EVOLUTION KERNELS FOR PHASE-SPACE DISTRIBUTIONS

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Different aspects of tunneling in the Wigner representation are studied. The evolution kernels for the Wigner function and for other phase-space distributions are considered and multidimensional tunneling is studied in the context of Fermi golden rule for transitions between potential surfaces. Marinov's path integral for the evolution kernel for the Wigner function is considered.

Contents

To the memory of Michael Marinov

Just a few years ago Prof. Michael Marinov was my teacher and D.Sc. advisor at the Technion, Israel Institute of Technology. We were a group of students, trying to understand the secrets of the universe, or at least of quantization, through many lectures, stimulating group meetings, seminars and — yes, hard work. Michael was a superb teacher much admired by all. He gave wonderful lectures on field theory, scattering theory, and quantum mechanics. I particularly remember his lectures on Grassmann algebra and on supersymmetry. This was a wonderland of truth and beauty. I shall always carry with me Michael's deep respect and admiration to nature and its laws which we try to understand through the adventure of science.

1 Introduction

In my work with Marinov we studied tunneling.[1-4] One object of our research was the evolution kernel of the Wigner function in one-dimensional potential scattering.[5] In my recent work I extended the treatment to other phase-space representations and to other physical conditions.[6,7] The Wigner function was used for various applications and many papers and reviews were written about it.[8-18] Traditionally, the similarity to classical distributions encouraged applications in semiclassical theories. Here, following my work with Marinov, I take a complementary view point emphasizing application of the Wigner representation to purely quantum effects with no classical counterpart. This work includes application to scattering, to wave-packet propagation, and to energy transfer processes within a single molecule including in particular nonclassical Frank-Condon factors and radiationless transitions in polyatomic molecules. What these different phenomena have in common is their nonclassical nature which is treated here within a phase-space Wigner function approach to tunneling.

Quantum propagators can be quite different from classical propagators. The classical equations of motion define classical trajectories in phase space for the coordinates, $q(t)$, and momenta, $p(t)$, as a function of the time t. The classical propagators for Liouville distributions in phase space are therefore δ functions over the classical trajectories defining a one-to-one mapping between single points of the initial and final distributions. In quantum mechanics, on the other hand, a single point of the phase-space distribution at one time can in principle be causally connected to many points of this phase-space distribution at another time. Furthermore, quantum propagators may include quantum jumps, sudden changes in the momentum or quick changes in the coordinate of the phase-space quasidistributions. Two points of the phase-space distribution at two different times can be causally connected even when no classical trajectory connects them. These essentially quantum features are the subject of this work.

2 Evolution kernel for the Wigner function

2.1 Propagators

A quantum state can be described by a wave function $\psi(q)$ or more generally by a density matrix $\hat{\rho}$ and its Weyl symbol — the Wigner function $\rho(q,p)$,

$$\rho(q,p) = \frac{1}{2\pi}\int \left\langle q+\frac{\eta}{2}\right| \hat{\rho} \left|q-\frac{\eta}{2}\right\rangle e^{-ip\eta} d\eta \; . \tag{1}$$

Here and in the following $\hbar = 1$ and all integrals run from $-\infty$ to ∞ unless otherwise specified. The evolution operator $\hat{U}(t) = \exp(-i\hat{H}t)$ gives the time evolution of the wave function $|\psi_t\rangle = \hat{U}(t)|\psi_0\rangle$ as well as that of the density operator $\hat{\rho}$: $\hat{\rho}_t = \hat{U}(t)\hat{\rho}_0\hat{U}^+(t)$. Propagators are defined to give this time evolution in some representation of the quantum state.

Feynman propagator, $\langle q|\hat{U}(t)|q_0\rangle$, gives the time evolution of the wave function in the coordinate representation

$$\psi_t(q) = \langle q|\psi_t\rangle = \int dq_0 \, \langle q|\hat{U}(t)|q_0\rangle\psi_0(q_0) \; , \tag{2}$$

and a similar propagator, $\langle p|\hat{U}(t)|p_0\rangle$, is defined in the momentum representation.

In an analogous way, the phase-space propagator $L_t(q,p;q_0,p_0)$ is defined to give the time evolution of the Wigner function,

$$\rho_t(x) = \int dx L_t(x,x_0)\rho_0(x_0) \; , \tag{3}$$

where $x \equiv (q,p)$.

The phase space propagator in terms of the propagators in the coordinate and in the momentum representations, respectively, is given by

$$\begin{aligned} &L_t(q,p;q_0,p_0) \qquad (4) \\ &= \frac{1}{2\pi}\int d\eta d\eta_0 e^{i(p\eta - p_0\eta_0)} \left\langle q-\frac{\eta}{2}|\hat{U}|q_0-\frac{\eta_0}{2}\right\rangle \left[\left\langle q+\frac{\eta}{2}|\hat{U}|q_0+\frac{\eta_0}{2}\right\rangle\right]^* \\ &= \frac{1}{2\pi}\int d\sigma d\sigma_0 e^{i(q\sigma - q_0\sigma_0)} \left\langle p+\frac{\sigma}{2}|\hat{U}|p_0+\frac{\sigma_0}{2}\right\rangle \left[\left\langle p-\frac{\sigma}{2}|\hat{U}|p_0-\frac{\sigma_0}{2}\right\rangle\right]^* . \end{aligned}$$

L is real and satisfies

$$\int dx L_t(x,x_0) = 1 = \int dx_0 L_t(x,x_0) ,$$
$$L_{t_1+t_2}(x,x_0) = \int dx' L_{t_2}(x,x') L_{t_1}(x',x_0) . \tag{5}$$

Two examples are: a free particle, for which

$$\langle q|\hat{U}|q_0\rangle = \sqrt{\frac{m}{2\pi it}} \exp\left[\frac{im}{2t}(q-q_0)^2\right] ,$$
$$\langle p|\hat{U}|p_0\rangle = \exp\left(-itp^2/2m\right)\delta(p-p_0) ,$$
$$L_t(q,p;q_0,p_0) = \delta(p-p_0)\delta\left(q-q_0-tp_0/m\right) , \tag{6}$$

and a harmonic oscillator (with $m=1$, $\omega=1$), for which

$$\langle q|\hat{U}|q_0\rangle = (2\pi i \sin t)^{-\frac{1}{2}} \exp\left[i\,\frac{(q^2+q_0^2)\cos t - 2qq_0}{2\sin t}\right] ,$$
$$\langle p|\hat{U}|p_0\rangle = (2\pi i \sin t)^{-\frac{1}{2}} \exp\left[i\,\frac{(p^2+p_0^2)\cos t - 2pp_0}{2\sin t}\right] ,$$
$$L_t(q,p;q_0,p_0) = \delta(p-p_0\cos t + q_0 \sin t)\delta(q - q_0\cos t - p_0 \sin t) . \tag{7}$$

The phase-space propagator provides an explicit distinction between classical and quantum dynamics. For any Hamiltonian $H = p^2/2m + V(q)$ with a potential $V(q)$ that is, at most, quadratic in the coordinate q, the phase-space propagator is a δ function on the classical paths. It is well known that in this case the classical and quantum dynamics are basically the same, as Wigner's integro-differential equation for quadratic potentials is equivalent to Liouville's classical equation. On the other hand, any deviation of L from a δ function is a manifestation of the difference between classical and quantum dynamics.

