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Equiprobability of large-energy classical paths for one-dimensional motion in potential wells of infinite depth

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Abstract. The semiclassical propagator in configuration space for a particle with one-dimensional motion in a potential well of infinite depth is investigated. It is shown that, if the motion's period and its derivative are asymptotically decreasing functions of the energy, the large-energy classical paths give the same contribution (in modulus) to the propagator, and are therefore asymptotically equiprobable. This extends the results previously obtained for the quartic anharmonic oscillator.

In a previous paper [1] the semiclassical propagator for the anharmonic quartic oscillator in configuration space was investigated by means of the Van Vleck formula, which gives it as a sum over all the denumerably infinite classical paths connecting two given points in the same time. It was found that the large-energy paths asymptotically give the same contribution, in modulus, to the semiclassical propagator, and therefore they tend to become equiprobable, while their energy increases. Moreover, the Van Vleck series diverges but in the general case it can be Cesaro resummed.

The aim of this paper is to show that the main results in [1] can be extended to a much more general class of potentials: indeed, in the one-dimensional case, they hold for any infinitely deep potential well if the motion's period and its derivative with respect to the energy are asymptotically monotonic decreasing functions of the energy when the latter goes to infinity. These conditions are satisfied, for instance, by any even-order polynomial potential well and, in order to clarify the hypothesis, this case will be examined in the following, the generalization being discussed at the appropriate places.

In the multi-dimensional case, analogous conclusions hold if the system is separable in some coordinate system and if the resulting one-dimensional motions satisfy the above specified conditions.

The results in [1] were obtained by means of direct analysis of the various quantities involved, while the present derivation is general.

Let us recall that the semiclassical approximation K_{WKB} for Feynman's propagator [2] in the configuration space is given [3, 4], in the one-dimensional case, by

$$K_{\mathrm{WKB}}(x_{\mathrm{B}}, t_{\mathrm{B}}; x_{\mathrm{A}}, t_{\mathrm{A}}) = \sum_{\alpha} \left|\frac{\mathrm{i}}{2\pi\hbar}\right|^{1/2} \left|\frac{\partial^2 S_\alpha}{\partial x_{\mathrm{A}} \partial x_{\mathrm{B}}}\right|^{1/2} \exp[\mathrm{i}(S_\alpha/\hbar - n_\alpha \pi/2)]. \quad (1)$$

Here the index α labels the classical paths, connecting the initial point x_{A} to the final point x_{B} in the same time $T = t_{\mathrm{B}} - t_{\mathrm{A}}$: in the following these will be denoted as ABT paths; S_α

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is the action for the αth path, $x_\alpha(t)$, i.e.

$$S_\alpha = \int_{t_A}^{t_B} L[x_\alpha(t), \dot{x}_\alpha(t), t]\, dt \tag{2}$$

L is the Lagrangian, and n_α is the number of the focal points along the path, which are the points where the second derivative $\partial^2 S_\alpha / \partial x_A \partial x_B$ diverges.

Let us consider a unit-mass particle with one-dimensional motion under the potential

$$V(x) = \sum_{j=0}^{N} a_j x^j \tag{3}$$

with even N ($\geqslant 4$, in order to exclude the trivial case of the harmonic oscillator) and $a_N > 0$.

As in [1], let us recall that the ABT paths are specified by their energies and in the general case can be divided into four classes, according to the signs of the initial and final momenta, which are $(+,+)$, $(+,-)$, $(-,+)$, $(-,-)$, respectively. Each class has a shortest member, plus all the paths obtained by adding an integer number m of complete oscillations.

