сообщения
объединенного
института
ядерных
исследований
дубна

E17-90-546

A.Radosz*, W.Magierski*

REAL TRAJECTORIES IN COMPLEX-TIME METHOD AND BARRIER PENETRATION-LIKE PHENOMENA

* Institute of Physics, Technical University of Wroclaw, Wybrzeze Wyspianskiego 27, 50-370 WROCLAW, Poland.

1990

1. Introduction

Problems involving barrier penetration phenomena might be discussed within a path integral formalism[1] by using propagator with complex-valued time parameter. Such an approach was firstly suggested by McLaughlin[2] (see also Ref.[3]) and next used by various authors e.g. Refs.[4-6] Eigenvalue problem in the case of double-well potential and the decay rate of the virtual level were studied in detail and results of ordinary quantum mechanics were obtained[7,8]. Although this method of real trajectories in complex time, leads to reasonable results which also agree with results of similar treatments[9-11] and which belong to regions determined by other predictions[12], there still have existed some questionable points.

Namely, in an eingenvalue problem, the energy levels, E_n, are found as zeros of the denominator of Green's function. In the first approximation for double-well potential (see below) the familiar splitting of energy levels[7]

$$E_n^{(\pm)} \cong E_n^{(o)} \pm \Delta E$$

might easily be found[4-6]. However, the exact solutions, E_n, obviously posses an imaginary part, so that they are not real! In the problem of decay of virtual level the decay rate is estimated by using a "smoothing procedure"[5] to exclude a dense part of spectrum. Any dense part may be predicted within treatment presented in Refs.[4-6] - zeros of the denominator of $G(E + i\delta)$ are rather well separated instead of forming dense spectrum. In Weiss and Haefner's approach[11]., where some quantitative differences in comparison with results of Refs.[4-6] were found, the above mentioned defects are also present.

The main purpose of this paper is to show that a proper way of summation over all closed (semi) clasical orbits in complex time[13-15] solves problems of this type. The energy eigenvalues E_n, both in the double-well and multiwell potentials, are real and a dense part of spectrum in a metastable state problem is actually present (and may be removed by a smoothing procedure). It will be shown that the method of real trajectories in complex time might also be used in discussion of (real) time-dependent phenomena. In the problem of the decay of virtual level, the escaping time of a particle from a metastable well is estimated, and it becomes in aggreament with inverse imaginary part of energy of false vacuum state. A phenomenon of jumping a particle between wells in the double-well potential will be reviewed as well.

To make the paper self - contained we start by short introduction of a method of real trajectories in complex time (Sec. 2). The eigenvalue problem for the double- and multiwell potentials (Sec. 3) and the problem of imaginary part of energy of a false vacuum state (Sec. 4) are then discused. In Sec. 5 the simplest cases of a time - dependent phenomena, escaping of a particle from a metastable well and jumping of a particle between two wells in the double-well potential, are considered and coincidence with results of indirect estimations of two earlier Sections is found. Final remarks are given in Sec. 6 and the details of summation over closed orbits are presented in Appendix.

2. Real trajectories and complex time-formalism

It is well-known that an agreement between semiclassical approximation of the path integral method[1], where the propagator

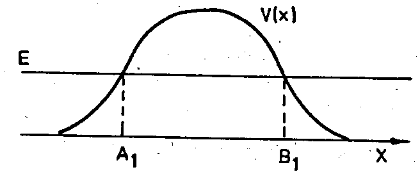
$K(x_2,x_1;T)$:

$$K(x_2,x_1;T)\equiv\langle x_2|\exp(-\tfrac{i}{\hbar}HT)|x_1\rangle=\int_{x(t_1=0)=x_1}^{x(t_2=T)=x_2} D[x(t)]\exp(-\tfrac{i}{\hbar}S[x]) \quad (2.1)$$

is dominated by trajectory of constant energy, and the WKB approximation of ordinary quantum mechanics, might be observed e.g. Ref[16]. Throughout this paper we shall discuss the case of particle with mass m within one-dimensional potential V(x), so that

$$S[x] = \int_0^T dt[\frac{m\dot{x}^2}{2} - V(x)].$$

It was shown by McLaughlin[2] that barrier penetration - like phenomena might be considered in the semiclassical approximation with time parameter extended onto complex plane (actually onto its lower, right part Im t ≤ 0, Re t ≥ 0). Such an approximation allows one to obtain propagator in the following form (see Fig. 1)