2.2 Phase-space propagator for barrier penetration

The phase-space propagator for barrier penetration is obtained by substituting in Eq. (4) the momentum propagator for one dimensional scattering, giving:

$$\begin{aligned} L_t(q,p;q_0,p_0) &= \delta(p-p_0)\frac{1}{2\pi}\int d\sigma e^{i\sigma(q_0+t\frac{p_0}{m}-q)}\, a(p_0-\sigma/2)\, a^*(p_0+\sigma/2) \\ &+ \delta(p+p_0)\frac{1}{2\pi}\int d\sigma e^{i\sigma(q_0+t\frac{p_0}{m}+q)}\, b(p_0-\sigma/2)\, b^*(p_0+\sigma/2) \\ &+ \left[\frac{1}{\pi}\, e^{2iqp_0 - 2i(q_0+t\frac{p_0}{m})p}\, b^*(p_0-p)\, a(p+p_0) + c.c.\right] , \end{aligned} \tag{8}$$

where $a(k)$ and $b(k)$ are the transmission and reflection amplitudes, respectively, for the time-independent Schrödinger equation. The integrals over σ converge since for real k $a(k)$ and $b(k)$ are physical amplitudes, regular and bounded:

$$\begin{aligned} 0 < |a(k)| < 1 \ , \quad |a(0)| = 0 \ , \quad |a(k \to \infty)| = 1 \ , \\ 0 < |b(k)| < 1 \ , \quad |b(0)| = 1 \ , \quad |b(k \to \infty)| = 0 \ . \end{aligned} \tag{9}$$

One can get a better understanding of the phase-space propagator by integrating in order to obtain either the coordinate or the momentum probability distributions. The probability of having a final momentum p is:

$$\begin{aligned} \mathcal{P}_t(p) &= \int_{-\infty}^{\infty} dq \rho_t(q,p) \\ &= |a(p)|^2 \int_{-\infty}^{\infty} dq_0 \rho_0(q_0,p) + |b(-p)|^2 \int_{-\infty}^{\infty} dq_0 \rho_0(q_0,-p) \\ &\quad + [b^*(-p)a(p) + b(-p)a^*(p)] \int_{-\infty}^{\infty} dq_0 \rho_0(q_0,0) \ . \end{aligned} \tag{10}$$

If the initial Wigner function has a well defined momentum, then $\rho_0(q_0,0) = 0$ and the last term vanishes, giving:

$$\mathcal{P}_t(p) = |a(p)|^2 \mathcal{P}_0(p) + |b(-p)|^2 \mathcal{P}_0(-p) \ , \tag{11}$$

where for a pure state $\mathcal{P}_t(p) = |\Psi_t(p)|^2$. In the same way, the probability of finding the particle in the final coordinate q is given by:

$$\begin{aligned} \mathcal{P}_t(q) &= \int dp \ \rho_t(q,p) = \int dq_0 dp_0 \rho_0(q_0,p_0) \\ &\quad \times \left\{ \frac{1}{2\pi} \int d\sigma \exp\left[i\sigma(q_f - q)\right] \ a(p_0 - \sigma/2)\, a^*(p_0 + \sigma/2) \right. \\ &\quad + \frac{1}{2\pi} \int d\sigma \exp\left[i\sigma(q_f + q)\right] \ b(p_0 - \sigma/2)\, b^*(p_0 + \sigma/2) \\ &\quad \left. + \left[\frac{\exp\left(i2qp_0\right)}{4\pi^2} \int d\sigma \exp\left(i\sigma q_f\right) \ b(p_0 - \sigma/2)\, a^*(p_0 + \sigma/2) + c.c. \right] \right\} \ , \\ q_f &\equiv q_0 + \frac{p_0}{m} t \ . \end{aligned} \tag{12}$$

If the time is large enough, so that $q_f \to \infty$ for every (q_0,p_0) for which $\rho_0(q_0,p_0) \neq 0$, the integrands oscillate rapidly, giving $\mathcal{P}_t(q) \to 0$ except for $q \sim q_f$ or $q \sim -q_f$. Here too, the last term does not contribute.

For any initial Wigner function that is prepared outside the potential range with a well defined momentum, and after a sufficiently long time, only the first two terms in the propagator contribute to $\rho_t(q,p)$. The phase-space propagator for Wigner functions with a well defined momentum, incident on a local potential barrier is therefore given by:

$$L_t(q,p;q_0,p_0) \quad = \quad \delta(p-p_0)T(q_f-q,p_0)+\delta(p+p_0)R(q_f+q,p_0) \ , \quad (13)$$

where

$$T(q_f-q,p_0) \equiv \int d\sigma\ t(\sigma) = \frac{1}{2\pi}\int d\sigma\, e^{i\sigma(q_f-q)}\, a(p_0-\sigma/2)\, a^*(p_0+\sigma/2) \ ,$$
$$R(q_f+q,p_0) \equiv \int d\sigma\ r(\sigma) = \frac{1}{2\pi}\int d\sigma\, e^{i\sigma(q_f+q)}\, b(p_0-\sigma/2)\, b^*(p_0+\sigma/2) \ . \quad (14)$$

The propagator has two distinct parts: a tunneling propagator in which the final momentum equals the initial one and a reflection propagator in which the momentum changes sign. Both are consistent with energy conservation. When any initial Wigner function is incident on the barrier the result after a long time will be two Wigner functions: one that has penetrated the barrier and moves in the original direction and one that has been reflected and moves in the opposite direction.

The tunneling propagator depends only on the initial momentum p_0, on the coordinate difference between free and actual motion q_f-q, and on the forward scattering amplitude $a(k)$. In the same way, the reflection propagator depends only on the initial momentum p_0, on the difference between the absolute value of the final coordinate and its value for free motion q_f+q, and on the backward scattering amplitude $b(k)$.

For a few barriers, $a(k)$ and $b(k)$, the transmission and reflection amplitudes respectively, are known from the exact solution of the time-independent Schrödinger equation. For these barriers one can substitute them and explicitly perform the integrations.

