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Multidimensional wave packet motion in quadratic potentials with and without friction: oscillation and barrier penetration

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Abstract. We study the motion of N-dimensional wave packets in quadratic potentials without friction and also under the influence of two different quantum frictional potentials. Differential equations for the coordinate and momentum uncertainties and for the correlations are presented and solutions for oscillatory motion and barrier penetration are given where possible. The barrier penetration probabilities are compared with each other.

1. Introduction

Ehrenfest's theorem holds rigorously if at most quadratic potentials are involved, i.e.

$$\langle \boldsymbol{x} \rangle = \bar{\boldsymbol{x}}, \tag{1.1a}$$

$$\langle \boldsymbol{p} \rangle = \bar{\boldsymbol{p}}, \tag{1.1b}$$

where here, and in the following, a bar denotes a classical quantity and angular brackets are expectation values. The centres of such quantum mechanical wave packets, hence, travel along classical trajectories which are solutions of Newton's equation of motion,

$$\dot{\bar{\boldsymbol{p}}} + \boldsymbol{\nabla} \bar{V} = 0, \tag{1.2}$$

provided that the potential has the form

$$\bar{V} = \tfrac{1}{2}\bar{\boldsymbol{x}}\mathbf{k}\bar{\boldsymbol{x}} + \boldsymbol{g}\mathbf{m}\bar{\boldsymbol{x}}. \tag{1.3}$$

Here, $\mathbf{k}$ is the symmetric stiffness matrix, $\mathbf{m}$ the symmetric matrix of inertia and $\boldsymbol{g}$ the vector of constant acceleration. The elements of $\mathbf{k}$, $\mathbf{m}$ and $\boldsymbol{g}$ do not depend on the coordinates or momenta and, except that $\mathbf{m}$ is positive definite and that the inverses of $\mathbf{k}$ and $\mathbf{m}$ exist, there are no other constraints superimposed. The solutions thus include cases where one or more eigenvalues of the stiffness matrix are negative, i.e. the motion on an inverted parabola or, more generally, in a multidimensional saddle-point surface. This corresponds quantum mechanically to the penetration of a quadratic barrier giving rise to the unfamiliar phenomenon that a Gaussian *wave packet* attacking a quadratic barrier does not split up into reflected and transmitted wave packets but rather stays Gaussian in shape and spreads in time (cf Weiner and Partom 1969 in one dimension and Weiner and Partom 1970 in several dimensions).

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This is in contrast to the penetration of *waves* through the same barrier or saddle surface (cf Hill and Wheeler 1953 in one and several dimensions).

It is one aim of this paper to give differential equations and their solutions for the time evolution of the coordinate and momentum spreading of wave packets in arbitrary quadratic potentials by using matrix notation. The other aim is to include frictional effects by considering instead of equation (1.2) the linearly damped equation of motion

$$\dot{\bar{\boldsymbol{p}}} + \mathbf{k}\bar{\boldsymbol{x}} + \mathbf{m}\boldsymbol{g} + \boldsymbol{\gamma}\bar{\boldsymbol{p}} = \mathbf{0}, \tag{1.4}$$

where the conservative potential (1.3) has already been employed and $\boldsymbol{\gamma}$ is the positive definite symmetric matrix of friction constants whose inverse need not necessarily exist. The classical time rate of change of the energy dissipation is then given by

$$\dot{\bar{E}} = -\tfrac{1}{2}\bar{\boldsymbol{p}}\mathbf{n}\boldsymbol{\gamma}\bar{\boldsymbol{p}}, \tag{1.5}$$

where $\mathbf{n} = \mathbf{m}^{-1}$ and the energy has been defined as potential energy (1.3) plus kinetic energy

$$\bar{T} = \tfrac{1}{2}\bar{\boldsymbol{p}}\mathbf{n}\bar{\boldsymbol{p}}. \tag{1.6}$$

Such linearly damped systems were recently taken into consideration in nuclear physics, for instance for the explanation of deep-inelastic heavy-ion scattering experiments or fission phenomena (for a review cf Hasse 1978). They are also of interest for models of Brownian motion in rate theories for solids (cf Weiner and Forman 1974). Their quantum mechanical counterparts, however, are not uniquely defined because non-conservative systems do not fit into the usual Hamilton formalism. Apart from the *linear* but explicitly time-dependent Hamiltonian of Kanai (1948) whose solutions conflict with the uncertainty principle (cf the discussion in Hasse 1975), yet two *non-linear* and Hermitean frictional potentials, W, are known which reproduce equation (1.4) in the Ehrenfest limit. The Hamiltonian, hence, reads

$$H = T + V + W, \tag{1.7}$$

with T and V as in equations (1.3) and (1.6) and $\bar{\boldsymbol{x}}$ replaced by $\boldsymbol{x}$ and $\bar{\boldsymbol{p}}$ by $\boldsymbol{p} = -\mathrm{i}\hbar\boldsymbol{\nabla}$. In the term W_{K}, due to Kostin (1972), the quantum analogue to the classical velocity is the hydrodynamic fluid velocity, i.e. the gradient of the phase of the wavefunction, giving rise to

$$W_{\mathrm{K}} = -\tfrac{1}{2}\mathrm{i}\hbar\gamma\left[\ln\left(\frac{\psi}{\psi^*}\right) - \left\langle\ln\left(\frac{\psi}{\psi^*}\right)\right\rangle\right]. \tag{1.8}$$