1. Semiclassical trajectory of constant energy with two turning points A, B.

$$\tilde{K}(x_2,x_1;t) \simeq [2\pi i k(x_2)k(x_2)]^{-\frac{1}{2}}\left[\left[\left(\int_{x_1}^{A_1} + \int_{B_1}^{x_2}\right)\frac{dx}{k^3(x)} - i\int_{A_1}^{B_1}\frac{dx}{\varkappa^3(x)}\right]^{-\frac{1}{2}}\right.$$

$$\exp(\tfrac{i}{\hbar}\tilde{S}), \quad (2.2)$$

where

$$k(x) = \frac{1}{\hbar}\sqrt{2m[E - V(x)]} \quad (2.2a)$$

$$\varkappa(x) = \frac{1}{\hbar}\sqrt{2m[V(x) - E]} \quad (2.2b)$$

$$\tilde{S} = \left(\int_{x_1}^{A_1} + \int_{B_1}^{x_2}\right)\hbar k(x)dx + i\hbar\int_{A_1}^{B_1}\varkappa(x)dx - Et \quad (2.2c)$$

$$t \equiv (t_R - it_I) \equiv \int_{x_1}^{x_2}\frac{dx}{\sqrt{\frac{2}{m}[E - V(x)]}} =$$

$$\left(\int_{x_1}^{A_1} + \int_{B_1}^{x_2}\right)\frac{dx}{\sqrt{\frac{2}{m}(E - V)}} - i\int_{A_1}^{B_1}\frac{dx}{\sqrt{\frac{2}{m}(V - E)}}. \quad (2.2d)$$

Propagator (2.2) is used in the asymptotical estimation of the Green's funcion G(x" x'|E)

$$G(x''\ x'|E) = \int_0^\infty \frac{dt}{2\pi\hbar}\tilde{K}(x''\ x';t)\exp\left[-\frac{i}{\hbar}(E + i\delta)t\right], \qquad (2.3)$$

where the contour of integration is deformed to pass the saddle point[2]

$$\frac{\partial}{\partial t}(\tilde{S} + Et) = 0. \qquad (2.4)$$

Finally $G(x''\ x'|E)$ is given as a sume over all fixed energy, path Eq.(2.4), with end points x' and x''

$$G(x''\ x'|E) = \frac{m}{2\pi\hbar}[k(x'')k(x')]^{-\frac{1}{2}}\sum_{paths}\prod_i f_i, \qquad (2.5)$$

where the factor f_i can be characterized via one of two sets of rules

1) propagation from x_a to x_b in a classically allowed region yields

$$\exp\left(i\int_{x_a}^{x_b}k(x)dx\right)$$

2) propagation from x_c to x_d in a classically forbiden region yelds

$$\exp\left(-\int_{x_c}^{x_d}\varkappa(x)dx\right)$$

and[4-6]

3') a factor (i) is yielded at each turning point[5,6] $E = V(x)$

or alternatively[13-15]

3") reflection at turning point $E = V(x)$ within classically allowed (forbiden) region yelds factor $-i(\frac{1}{2})$.

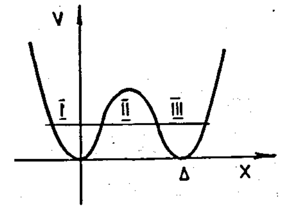
It turned out that rules 1-3') and 1-3") yielded the same results up to the first order approximation in the case of double-well potential. However, higher order corrections, which are not discussed, usually behave in different ways within 1-3') and 1-3") sets of rules.

3. The eigenvalue problem

The energy eigenvalues, E_n, may be found as the poles of Green's function $G(E)$[18,10]

$$G(E) = \int dx G(x,x|E) \qquad (3.1)$$

In the most simple, non-trivial case, of the double-well potential $V(x)$ (see Fig.2) the denominator of $G(E)$ calculated according to



2. Symmetric double-well potential.

rules 3') and 3") has the following form (see Appendix)

$$a)\quad G^{-1}(E) \sim (1 + a_1^2)(1 + a_2^2) + b_I^2 \qquad (3.2a)$$

$$b)\quad G^{-1}(E) \sim (1 + a_1^2)(1 + a_2^2) + \frac{1}{4}b_I^2(1 - a_1^2)(1 - a_2^2) \qquad (3.2b)$$

respectively, where

$$a_i = \exp(-iW_i), \quad (i = 1, 2) \qquad (3.3a)$$

$$b_I = \exp(-W_I) \qquad (3.3b)$$

$$W_i = \int_{B_{i-1}}^{A_i}k(x)dx, \quad (i = 1, 2) \qquad (3.3c)$$

$$W_I = \int_{A_1}^{B_1}\varkappa(x)dx \qquad (3.3d)$$

Let us shortly discuss the main differences between formula (3.2a) and (3.2b), in symmetric and asymmetric cases.

1. Symmetric double-well potential.

The properties of potential

$$V(x) = \frac{B}{4}(x^2 - \frac{A}{B})^2 \qquad (3.4)$$

have been widely discussed[5-7,15,19,20] and it is said that low-lying levels are splitted into pairs due to the tunneling effect. In this case

$$a_1^2 = a_2^2 \equiv a^2,$$

and low-lying energy levels, $E = E_n$,

$$G(E_n) = 0, \qquad (3.5)$$

in the zeroth order approximation, $E = E_n^0$, $b_I^2 = 0$

$$1 + a^2 = 0, \qquad (3.6a)$$

$$W_1(E_n^0) = (n + \frac{1}{2})\pi, \qquad (3.6b)$$

and in the first order approximation, $E = E_n^{\pm}$, $b_I^2 \neq 0$

$$(1 - a^2) \simeq 2 \qquad (3.7a)$$

$$(1 + a^2)^2 + \frac{1}{4}b_I^2(1 - a^2)^2 \simeq (1 + a^2)^2 + b_I^2 = 0 \qquad (3.7b)$$