The paths' energies E are the solutions of the equation

$$T = \pm \int_{x_A}^{x_B} \frac{dx}{\sqrt{(2(E - V(x)))}} \tag{4}$$

for given x_A, x_B, T. Let us define τ^K as

$$\tau^K = \int_0^{x_K} \frac{dx}{\sqrt{(2(E - V(x)))}} \tag{5}$$

where $\tau^K = \tau^K(E)$ is the time needed for the particle to go from the origin to the point x_K along the direct path of energy E. In order to clarify this let us suppose $0 \leqslant x_A \leqslant x_B$. Then equation (4) can be written

$$T = \sigma_{Bi}\tau^B + \sigma_{Ai}\tau^A + 2\delta_{i2}\tau^R + 2\delta_{i3}\tau^L + (m + \delta_{i4})P(E) \tag{6}$$

where $P(E)$ denotes the period of the path with energy E, m is the number of complete oscillations, τ^R and τ^L denote the times needed for the particle to go from the origin to the right (x_R) and to the left (x_L) turning point, respectively; the index $i = 1, \ldots, 4$ refers to the path's class, $\sigma_{Bi} = 1, -1, 1, -1$, $\sigma_{Ai} = -1, -1, 1, 1$, and δ_{ij} denotes the Kronecker delta. Let us investigate equation (6) for large values of the energy. In this case, the turning points approach $\pm b$, where

$$b \sim \sqrt[N]{\frac{E}{a_N}} \qquad (E \to \infty). \tag{7}$$

Here, as usual [5], the symbol $\sim$ denotes an asymptotic representation, i.e. $f(x) \sim ag(x)$, as $x \to \infty$, where a is a constant, is equivalent to $f(x) = ag(x) + o(g(x))$ as $x \to \infty$. Moreover, when $E \gg 1$, the period $P(E)$ approaches $4\tau^b$ and, from equation (4), it is asymptotically given by

$$P(E) \sim cE^{(2-N)/(2N)} \qquad (E \to \infty) \tag{8}$$

where c is a constant.

Therefore, for given x_A, x_B, T, m and i, when the energy becomes large, the right-hand side of equation (6) is a monotonic decreasing function of E; hence this equation admits a unique solution $E_{m,i}(x_A, x_B, T)$ for each integer m greater than a minimum value $m_{\min}(i)$. This is also true for more general non-polynomial potentials if $P(E)$ has an asymptotic monotonic decreasing dependence on E. In conclusion, for each class there is a countable family of ABT paths. Moreover, from the equations (6) and (8) it follows that

$$E \sim \left(\frac{cm}{T}\right)^{2N/(N-2)} \qquad (E \to \infty). \tag{9}$$

The amplitude $A_{m,i}$ of the path's contribution to the semiclassical propagator is given by

$$A_{m,i} = \left|\frac{\mathrm{i}}{2\pi\hbar}\right|^{1/2} \left|\frac{\partial^2 S_{m,i}}{\partial x_A \partial x_B}\right|^{1/2} \tag{10}$$

where the action $S_{m,i}$ is

$$S_{m,i} = \int_{x_A}^{x_B} p\,\mathrm{d}x - E_{m,i}T = W_{m,i} - E_{m,i}T \tag{11}$$

and $W_{m,i}$, the Hamiltonian's characteristic function, can be written as

$$W_{m,i} = \sigma_{Bi} w^B + \sigma_{Ai} w^A + 2\delta_{i2} w^R + 2\delta_{i3} w^L + (m + \delta_{i4}) J(E). \tag{12}$$

In the last equation w^K is defined as

$$w^K = \int_0^{x_K} \sqrt{(2(E - V(x)))\,\mathrm{d}x} \tag{13}$$

where the integral is done along the direct path from the origin to the point x_K, and $J(E)$ is the action variable

$$J(E) = 2\int_{x_L}^{x_R} p\,\mathrm{d}x. \tag{14}$$

The term $mJ(E)$ in the right-hand side of equation (12) gives the contribution to W from m complete oscillations.

