\left[\frac{x_0 + i(k_0-k)\lambda^2}{\sqrt{2}\lambda}\right]\right), \qquad (A16a)$$

and

$$b_-(k) \equiv i\left(\frac{\lambda}{2\sqrt{\pi}}\right)^{1/2}\exp\left[i(k_0-k)x_0-\frac{\lambda^2}{2}(k_0-k)^2\right]. \tag{A16b}$$

The error function in Eq. (A16a) is defined by

$$\mathrm{Erf}(z)=\frac{2}{\sqrt{\pi}}\int_0^z \mathrm{d}t\, e^{-t^2}. \tag{A17}$$

Equations (A15) and (A16) further imply

$$a_\pm(k)=-a_\pm(-k). \tag{A18}$$

Introducing the abbreviation

$$\beta \equiv \frac{\hbar}{2m}, \tag{A19}$$

the general solution (A12) can be written as

$$\psi(t,x)=I_+(t,x)+I_-(t,x), \tag{A20}$$

where

$$I_+(t,x) \equiv \int_0^\infty \mathrm{d}k\, a_+(k)\phi_k^+(x)e^{-i\beta k^2 t}, \tag{A21a}$$

$$I_-(t,x) \equiv \int_0^\infty \mathrm{d}k\, a_-(k)\phi_k^-(x)e^{-i\beta k^2 t}. \tag{A21b}$$

By using Eq. (A15b) and inserting the explicit expression for $\phi_k^-(x)$, we find

$$\begin{aligned}
I_-(t,x) &= \frac{1}{\sqrt{\pi}}\int_0^\infty \mathrm{d}k[b_-(k)-b_-(-k)]\sin(kx)e^{-i\beta k^2 t}\\
&= \frac{1}{2\sqrt{\pi}}\int_{-\infty}^\infty \mathrm{d}k\,[b_-(k)-b_-(-k)]\sin(kx)e^{-i\beta k^2 t}\\
&= \frac{1}{\sqrt{\pi}}\int_{-\infty}^\infty \mathrm{d}k b_-(k)\sin(kx)e^{-i\beta k^2 t}\\
&\overset{\text{(A16b)}}{=} i\left(\frac{\lambda}{2\sqrt{\pi^3}}\right)^{1/2}\int_{-\infty}^\infty \mathrm{d}k\,\sin(kx)\\
&\quad\times\exp\left[i(k_0-k)x_0-\frac{\lambda^2}{2}(k_0-k)^2-i\beta k^2 t\right].
\end{aligned} \tag{A22}$$

The integral (A22) can be calculated:

$$\begin{aligned}
I_-(t,x) &= \left[\frac{\lambda}{4\sqrt{\pi}(\lambda^2+2i\beta t)}\right]^{1/2}\exp\left(ik_0x_0-\frac{\lambda^2k_0^2}{2}\right)\\
&\quad\times\left\{\exp\left[-\frac{1}{2}\frac{(x_0-x+ik_0\lambda^2)^2}{\lambda^2+2i\beta t}\right]\right.\\
&\quad\left.-\exp\left[-\frac{1}{2}\frac{(x_0+x+ik_0\lambda^2)^2}{\lambda^2+2i\beta t}\right]\right\},
\end{aligned}$$

where, in particular,

$$\begin{aligned}
I_-(0,x) &= \left(\frac{1}{4\sqrt{\pi}\lambda}\right)^{1/2}\left\{\exp\left[-\frac{(x_0-x)^2}{2\lambda^2}+ik_0x\right]\right.\\
&\quad\left.-\exp\left[-\frac{(x_0+x)^2}{2\lambda^2}-ik_0x\right]\right\}.
\end{aligned}$$

Unfortunately, because of the error function in Eq. (A16a), the remaining integral $I_+(t,x)$ cannot explicitly be solved.

Therefore, we shall next try to find a convenient integral representation of the solution $\psi(t,x)$ by considering a special limit case.

3. Limit case $|x_0| \gg \lambda$

In the following we shall consider the limit case

$$x_0<0, \quad k_0>0, \quad \left|\frac{x_0}{\sqrt{2}\lambda}\right| \gg 1. \tag{A23}$$

This means that (i) the wave packet approaches the barrier from the left and (ii) the spatial probability is initially concentrated in the region $x<0$. By virtue of

$$\lim_{x\to-\infty}\mathrm{Erf}(x+iy)=-1, \quad x,y\in\mathbb{R}, \tag{A24}$$

we obtain in the limit case (A23) from Eq. (A16a)

$$b_+(k) \simeq \left(\frac{\lambda}{2\sqrt{\pi}}\right)^{1/2}\frac{k+i\kappa}{\sqrt{k^2+\kappa^2}}\exp\left[i(k_0-k)x_0-\frac{\lambda^2}{2}(k_0-k)^2\right]. \tag{A25}$$