$$E_n^{\pm} = E_n^0 \pm \Delta E_n \qquad (3.7c)$$

$$\Delta E_n = \frac{1}{2}\left(\frac{\partial W_1}{\partial E}\right)\Bigg|_{E_n^0}^{-1} e^{-W_I(E_n^0)} \equiv \frac{h\omega}{2\pi}e^{-W_I(E_n^0)} \qquad (3.7d)$$

are the same within rules 3') and 3")[17]. However the meaning of results (3.2a) and (3.2b) is different! Let us note that for real E

$$|a^2| = 1$$

and Eq. (3.5) in the first case (3.2a)

$$(1 + a^2)^2 = -b_I^2 < 0 \qquad (3.8)$$

has no real solutions. Its real solutions $E_n^{\pm}$, Eq. (3.7c), exist only in the first order approximation, whereas higher order corrections must be complex. On the other hand, Eq. (3.5) in the second case (3.2b)

$$(1 + a^2)^2 = -\frac{1}{4}b_I^2(1 - a^2)^2 \qquad (3.9a)$$

might be rewritten as

$$\mathrm{ctg}^2[W_1(E)] = \frac{1}{4}\exp[-W_I(E)] \,. \qquad (3.9b)$$

Solution of Eq. (3.9b) real (obviously each term in expansion with respect eventually small parameter b_I is also real) and being gathered into characteristic pairs deep enough within wells, might be arranged in a less regular way for higher levels. The difference between results of treatement 3') and 3") is more apparent in the case of

2. Asymmetric double-well potential.

There is no any reasonable approximation which might lead to real energy levels E_n, within rule 3')

$$(1 + a_1^2)(1 + a_2^2) + b_I^2 = 0 \qquad (3.10)$$

in such a case (see Fig. 3). On the other hand within 3"), real solution of eigenvalue problem (see Eq. (3.2b))

$$(1 + a_1^2)(1 + a_2^2) + \frac{1}{4}b_I^2(1 - a_1^2)(1 - a_2^2) = 0 \qquad (3.11)$$

obviously exist as solution of an equivalent equation

$$\mathrm{ctg}[W_1(E)]\,\mathrm{ctg}[W_2(E)] = \frac{1}{4}b_I^2 = \frac{1}{4}\exp[-2W_I(E)] \qquad (3.11a)$$

Plot of funcion $\mathrm{ctg}\alpha$ guarantees a finite sequence of such solutions E_n (<V_0). Higher levels, $E > V_0$ are found from a familiar equation

$$1 + a^2 = 0, \quad (W(E) = (n + \tfrac{1}{2})\pi h). \qquad (3.12)$$

The method 1-3") summation over all closed orbits presented in Appendix might be used in the case of multiwell potential. In the case of three-well potential, one has to assume that there are two addidional turning points B_2 and A_3 (see Fig. 4). Therefore, in the right-hand side of Eq. (3.2b) one should change

$$a_2^2 \to A_2^2 = a_2^2(1 + e^{i\frac{\pi}{2}}O_{A_2}) = a_2^2\left[1 - \frac{2(\frac{1}{2}b_{II})^2(1 - a_3^2)}{(1 + a_3^2) + \frac{1}{2}b_2^2(1 - a_3^2)}\right], \qquad (3.13)$$

where

$$b_{II} = \exp[-W_{II}(E)], \qquad W_{II}(E) = h\int_{A_2}^{B_2}\varkappa(x)\,dx$$

$$a_3 = \exp[iW_3(E)], \qquad W_3(E) = \hbar\int_{B_2}^{A_3}k(x)\,dx \,.$$

Energy levels are found as solution of the following equation

$$0 = (1 + a_1^2)(1 + a_2^2)(1 + a_3^2) + (1 + a_1^2)(\tfrac{1}{2}b_{II})^2(1 - a_2^2)(1 - a_3^2)$$

$$+ (1 + a_2^2)(\tfrac{1}{2}b_I)^2(\tfrac{1}{2}b_{II})^2(1 - a_1^2)(1 - a_3^2)$$

$$+ (1 + a_3^2)(\tfrac{1}{2}b_I)^2(1 - a_1^2)(1 - a_2^2) \qquad (3.14)$$

and one can rather easy show that Eq. (3.14) has real solution found from

$$\mathrm{ctg}[W_1(E)]\mathrm{ctg}[W_2(E)]\mathrm{ctg}[W_3(E)] = (\tfrac{1}{2}b_{II})^2\mathrm{ctg}[W_1(E)]$$

$$+ \tfrac{1}{2}(b_I)^2\mathrm{ctg}[W_3(E)] + (\tfrac{1}{2}b_I)^2(\tfrac{1}{2}b_{II})^2\mathrm{ctg}[W_2(E)] \,. \qquad (3.15)$$

In the case of one large barrier, e.g. $b_I \simeq 0$, Eq. (3.15) leads to the formulae for energy levels in a separate single well

$$\mathrm{ctg}W_1 = 0 \qquad (3.16a)$$

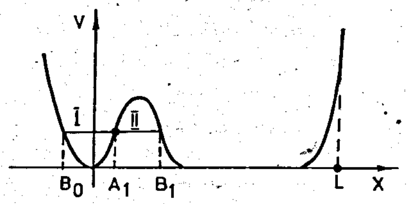
and double-well

$$\mathrm{ctg}W_2\,\mathrm{ctg}W_3 = \frac{1}{4}b_{II}^2 \qquad (3.16b)$$

as one is expected.

