

Boundary effects on the sojourn time of two-dimensional inverted inverse quadratic oscillator in a wedge

LE Jiayi, CHEN Yin, PAN Xiaoyin*

(School of Physical Science and Technology, Ningbo University, Ningbo 315211, China)

Abstract: By employing the Feynman path-integral approach, we investigate the sojourn time of the two-dimensional inverted inverse quadratic oscillator in a wedge with external angle $a\pi$ ($0 \leq a < 2$). The exact expressions for the wave function and the corresponding density are obtained analytically, then the sojourn time as a function of a is calculated numerically. It is shown that the sojourn time monotonically increases as the external angle increases, but there is a big jump in the limit of $a \rightarrow 2$ implying that there is a huge difference between the case when the wedge becomes a singular line and the one without a wedge. In other words, although a singular line does not occupy any area in the two-dimensional space, the sojourn time can still be reduced dramatically due to the existence of the singular line, which may indicate the importance of the boundary condition.

Key words: boundary effect; sojourn time; path-integral; wedge

CLC number: O413.1

Document code: A

Article ID: 1001-5132 (2022) 01-0105-07

1 Introduction

Boundary conditions play important roles in almost all areas of classical and quantum physics, including classical electrodynamics^[1], quantum field theory^[2] and its applications on condensed matter (such as quantum Hall effect^[3-6], quantum dots and wires^[7-11], graphene^[12-14], etc), and fundamental physics like quantum gravity^[15] and cosmology^[16], as well as in quantum mechanics (QM)^[17]. It is well known that the original approach to QM due to Heisenberg and Schrödinger is based on the Hamiltonian formalism, while the Feynman's path integral method^[18-20] is a Lagrangian approach. However, Feynman's approach becomes more intricate than the Hamiltonian operator approach and requires a sophisticated implementation

for systems constrained to bounded domains^[21].

The wedge problem, namely the propagation of radiation or particles in the presence of a wedge, as a typical example that shows the significance of boundary condition both in classical and quantum physics has a long history. The earlier work could date back to Sommerfeld's^[22] calculation of diffraction of light by a wedge in 1896. Later, Pauli also studied the wedge problem^[23] in the context of diffraction of light.

The quantum version of the wedge problem has been attacked by several groups using path integral techniques independently. Crandall^[24] and DeWitt-Morette^[25] calculated the propagator for a free particle interacting with a rational wedge. Schulman^[26] and Wiegell et al^[27] obtain, respectively, the exact propagator of a free particle interacting with a harmonic oscillator,

收稿日期: 2021-10-08.

宁波大学学报(理工版)网址: <http://journallg.nbu.edu.cn/>

基金项目: 国家自然科学基金(11375090).

第一作者: 乐家怡(1996-), 女, 浙江慈溪人, 在读硕士研究生, 主要研究方向: 量子力学. E-mail: 592981258@qq.com

*通信作者: 潘孝胤(1974-), 男, 浙江宁海人, 研究员, 主要研究方向: 凝聚态理论. E-mail: panxiaoyin@nbu.edu.cn

both interacting with an infinite half-plane barrier. Later Cheng^[28] generalized their results to the case in the additional presence of a harmonic oscillator potential, the case when the wedge is irrational^[29], and further to the case of a two-dimensional inverse quadratic oscillator interacting with a wedge^[30].

On the other hand, the calculation of sojourn time which measures the limited time for a particle to sojourn near an unstable equilibrium, is a fundamental problem in quantum mechanics^[31-36]. The problem is often idealized drastically and reduces to the behavior of a particle in an inverted harmonic oscillator potential which is exactly solvable and has wide applications in many areas such as evolution of cosmology^[37], reactive scattering^[38], masers^[39], and can serve as a test ground for various approximation methods^[40]. Especially, the AB effect on the sojourn time of an inverted two-dimensional (2D) harmonic oscillator under a perpendicular uniform magnetic field has been studied recently^[41], and the quantum effect of the integer part of the flux quantum number is manifested for the first time.