Since W_{K} is not of the form of a scalar product, it cannot be generalised to non-isotropic friction in more dimensions (γ is a scalar). The other term considered, the general frictional potential W_{G}, whose functional form is due to Süssmann (1973), cf also Albrecht (1975), Hasse (1975) and Kostin (1975), is based on the supposition that the quantum analogue to the classical momentum is the momentum operator. This friction potential reads

$$W_{\mathrm{G}} = \gamma\left[\langle p\rangle(x - \langle x\rangle) + \tfrac{1}{2}c[x - \langle x\rangle, p - \langle p\rangle]_+\right] \tag{1.9a}$$

in one dimension. Here $[\ ,\ ]_+$ is the anticommutator and c is an arbitrary real constant which does not enter in the classical equation of motion but rather allows for fluctuations. Its generalisation to more degrees of freedom and anisotropic friction is straightforward. Employing equation (1.1) here and in what follows, which is still valid under friction for quadratic potentials, equation (1.9*a*) becomes

$$W_G = \bar{p}\gamma(x-\bar{x}) + \tfrac{1}{2}c[(x-\bar{x})\gamma(p-\bar{p}) + (p-\bar{p})\gamma(x-\bar{x})]$$
$$= (x-\bar{x})\gamma[cp + (1-c)\bar{p}] - \tfrac{1}{2}\mathrm{i}\hbar c\,\mathrm{Tr}(\gamma). \qquad (1.9b)$$

In § 2 we will be concerned with the spreading of multidimensional wave packets under the action of the general frictional potential. Analogous results with Kostin's friction will be given in § 3 and solutions for both types of frictional potentials are presented in § 4.

2. General frictional potential

The mean square deviations of the expectation values of the coordinates and momenta and their correlations are defined by† (cf Messiah 1964 for the one-dimensional case)

$$\chi = \langle x \circ x\rangle - \bar{x}\circ\bar{x} \qquad (2.1a)$$

$$\phi = \langle p \circ p\rangle - \bar{p}\circ\bar{p} \qquad (2.1b)$$

$$\sigma = \langle x \circ p\rangle - \bar{x}\circ\bar{p} - \tfrac{1}{2}\mathrm{i}\hbar\mathbf{1}. \qquad (2.1c)$$

The matrices χ and ϕ are real and symmetric by definition, whereas σ is not symmetric. By virtue of the commutation relations,

$$p\circ x - \widetilde{x\circ p} = -\mathrm{i}\hbar\mathbf{1}, \qquad (2.2)$$

however, σ is real and its transpose is given by

$$\tilde{\sigma} = \langle p\circ x\rangle - \bar{p}\circ\bar{x} + \tfrac{1}{2}\mathrm{i}\hbar\mathbf{1}. \qquad (2.1d)$$

In the next subsections differential equations are established for these three functions of time under the action of the time-dependent Schrödinger equation with the frictional potential (1.9*b*).

2.1. *General wave packets*

Without particular knowledge of the solution of the Schrödinger equation the evolution in time of the position and momentum uncertainties and their correlations is obtained by use of the equation of motion of operator expectation values:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\mathbf{A}\rangle = \left\langle\frac{\partial\mathbf{A}}{\partial t}\right\rangle - \frac{\mathrm{i}}{\hbar}\langle[\mathbf{A}, H]\rangle. \qquad (2.3)$$

Employing for $\mathbf{A}$ the operators $x\circ x$, $p\circ p$ and $x\circ p$, respectively, one gets

$$\dot{\chi} = \sigma\mathbf{n} + \mathbf{n}\tilde{\sigma} + \gamma'\chi + \chi\gamma' \qquad (2.4a)$$

$$-\dot{\phi} = \mathbf{k}\sigma + \tilde{\sigma}\mathbf{k} + \gamma'\phi + \phi\gamma' \qquad (2.4b)$$

$$\dot{\sigma} = \mathbf{n}\phi - \chi\mathbf{k} + \gamma'\sigma - \sigma\gamma'. \qquad (2.4c)$$

† Notation: The tensor product, $\mathbf{A} = a\circ b$, is defined by $A_{ij} = a_i b_j$. Transposition is indicated by $\tilde{\mathbf{A}}$ with $\tilde{A}_{ij} = A_{ji}$. The unit matrix with elements δ_{ij} is denoted by $\mathbf{1}$.

Here only the combination $\boldsymbol{\gamma}' = c\boldsymbol{\gamma}$ enters which means that in the special case $c = 0$ (Albrecht 1975) wave packets spread at the same rate as in the undamped case although their centres travel along damped classical trajectories. Secondly, the constant acceleration, $\boldsymbol{g}$, does not enter at all.