For a general potential barrier $a(k)$ and $b(k)$ are unknown. However, their analytic properties in the complex k plane can be deduced from the theory of differential equations, and used in order to obtain a universal form for T and R. For real k, $a(k)$ and $b(k)$ are regular and bounded. We have shown that they are also regular in the immediate neighborhood of the real k axis. The singularities of $a(k)$ and $b(k)$ are poles, which are all at finite distances from the real k axis, and an essential singularity at infinity. Furthermore, $a(k)$ is analytic in the upper half of the complex k plane. The fact that $a(k)$ has no singularities for $\Im k > 0$ is related to causality.[1]

The transmission $T \neq 0$ only for $q \sim q_f \gg 0$, and the reflection $R \neq 0$ only for $q \sim -q_f \ll 0$. The coefficient of σ in the exponent, $q_f - |q|$, has a clear physical meaning, it is the path delay: the difference between the final coordinate q and the coordinate a free particle would assume if it has passed through the barrier without noticing it, q_f, or if it has been reflected from an infinite wall at the middle of the barrier, $-q_f$. For $q_f > |q|$, or for $q_f < |q|$, one can close the contour in the upper half, or the lower half, of the complex σ plane, respectively, and use Caushy's theorem in order to perform the integrations. T and R can be given, in this way, by a sum over the residues at the poles of the integrands in the complex σ plane. The singularities of the integrands $t(\sigma)$, $r(\sigma)$ are induced by the singularities of $a(k)$ and $b(k)$. Each singular point in the complex k plane induces two singular points in the complex σ plane, located symmetrically on both sides of the imaginary σ axis, with complex conjugates contributions to the integrals, with opposite signs.

If, for example, $b(k)$ has a singularity in the complex k plane at $k = \kappa$, then $r(\sigma)$ will have two induced singularities of the same kind in the complex σ plane, at $\sigma_1 = 2(p_0 - \kappa)$ and at $\sigma_2 = -2(p_0 - \kappa^*)$. If, the singularity is a simple pole with the residue K, the residue of $r(\sigma)$ at σ_1 will be $-2K\, b^*(2p_0 - \kappa^*)\exp[i2(p_0-\kappa)(q_f+q)]$ while the residue of $r(\sigma)$ at σ_2 will be $2K^*\, b(2p_0 - \kappa^*)\exp[-i2(p_0-\kappa^*)(q_f+q)]$. Using the notation:

$$Be^{-i\beta} \equiv 4K^*\ b(2p_0 - \kappa^*)\ , \tag{15}$$

this two residues, multiplied by $(2\pi i)$, add up to

$$2\pi B e^{2\Im\kappa(q_f+q)} \sin\left[2(p_0 - \Re\kappa)(q_f+q) + \beta\right]\ . \tag{16}$$

In the same way, if $a(k)$ has a simple pole at $k = \kappa$ with the residue K, then $t(\sigma)$ will have two induced poles at $\sigma_1 = 2(p_0-\kappa)$ and at $\sigma_2 = -2(p_0-\kappa^*)$ whose two residues, multiplied by $(2\pi i)$, add up to

$$2\pi A e^{2\Im\kappa(q_f-q)} \sin\left[2(p_0 - \Re\kappa)(q_f-q) + \alpha\right]\ , \tag{17}$$

where

$$Ae^{-i\alpha} \equiv -4K^*\ a(2p_0 - \kappa^*)\ . \tag{18}$$

We have deduced from causality that $a(k)$ has no singularities for $\Im k > 0$. This implies that the t has no singularities in the lower half of the complex σ plane and

$$T\left(q_0 + tp_0/m - q < 0\right) = 0\ . \tag{19}$$

Given a point in the initial Wigner function, with the initial coordinate q_0 and the initial momentum p_0, the final coordinate, as obtained by the asymptotic phase-space propagator we have found, can not exceed its value for free motion, or causality will be violated.

Finally, the universal form for the transmission and reflection propagators for barrier penetration in phase space is given by:

$$\begin{aligned}
&T(q_f - q, p_0) = \delta(q_f - q) \\
&\quad -\Theta(q_f - q) \sum_n A_n e^{2\Im\kappa_n (q_f - q)} \sin[2(p_0 - \Re\kappa_n)(q_f - q) + \alpha_n] \ , \\
&R(q_f + q, p_0) = \\
&\quad \Theta(q_f + q) \sum_m B_m e^{2\Im\kappa_m (q_f + q)} \sin[2(p_0 - \Re\kappa_m)(q_f + q) + \beta_m] \\
&\quad +\Theta[-(q_f + q)] \sum_l C_l e^{2\Im\kappa_l (q_f + q)} \sin[2(p_0 - \Re\kappa_l)(q_f + q) + \gamma_l] \ , \quad (20)
\end{aligned}$$

where n numbers the singularities of $a(k)$ with $\Im k < 0$, m numbers the singularities of $b(k)$ with $\Im k < 0$, and l numbers the singularities of $b(k)$ with $\Im k > 0$. Furthermore, κ_n, κ_m, and κ_l are the positions of these singularities in the complex k plane. For a given potential barrier they are constant parameters, while A_n, α_n, B_m, β_m, C_l and γ_l are functions of p_0, whose exact forms are determined by the details of the barrier's shape.

The coordinate dependence of the propagators has the same functional form for every local potential. The propagators are functions of the path-delay, $q_0 + tp_0/m - |q|$, which is the coordinate difference between free and actual motion. The probability for a large path-delay decreases exponentially, but the most probable path-delay is not zero, since the exponential decline is modulated by an oscillatory term. The rate of the exponential decline, and the frequency of the oscillations, are given by the distance of the singularities of the transition and reflection amplitudes, in the complex momentum plane, from the imaginary and real axis, respectively. The coefficients and the phase-shifts depend on the details of the barrier shape and on the initial momentum.

It is important to note that the phase-space propagator is not a δ function. Each point in the initial Wigner function is propagated, not into a single point, but into a region of points in the final Wigner function. This is a manifestation of the difference between classical and quantum dynamics during barrier penetration. Notice that, asymptotically, after the particle had passed the barrier or has been reflected from it, the propagation in time is a simple coordinate translation, where each point in the final Wigner functions is translated with a different velocity, given classically by its momentum.

2.3 Two limits: semiclassical versus sudden approximation

In this section two complementary limits for our propagator will be considered: the semiclassical limit, and the limit of a δ function potential barrier, where the semiclassical approximation fails. The phase-space propagator was expressed above via sums over the singularities of the amplitudes. For a general potential barrier these are usually infinite sums. We will show that in the limit of a sharp barrier only the first terms in these sums contribute, while in the semiclassical approximation the various terms acquire large phases and are equally important.