4. Decay of a metastable state

The decay of a metastable state-problem may be discussed in the model of asymmetrical double-well potential (Fig.3). It has usually



3. Asymmetric double-well potential.

been assumed[5,6,11] that the infinite wall in the right well at $x = L$ is for away and/or might eventually be removed to infinity, $L \to \infty$. According to 1-3'), equation for energy levels (3.10) was obtained, and in the zeroth order

$$b_I = 0,$$

discrete spectrum in the left well

$$W_1(E_l^0) = (l + \tfrac{1}{2})\pi, \qquad (4.1)$$

and quasicontinous spectrum in the right well

$$W_2(E_r^0) \approx \frac{1}{h} L\sqrt{2mE_r^0} = (r + \tfrac{1}{2})\pi, \qquad (4.2)$$

were found. Then, the smoothing procedure for density of states $\rho_\gamma(E)$[5,6]

$$\rho_\gamma(E) = \frac{1}{\pi} \mathrm{Im}G(E + i\gamma)$$

provided complex poles, in the first order in b_I, for E_l

$$E_l \cong \mathrm{Re}E_l - i\Gamma_l \approx E_l^0 - i\Gamma_l$$

$$\Gamma_l = \frac{1}{2}\left(\frac{\partial W_1}{\partial E}\right)\Big|_{E_l^0}^{-1} e^{-2W_I(E_l^0)} \equiv \frac{h\omega(E_l^0)}{2\pi} e^{-2W_I(E_l^0)}. \qquad (4.3)$$

However, as is has been discussed in previous section there is no real solution of Eq. (3.10) in this case also in the first order approximation in b_I ($\ll 1$). Therefore, a quasicontinous spectrum is only zeroth-order approximation effect and there is no any reason to consider smoothed density function. On the other hand, Holstein[15] assumed that the wall in the right well is at infinity and "no reflection is allowed". Then

$$a_2 = 0 \qquad (4.4)$$

and Eq. (3.11) leads to the formulae

$$E_n \cong E_n^0 - i\Gamma_n \qquad (4.5)$$

$$\Gamma_n = \frac{1}{4}\left(\frac{\partial W_1}{\partial E}\right)\Big|_{E_n^0}^{-1} e^{-2W_I(E_n^0)} \qquad (4.6)$$

which reproduces WKB-type result and differs from Patrascioiu results (4.3) by factor $\frac{1}{2}$.

One can show that inconsequences of the former treatment 1-3'), Eqs. (4.1 - 3), do not appear in a later one 1-3") and it is not necessary within this approach to remove a wall to infinity.

The spectrum of energy levels determined by Eq. (3.11) turns out to be quasicontinuous in the case of large asymmetry

$$\mathrm{ctg}(W_1(E))\,\mathrm{ctg}(\tfrac{1}{2}L\sqrt{2mE}) = \tfrac{1}{4}\exp[-2W_I(E)] \qquad (4.7a)$$

$$(E_{n+1} - E_n) \sim \frac{1}{L^2} \qquad (4.7b)$$

with fluctuations of density states around

$$E \sim E_l^0$$

(Eq. (4.1)). One finds that smoothed density function $\rho_\gamma(E)(= \frac{1}{\pi}\mathrm{Im}G(E + i\gamma)$, with

$$\gamma \gg \Delta E_n = E_{n+1} - E_n \sim \frac{1}{L^2}, \qquad (4.8)$$

$$a_2 = \exp[iW_2(E + i\gamma)] \approx 0, \qquad (4.9)$$

has pols in the complex E-plane (Eq. (3.11))

$$(1 + a_1^2) + \tfrac{1}{4}(1 - a_1^2)b_1^2 = 0, \qquad (4.10)$$

and in the first order approximation in b_1

$$E_l = E_l^0 - i\Gamma_l,$$

where E_l^0 and Γ_l are given by Eqs.(4.1) and (4.6), respectively. Higher order corrections may be found from Eq. (4.10) and they fulfill the condition of asymptotic expansion found by Combes et al[12]. Let us note that the smoothin procedure (4.8 and 9) is equivalent to the summation over all trajectories belonging to the region $x_1 - x_2$ (Fig. 3). This will help us in direct interpretation of $\frac{1}{h}\Gamma_0$ as the inverse life-time of a particle in the left well.