In order to find the role played by the boundary condition on the sojourn time, in the present work we study the sojourn time of the 2D inverted inverse quadratic oscillator interacting with a wedge. This model describes a particle confined in an inverted harmonic oscillator, plus an additional potential g/r^2 with $g > 0$ (which can be used to describe a quantum antidot^[42]) interacting with the wedge.

2 The model and evolution of the Gaussian wave packet

Consider a system of an electron of charge $q = -e$ and mass μ confined by an inverted 2D harmonic oscillator potential in a wedge along the z -axis with external angle $a\pi$, see Fig. 1. Then with $\mathbf{r}(r, \theta) = (x, y)^T$ denoting the 2D position vector, the Hamiltonian (in international units) of the so called inverse quadratic oscillator model, which is an inverted harmonic oscillator interacting with an inverse square

potential, takes the form:

$$\hat{H}_0 = \frac{1}{2\mu} \hat{p}^2 - \frac{1}{2} \mu \omega_0^2 (x^2 + y^2) + \frac{g}{r^2}, \quad (1)$$

where $g > 0$ is the strength of the inverse square potential, $r^2 = x^2 + y^2$. Thus, the particle moves only in the x - y plane with an infinite barrier at angle $\theta = 0$ and $a\pi$, i.e. the wave function Ψ must vanish at $\theta = 0$ and $a\pi$. This boundary condition is obviously different from the case in the absence of the wedge, which has a periodic boundary condition $\Psi(r, \theta = 0) = \Psi(r, \theta = 2\pi)$. As we shall see below, the change of boundary condition will change the sojourn time dramatically.

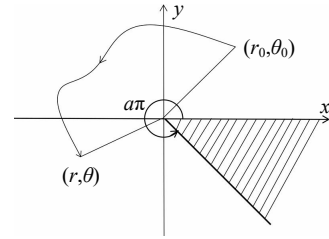


Fig. 1 Schematic of a particle confined in a wedge centered at the origin of the (r, θ) plane

Note that the above Hamiltonian can be obtained by replacing ω_0 with $i\omega_0$ from the Hamiltonian describing a two-dimensional inverse quadratic oscillator interacting with a wedge^[29], thus the propagator of the system can be readily obtained in a similar manner, in polar coordinates as

$$K_a(\mathbf{r}, \mathbf{r}_0; t, 0) = \frac{\mu \omega_0 \exp\left[\frac{i\mu \omega_0}{2\hbar} (r^2 + r_0^2) \coth \omega_0 t\right]}{2a\pi i \hbar \sinh \omega_0 t} \times \\ 4 \sum_{l=1}^{\infty} \sin\left(\frac{l\theta}{a}\right) \sin\left(\frac{l\theta_0}{a}\right) I_{\nu(l)}\left(\frac{\mu \omega_0 r r_0}{i\hbar \sinh \omega_0 t}\right), \quad (1)$$

where $\nu(l) = [(l/a)^2 + 2\mu g / \hbar^2]^{1/2}$.

It is evident that the propagator vanishes at the boundary, i.e., when angle $\theta = 0$ and $a\pi$. It should also be pointed out that in the limit of $a \rightarrow 2$, this propagator does not reduce to the one for the case when there is no wedge, which reads

$$K(\mathbf{r}, \mathbf{r}_0; t, 0) = \frac{\mu \omega_0 \exp\left[\frac{i\mu \omega_0}{2\hbar} (r^2 + r_0^2) \coth \omega_0 t\right]}{2\pi i \hbar \sinh \omega_0 t} \times \\ \sum_{n=-\infty}^{\infty} e^{in(\theta - \theta_0)} I_{\nu(n)}\left(\frac{\mu \omega_0 r r_0}{i\hbar \sinh \omega_0 t}\right). \quad (2)$$