Using this approximate expression, we can rewrite $I_+(t,x)$ from Eq. (A21a). Inserting Eq. (A15a) and the explicit expression for $\phi_k^+(x)$, we find

$$\begin{aligned}
I_+(t,x) &= \frac{1}{\sqrt{\pi}}\int_0^\infty \mathrm{d}k[b_+(k)-b_+(-k)]e^{-i\beta k^2 t}\\
&\quad\times\cos\left[k|x|+\arctan\left(\frac{\kappa}{k}\right)\right],\\
&= \frac{1}{\sqrt{\pi}}\int_0^\infty \mathrm{d}k[b_+(k)-b_+(-k)]e^{-i\beta k^2 t}\\
&\quad\times\left[\frac{k\cos(k|x|)-\kappa\sin(k|x|)}{\sqrt{k^2+\kappa^2}}\right].
\end{aligned}$$

Since the integrand is an even function with respect to k, we obtain

$$\begin{aligned}
I_+(t,x) &= \frac{1}{2\sqrt{\pi}}\int_{-\infty}^\infty \mathrm{d}k[b_+(k)-b_+(-k)]e^{-i\beta k^2 t}\\
&\quad\times\left[\frac{k\cos(k|x|)-\kappa\sin(k|x|)}{\sqrt{k^2+\kappa^2}}\right]\\
&= \frac{1}{\sqrt{\pi}}\int_{-\infty}^\infty \mathrm{d}k\, b_+(k)e^{-i\beta k^2 t}\left[\frac{k\cos(k|x|)-\kappa\sin(k|x|)}{\sqrt{k^2+\kappa^2}}\right].
\end{aligned}$$

Inserting Eq. (A25) for $b_+(k)$, we have

$$I_+(t,x) \simeq \left(\frac{\lambda}{2\sqrt{\pi^3}}\right)^{1/2}\int_{-\infty}^{\infty} \mathrm{d}k \frac{k+i\kappa}{k^2+\kappa^2}[k\cos(k|x|) - \kappa\sin(k|x|)]\exp\left[i(k_0-k)x_0 - \frac{\lambda^2}{2}(k_0-k)^2 - i\beta k^2 t\right]. \quad \text{(A26)}$$

Combining Eqs. (A22) and (A26) we get

$$\psi(t,x) \simeq \left(\frac{\lambda}{2\sqrt{\pi^3}}\right)^{1/2}\int_{-\infty}^{\infty} \mathrm{d}k\, A(k,x)\exp\left[i(k_0-k)x_0 - \frac{\lambda^2}{2}(k_0 - k)^2 - i\beta k^2 t\right],$$

where

$$A(k,x) = \frac{k\cos(k|x|) - \kappa\sin(k|x|)}{k-i\kappa} + i\sin(kx) = \frac{k[\cos(k|x|) + i\sin(kx)] + \kappa[\sin(kx) - \sin(k|x|)]}{k-i\kappa}.$$

For $x \geqslant 0$ we have $|x| = x$ and, thus,

$$A(k,x)_{x\geqslant 0} = \frac{k}{k-i\kappa}\exp(ikx),$$

whereas for $x<0$ we have $|x| = -x$, yielding

$$A(k,x)_{x<0} = \frac{k}{k-i\kappa}\exp(ikx) + \frac{2\kappa}{k-i\kappa}\sin(kx).$$

Formally, the above results can be summarized as follows:

$$\psi(t,x) \simeq \left(\frac{\lambda}{2\sqrt{\pi^3}}\right)^{1/2}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{i(k_0-k)x_0-(\lambda^2/2)(k_0-k)^2-i\beta k^2 t} \times \left[\frac{k}{k-i\kappa}\exp(ikx) + \Theta(-x)\frac{2\kappa}{k-i\kappa}\sin(kx)\right], \quad \text{(A27)}$$

where the step function $\Theta(x)$ is defined by

$$\Theta(x) \equiv \begin{cases} 1, & x \geqslant 0, \\ 0, & x<0. \end{cases} \quad \text{(A28)}$$

Finally, we can reparametrize

$$\lambda = \sqrt{2\alpha},$$

which allows us to rewrite the solution (A27) as

$$\psi(t,x) \simeq \left(\frac{\alpha}{2\pi^3}\right)^{1/4}\int_{-\infty}^{\infty} \mathrm{d}k\, e^{i(k_0-k)x_0-\alpha(k_0-k)^2-i\beta k^2 t} \times \left[\frac{k}{k-i\kappa}\exp(ikx) + \Theta(-x)\frac{2\kappa}{k-i\kappa}\sin(kx)\right], \quad \text{(A29)}$$

where α and β play the same role as, e.g., in Eq. (10). Note that in the limit case $\kappa \to 0$, the solution (A29) correctly reduces to the free-particle solution (10).

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