From equations (11) and (12) it follows that

$$\frac{\partial S_{m,i}}{\partial x_A} = \left(\sigma_{Bi}\frac{\partial w^B}{\partial E} + \sigma_{Ai}\frac{\partial w^A}{\partial E} + 2\delta_{i2}\frac{\partial w^R}{\partial E} + 2\delta_{i3}\frac{\partial w^L}{\partial E} + (m + \delta_{i4})\frac{\partial J}{\partial E} - T\right)\frac{\partial E}{\partial x_A} + \sigma_{Ai}\frac{\partial w^A}{\partial x_A} \tag{15}$$

but the sum in parentheses on the right-hand side is identically zero, due to equation (6), since $\partial J/\partial E = P(E)$, and $\partial w^K/\partial E = \tau^K$. Therefore

$$\left|\frac{\partial^2 S_{m,i}}{\partial x_A \partial x_B}\right| = \left|\frac{\partial^2 w^A}{\partial x_A \partial E}\frac{\partial E}{\partial x_B}\right|. \tag{16}$$

From equation (13) it follows that

$$\frac{\partial^2 w^{\mathrm{A}}}{\partial x_{\mathrm{A}} \partial E} \sim \frac{1}{\sqrt{(2E)}}. \tag{17}$$

Moreover, from equation (6),

$$\frac{\partial E}{\partial x_{\mathrm{B}}} = \frac{-\sigma_{\mathrm{B}i} \dfrac{\partial \tau^{\mathrm{B}}}{\partial x_{\mathrm{B}}}}{\left[\sigma_{\mathrm{B}i} \dfrac{\partial \tau^{\mathrm{B}}}{\partial E} + \sigma_{\mathrm{A}i} \dfrac{\partial \tau^{\mathrm{A}}}{\partial E} + 2\delta_{i2} \dfrac{\partial w^{\mathrm{R}}}{\partial E} + 2\delta_{i3} \dfrac{\partial w^{\mathrm{L}}}{\partial E} + (m + \delta_i) \dfrac{\partial P}{\partial E}\right]}. \tag{18}$$

In order to investigate the behaviour of $\partial E/\partial x_{\mathrm{B}}$ for large energy, we need the asymptotic representation of $\partial P/\partial E$; now, it is well known that it is not always possible to differentiate an asymptotic representation such as equation (8), and for a generic potential one has to assume the independent existence of an asymptotic expansion for $\partial P/\partial E$ or equivalent conditions [6]; however, it is easy to see that these conditions are fulfilled for polynomial potentials as given in equation (3) so that, from equation (8),

$$\frac{\partial P}{\partial E} \sim \frac{c(2-N)}{2N} E^{(2-3N)/(2N)}. \tag{19}$$

From equations (5) and (19) it follows that for large E, the leading term in the denominator in equation (18) is $m(\partial P/\partial E)$ with asymptotic behaviour

$$m \frac{\partial P}{\partial E} \sim T \frac{(2-N)}{2N} E^{-1}. \tag{20}$$

Putting together equations (16)–(18) and (20) it follows that, for large values of the energy,

$$A_{m,i} \sim \left(\frac{1}{2\pi\hbar}\right)^{1/2} \left(\frac{N}{(N-2)} \frac{1}{T}\right)^{1/2} \qquad (E \to \infty). \tag{21}$$

This equation shows that the asymptotic amplitude of the ABT paths' contributions to the semiclassical propagator does not depend on the path's energy: the ABT paths are therefore asymptotically equiprobable, and the results found in [1] for the $N = 4$ case, by directly computing the various quantities, are extended in this way to this more general case. The asymptotic equiprobability of the classical paths therefore appears to be a general property of one-dimensional motion in an infinitely deep potential well, under the above specified conditions. The physical interpretation of this result is the following: the amplitude of a classical path's contribution to the semiclassical propagator is a measure of the number of neighbouring constructively interfering paths, and this number, which is *a priori* different for the various paths, becomes asymptotically the same, while the path's energy increases.

This result also implies that the series (1) for the semiclassical propagator does not converge, but it can, in general, be resummed due to phase cancellation, as shown in the case of a quartic oscillator in [1].

These conclusions hold as long as x_{B} is not conjugate to x_{A} with respect to a path $x_i(t)$. In the latter case, the corresponding amplitude will diverge, as shown in [1], and that path's contribution will dominate the entire Van Vleck's series. This path will therefore be favoured with respect to the others. The discussion of this point is similar to the one given in [1], and will therefore be omitted here.

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