This set of coupled matrix differential equations can be simplified in two cases. If $\boldsymbol{\gamma} = \mathbf{0}$ or $c = 0$ one obtains

$$\overset{\bullet}{\boldsymbol{\chi}} + 2(\boldsymbol{\omega}^2\ddot{\boldsymbol{\chi}} + \ddot{\boldsymbol{\chi}}\tilde{\boldsymbol{\omega}}^2) + (\boldsymbol{\omega}^4\boldsymbol{\chi} - 2\boldsymbol{\omega}^2\boldsymbol{\chi}\tilde{\boldsymbol{\omega}}^2 + \boldsymbol{\chi}\tilde{\boldsymbol{\omega}}^4) = \mathbf{0}, \tag{2.5}$$

where $\boldsymbol{\omega}^2 = \mathbf{nk}$ is the square of the frequency matrix. Furthermore, the one-dimensional case with friction obeys

$$\dddot{\chi} + 4(\omega^2 - \gamma'^2)\dot{\chi} = 0. \tag{2.6}$$

2.2. Gaussian wave packets

The differential equations (2.4) contain solutions which do not obey the Heisenberg uncertainty equation,

$$\chi_{ii}\phi_{ii} \geqslant \tfrac{1}{4}\hbar^2. \tag{2.7}$$

For this reason and for the sake of simplicity it is advantageous to restrict oneself to Gaussian wave packet solutions. If the N-dimensional complex but symmetric width matrix $\boldsymbol{\alpha}$ is employed, we have

$$\psi(\boldsymbol{x}, t) = N(t)\exp\left[-\frac{1}{2}(\boldsymbol{x} - \bar{\boldsymbol{x}})\boldsymbol{\alpha}^{-1}(\boldsymbol{x} - \bar{\boldsymbol{x}}) + \frac{i}{\hbar}(\bar{\boldsymbol{p}}(\boldsymbol{x} - \bar{\boldsymbol{x}}) + \theta(t))\right], \tag{2.8}$$

where the normalisation function is

$$N(t) = \left(\frac{2\det(\mathrm{Re}(\boldsymbol{\alpha}^{-1}))}{(2\pi)^N}\right)^{1/4}. \tag{2.9}$$

The time-dependent phase $\theta(t)$ and also $\boldsymbol{\alpha}(t)$ are determined from the Schrödinger equation,

$$\dot{\boldsymbol{\alpha}} = \mathrm{i}\hbar\mathbf{n} - \frac{\mathrm{i}}{\hbar}\boldsymbol{\alpha}\mathbf{k}\boldsymbol{\alpha} + \boldsymbol{\alpha}\boldsymbol{\gamma}' + \boldsymbol{\gamma}'\boldsymbol{\alpha}, \tag{2.10a}$$

$$\dot{\theta} = \bar{L} - \tfrac{1}{4}\hbar^2\,\mathrm{Tr}(\mathbf{n}\boldsymbol{\chi}^{-1}), \tag{2.10b}$$

where $\bar{L} = \bar{T} - \bar{V}$ is the classical Lagrangian. The wave packet's position, momentum and correlation uncertainty are related to $\boldsymbol{\alpha}$ as follows,

$$\boldsymbol{\chi} = \tfrac{1}{2}(\mathrm{Re}(\boldsymbol{\alpha}^{-1}))^{-1} \tag{2.11a}$$

$$\boldsymbol{\phi} = \tfrac{1}{2}\hbar^2(\mathrm{Re}(\boldsymbol{\alpha}))^{-1} \tag{2.11b}$$

$$\boldsymbol{\sigma} = \tfrac{1}{2}\hbar\,\mathrm{Im}(\boldsymbol{\alpha})(\mathrm{Re}(\boldsymbol{\alpha}))^{-1}, \tag{2.11c}$$

from which one obtains immediately the condition which restricts general solutions to Gaussians,

$$\boldsymbol{\chi}\boldsymbol{\phi} = \boldsymbol{\sigma}^2 + \tfrac{1}{4}\hbar^2\mathbf{1}. \tag{2.12}$$

If equation (2.12) is employed, the linear fourth-order differential equation for the one-dimensional case reduces to the second-order non-linear equation

$$2\chi\ddot{\chi}-\dot{\chi}^2+4(\omega^2-\gamma'^2)\chi^2=\hbar^2/m^2. \tag{2.13}$$

On the other hand, if $\boldsymbol{\alpha}$ is split up into real and imaginary parts according to

$$\boldsymbol{\alpha}^{-1}=\tfrac{1}{2}\boldsymbol{\chi}^{-1}-\frac{\mathrm{i}}{\hbar}\boldsymbol{\beta}, \tag{2.14}$$

so that $\boldsymbol{\beta}^{-1}$ has the meaning of the width of the phase of the wave packet, equation (2.10a) becomes identical to the coupled set of equations

$$\dot{\boldsymbol{\chi}}=\mathbf{n}\boldsymbol{\beta}\boldsymbol{\chi}+\boldsymbol{\chi}\boldsymbol{\beta}\mathbf{n}+\boldsymbol{\gamma}'\boldsymbol{\chi}+\boldsymbol{\chi}\boldsymbol{\gamma}', \tag{2.15a}$$

$$\boldsymbol{\beta}+\boldsymbol{\beta}\mathbf{n}\boldsymbol{\beta}+\mathbf{k}+\boldsymbol{\gamma}'\boldsymbol{\beta}+\boldsymbol{\beta}\boldsymbol{\gamma}'=\tfrac{1}{4}\hbar^2\boldsymbol{\chi}^{-1}\mathbf{n}\boldsymbol{\chi}^{-1}. \tag{2.15b}$$

The quantity $\boldsymbol{\beta}$ is related to the other functions according to

$$\boldsymbol{\sigma}=\boldsymbol{\chi}\boldsymbol{\beta} \tag{2.16a}$$

$$\boldsymbol{\phi}=\tfrac{1}{4}\hbar^2\boldsymbol{\chi}^{-1}+\boldsymbol{\beta}\boldsymbol{\chi}\boldsymbol{\beta}. \tag{2.16b}$$

Unfortunately, $\boldsymbol{\beta}$ cannot be eliminated from (2.15) to yield a matrix equation of the form (2.13).