5. Life-time of a false vaccum state

In this section we shall show that the method of complex time and real trajectories can be used in discussion of explicitly time-dependent phenomena. Let us estimate the time of decay a metastable state formulating the problem as follows:

How much time does the particle originally placed in the left well (Fig. 3) need, to escape throught a potential barrier? One can say that we are interested in a time evolution of (an appropriate) wave packet, localized at $t = 0$ somewhere around $x = 0$. In this case propagator $K(x'',x':T)$ is evaluated as a Laplace transform of a Green's function $G(x'',x'|E)$

$$K(x'',x';T) = \int_0^\infty e^{\frac{i}{\hbar}ET} G(x'',x'|E)dE. \tag{5.1}$$

According to the results of Secs. 2 and 4 $G(x'',x'|E)$ is a sume over all trajectories of constant energy, Eq. (2.5), starting (x') and ending (x'') within classically allowed region x_1 y_1, and eventually penetrating classically forbiden region y_1 x_2.

Therefore,

$$G(x'',x'|E) = \sum_{n=0}^{\infty} G_0^{(n)}(x'',x'|E)\left[1 + e^{i\frac{\pi}{2}} O_{B1}\right]^n$$
$$= \sum_{n=0}^{\infty} G_0^n(x'',x'|E)\left[1 - 2\frac{\frac{1}{4}b_I^2}{1+\frac{1}{4}b_I^2}\right]^n, \tag{5.2}$$

n-th trajectory comes n-times to the point y_1 from a classically allowed region x_1y_1. Inserting result (5.2) into Eq. (5.1) and using stationary phase approximation [13,16] one obtains

$$K(x'',x';T) = K_0^{(p)}(x'',x';T)\left[1-2\frac{\frac{1}{4}b_I^2}{1+\frac{1}{4}b_I^2}\right]^p\Bigg|_{E=\bar E}, \tag{5.3}$$

where $\bar E$ is defined by stationary condition

$$T = \int_{x'_{(p)}}^{x''} \frac{dx}{\sqrt{\frac{2}{m}(\bar E - V)}}, \tag{5.3a}$$

(p) fixes an appropiate trajectory (p - classical reflections at y_1), and

$$K_0^{(p)}(x'',x';T) = \left[\frac{1}{2\pi i\hbar^3}\right]^{\frac{1}{2}}(k(x'')k(x'))^{-\frac{1}{2}}\left[\int_{x'_{(p)}}^{x''}\frac{dx}{\sqrt{2m(\bar E - V)}^3}\right]^{-\frac{1}{2}}$$
$$\exp\left\{\frac{i}{\hbar}\left[\int_{x'_{(p)}}^{x}\sqrt{2m(\bar E - V)}dx - ET\right]\right\} \tag{5.3b}$$

At that point one can again invoke a suggestion of previous Section and choose as a "false vacuum" state a ground state of a left well. Thus, using a harmonic approximation in $K_0^{(p)}(x'',x';T)$

$$V(x) \simeq \frac{1}{2}V''(0)x^2 \equiv \frac{1}{2}m\omega^2x^2 \tag{5.4a}$$

and placing originally the particle in a state $_0(x)$

$$\Psi_0(x) = \left[\frac{\pi^2\hbar}{m\omega}\right]^{\frac{1}{4}}\exp\left[-\frac{1}{2}\left[\frac{m\omega}{\hbar}\right]x^2\right] \tag{5.4b}$$

one finds

$$\Psi(x'',T) = \int dx' K(x'',x';T)\Psi_0(x') = e^{i\frac{\omega T}{2}}\Psi_0(x'')\left[1 - 2\frac{\frac{1}{4}b_I^2}{1+\frac{1}{4}b_I^2}\right]^p_{\bar E=0}. \tag{5.5}$$

where integral in the above equation is, as usually, taken within saddle point approximation [2,13,16]. Amplitude of probability of finding a particle in an original state Ψ_0 after time t

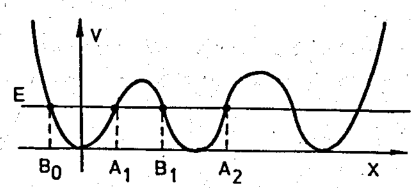
$$A_1 = \left|\int dx\Psi_0(x)\Psi(x,t)\right| = \left[1-2\frac{\frac{1}{4}b_I^2}{1+\frac{1}{4}b_I^2}\right]^p_{\bar E=0} \tag{5.6}$$

in the limit of small $b_I(\ll 1)$, vanishes exponentially, $A_1 \sim e^{-1}$, for large enough p

$$p \sim \bar p = \left[2\frac{\frac{1}{4}b_I^2}{1+\frac{1}{4}b_I^2}\right]^{-1} \approx \left[\frac{1}{2}e^{-2W_I(E=0)}\right]^{-1}. \tag{5.7}$$