To calculate the sojourn time near the origin, we consider the time evolution of a normalized Gaussian wave packet initially centered at the origin, for $0 \leq \theta \leq a\pi$,

$$\Psi(r_0, \theta_0) = \lambda_0 e^{-\frac{\lambda_0^2}{2} r_0^2} F(\theta_0) / \sqrt{a\pi/2}, \quad (3)$$

where λ_0 is a parameter that represents the width of the wave packet, $F(\theta) = 1$ when $0 < \theta < a\pi$ and zero when at the boundary $\theta = 0, a\pi$. Actually one can expand $F(\theta)$ as

$$F(\theta) = \frac{2}{a\pi} \sum_{n=1}^{\infty} F_n \sin\left(\frac{n\theta}{a}\right), \quad (4)$$

with $F_n = \int_0^{a\pi} \sin\left(\frac{n\theta}{a}\right) d\theta = a \frac{[1 - (-1)^n]}{n}$. In principle,

$F(\theta)$ has discontinuities at $\theta_0 = 0, a\pi$. However, the summation can only go from $k=1$ to a large number N in practice, thus $F(\theta)$ is continuous at the boundary (for more details, please see the discussions in the last section). Then by employing Feynman path integral method^[19-20], we can obtain the wave packet at time t as

$$\begin{aligned} \Psi_a(\mathbf{r}, t) = & \int K_a(\mathbf{r}, \mathbf{r}_0; t, 0) \Psi(\mathbf{r}_0) d\mathbf{r}_0 = \frac{4\lambda_0}{\sqrt{a\pi/2}} \times \\ & \left(\frac{\mu\omega_0}{2a\pi i \hbar \sinh \omega_0 t} \right) \exp\left[\frac{i\mu\omega_0}{2\hbar} r^2 \coth \omega_0 t \right] \times \\ & \int_0^{a\pi} r_0 dr_0 \int_0^{a\pi} d\theta_0 \sum_{l=1}^{\infty} \sin\left(\frac{l\theta}{a}\right) \sin\left(\frac{l\theta_0}{a}\right) \times \\ & e^{-\frac{\lambda_0^2}{2} r_0^2 - \frac{i\mu\omega_0}{2\hbar} r_0^2 \coth \omega_0 t} I_{\nu_l} \left(\frac{\mu\omega_0 r r_0}{i\hbar \sinh \omega_0 t} \right). \end{aligned} \quad (5)$$

Integrating out θ_0 in above equation yields

$$\begin{aligned} \Psi_a(\mathbf{r}, t) = & \frac{8\lambda_0}{\pi\sqrt{a\pi/2}} \frac{\mathcal{B}}{r} \exp\left[\frac{i\mu\omega_0}{2\hbar} r^2 \coth \omega_0 t \right] \times \\ & \sum_{k=0}^{\infty} \frac{\sin(2k+1)\theta}{2k+1} \int_0^{a\pi} r_0 dr_0 e^{-\mathcal{A} r_0^2} I_{\nu(2k+1)}(2\mathcal{B}r_0), \end{aligned} \quad (6)$$

where $\mathcal{A} = \frac{\lambda_0^2}{2} - \frac{i\mu\omega_0}{2\hbar} \coth \omega_0 t$, $\mathcal{B} = \frac{\mu\omega_0 r}{2i\hbar \sinh \omega_0 t}$.

Employ the following identity^[43],

$$\int_0^{\infty} e^{-\alpha x} I_{\nu}(2\beta\sqrt{x}) dx = \frac{\Gamma(\nu/2+1) e^{2\alpha}}{\beta\sqrt{\alpha}\Gamma(\nu+1)} M_{-\frac{1}{2}, \nu} \left(\frac{\beta^2}{\alpha} \right), \quad (7)$$

where $M_{k,m}(z)$ is the Whittaker's function^[44], which is defined as

$$M_{k,m}(z) = e^{-z/2} z^{m+1/2} {}_1F_1(m-k+1/2; 1+2m; z), \quad (8)$$

with ${}_1F_1(\alpha; \gamma; z)$ being the Kummer function^[44].