3. Kostin's frictional potential

The functions $\boldsymbol{\chi}$, $\boldsymbol{\phi}$ and $\boldsymbol{\sigma}$ are not sufficient to determine a set of matrix equations like equation (2.4) for arbitrary wave packets under the influence of Kostin's friction, equation (1.8), because the expectation value of the second derivative of the phase cannot in general be expressed by them. For Gaussian wave packets with their simple phases, however, one obtains, with the same procedure as indicated above,

$$\dot{\boldsymbol{\chi}}=\boldsymbol{\sigma}\mathbf{n}+\mathbf{n}\tilde{\boldsymbol{\sigma}} \tag{3.1a}$$

$$-\dot{\boldsymbol{\phi}}=\mathbf{k}\boldsymbol{\sigma}+\tilde{\boldsymbol{\sigma}}\mathbf{k}+2\gamma(\boldsymbol{\phi}-\tfrac{1}{4}\hbar^2\boldsymbol{\chi}^{-1}) \tag{3.1b}$$

$$\dot{\boldsymbol{\sigma}}=\mathbf{n}\boldsymbol{\phi}-\boldsymbol{\chi}\mathbf{k}-\gamma\boldsymbol{\sigma}. \tag{3.1c}$$

Similarly, the equivalent to equation (2.10) is

$$\dot{\boldsymbol{\alpha}}=\mathrm{i}\hbar\mathbf{n}-\frac{\mathrm{i}}{\hbar}\boldsymbol{\alpha}\mathbf{k}\boldsymbol{\alpha}+\mathrm{i}\gamma\boldsymbol{\alpha}\,\mathrm{Im}(\boldsymbol{\alpha}^{-1})\boldsymbol{\alpha} \tag{3.2a}$$

$$\dot{\theta}=\bar{L}-\mathrm{Tr}(\tfrac{1}{4}\hbar^2\mathbf{n}\boldsymbol{\chi}^{-1}-\tfrac{1}{2}\gamma\mathbf{n}^{-1}\dot{\boldsymbol{\chi}}), \tag{3.2b}$$

and the one equivalent to equation (2.15) is

$$\dot{\boldsymbol{\chi}}=\mathbf{n}\boldsymbol{\beta}\boldsymbol{\chi}+\boldsymbol{\chi}\boldsymbol{\beta}\mathbf{n} \tag{3.3a}$$

$$\dot{\boldsymbol{\beta}}+\boldsymbol{\beta}\mathbf{n}\boldsymbol{\beta}+\mathbf{k}+\gamma\boldsymbol{\beta}=\tfrac{1}{4}\hbar^2\boldsymbol{\chi}^{-1}\mathbf{n}\boldsymbol{\chi}^{-1}. \tag{3.3b}$$

Finally, the one-dimensional case obeys the non-linear differential equation similar to equation (2.13),

$$2\chi\ddot{\chi}-\dot{\chi}^2+4\omega^2\chi^2+2\gamma\chi\dot{\chi}=\hbar^2/m^2. \tag{3.4}$$

4. Solutions

The inertias, stiffnesses and friction constants are in general non-isotropic, i.e. non-diagonal with respect to the coordinates $\bar{x}$. However, if the linear frictional force is proportional to the mass (as well as to the velocity), the same transformation which diagonalises the inertia and the stiffness matrix also diagonalises the friction matrix (Goldstein 1959). The form (1.4) of the classical equations of motion suggests therefore already that $\mathbf{k}$, $\mathbf{m}$ and $\boldsymbol{\gamma}$ are diagonal. On the other hand, if the components of $\bar{x}$ are regarded as generalised coordinates, they will usually be chosen in such a way that the equations of motion are decoupled. In the following we will therefore assume with a slight loss of generality that $\mathbf{k}$, $\mathbf{m}$ and $\boldsymbol{\gamma}$ and, hence, also $\mathbf{n}$ and $\boldsymbol{\omega}^2$ are diagonal with elements k_i, m_i, γ_i, n_i and ω_i^2, respectively. Furthermore, since the linear force $\mathbf{m}\boldsymbol{g}$ does not enter in the spreading of the wave packets, it is omitted completely.

4.1. *General friction, N-dimensional Gaussian wave packets*

The set of real linear differential equations (2.4) together with the condition (2.12) is equivalent to the complex non-linear differential equation (2.10*a*). Since (2.4) has only exponential (or oscillatory) solutions, those of equation (2.10*a*) therefore must be of the same functional form. The condition (2.12), hence, although valid for all times, restricts only the initial conditions to certain values. As a consequence, in order to find the Gaussian wave packet solutions, it suffices to find the solutions of the simpler set (2.4) and then to employ (2.12) at $t = 0$.