On the other hand, large p means (see Eq. (5.3a)):

$$T \sim p\,\frac{2\pi}{\omega}, \tag{5.8}$$



4. Multi-(three)-well potential.

so that, time τ_o the particle needs to escape from the left well is

$$\tau_o \sim \frac{2\pi}{\omega}\,\bar{p} = \frac{2\pi}{\omega}\left(\frac{1}{2}b_1^2\right)^{-1} = 4h\left(\frac{\partial W_1(E)}{\partial E}\right)\Bigg|_{E=E_o=h\omega/2} \exp[2W_I(E=0)]\ , \qquad (5.9)$$

the same, with a good accuracy, as the inverse width of a false vacuum state $\left(\frac{1}{h}\Gamma_o\right)^{-1}$ found in previous Section, Eqs.(4.6) and (4.11). The limitations of the above approach are obvious. In propagator $K(x'',x';T)$, Eq.(5.1), we have omitted the contribution associated with propagation through the classically allowed region $x_2\ y_2$ (see Fig.3 and Eq.(5.2)). It takes at least time interval $\bar{t}$

$$\bar{t} = 2T_r(E_o) = 2\int_{x_2}^{y_2}\frac{dx}{\sqrt{\frac{2}{m}(E-V)}} \approx 2\left(\frac{h\omega}{m}\right)^{-\frac{1}{2}}L\ , \qquad (5.10)$$

and the approach is expected to be valid only if the following condition

$$\tau_o \ll \bar{t} = 2T_r(E_o) \qquad (5.11)$$

is satisfied (see also Ref.[5]).

At last we shall discuss another time-dependent phenomenon: we estimate time the particle needs for jumping from one well to the other one in the symmetric double-well potential case. The two-lowest level approximation, $\Psi_+(E_+)$, $\Psi_-(E_-)$, produces an obvious result[1,20].

By assumption $\Psi_L(\Psi_R)$ is a wave function localized in the left (right) well and

$$\Psi_{L(R)} = \frac{1}{\sqrt{2}}\,(\Psi_+ (\mp)\, \Psi_-)\ . \qquad (5.12)$$

The amplitude of probability of transition from the left to the right well is

$$\langle\Psi_R|e^{iHt/h}|\Psi_L\rangle = ie^{iE_ot/h}\sin\,(\Delta E_o t/h) \qquad (5.13)$$

so that the particle initially localized in the left well may be found in the right well after time t_o (c.f. Eq.(3.7d))

$$t_o \sim \frac{h}{\Delta E_o} = 2\frac{2\pi}{\omega}e^{W_I(E_o=h\omega/2)}, \qquad (5.14)$$

In our method where approximations have quite different sense than two-lowest level cut-off, the Green's function $G(x'',x'|E)$ involving

trajectories starting in the left well (x') and ending in the right well (x'') might easily be found, at least in the lowest (first) order in b_1:

$$G(x'',x'|E) \approx \left[\sum_{n_1=0}^{\infty} G^{(n_1)}(y_1,x'|E)\right]b_1(E)\left[\sum_{n_2=0}^{\infty} G^{(n_2)}(x'',x_2|E)\right] \qquad (5.15)$$

where n_1 (n_2) denotes the number of closed loops within the left (right) well. As the wells are symmetric, one obtains in this case:

$$G(x'',x'|E) = iG^{(0)}(y'',x'|E)\; b_I(E)\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\exp(-i[2(n_1+n_2)-1]W_1(E))\ , \qquad (5.16)$$

where

$$y'' = x'' - \Delta$$

$$G^{(0)}(y'',x'|E) = \exp\left[i\int_{x'}^{y''}k(x)\,dx\right]\ . \qquad (5.16a)$$

Therefore, propagator $K(x'',x';T)$, Eq.(5.1), calculated in approximation (5.16) is determined as follows:

$$K(x'',x';T) = K_o^{(n_o)}(x''-\Delta,x';T)\,b_I(\bar{E})(n_o+1)\ , \qquad (5.17)$$

where $\bar{E}$ is defined by equation

$$T = \int_{x'}^{y''}\frac{dx}{\sqrt{\frac{2}{m}(\bar{E}-V)}} + \left(2n_o-\frac{1}{2}\right)\oint\frac{dx}{\sqrt{\frac{2}{m}(\bar{E}-V)}}\ . \qquad (5.18)$$

As the transition amplitude, A, of the particle from the left well:

$$\Psi_o(x)\equiv\Psi_L(x) = \left(\frac{\pi^2 h}{m\omega}\right)^{\frac{1}{4}}\exp\left(-\frac{1}{2}\frac{m\omega}{h}x^2\right) \qquad (5.19)$$

to the right well, $\Psi_R(x) = \Psi_L(x-\Delta)$ after time T, is determined by propagator (5.17), thus

$$\begin{aligned} A &= \left|\int\Psi_R(x)\Psi(x,T)\,dx\right| = \left|\int dx\,\Psi_R(x)\int dx'\,K(x,x';T)\Psi_L(x')\right| \\ &= \left|\int dx\,\Psi_R(x)(n_o+1)\,b_I(\bar{E}=0)\,e^{i\omega T/2}\Psi(x-\Delta)\right| \\ &= \left|(n_o+1)\,b_I(\bar{E}=0)\,e^{i\omega T/2}\right|, \end{aligned} \qquad (5.20)$$

Therefore, the probability P_{tr} of transition from the left well to the right well

$$P_{tr} = A^2 = |(n_o+1)b_I(E=0)|^2 \sim 1 \qquad (5.21)$$

for

$$n_o \sim b_I^{-1}. \qquad (5.22)$$

This means that after time t_o

$$t_o \sim n_o 2\frac{2\pi}{\omega} = 2\frac{2\pi}{\omega}\exp[W_I(E=0)] \qquad (5.23)$$

a particle is expected to appear in the right well. This estimation, (5.23), is in a good accuracy with result of above cited two lowest-level approximation (5.14).