Carrying out the integral in Eq. (6) yields

$$\begin{aligned} \Psi_a(\mathbf{r}, t) = & \frac{4\lambda_0 e^{\frac{i\mu\omega_0 r^2}{2\hbar} \coth \omega_0 t}}{r\pi\sqrt{(a\pi/2)\mathcal{A}}} \sum_{k=0}^{\infty} \sin(\gamma\theta) \frac{z^{\frac{\bar{\nu}+1}{2}}}{2k+1} \times \\ & \frac{\Gamma(\bar{\nu}/2+1)}{\Gamma(\bar{\nu}+1)} {}_1F_1(\bar{\nu}/2+1; \bar{\nu}+1; z), \end{aligned} \quad (9)$$

where $\gamma = (2k+1)/a$ is a function of k , $\bar{\nu} = \nu(2k+1)$,

$z = \frac{\mathcal{B}^2}{\mathcal{A}} = Cr^2$ with $C = -\frac{(\mu\omega_0)^2}{4\hbar^2 \mathcal{A} \sinh^2 \omega_0 t}$ being a complex function of t .

When the wedge is absent, we choose $F(\theta_0) = F_0(\theta_0) = 1$ for $0 \leq \theta_0 \leq 2\pi$ (this function is continuous at $\theta_0 = 0, 2\pi$). By using the propagator of Eq. (3), similar calculation yields the following wave function,

$$\begin{aligned} \Psi(\mathbf{r}, t) = & \frac{\lambda_0 e^{\frac{i\mu\omega_0 r^2}{2\hbar} \coth \omega_0 t}}{r\sqrt{\pi\mathcal{A}}} z^{\frac{(1+\nu(0))}{2}} \frac{\Gamma(\nu(0)/2+1)}{\Gamma(\nu(0)+1)} \times \\ & {}_1F_1(\nu(0)/2+1; \nu(0)+1; z), \end{aligned} \quad (10)$$

with $\nu(0) = \sqrt{2\mu g} / \hbar$.

3 Calculation of the sojourn time and numerical results

From the wave function of Eq. (9) we can obtain the corresponding density,

$$\begin{aligned} \rho_a(\mathbf{r}, t) = & \frac{32\lambda_0^2}{a\pi^3 |\mathcal{A}| r^2} \left| \sum_{k=0}^{\infty} \sin(\gamma\theta) \frac{z^{\frac{\bar{\nu}+1}{2}}}{2k+1} \right. \\ & \left. \frac{\Gamma(\bar{\nu}/2+1)}{\Gamma(\bar{\nu}+1)} {}_1F_1(\bar{\nu}/2+1; \bar{\nu}+1; z) \right|^2, \end{aligned} \quad (11)$$

then the probability so that the particle is still in a sector around the origin with radius R , angle $a\pi$ at time t is

$$Q_a(R, t) = \int_0^{a\pi} d\theta \int_0^R r dr \rho_a(\mathbf{r}, t), \quad (12)$$

which describes the descent from equilibrium in detail. Substitution of Eq. (12) into Eq. (13) and performing the angle integral yields

$$\begin{aligned} Q_a(R, t) = & \sum_{k=0}^{\infty} \int_0^R dr \frac{16\lambda_0^2 |\mathcal{C}|^{(\bar{\nu}+1)} r^{(2\bar{\nu}+1)}}{\pi^2 (2k+1)^2 |\mathcal{A}|} \times \\ & \left| \frac{\Gamma(\bar{\nu}/2+1)}{\Gamma(\bar{\nu}+1)} {}_1F_1(\bar{\nu}/2+1; \bar{\nu}+1; z) \right|^2. \end{aligned} \quad (13)$$

For comparison, we also give the result for the case when the wedge is absent. In this case

$$\rho(r, t) = \frac{\lambda_0^2}{\pi |\mathcal{A}| r^2} \left| z^{\frac{\nu(0)+1}{2}} \frac{\Gamma(\nu(0)/2+1)}{\Gamma(\nu(0)+1)} \right|^2 \times \\ \left| {}_1F_1(\nu(0)/2+1; \nu(0)+1; z) \right|^2, \quad (14)$$

and

$$Q(R, t) = \int_0^{2\pi} d\theta \int_0^R r dr \rho(r, t). \quad (15)$$

In the case of $g \rightarrow 0$, above results further reduce to

$$\rho(r, t)|_{g=0} = \frac{\lambda_0^2 |C|}{\pi |\mathcal{A}|} e^{(C+C^*)r^2}, \quad (16)$$

and

$$Q(R, t)|_{g=0} = 1 - e^{(C+C^*)R^2}. \quad (17)$$

It is evident that in the limit of $R \rightarrow \infty$, $Q(R, t)|_{g=0} \rightarrow 1$ as required.