In the limit where the area under the barrier is kept constant while its width tends to zero and its height to infinity, the potential approaches a δ function:

$$V^\delta(q) = \Omega\delta(q) \ , \tag{21}$$

(taking, for simplicity, $m = 1$). The amplitudes for this potential are:

$$a^\delta(k) = \frac{k}{k + i\Omega} \ , \qquad b^\delta(k) = \frac{i\Omega}{k + i\Omega} \ . \tag{22}$$

Both have only one simple pole in the complex k plane at $\kappa = -i\Omega$. Applying the formalism described above, the phase-space propagator for this barrier is:

$$\begin{aligned}
&L_t^\delta(q,p;q_0,p_0) = \delta(p-p_0)T^\delta(q_f-q,p_0) + \delta(p+p_0)R^\delta(q_f+q,p_0) \ , \\
&T^\delta(q_f-q,p_0) = \delta(q_f-q) \\
&\qquad\qquad - \ \Theta(q_f-q)A^\delta(p_0)\exp\left[-2\Omega(q_f-q)\right] \ \sin\left[2p_0(q_f-q)+\alpha^\delta\right] \ , \\
&R^\delta(q_f+q,p_0) = \Theta(q_f+q) \ B^\delta(p_0)\sin\left[2p_0(q_f+q)\right] \ , \\
&A^\delta(p_0) = 2\Omega\sqrt{(2p_0)^2+\Omega^2}/p_0 \ , \quad B^\delta(p_0) = 2\Omega^2/p_0 \ , \\
&\alpha^\delta = -\arctan\left(2p_0/\Omega\right) \ .
\end{aligned} \tag{23}$$

In the opposite limit of a wide and smooth barrier and when the initial momentum is small compared to the barrier's height, the semiclassical approximation to barrier penetration, WKB, applies. To leading order in this approximation the transition amplitude is given by:

$$\begin{aligned}
&a^{sc}(k) = \exp\left[\varphi(k)\right] \ , \\
&\varphi(k) = i\int_{-\infty}^{\infty}\left[\sqrt{k^2-2mV(q)}-k\right]dq \ , \\
&|a^{sc}(k)|^2 = \exp\left[-2\int_{q_<}^{q_>}\sqrt{2mV(q)-k^2}dq\right] \ ,
\end{aligned} \tag{24}$$

where $q_>(k)$ and $q_<(k)$ are the turning points. One can see that in the semiclassical approximation, the integrand of the transmission propagator, $a^{sc}(p_0-\sigma/2)\,a^{sc*}(p_0+\sigma/2)$, analytically continued off the real σ axis is an entire function of σ whose only singularity is an essential singularity at infinity. The result of Eq. (20) does not apply since the residue theorem can not be used in order to calculate the phase-space propagator. One should go back and substitute $a^{sc}(k)$ in Eq. (14), obtaining:

$$T^{sc} = \frac{1}{2\pi}\int d\sigma \exp\left[i\sigma(q_f-q)+\varphi(p_0-\sigma/2)+\varphi^*(p_0+\sigma/2)\right] \ . \tag{25}$$

For potential barriers, $V(q)$, which are wide and smooth enough so that φ can be expanded as a converging power series of σ around p_0, one has:

$$\begin{aligned}
&\varphi(p_0-\sigma/2)+\varphi^*(p_0+\sigma/2) = \varphi_0 - i\varphi_1\sigma + \varphi_2\sigma^2 - i\varphi_3\sigma^3 + \dots \qquad ,\\
&\varphi_0 = 2\Re\varphi(p_0) \ , \quad \varphi_1 = \Im\varphi^{'}(p_0) \ , \quad \varphi_2 = \frac{\Re\varphi^{''}(p_0)}{4} \ , \quad \varphi_3 = \frac{\Im\varphi^{'''}(p_0)}{24} \ ,\\
&\varphi_{2n} = \frac{\Re\varphi^{(2n)}(p_0)}{2^{2n-1}(2n)!} \ , \quad \varphi_{2n+1} = \frac{\Im\varphi^{(2n+1)}(p_0)}{2^{2n}(2n+1)!} \ .
\end{aligned} \tag{26}$$

Neglecting all orders of σ but one, a δ function is obtained:

$$\begin{aligned}
T^{sc} &= |a^{sc}(p_0)|^2 \int_{-\infty}^{\infty} d\sigma \exp\left[i\sigma(q_f-q-\varphi_1)\right] \qquad (27)\\
&= \exp\left(-2\int_{q_<}^{q_>}\sqrt{2mV(q)-p_0^2}\;dq\right)\delta\left[q-\left(q_0+\frac{p_0}{m}t-\Im\varphi^{'}(p_0)\right)\right] \ .
\end{aligned}$$

In this limit the propagation is similar to classical propagation with a time delay given by the first derivative of the phase shift $\varphi_1 = \Im\varphi^{'}(p_0)$.

Keeping terms up to σ^3 gives,

$$T^{sc} \simeq |a^{sc}(p_0)|^2\frac{1}{\pi}\int_0^{\infty} d\sigma e^{\varphi_2\sigma^2}\cos\left[\sigma(q_f-q-\varphi_1)-\sigma^3\varphi_3\right] \ . \tag{28}$$

Application of this semiclassical approximation to a general barrier may be subtle as this integral converges only for $\varphi_2 \le 0$. In fact, φ acquire additional phase shifts at the turning points whenever the barrier is not smooth enough. However, for "well-behaved" barriers, for which $\varphi_2 \le 0$, an Airy function, sometimes modified by an exponential decline, is obtained, which is typical to semiclassical Wigner functions. This was demonstrated for the Poschl-Teller barrier.[2]

The semiclassical propagator obtained in this way does not display the properties of the exact propagators. These deviations are artifacts of the approximation, not real properties of the quantum propagation.

3 Propagation of other phase-space distributions

3.1 Phase-space representations

Different representations of quantum mechanics in phase space were introduced over the years. A simple definition for most of these representations can be given in the following way:

$$\begin{aligned} \varrho_t^{\zeta}(q,p) &= \frac{1}{4\pi^2}\int d\xi \int d\eta \int dq' \left\langle q' + \frac{\hbar}{2}\eta \right| \hat{\rho}_t \left| q' - \frac{\hbar}{2}\eta \right\rangle \\ &\quad \times \zeta(\xi,\eta)\exp[i\xi(q'-q) - i\eta p]\,, \end{aligned} \tag{29}$$

where $\hat{\rho}$ is the density matrix.[15] In this section we do not set $\hbar = 1$. The function $\zeta(\xi,\eta)$ defines the representation. Not every $\zeta(\xi,\eta)$ is allowed.[12,16] We focus on the best known and most used phase-space representations: the Wigner function, the standard-ordered function, the Kirkwood (antistandard-ordered) function, the P function, and the Husimi function, for which $\zeta(\xi,\eta)$ is respectively given by:

$$\zeta^{\mathrm{W}}(\xi,\eta) = 1\,, \tag{30}$$

$$\zeta^{\mathrm{S}}(\xi,\eta) = \exp\left[-i\frac{\hbar}{2}\,\xi\eta\right]\,, \tag{31}$$

$$\zeta^{\mathrm{K}}(\xi,\eta) = \exp\left[i\frac{\hbar}{2}\,\xi\eta\right]\,, \tag{32}$$

$$\zeta^{\mathrm{P}}(\xi,\eta) = \exp\left[\frac{\hbar}{4m\kappa}\xi^2\right]\exp\left[\frac{\hbar m\kappa}{4}\eta^2\right]\,, \tag{33}$$

$$\zeta^{\mathrm{H}}(\xi,\eta) = \exp\left[-\frac{\hbar}{4m\kappa}\xi^2\right]\exp\left[-\frac{\hbar m\kappa}{4}\eta^2\right]\,, \tag{34}$$

where κ and m are constants defining the representation. The Glauber Q function is a special case of the Husimi function. Other phase-space distribution, e.g. with singular kernels are not considered here but can be considered as well.[16]