6. Conclusion

In this paper various aspects of complex time and real trajectories method have been discussed. It was shown earlier that this approximation might be useful in diferent problems, reproducing WKB-type results and as, trajectory of constant energy plays distinguished role both local and global properties of single particle potential V(x) are taken into account, as one expects in a semiclassical approximation. However, the validity of this method seemed to be questionable because of some unclear points, among whose, the problem of reality energy eigenvalues was the most impressive. It was shown here that following a proper way of summation over closed orbits, one can not only remove these difficulties but also extend the region of applicability of the method. Namely, in the symmetric double-well potential case one obtains the equation which yields real energy eigenvalues E_n, as it should be, and contrary to WKB-type approximation, there is no any limitation to the low-lying levels. In the case of asymmetric double-well potential the equation for energy eigenvalues still produces sequence of real numbers and in the limit of large asymmetry a quasicontinuous spectrum is found. Therefore, the smoothing procedure can actually be used to estimate a width of a false

ground state. The results for symmetric and asymmetric potentials are in agreement with mathematically well-justified predictions[12].

We also have shown that extension of a time parameter onto the complex plane is useful in estimation of G(x",x'|E) and does not prevent us to discuss (real) time-dependent phenomena. Two of this type problems have been considered. The direct estimation of life-time in a metastable state and time of jumping between wells for particle in asymmetric and symmetric potentials, respectively, turned out to be in good agreement with indirect estimations. In a natural way, the criterion of almost impossible phenomenon which takes place with exponentially small probability, $p < e^{-1}$, has appeared.

We want to emphasize that the method of complex time and real trajectories seems to be consistent, semiclassical, approximation which might be used in studies of barrier penetration-like phenomena. Some of its predictions should however, still be investigated. First of all it ought to be verified out of the range of applicability of standard WKB approximation, so the energy eigenvalue spectrum near local maxima of potential V(x) should be studied (see also Ref.[21]). One can expect that further studies would improve consitency between direct, Eq.(5.9), and indirect, Eq.(4.6) (see also Eqs.(5.23) and (5.14)) predictions for time-dependent phenomena. Another time dependent phenomenon, tunneling effect, is beyond the scope of this paper and will be discussed elsewhere but as the result is in that case rather unexpected and differs from the well-known results. We feel that the range of the applicability above considered method is yet far from being well-established.

Acknowledment

One of us (A.R.) is greatly indebted to Prof. J.Czerwonko and Prof. P.Eksner for encouraging and discouraging, respectively, discussions.

Appendix

On the example of the double-well (see Fig.3) potential we show how the Green's function $G(E)$ might be calculated. As the summation over all closed orbits should be done in $G(E)$, one can write it down in this case [4,5,11,15]

$$G(E) = G_1(E) + G_I(E) + G_2(E), \qquad (A.1)$$

where

$$G_\mu(E) = T_\mu(E) \sum_{paths} \exp[iW_{path}(E)], \quad (\mu = 1,2,I) \qquad (A.2)$$

$$T_i(E) = 2\int_{B_{i-1}}^{A_i} \frac{dx}{\sqrt{\frac{2}{m}(E - V(x))}}, \quad (i = 1,2) \qquad (A.3a)$$

$$T_I(E) = (-i)2\int_{A_1}^{B_1} \frac{dx}{\sqrt{\frac{2}{m}(V(x) - E)}}. \qquad (A.3b)$$

Then, one finds

$$G_1(E) = T_1(E)a_1^2e^{-i\pi/2}(e^{-i\pi/2} + O_{A_1})$$
$$\{1 + a_1^2e^{-i\pi/2}(e^{-i\pi/2} + O_{A_1})\{\ldots\}\ldots\} =$$
$$= -T_1(E)\frac{a_1^2(1 + e^{i\pi/2}O_{A_1})}{1 + a_1^2(1 + e^{i\pi/2}O_{A_1})}, \qquad (A.4)$$

where O_{A_1}, contribution from all trajectories starting and ending at A_1 and passing region right of A_1, might be calculated according to

a) 1 – 3') rules

$$O_{A_1} = O'_{A_1} = e^{-i\pi/2}b_I^2(e^{-i\pi/2} + O'_{B_1})\{e^{-i\pi/2} + e^{-i\pi/2}b_I^2$$
$$(e^{-i\pi/2} + O'_{B_1})\{\ldots\}\ldots\} =$$
$$= -e^{-i\pi/2}\frac{b_I^2(1 + e^{i\pi/2}O'_{B_1})}{1 + b_I^2(1 + e^{i\pi/2}O'_{B_1})}, \qquad (A.5a)$$

or, to

b) 1 – 3") rules

$$O_{A_1} = O''_{A_1} = b_I^2(\tfrac{1}{2}e^{i\pi/2} + O''_{B_1})\{1 + \tfrac{1}{2}b_I^2e^{i\pi/2}(\tfrac{1}{2}e^{i\pi/2} + O''_{B_1})\{\ldots\}\ldots\}$$
$$= -e^{-i\pi/2}\, 2\,\frac{\frac{1}{4}b_I^2(1 + 2e^{-i\pi/2}O''_{B_1})}{1 + \frac{1}{4}b_I^2(1 + 2e^{-i\pi/2}O''_{B_1})}. \qquad (A.5b)$$