Under these conditions, equation (2.4) becomes

$$\dot{\chi}_{ij} = n_j\sigma_{ij} + n_i\sigma_{ji} + (\gamma_i' + \gamma_j')\chi_{ij} \tag{4.1a}$$

$$-\dot{\phi}_{ij} = k_i\sigma_{ij} + k_j\sigma_{ji} + (\gamma_i' + \gamma_j')\phi_{ij} \tag{4.1b}$$

$$\dot{\sigma}_{ij} = n_i\phi_{ij} - k_j\chi_{ij} + (\gamma_i' - \gamma_j')\sigma_{ij}. \tag{4.1c}$$

By making *ansatzes* of harmonic time dependences for the quantities χ_{ij}, ϕ_{ij}, σ_{ij} one obtains immediately the eigenfrequencies $\pm(\nu_i' \pm \nu_j')$, where

$$\nu_i' = (\omega_i^2 - \gamma_i'^2)^{1/2}. \tag{4.2}$$

However, if one of the stiffnesses is negative, i.e. if one ω_i^2 is negative, we shall employ the notation

$$\mu_i' = (\omega_i^2 + \gamma_i'^2)^{1/2} \tag{4.3}$$

so that in all subsequent formulae, ν_i' is to be replaced by $\mathrm{i}\mu_i'$.

As concerns the initial conditions, equation (2.12) and its derivative with respect to time connect $\boldsymbol{\phi}(0)$ and $\dot{\boldsymbol{\phi}}(0)$ to $\boldsymbol{\chi}(0)$ and $\dot{\boldsymbol{\chi}}(0)$, so that the only free parameters are $\boldsymbol{\chi}(0)$ and $\dot{\boldsymbol{\chi}}(0)$. Among these, only two cases are of physical interest: (i) the wave packet has no initial spreading velocity, i.e. $\dot{\boldsymbol{\chi}}(0) = \mathbf{0}$; and (ii) the wave packet has an initial minimum uncertainty product, i.e. $\boldsymbol{\chi}(0)\boldsymbol{\phi}(0) = \frac{1}{4}\hbar^2\mathbf{1}$. The latter condition, in turn, means $\boldsymbol{\sigma}(0) = \mathbf{0}$ by equation (2.12) and, consequently, $\dot{\boldsymbol{\chi}}(0) = \boldsymbol{\gamma}'\boldsymbol{\chi}(0) + \boldsymbol{\chi}(0)\boldsymbol{\gamma}'$ by equation (2.4*a*),

$$\text{(i)} \qquad \chi_{ij}(0) = \chi_{ij}^0, \qquad \dot{\chi}_{ij}(0) = 0 \tag{4.4a}$$

$$\text{(ii)} \qquad \chi_{ij}(0) = \chi_{ij}^0, \qquad \dot{\chi}_{ij}(0) = (\gamma_i' + \gamma_j')\chi_{ij}^0. \tag{4.4b}$$

Note that (i) and (ii) become equivalent if $\boldsymbol{\gamma}' = \mathbf{0}$, i.e. if there is no damping or if $c = 0$. The full solutions with the set (i) of initial conditions now read

$$\chi_{ij} = \chi_{ij}^0 \cos(\nu_i' t)\cos(\nu_j' t) + \phi_{ij}^0 \frac{n_i n_j}{\nu_i' \nu_j'} \sin(\nu_i' t)\sin(\nu_j' t) \tag{4.5a}$$

$$\phi_{ij} = \chi_{ij}^0 \frac{\nu_i' \nu_j'}{n_i n_j}\left(\sin(\nu_i' t) + \frac{\gamma_i'}{\nu_i'}\cos(\nu_i' t)\right)\left(\sin(\nu_j' t) + \frac{\gamma_j'}{\nu_j'}\cos(\nu_j' t)\right)$$
$$+ \phi_{ij}^0\left(\cos(\nu_i' t) - \frac{\gamma_i'}{\nu_i'}\sin(\nu_i' t)\right)\left(\cos(\nu_j' t) - \frac{\gamma_j'}{\nu_j'}\sin(\nu_j' t)\right) \tag{4.5b}$$

$$\sigma_{ij} = -\chi_{ij}^0 \frac{\nu_j'}{n_j}\cos(\nu_i' t)\left(\sin(\nu_j' t) + \frac{\gamma_j'}{\nu_j'}\cos(\nu_j' t)\right) + \phi_{ij}^0 \frac{n_i}{\nu_i'}\sin(\nu_i' t)\left(\cos(\nu_j' t) - \frac{\gamma_j'}{\nu_j'}\sin(\nu_j' t)\right), \tag{4.5c}$$

where the condition (2.12) at $t = 0$ demands $\boldsymbol{\phi}^0 \neq \boldsymbol{\phi}(0)$ but $\boldsymbol{\chi}^0 \boldsymbol{\phi}^0 = \frac{1}{4}\hbar^2 \mathbf{1}$, i.e.

$$\phi_{ij}^0 = \tfrac{1}{4}\hbar^2 (\chi_{ij}^0)^{-1}. \tag{4.6}$$

The solutions (4.5) contain an interesting special case well known from undamped oscillatory motion, namely if

$$\chi_{ij}^0 = \frac{1}{2}\hbar \frac{n_i}{\nu_i'}\delta_{ij}, \tag{4.7}$$

then the inverse matrix elements become equal to the reciprocal elements and all functions stay diagonal and constant in time,

$$\chi_{ij} = \frac{1}{2}\hbar \frac{n_i}{\nu_i'}\delta_{ij}, \qquad \phi_{ij} = \frac{1}{2}\hbar \frac{\omega_i^2}{n_i \nu_i'}\delta_{ij}, \qquad \sigma_{ij} = -\frac{1}{2}\hbar \frac{\gamma_i'}{\nu_i'}\delta_{ij}. \tag{4.8}$$