Time evolution can be considered in phase space in terms of evolution kernels for each one of these phase-space quasi-distributions. For each phase-space distributions a phase-space propagator is defined as the evolution kernel in the following way:

$$\varrho_t^\zeta(q,p) = \int dq_0 \int dp_0 \; \mathcal{L}_t^\zeta(q,p;q_0,p_0)\varrho_0^\zeta(q_0,p_0)\,. \tag{35}$$

3.2 Free propagation

The free propagator depends on the representation. In the classical limit of $\hbar \to 0$ we recover for all the representations the simple propagator:

$$\lim_{\hbar\to 0} \mathcal{L}_t^\zeta(q,p;q_0,p_0) = \delta(p-p_0)\delta(q_0 + \frac{p}{m}\,t - q)\;, \tag{36}$$

but for finite $\hbar$ the propagators are not the simple delta function of free classical propagation. Unique in this respect is the free propagator for the Wigner function whose simple form is exact in the quantum regime as well as in the classical one:

$$\mathcal{L}_t^{\mathrm{W}}(q,p;q_0,p_0) = \delta(p-p_0)\delta(q_0 + \frac{p}{m}\,t - q)\;. \tag{37}$$

In all the other representation the integrals defining the free propagator diverge for finite $\hbar$. Nevertheless, the propagators defined by these divergent integrals are well defined distributions. In particular, they are normalized and integrable. In all the representations, excluding Wigner, there is a competition between the limits of large time and small $\hbar$ and deviations of the free propagators from their classical limit grow with time.

The free propagators for the standard-ordered function and the Kirkwood (antistandard-ordered) functions are, respectively:

$$\begin{aligned}
\mathcal{L}_t^{\mathrm{S/K}}(q,p;q_0,p_0) &= \frac{\delta(p_0-p)}{2\pi}\int d\xi \exp\left[i\xi\left(q_0+\frac{p}{m}\,t-q\right) \pm i\frac{\hbar t}{2m}\xi^2\right] &(38)\\
&= \delta(p_0-p)\sqrt{\frac{\pm im}{2\pi t\hbar}}\;\exp\left[\frac{\mp im}{2t\hbar}(q_0+\frac{p}{m}\,t-q)^2\right]\;, &(39)
\end{aligned}$$

where the integral representation of Eq. (38) is exact while the expression in Eq. (39) was obtained after a regularization. The free propagators for the P function and the Husimi distribution are:

$$\begin{aligned}
\mathcal{L}_t^{\mathrm{H}}(q,p;q_0,p_0) &= -\frac{1}{2\pi}\sqrt{\frac{1}{\pi m\hbar\kappa}}\exp\left[-\frac{m}{\hbar\kappa t^2}\left(q_0+\frac{p}{m}\,t-q\right)^2\right] \\
&\quad\times\int d\eta \exp\left[-i\eta\left(q_0+\frac{p}{m}\,t-q\right)+\frac{\hbar\kappa t^2}{4m}\eta^2\right] &(40)\\
&= -\mathcal{L}_t^{\mathrm{P}}(q,p_0;q_0,p)\;. &(41)
\end{aligned}$$

The difference between the Wigner representation and other representations here is striking. Free propagation in all other representations is based on interference. The value of each initial point contributes to the values of many final points and the value of each final point is determined by the values of many initial points. The Wigner function is the only phase-space function freely propagating in a completely classical way.

Furthermore, while the propagators for the Wigner, standard-ordered, and Kirkwood functions explicitly display momentum conservation with $\delta(p-p_0)$ and a symmetry between initial and final coordinates and momenta, the propagators for the P function and the Husimi function do not have these properties. In fact the propagation of the Husimi function seems to be carried out with a Gaussian distribution of momenta around the final momentum, while the relation to the initial momentum is ill defined, and the reverse applies to the propagation of the P function. Clearly momentum is conserved regardless of the representation chosen to describe the process. Integration of the time evolution in all these representations would give the same result for any observable consequences of momentum conservation. In some representations, however, momentum is conserved explicitly in the evolution kernel: the value of these quasidistributions at a phase-space point propagates only into phase-space points with the same momentum. In other representations the intrinsic property of momentum conservation is obscured. The point-to-point influence functional does not display it and it is recovered only after integration.

3.3 Scattering

If the propagation is asymptotically free yet includes a small region of interaction, a scattering matrix can be defined. For single channel scattering, as well as for the elastic channel of multichannel scattering, a single amplitude $a(p)$ defines the propagation. The propagators in the different representations are:

$$\begin{aligned}\mathcal{L}_t^{\mathrm{W}}(q,p;q_0,p_0) &= \delta(p-p_0)\frac{1}{2\pi}\int d\xi\ a(p+\hbar\xi/2)a^*(p-\hbar\xi/2)\\ &\quad\times\exp\left[i\xi\left(q-q_0-tu^{\mathrm{W}}(p,\xi)\right)\right]\ ,\end{aligned}\tag{42}$$

$$\begin{aligned}\mathcal{L}_t^{\mathrm{S}}(q,p;q_0,p_0) &= \delta(p-p_0)\frac{1}{2\pi}\int d\xi\, a(p)a^*(p-\hbar\xi)\\ &\quad\times\exp\left[i\xi\left(q-q_0-tu^{\mathrm{S}}(p,\xi)\right)\right]\ ,\end{aligned}\tag{43}$$

$$\begin{aligned}\mathcal{L}_t^{\mathrm{K}}(q,p;q_0,p_0) &= \delta(p-p_0)\frac{1}{2\pi}\int d\xi\, a(p+\hbar\xi)a^*(p)\\ &\quad\times\exp\left[i\xi\left(q-q_0-tu^{\mathrm{K}}(p,\xi)\right)\right]\ ,\end{aligned}\tag{44}$$

$$\mathcal{L}_t^{\mathrm{P}}(q,p;q_0,p_0) = \int dp_1\, \frac{1}{\sqrt{\pi m\kappa\hbar}} \exp\left[-\frac{1}{m\kappa\hbar}(p_0-p_1)^2\right] \tag{45}$$

$$\times \frac{1}{2\pi}\int d\eta\, \exp\left[i\;\eta(p_1-p)\right]\; \exp\left[\frac{\hbar m\kappa}{4}\eta^2\right]$$

$$\times \frac{1}{2\pi}\int d\xi\, a(p_1+\hbar\xi/2)\, a^*(p_1-\hbar\xi/2)\exp\left[i\;\xi\left(q-q_0-tu^{\mathrm{W}}(p_1,\xi)\right)\right]$$

$$= \mathcal{L}_t^{\mathrm{H}}(q,p_0;q_0,p)\,. \tag{46}$$

where we have introduced the auxiliary velocity functions:

$$u^{\mathrm{W}}(p,\xi) = \frac{p}{m}\,, \tag{47}$$

$$u^{\mathrm{K}}(p,\xi) = \frac{p}{m}+\frac{\hbar\xi}{2m}\,, \tag{48}$$

$$u^{\mathrm{S}}(p,\xi) = \frac{p}{m}-\frac{\hbar\xi}{2m}\,. \tag{49}$$

Note that while $u^{\mathrm{W}}(p,\xi)$ does not depend on ξ, $u^{\mathrm{K/S}}(p,\xi)$ do. The propagators for single channel scattering in the different phase-space representations are given by bilinear integral transforms of the scattering amplitude. They provide different mappings from the energy domain where the amplitudes are defined to the time domain where the propagators act. Mappings between the energy and time domains are particularly interesting for the discussion of causality.