Adopting the definition as that in Ref. [31], we have the expression for the sojourn time,

$$T_a(R) = \int_0^\infty dt Q_a(R, t). \quad (18)$$

Unfortunately, the integral in Eq. (19) cannot be performed analytically, in order to investigate the effects of the wedge, we have to resort to numerical calculations.

In the numerical calculations, the summation of k from 1 to infinity is replaced by 1 to N . In other words, the function $F(\theta)$ of Eq. (5) is approximated by

$$F'(\theta) = \frac{2}{a\pi} \sum_{n=1}^N F_n \sin\left(\frac{n\theta}{a}\right), \quad (19)$$

where N is a large integer number. The results for $N=100$ (which is essentially the same as $N \rightarrow \infty$ since the difference between the two cases is too small to detect) are presented in Fig. 2. From the graph, it is clear that the sojourn time monotonically increases as the external angle increases as expected. Of particular interest is the case when $a \rightarrow 2$ as shown in Fig. 3. In this case the wedge becomes a singular line and does not occupy any area. It appears that the sojourn time in this case should not differ much from the case without a wedge. However, from the results presented in Fig. 2, it is evident that the sojourn time T has a big jump at $a=2$ (for instance, at $g=0$, the value of T jumps from 0.309 1 to 1.299 4, while the value of T jumps from 0.097 0 to 0.150 0 for $g=3$, see more in Table 1), implying that there is a huge difference between the case

when the wedge becomes a singular line and the one without a wedge. In other words, a singular line which does not occupy any area in 2D space, but counter-intuitively can reduce the sojourn time dramatically to about or more than 30 percentage less. Namely, the time for the particle to stay in the circle with radius $R=1$ is reduced to less than 70 percentage of the original value $T_{a=2}$ when the circle is cut by a singular line. Particularly, the sojourn time $T_{a \rightarrow 2}$ is reduced to about 24 percentage of the value of $T_{a=2}$ in the case when $g=0$. This surprising huge amount of difference indicates that the boundary indeed plays an important role in this problem.

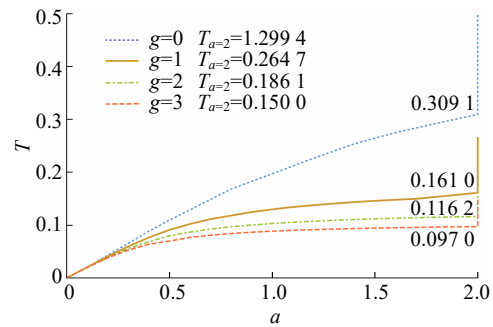


Fig. 2 Sojourn time as a function of the a at different values of g ($\mu = \hbar = q = \lambda_0 = \omega_0 = R = 1$)

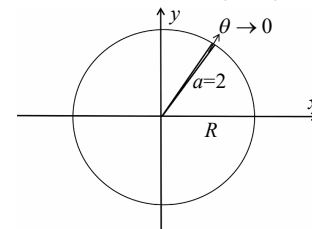


Fig. 3 The wedge in the limit of $a \rightarrow 2$

Table 1 The values of the sojourn $T(R=1)$ at $a=2$ and $a \rightarrow 2$ for different values of g

g	$T_{a \rightarrow 2}$	$T_{a=2}$	$T_{a \rightarrow 2} / T_{a=2}$
0	0.309 1	1.299 4	0.237 9
1	0.161 0	0.264 7	0.608 4
2	0.116 2	0.186 1	0.624 3
3	0.097 0	0.150 0	0.646 5
4	0.083 2	0.128 4	0.647 5
5	0.075 0	0.113 8	0.658 7
10	0.052 7	0.078 3	0.673 1
20	0.037 5	0.054 1	0.692 8
100	0.016 4	0.023 1	0.709 1