Equation (4.7), however, can only be fulfilled for oscillatory motion, because otherwise χ_{ij}^0 would become imaginary. On the other hand, employing the set (ii) of initial conditions yields the solutions

$$\chi_{ij} = \chi_{ij}^0\left(\cos(\nu_i' t) + \frac{\gamma_i'}{\nu_i'}\sin(\nu_i' t)\right)\left(\cos(\nu_j' t) + \frac{\gamma_j'}{\nu_j'}\sin(\nu_j' t)\right) + \phi_{ij}^0 \frac{n_i n_j}{\nu_i' \nu_j'}\sin(\nu_i' t)\sin(\nu_j' t) \tag{4.9a}$$

$$\phi_{ij} = \chi_{ij}^0 \frac{k_i k_j}{\nu_i' \nu_j'}\sin(\nu_i' t)\sin(\nu_j' t) + \phi_{ij}^0\left(\cos(\nu_i' t) - \frac{\gamma_i'}{\nu_i'}\sin(\nu_i' t)\right)\left(\cos(\nu_j' t) - \frac{\gamma_j'}{\nu_j'}\sin(\nu_j' t)\right) \tag{4.9b}$$

$$\sigma_{ij} = -\chi_{ij}^0 \frac{k_j}{\nu_j'}\left(\cos(\nu_i' t) + \frac{\gamma_i'}{\nu_i'}\sin(\nu_i' t)\right)\sin(\nu_j' t) + \phi_{ij}^0 \frac{n_i}{\nu_i'}\sin(\nu_i' t)\left(\cos(\nu_j' t) - \frac{\gamma_j'}{\nu_j'}\sin(\nu_j' t)\right). \tag{4.9c}$$

4.2. General friction, barrier penetration

The probability of barrier penetration as defined and evaluated in the appendix depends only upon the classical motion of the centre and the spreading of the wave packet in the direction of the barrier. We can therefore drop the subscripts 1 and 1, 1 and write

$$P(t) = \tfrac{1}{2}\,\mathrm{erfc}[-\bar{x}(t)/(2\chi(t))^{1/2}]. \tag{4.10}$$

The classical motion, $\bar{x}(t)$, is the solution of equation (1.4),

$$\bar{x}(t)=\left(\bar{x}^0\cosh(\mu t)+\frac{\dot{\bar{x}}^0+\frac{1}{2}\gamma\bar{x}^0}{\mu}\sinh(\mu t)\right)e^{\frac{1}{2}\gamma t}, \tag{4.11}$$

where $\mu=(\omega^2+\gamma^2/4)^{1/2}$ and $\omega^2=-k/m>0$, and the one-dimensional spreading law with the set (i) of initial conditions,

$$\chi(t)=\chi^0\cosh^2(\mu' t)+\frac{\hbar^2}{4m^2\mu'^2\chi^0}\sinh^2(\mu' t), \tag{4.12}$$

where $\mu'=(\omega^2+c^2\gamma^2)^{1/2}$, results from equations (4.5*a*) with (4.6).

In the limit of large times, the argument of the error function becomes proportional to

$$\exp(\mu-\mu'-\tfrac{1}{2}\gamma)t, \tag{4.13}$$

which tends to zero for both of the physically relevant cases $c=0$ (Albrecht 1975) and $c=\frac{1}{2}$ (Hasse 1975). Thus $P(t)\to\frac{1}{2}$ and the wave packet spreads faster over all space than its centre moves.

If friction is absent, however, the expression (4.13) is equal to unity, which results in a finite value of the argument of the error function and the asymptotic value of the barrier penetrability (cf Weiner and Partom 1969),

$$P(t)\to\frac{1}{2}\operatorname{erfc}\left(-\frac{\omega\bar{x}^0+\dot{\bar{x}}^0}{\omega(2\chi^0+\hbar^2/2m^2\omega^2\chi^0)^{1/2}}\right). \tag{4.14}$$

The existence of this finite value hinges on the fact that the wave packet moves asymptotically with the same law as it spreads.

4.3. *Kostin friction, barrier penetration*

Except for the trivial constants

$$\chi_{ij}=\frac{1}{2}\hbar\frac{n_i}{\omega_i}\delta_{ij},\qquad \phi_{ij}=\frac{1}{2}\hbar\frac{\omega_i}{n_i}\delta_{ij},\qquad \sigma_{ij}=0 \tag{4.15}$$

if oscillatory motion is concerned, no elementary solutions of the differential equations (3.1) through (3.4) are known. For barrier penetration, however, the asymptotic form

$$\chi(t)\propto e^{(2\mu-\gamma)t} \tag{4.16}$$

is easily obtained from (3.4) by replacing ω^2 by $-\omega^2$ and setting the right-hand side equal to zero. Thus $(2\chi(t))^{1/2}$ obeys asymptotically the same law as $\bar{x}(t)$ and $P(\infty)$ will assume a definite value other than $\frac{1}{2}$. The constant of proportionality in (4.16) can only be determined approximately. Weiner and Forman (1974), for example, rewrite equation (3.4) in such a way that the linear portion of it with the correct asymptotic behaviour equals a right-hand side which is then replaced by its initial value. With the set (i) of initial conditions we get

$$\ddot{\chi}-4\omega^2\chi+2\gamma\dot{\chi}=\frac{\hbar^2}{2m^2\chi}+\frac{\dot{\chi}^2}{2\chi}+\gamma\dot{\chi}-2\omega^2\chi\approx\frac{\hbar^2}{2m^2\chi^0}-2\omega^2\chi^0. \tag{4.17}$$