The scattering amplitude $a(p)$ and its properties depend on the specific problem considered. It often has the following properties when analytically continued into the complex momentum plane:

- $a^*(p) = a(-p)$, or $a^*(p) = -a(-p)$.
- $a(p)$ is analytic in the upper half of the complex p plane .
- $a(p) \to 1$ as $|p| \to \infty$.

These properties were proven for the Schrödinger equation with a positive potential,[1] but are more general. Whenever the transition amplitude has these properties, the propagators can be written with $a(-p+\hbar\xi)$ instead of $a^*(p-\hbar\xi)$ etc. The integral over ξ can then be considered as a contour integral in the complex ξ plane. Because $a(-p\pm\hbar\xi)$ and $a(-p\pm\hbar\xi/2)$ are analytic in the upper ξ plane it is possible to deform the contour of $\int_{-\infty}^{\infty} d\xi$ to the arc at infinity of the upper ξ plane, where $|a| \to 1$. In general, this will not give any simple result or insight. The integral over the arc at infinity can assume very complicated forms and would often diverge for an arbitrary dependence of the auxiliary u functions on ξ. Only for cases in which $u(p,\xi) = v(p)$ does not depend on ξ, a simple result follows. In these cases the integral over ξ would vanish identically for $q > q_0 + tv(p)$. For $q < q_0 + tv(p)$ different velocity functions, different scattering amplitudes, and different representations would all give different propagators but under the assumptions specified above all these different propagators will vanish for coordinates too far apart at times that are too short. The limit on the propagation is then locally set by the velocity $v(p)$.

The manifestation in phase space of the analytical properties of the scattering matrix then depends on the representation. In previous section we have shown that in the Wigner representation:

$$\mathcal{L}_t^{\mathrm{W}}(q > q_0 + tp/m) = 0 \,. \tag{50}$$

This property of the Wigner function tells us that no information can be transferred faster than free motion as long as the assumptions regarding the analytical properties of the scattering amplitude hold.[2,5] In this section we have checked for this property in the other phase-space representations and found that no such simple restriction applies to the other phase-space propagators. In them, the velocity functions u depend on ξ, and the contributions from the arcs at infinity diverge. We note however that the reason for the lost simplicity is not in the scattering process but rather in the free propagation which is so simple for the Wigner function yet so complicated for the other phase-space quasi-distributions. Note that the Husimi function propagator as was noticed before does not explicitly display momentum conservation. As a result, while it is confined by classical free propagation, this free propagation can be with any momentum, hence the propagation velocity is not really confined.

4 Fermi golden rule in phase space

In the previous sections propagation in phase space was considered in one dimension and with a given Hamiltonian. The advantage of the Wigner representation was demonstrated. In this section we a priori restrict the discussion to the Wigner representation, yet include the more complicated dynamics of transitions between multidimensional potential energy surfaces.

Radiationless transitions in molecules,[19] and output coupling from a Bose-Einstein Condensate to form an atom laser,[20,21] are very different physical processes. Yet they share essential features: both involve an irreversible transition between distinct energy surfaces in multidimensional complex systems. We consider these processes in the Wigner phase-space representation. Fermi

Golden Rule in phase space gives:

$$\frac{2\pi}{\hbar}\kappa^2 \mathrm{Tr}\left[\hat{\varrho}_i{}' \hat{\varrho}_f\right] = \frac{2\pi}{\hbar}\kappa^2 \int dq dp \rho_f(q,p)\rho_i'(q,p) \tag{51}$$

for the transition rate. Here κ^2 is an integral over the electronic degrees of freedom, $\rho_i'(q,p)$ is the Wigner transform of the incoming state density matrix, $\hat{\varrho}_i{}'$, and $\rho_f(q,p)$ is the Wigner transform of the outgoing state density matrix, $\hat{\varrho}_f$. The incoming density matrix is $\hat{\varrho}_i{}' = \hat{\lambda}\hat{\varrho}_i\hat{\lambda}^\dagger$ where $\hat{\varrho}_i$ is the initial density matrix and $\hat{\lambda}$ is the coupling operator. For a pure initial state $\hat{\varrho}_i = |\psi_i\rangle\langle\psi_i|$ where ψ_i is an eigenfunction of $\hat{H}_i$. The manifold of final states $\{\varphi_k\}$ includes all eigenfunctions of $\hat{H}_f$ with a given energy:

$$\hat{\varrho}_f = \Sigma_{E_k=E}\ |\varphi_k\rangle\langle\varphi_k| = \delta\left(E - \hat{H}_f\right)\ ,$$

where $E = E_i$ for radiationless transitions and $E = E_i \pm \hbar\omega$ for radiative transitions. The initial and final hamiltonians $\hat{H}_i$ and $\hat{H}_f$ differ because of an electronic transition in molecules and a change of hyperfine state of an output coupled atom in the BEC.

The phase-space overlap integral of Eq. (51) is a subject of our study[6] as well as of previous works.[22,23] The integral yields an approximation for the rate, while a study of the integrand shows where in phase space the transition occurs. For the cases in which the surfaces do not cross in classically allowed points, surface jumping to the point or region in phase space that dominate the overlap integral, constitute the dominant relaxation channel in multi-channel and multidimensional relaxation processes.[6]

4.1 Radiationless transitions in polyatomic molecules

Relaxation of electronically excited molecules plays a part in many chemical processes. In a radiative transition the population on the upper surface undergoes a vertical transition according to the Condon principle. A photon is emitted with a frequency that overcomes the energy gap between the surface potentials. The initial conditions for the nuclear dynamics on the ground surface potential are given by the position and momentum of the wave packet on the upper surface. The Condon principle applies as well to radiationless transition in the case where the surfaces cross in a classically allowed position. In this case, the population transfer between the surfaces is in the region where the electronic surfaces cross and the electronic energy of the excited molecule is transferred to the molecular internal vibrational degrees of freedom smoothly, without the nuclei jumping in either position or momentum discontinuously.

We consider a radiationless transition between nested surface potentials where the two surface potentials do not cross in a classically allowed region. If the radiative transition channel is not available a vertical transition is impossible and the molecule must decay by a sudden change of its nuclei position or momentum. We call this process *surface jumping* where the jumping we refer to is a quantum jump and can be related to the general non-classical phenomena of tunneling.