Moreover, as the strength of the inverse square potential, namely the value of g increases, the sojourn time decreases. This behaviour of T as a function of g is also reflected at $a = 2$, which we present in Fig. 4. The reason behind is that the inverse square potential g/r^2 provides a repulsive force $2g/r^3$, the force increases as g increases and tends to push away the particle, hence the sojourn time decreases as g increases. It is also clear from Table 1, that the value of $T_{a \rightarrow 2}/T_{a=2}$ increases as the value of g increases, i.e., the boundary effect becomes less obvious as the value of g increases.

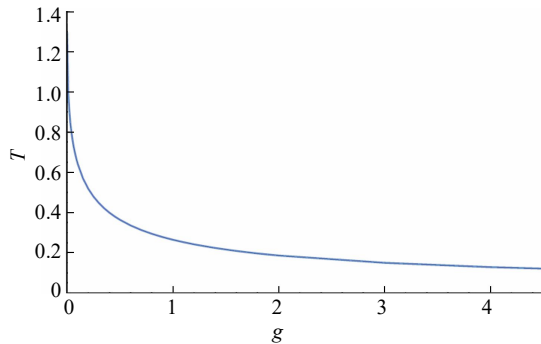


Fig. 4 Sojourn time as a function of g at $a = 2$ in the absence of the wedge ($\mu = \hbar = q = \lambda_0 = \omega_0 = 1$)

4 Discussions and concluding remarks

From the procedure of calculations, it is clear that the difference between the case $a = 2$ (without a wedge) and $a \rightarrow 2$ (an infinitely narrow wedge) is caused by two factors. Firstly, the propagators used for each case are different (see Eq.s (2) and (3)). Secondly, the original wave functions used are also different. It should be pointed out that the calculation for the case $a = 2$, the original wave function is equivalent to the case that we choose $F(\theta) = F_0(\theta) = 1$ in Eq. (4) for $0 \leq \theta_0 \leq 2\pi$. As shown by the dashed lines in Figs. 5~7, this function is always a continuous function at $\theta = 0, 2\pi$, namely $F_0(0) = F_0(2\pi) = 1$. On the other hand, $F(\theta)$ of Eq. (5) is discontinuous at $\theta = 0, 2\pi$, i.e. $F(\theta) = 0$ when $\theta = 0, 2\pi$ while $F(\theta) = 1$ when $0 < \theta < 2\pi$.

In the practical calculations, $F(\theta)$ of Eq. (5) is replaced by $F'(\theta)$ of Eq. (20) which is then a continuous function. We plot $F'(\theta)$ for $N = 1\,000, 5\,000, 10\,000$

with $a = 2$ in Figs. 5~7 respectively. It is evident from the graphs, $F'(\theta)$ oscillates rapidly near the boundary. As N increases, the amplitudes as well as the frequencies of oscillation decrease. In the limit of $N \rightarrow \infty$, it becomes the dashed line which denotes $F(\theta)$ of Eq. (5).