This has the solution

$$4\chi(t) \approx \left(2\chi^0 - \frac{\hbar^2}{2m^2\omega^2\chi^0}\right) + \left(2\chi^0 + \frac{\hbar^2}{2m^2\omega^2\chi^0}\right)\left(\cosh(2\mu t) + \frac{\gamma}{2\mu}\sinh(2\mu t)\right) e^{-\gamma t}, \tag{4.18}$$

and the asymptotic probability of barrier penetration becomes

$$P(t) \to \frac{1}{2}\,\mathrm{erfc}\left(-\frac{(\mu + \frac{1}{2}\gamma)\bar{x}^0 + \dot{\bar{x}}^0}{[\mu(\mu + \frac{1}{2}\gamma)(2\chi^0 + \hbar^2/2m^2\omega^2\chi^0)]^{1/2}}\right). \tag{4.19}$$

Another approximate solution results from replacing the disturbing linear first derivative with respect to time by its asymptotic value,

$$2\chi\ddot{\chi} - \dot{\chi}^2 - (2\mu - \gamma)^2\chi^2 = \hbar^2/m^2. \tag{4.20}$$

Then we get the solution

$$4\chi(t) \approx \left(2\chi^0 - \frac{\hbar^2}{2m^2(\mu - \frac{1}{2}\gamma)^2\chi^0}\right) + \left(2\chi^0 + \frac{\hbar^2}{2m^2(\mu - \frac{1}{2}\gamma)^2\chi^0}\right)\cosh[(2\mu - \gamma)t], \tag{4.21}$$

leading to

$$P(t) \to \frac{1}{2}\,\mathrm{erfc}\left(-\frac{(\mu + \frac{1}{2}\gamma)\bar{x}^0 + \dot{\bar{x}}^0}{\mu[2\chi^0 + \hbar^2/2m^2(\mu - \frac{1}{2}\gamma)^2\chi^0]^{1/2}}\right). \tag{4.22}$$

A comparison of the two different results of the time-dependent probability of barrier penetration, equation (4.10) with (4.11) and (4.18), (4.21), and an exact numerical solution is provided in figure 1. The arbitrary units of time and length are T and L, respectively, and the constants involved are chosen as $\bar{x}^0 = -4L$, $2\chi^0 = L^2$, $\omega = 1/T$, $\gamma = 0{\cdot}3/T$, $\hbar/m = L^2/T$ and part (a) corresponds to the initial condition $\dot{\bar{x}} = 0$, whereas part (b) corresponds to $\dot{\bar{x}}^0 = 3L/T$. In both cases a slight improvement is achieved by use of equation (4.21) instead of equation (4.18) of Weiner and

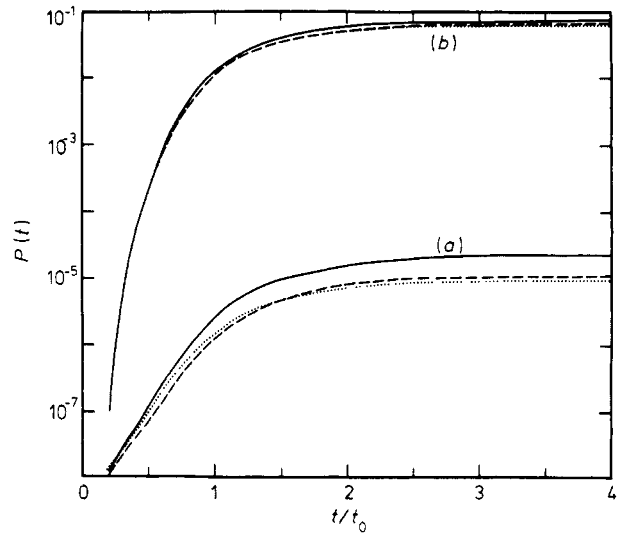

Figure 1. The time-dependent probability of barrier penetration under Kostin's friction for two different initial conditions. See text for units and constants. Full curve, exact numerical solution; broken curve, Hasse equation (4.21); dotted curve, Weiner and Forman equation (4.18).

Forman (1974). The difference becomes relatively larger the smaller the penetrability is. Using the property that $\mathrm{erfc}(x) \propto x$ for small arguments, the ratio of (4.22) to (4.19) becomes $(1+\gamma/2\mu)^{1/2}$ which amounts to 7% for the above given parameters.

5. Summary

We have formulated in general the motion and the spreading of wave packets in quadratic potentials by establishing coupled differential equations in time for the position and momentum uncertainties and the correlation between them. Arbitrary as well as Gaussian wave packets were considered in oscillator and inverted oscillator potentials. Linear potentials are also included, but they do not influence the spreading. Special emphasis has been put on the use of frictional Schrödinger equations although the frictionless case is also included. Thereby two different quantum frictional potentials were employed, namely the fluid dynamical analogue of Kostin (1972) and the general frictional potential which was initiated by Süssmann (1973).