One of the crucial steps in the formal description of the transition between the surfaces involve the calculation of the Frank-Condon (FC) overlap integrals between the initial and final vibronic states. The value of the FC integral serves as a measure for the probability of the transition and when several modes of vibration are competing for the electronic energy the relative FC factors can be a defining parameter for the division of the energy. For a radiationless transition it can be shown, using the reflection principle, or by using the stationary phase approximation, that for the case of crossing surfaces the contribution to the FC integral is maximal in the region where the electronic states cross. The integral defining the FC factor is controlled by the vicinity of this leakage point. *Surface jumping* occurs for the cases in which the electronic surfaces do not cross in classically allowed points, the FC factor is exponentially small, the reflection principle does not apply, and there is no straightforward way to predict which region in space would dominates the FC factor.

We suggest a simple method for calculating such weak Franck-Condon factors. The Wigner transform of the wavefunction on an initial Born-Oppenheimer state is calculated for the donor potential surface and projected onto the acceptor energy surface energy shell. The integrated projection yields an approximation for the relevant Franck-Condon factors, while the phase-space integrand shows where in phase space the leakage occurs between the donor and acceptor states. This in turn determines the initial conditions on the acceptor surface for subsequent internal vibrational relaxation and energy flow.

A model of the $S_2 \rightarrow S_0$ vibronic relaxation transition of the benzene molecule where 30 modes of vibration compete for the electronic energy was studied within this approach. For this model, we have shown that almost all the energy must go to a single $C-H$ local stretching. The initial conditions for vibrations of this mode will be a coordinate jump of the hydrogen atom toward the ring. All the other modes undergo an almost vertical transition, where the energy that they take is proportional to their equilibrium displacement between the two surfaces.

Our analysis shows that, almost by definition, this is a general phenomena:

surface jumping in radiationless transitions in polyatomic molecules involves an excitation of one degree of freedom of the system which takes most of the energy while the rest of the degrees of freedom undergo a vertical or an almost vertical transition. For larger energy gaps - more energy is transferred to this dominant accepting mode, which need not be a normal mode of the system.

4.2 Radiative decay

A similar situation occurs in radiative transitions when the energy of the photon is too big or too small to account for the energy difference between the surfaces, i.e. in the wings of an absorption band.[22] If we quantize the radiation field, it becomes clear that induced radiative transitions are very similar to radiationless decay, in that a given level (molecule + photon) is weakly coupled to a dense set of quasidegenerate levels (excited molecule+ one less photon). In an electronic absorption for example, we can raise the lower potential energy surface by $\hbar\omega$, where ω is the frequency of the light; using the radiation coupling as the perturbation, we can now treat the coupling as if it were radiationless. Radiative transitions are thus more experimentally flexible than radiationless ones, in that the photon energy can be used to put the two surfaces out of contact with each other. This corresponds spectroscopically to being the red or blue wings of the absorption band.

4.3 Transitions from a thermal state

A semiclassical approximation for the transfer rate of a thermal distribution of atoms or molecules between two potential surfaces under the influence of an external electromagnetic field is obtained by projecting the initial thermal phase-space distribution into a set of energy surfaces corresponding to the initial energy distribution shifted by the energy supplied by the external field. To leading order, the transition rate from a thermal state is given by

$$\Gamma_T(\Delta) \approx \frac{2\pi\kappa^2}{\hbar}\frac{1}{(2\pi\hbar)^d}\int dq \int dp\, P_T(H_i)\,\delta(H_f - H_i - \hbar\Delta)\,, \tag{52}$$

which farther simplifies in cases where $H(q,p) = p^2/2m + V(q)$ to

$$\Gamma_T(\Delta) \approx \frac{2\pi\kappa^2}{\hbar}\frac{1}{(2\pi\hbar)^d}\int dq\,\delta(V_f - V_i - \hbar\Delta)\int dp\, P_T(H_i)\,, \tag{53}$$

where κ is the electronic term, Δ is the detuning between the frequency of the electromagnetic field and the splitting between the levels, $P_T(E)$ is the thermal occupation probability of a state in the initial potential surface with energy E and $H_i(q,p)$ and $H_f(q,p)$ are the phase-space representations of the Hamiltonians corresponding to the two potential surfaces.

This forms the basis for a calculation of the transfer rate of a gas of atoms or molecules with initial Boltzmann or Bose-Einstein thermal distributions. We have applied it to the calculation of finite temperature effects on weak output coupling of a magnetically trapped atomic bose gas so as to form an atom laser, where the different surfaces correspond to different hyperfine levels of the atoms; as well as to model systems where the approximate results were successfully compared with exact quantum calculations.

5 Path integral for the propagator

The path integral[24] was a subject close to Marinov's heart. His report[25] is a classic monograph on this subject. In his recent paper[14] and lecture notes[26] Marinov developed a new type of phase-space path integral for the evolution kernel of the Wigner function.

There were several issues motivating this work. Mostly, Marinov wanted a path integral that would preserve the canonical invariance of the theory and would not introduce a polarization in phase space. He was concerned with the fact that Feynman's path integral for the evolution kernel in real space introduces such a polarization, and wrote:

> "The problem here is that the trajectories in the phase space must belong to a special class, determined in a non-invariant manner"

and therefore:

> "One could not get the standard path integral for coordinate spaces having a non-Euclidean topology".[26]

In this section I revisit Marinov's path integral and study some of its properties.

5.1 General structure

A path integral for the phase-space propagator of the Wigner function was developed by Marinov. He has shown that for $H = p^2/2m + V(q)$ the phase-space propagator is

$$L_t(q,p;q_0,p_0) = \lim_{N\to\infty} \prod_{\nu=1}^{N-1} \left[\int dq_\nu \int dp_\nu \right] \prod_{\nu=1}^{N} \delta \left[(q_\nu - q_{\nu-1}) - \frac{t}{N} \frac{p_\nu + p_{\nu-1}}{2m} \right]$$

$$\times \prod_{\nu=1}^{N} \left[\int \frac{d\eta_\nu}{2\pi} \exp\Big\{ -i \Big[\eta_\nu (p_\nu - p_{\nu-1}) \right.$$

$$\left. + \frac{t}{N} \left(V \left(\frac{q_\nu + q_{\nu-1} + \eta_\nu}{2} \right) - V \left(\frac{q_\nu + q_{\nu-1} - \eta_\nu}{2} \right) \right) \Big] \Big\} \right] \tag{54}$$

where $p_n = p$ and $q_N = q$. We will see that sometimes this path integral reduces to a sum over classical trajectories, in other cases it is dominated by classical trajectories but allows for some quantum fluctuations around the classical paths, and finally, it includes the possibility for quantum jumps, which can even dominate if no classical paths exist.

5.2 Classical trajectories

For potentials that are at most quadratic in the coordinate, the phase-space propagator is a δ function on the classical paths. It is easy to verify this property starting from the path integral.