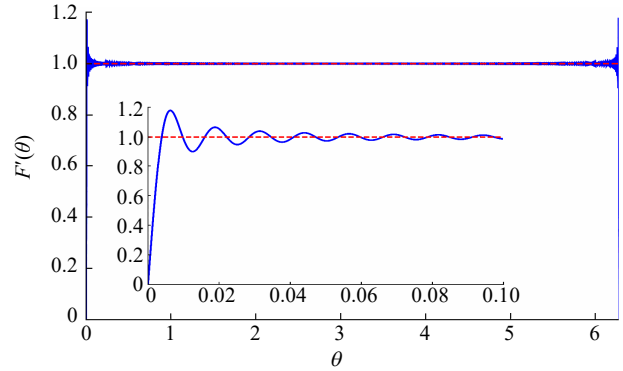


Fig. 5 The plot of function $F'(\theta)$ for $N = 1\,000$, $a = 2$

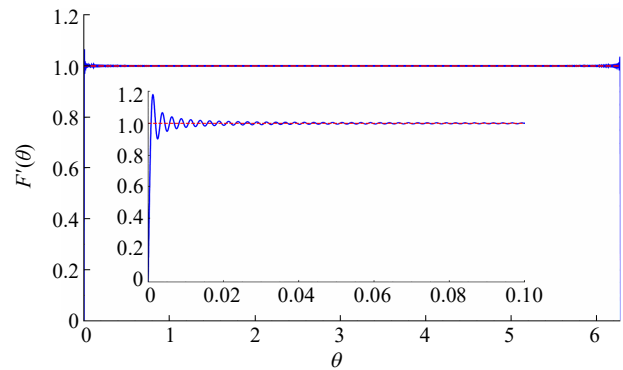


Fig. 6 The plot of function $F'(\theta)$ for $N = 5\,000$, $a = 2$

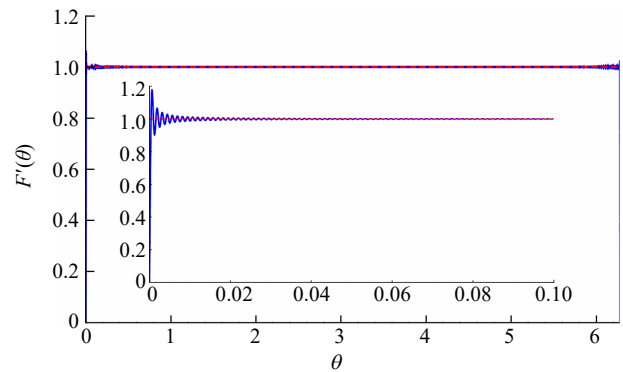


Fig. 7 The plot of function $F'(\theta)$ for $N = 10\,000$, $a = 2$

On the other hand, notice that the numbers in Table 1 obtained if we choose $N = 100$ are essentially the same as those obtained if we choose $N = 200$. This indicates that the difference in the initial wave functions for $N = 100$ and $N = 200$ is diminished if we use the same propagator to do the calculations. Hence, the boundary effect for $a = 2$ and $a \rightarrow 2$ are mainly

caused by the different propagators used.

In summary, by employing Feynman path integral approach, we have investigated the two-dimensional inverted inverse quadratic oscillator in a wedge. Our results show that the sojourn time is a monotonically decreasing function of the strength of the inverse square potential g irrespective of whether the wedge is absent or present. The sojourn time T has a big jump from the case when the wedge becomes a singular line (in the limit of $a \rightarrow 2$), to the case when the wedge is absent ($a = 2$), implying that the boundary indeed plays an important role in this problem. Moreover, the effect of boundary condition becomes less obvious as the value of the strength of the inverse square potential g increases.

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边界对二维反谐振子在平方反比势和楔子中逗留时间的影响

乐家怡, 陈寅, 潘孝胤*

(宁波大学 物理科学与技术学院, 浙江 宁波 315211)

摘要: 本文研究了二维反谐振子在平方反比势和外角为 $a\pi$ ($0 \leq a < 2$) 的楔子中的逗留时间, 利用费曼路径积分法得到了波函数和相应密度的精确表达式, 进一步利用数值积分方法计算了逗留时间与 a 的函数. 结果表明, 随着外角增加, 逗留时间单调递增. 在 $a \rightarrow 2$ 的极限上有一个很大的跳跃, 这意味着当楔子成为奇异线时, 与没有楔子时存在着很大的差异. 换句话说, 尽管奇异线在二维空间中并不占据任何区域, 但是由于奇异线的存在, 使得逗留时间大大缩短, 从而说明了边界条件的重要性.

关键词: 边界效应; 逗留时间; 路径积分; 楔子

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