In particular, analytic solutions of the evolution in time of the wave packets and of the barrier penetrability are given if the wave packets are under the influence of the general frictional potential. Here the barrier penetrability tends asymptotically towards $\frac{1}{2}$ except for the case that friction is absent. On the other hand, if Kostin's frictional potential is employed, the differential equations have no solutions in closed form, but an improved asymptotic value of the barrier penetrability is derived which is then compared with a numerical solution and with another approximation of Weiner and Forman (1974). This value is in general different from $\frac{1}{2}$ which is a consequence of the fact that such wave packets spread in time with the same law as their centres move. From these results, however, one cannot draw a conclusion whether one or the other frictional potential is physically more relevant because in physics only piecewise inverted quadratic potentials are realised and, hence, the asymptotic values of the barrier penetration probabilities are never attained.

As applications of these frictional Hamiltonians and of the formalism and results presented in this paper we primarily mention nuclear deep-inelastic heavy-ion reactions and nuclear fission where energy is transferred from the collective motion into the intrinsic degrees of freedom (cf Hasse 1978). Similarly in molecular physics, theories of non-adiabatic molecular collisions (Tully and Preston 1971) and in solid state physics, models of Brownian motion for rate theories in solids (Weiner and Forman 1974) can be modified by including quantum friction. Also Brownian motion and transport phenomena in general (Kostin 1972) are interesting subjects of investigation.

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I should like to thank Dr J H Weiner for bringing his work to my attention.

Appendix. The barrier penetration formula

The time-dependent barrier penetration probability, $P(t)$, is defined as the fraction of the wave packet's squared amplitude which is beyond the barrier's top. Let x_1 be the direction of the barrier and the top be located at $x_1 = 0$, then

$$P(t) = \int_0^\infty dx_1 \int_{-\infty}^{+\infty} dx_2 \cdots \int_{-\infty}^{+\infty} dx_N |\psi(x_1, \ldots, x_N)|^2. \tag{A.1}$$

Using Gaussian wave packets and the transformation $y_i = x_i - \bar{x}_i$, $i = 1, \ldots, N$, this reduces to

$$P(t) = (2\pi)^{-N/2}(\det(\boldsymbol{\eta}))^{1/2} \int_{-\bar{x}_1}^\infty dy_1 \int_{-\infty}^{+\infty} dy_2 \ldots \int_{-\infty}^{+\infty} dy_N \exp\Big(-\tfrac{1}{2}\sum_{ij} y_i \eta_{ij} y_j\Big), \tag{A.2}$$

where $\boldsymbol{\eta} = \boldsymbol{\chi}^{-1}$. Equation (A.2) is evaluated by employing another transformation, $z_\alpha = y_\alpha + f_\alpha$, where greek indices now run only over the oscillators, $\alpha = 2, \ldots, N$, and

$$f_\alpha = y_1 \sum_\beta \eta'^{-1}_{\alpha\beta} \eta_{1\beta}. \tag{A.3}$$

Here $\boldsymbol{\eta}'$ is the minor which is left over after erasing the first row and first column of $\boldsymbol{\eta}$. With the identity

$$\sum_{\alpha,\beta} y_\alpha \eta_{\alpha\beta} f_\beta = y_1 \sum_\alpha \eta_{1\alpha} y_\alpha \tag{A.4}$$

equation (A.2) becomes

$$P(t) = [(2\pi)^{-N} \det(\boldsymbol{\eta})]^{1/2} \int_{-\bar{x}_1}^\infty dy_1 \exp\Big[-\tfrac{1}{2}y_1^2\Big(\eta_{11} - \sum_{\alpha,\beta} \eta_{1\alpha}\eta'^{-1}_{\alpha\beta}\eta_{\beta 1}\Big)\Big]$$
$$\times \int_{+\infty}^{+\infty} dz_2 \ldots \int_{-\infty}^{+\infty} dz_N \exp\Big(-\tfrac{1}{2}\sum_{\alpha,\beta} z_\alpha \eta_{\alpha\beta} z_\beta\Big). \tag{A.5}$$

The second line of equation (A.5) is simply the normalisation of an $(N-1)$-dimensional Gaussian wave packet, $[(2\pi)^{N-1}/\det(\boldsymbol{\eta}')]^{1/2}$, so that equation (A.5) simplifies even further,

$$P(t) = [\det(\boldsymbol{\eta})/2\pi \det(\boldsymbol{\eta}')]^{1/2} \int_{-\bar{x}_1}^\infty dy_1 \exp\Big[-\tfrac{1}{2}y_1^2\Big(\eta_{11} - \sum_{\alpha,\beta} \eta_{1\alpha}\eta'^{-1}_{\alpha\beta}\eta_{\beta 1}\Big)\Big]. \tag{A.6}$$

Finally, the expression in the argument of (A.6) is just the ratio of the two determinants, which is given by

$$\eta_{11} - \sum_{\alpha,\beta} \eta_{1\alpha}\eta'^{-1}_{\alpha\beta}\eta_{\beta 1} = \det(\boldsymbol{\eta})/\det(\boldsymbol{\eta}') = 1/\eta^{-1}_{11} = 1/\chi_{11}. \tag{A.7}$$

The remaining integral,

$$P(t) = (2\pi\chi_{11})^{-1/2} \int_{-\bar{x}_1}^\infty dy_1 \exp(-y_1^2/2\chi_{11}), \tag{A.8}$$

can be evaluated by use of the associated error function,

$$P(t) = \tfrac{1}{2}\operatorname{erfc}[-\bar{x}_1/(2\chi_{11})^{1/2}] \tag{A.9}$$

a result quoted by Rice (1945).

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