O_{B_1} is contribution from all orbits starting and ending at B_1 and passing the region right of B_1 (see Fig.3). Formula for O'_{B_1} and O''_{B_1}

a) $$O'_{B_1} = e^{-i\pi/2}\, a_2^2\, e^{-i\pi/2}(e^{-i\pi/2} + e^{-i\pi/2}\, a_2^2\, e^{-i\pi/2}$$
$$(e^{-i\pi/2} + \ldots)\ldots) = -e^{-i\pi/2}\frac{a_2^2}{1 + a_2^2}, \qquad (A.6a)$$

b) $$O''_{B_1} = a_2^2\, e^{-i\pi/2}(1 + e^{-i\pi/2}\, a_2^2\, e^{-i\pi/2}(1 + \ldots)\ldots)$$
$$= -e^{-i\pi/2}\frac{a_2^2}{1 + a_2^2}, \qquad (A.6b)$$

are found to be the same. Inserting results (A.6) and (A.5) into (A.4) and repeating the procedure for $G_2(E)$ and $G_I(E)$, we finally obtain

$$G'(E) = -\frac{T_1(E)\, a_1^2\,(1 + a_2^2) + T_I(E)\, b_I^2 + T_2(E)\, a_2^2\,(1 + a_1^2)}{(1 + a_1^2)(1 + a_2^2) + b_I^2}. \qquad (A.7a)$$

$$G''(E) = -\left\{\frac{T_1(E)\, a_1^2\,[(1 + a_2^2) - \frac{1}{4}\, b_I^2\,(1 - a_2^2)]}{(1 + a_1^2)(1 + a_2^2) + \frac{1}{4}\, b_I^2\,(1 - a_1^2)(1 - a_2^2)}\right.$$
$$+ \frac{T_I(E)\,\frac{1}{4}\, b_I^2\,(1 - a_1^2)(1 - a_2^2)}{(1 + a_1^2)(1 + a_2^2) + \frac{1}{4}\, b_I^2\,(1 - a_1^2)(1 - a_2^2)}$$
$$\left.+ \frac{T_2(E)\, a_2^2\,[(1 + a_1^2) - \frac{1}{4}\, b_I^2\,(1 - a_1^2)]}{(1 + a_1^2)(1 + a_2^2) + \frac{1}{4}\, b_I^2\,(1 - a_1^2)(1 - a_2^2)}\right\}. \qquad (A.7b)$$

References

1. R.P.Feynman and A.R.Hibbs, Quantum mechanics and path integrals (McGraw-Hill, New York, 1965).
2. D.W.McLaughlin, J.Math.Phys. 13, 1099 (1972).
3. K.F.Freed, J.Chem.Phys. 56, 692 (1971).
4. S.Levit, J.W.Negele and Z.Paltiel, Phys.Rev.C 22, 1979 (1980).
5. A.Patrascioiu, Phys.Rev.D 24, 496 (1981).
6. A.Lapedes and E.Mottola, Nucl.Phys.B 203, 58 (1982).
7. A.Martin Sánchez and J.Diaz Bejarano, J.Phys.A: Math.Gen. 19, 887 (1986).
8. J.A.Caballero Carretero and A.Martin Sánchez, J.Math.Phys. 28, 636 (1987).
9. E.Gildener and A.Patrascioiu, Phys.Rev.D 16, 423 (1977).
10. R.Rajaraman, Solitons and Instantons (North-Holland, 1982).
11. U.Weiss and W.Haefner, Phys.Rev.D 27, 2916 (1983).
12. J.M.Combes, P.Duclos, M.Klein and R.Seiler, Commun.Math.Phys. 110, 215 (1987).
13. B.R.Holstein and A.R.Swift, Am.J.Phys. 50, 833 (1982).
14. B.R.Holstein, Am.J.Phys. 51, 897 (1983).
15. B.R.Holstein, J.Phys.C: Solid State Phys. 19, L279 (1986).
16. B.R.Holstein and A.R.Swift, Am.J.Phys. 50, 829 (1982).
17. A.Radosz, J.Phys.C: Solid State Phys. 19, L345 (1986).
18. R.Dashen, B.Hasslacher and A.Neveu, Phys.Rev.D 10, 4114 (1974).
19. A.Radosz, J.Phys.C: Solid State Phys. 18, L189 (1985).
20. A.J.Leggett, S.Chakravarty, A.T.Dorsey, M.P.A.Fisher, A.Garg and W.Zwerger, Rev.Mod.Phys. 59, 1 (1987).
21. A.Radosz J.Phys.C: Solid State Phys. 19, L31 (1986).

Received by Publishing Department
on December 5, 1990.