For the simplest case of a free particle $V = 0$ and

$$L_t^0(q,p;q_0,p_0) = \lim_{N\to\infty} \prod_{\nu=1}^{N-1} \left[\int dq_\nu \int dp_\nu \right] \prod_{\nu=1}^{N} \Big\{ \delta \Big[(q_\nu - q_{\nu-1})$$

$$- \frac{t}{N} \frac{(p_\nu + p_{\nu-1})}{2m} \Big] \delta(p_\nu - p_{\nu-1}) \Big\} = \delta(p - p_0) \delta \left(q - q_0 - \frac{p_0}{m} t \right). \tag{55}$$

For a potential which is at most quadratic in q, $V(q+\eta/2) - V(q-\eta/2) = \eta\, \partial V/\partial q$,

$$L_t^{\text{quad.}}(q,p;q_0,p_0) = \lim_{N\to\infty} \prod_{\nu=1}^{N-1} \left[\int dq_\nu \int dp_\nu \right] \prod_{\nu=1}^{N} \Big\{ \delta \Big[(q_\nu - q_{\nu-1})$$

$$- \frac{t}{N} \frac{p_\nu + p_{\nu-1}}{2m} \Big] \delta \left(p_\nu - p_{\nu-1} + \frac{t}{N} \frac{\partial V}{\partial q} \right) \Big\} = \delta(p - p_{cl}) \delta(q - q_{cl}). \tag{56}$$

When the potential is not quadratic, quantum fluctuations start to play a role. A semiclassical approximation, expanding the exponent to second order in the coordinates, shows that the propagator is dominated by the classical paths, yet this treatment is restricted to those cases where such an expansion is justified. Quantum corrections can then be analyzed by keeping higher order terms in the expansion, giving the propagator a finite width around the classical path. What if the expansion is wrong, say because it is mathematically ill defined, or when no classical path exists? An alternative approach to quantum effects can be developed by resuming the path integral as a sum over momenta jumps. This approach is introduced in the next subsection.

5.3 Quantum fluctuations and quantum jumps

The integral over η includes the possibility for quantum fluctuations and quantum jumps.

For simplicity, let us focus on cases where the potential is 0 or V_0 on different segments of space so that $\partial V/\partial q$ is either 0 or ill defined. In these cases $V\left[\left(q_\nu+q_{\nu-1}+\eta_\nu\right)/2\right]-V\left[\left(q_\nu+q_{\nu-1}-\eta_\nu\right)/2\right]$ is 0, V_0 or $-V_0$ for different values of $q_\nu+q_{\nu-1}$ and η. The integral over η can be calculated exactly to give a sum over such functions as $\sin\left[(p_\nu-p_{\nu-1})(q_\nu+q_{\nu-1})\right]/(p_\nu-p_{\nu-1})$ with different coefficients depending on the values of $\bar{q}_\nu=(q_\nu+q_{\nu-1})/2$, $\tilde{p}_\nu=p_\nu-p_{\nu-1}$ and on the coordinate segments defining the potential. In general:

$$F_\nu \equiv \int \frac{d\eta_\nu}{2\pi}\exp\left\{-i\left[\eta_\nu\tilde{p}_\nu+\frac{t}{N}\left(V\left(\bar{q}_\nu+\frac{\eta_\nu}{2}\right)-V\left(\bar{q}_\nu-\frac{\eta_\nu}{2}\right)\right)\right]\right\}-\delta(\tilde{p}_\nu)\ . \quad (57)$$

Different potentials would give different functions $F_\nu=F_\nu(\tilde{p}_\nu;\bar{q}_\nu)$.

With this definition, the trajectories can be redefined and resummed by the number σ of steps in which the momentum changes or *jumps*, the time intervals $\nu_1,\ \ldots,\ \nu_\sigma$ in which the jumps occur and the size of these momentum jumps $\alpha_1,\ \ldots,\ \alpha_\sigma$,

$$\begin{aligned}
L_t(q,p;q_0,p_0) &= \lim_{N\to\infty}\sum_{\sigma=0}^{N}\sum_{\nu_1=1}^{N}\int d\alpha_1\sum_{\nu_2=\nu_1+1}^{N}\int d\alpha_2 \ldots \sum_{\nu_\sigma}^{N}\int d\alpha_\sigma \\
&\times\prod_{\nu=1}^{N-1}\left[\int dq_\nu\int dp_\nu\right]\prod_{\nu=1}^{N}\delta\left[(q_\nu-q_{\nu-1})-\frac{t}{N}\frac{p_\nu+p_{\nu-1}}{2m}\right] \\
&\times\prod_{\nu\neq\nu_1,\ldots\nu_\sigma}\delta(p_\nu-p_{\nu-1})\prod_{\nu=\nu_1,\ldots\nu_\sigma}\delta(p_\nu-p_{\nu-1}-\alpha_i)F_\nu(\alpha_i;q_\nu+q_{\nu-1}) \\
&= \lim_{N\to\infty}\sum_{\sigma=0}^{N}\sum_{\nu_1=1}^{N}\int d\alpha_1 F_1(\nu_1,\alpha_1;q_0,p_0) \\
&\times\sum_{\nu_2=\nu_1+1}^{N}\int d\alpha_2 F_2(\nu_1,\nu_2,\alpha_1,\alpha_2;q_0,p_0) \\
&\times\ldots\sum_{\nu_\sigma}^{N}\int d\alpha_\sigma F_\sigma(\nu_1,\ldots,\nu_\sigma,\alpha_1,\ldots,\alpha_\sigma;q_0,p_0) \\
&\times\delta\left[q-q_0-\frac{t}{m}\left(p_0+\sum_{i=1}^{\sigma}\frac{\nu_i}{N}\alpha_i\right)\right]\delta\left(p-p_0-\sum_{i=1}^{\sigma}\alpha_i\right)\ . \qquad (58)
\end{aligned}$$

The functions $F_{2,3,\ldots,\sigma}$ depend on ν_1 and α_1 because $q_{2,3,\ldots,\sigma}$ do.

This new form for Marinov's path integral is conceptually very simple. Each point in the Wigner function is propagated by an evolution kernel which is a sum over simple trajectories. Each trajectory is characterized by the number, times, and strength of sudden changes of its momentum. In between the jumps the path is a free particle path, and with each jump comes a factor F which depends on the position of the jump and on the potential in an essentially non-local way. The difficulty in calculating propagators for specific potentials is two-fold: first one has to find the factors F and second to sum over the infinite number of paths.

6 Conclusions

Quantum mechanics can be studied in many different representations. The physical results of an experiment or the theoretical predictions for an observable effect do not depend on the representation chosen but a clever choice often simplifies the analysis and sometimes helps our physical intuition. In this work several cases where considered where fundamental or complicated problems considerably simplify in the Wigner representation. Several questions remain:

- In studying the propagator of section 2 above we have neglected a third term which appeared in addition to tunneling and reflection. Preliminary studies indicate that this third term is responsible for transient ringing effects at the barrier region. Farther work is needed to resolve the properties of these ringing effects.
- The transition rates according to Fermi Golden Rule was applied within a Born-Oppenheimer approximation, yet it may be more general. Extending the treatment beyond the adiabatic approximation is worth looking into.
- The path integral for the propagator was written as a sum over momentum jumps. Summation of the paths to rederive the closed form expression for the propagator in the limit of a narrow barrier and large time, remains to be done.

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