行政院國家科學委員會補助專題研究計畫成果報告

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中　華　民　國　九十一年　十　月二十五日

摘　　要

在本計劃支助下，我們完成了一項有關隨時間變化位場下一個系統的量子亞穩性的研究。結果已發表在

Physical Review A, Vol. 65, (2002) pg. 022111

關鍵詞：量子亞穩性

ABSTRACT

We have completed a study on the quantum metastability of a system under the influence of a class of time-dependent potential. The result has been published in :

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Key words: Quantum metastability

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Quantum metastability in a class of moving potentials

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In this paper we consider quantum metastability in a class of moving potentials introduced by Berry and Klein. This class of potential has height and width scaled in a specific way so that it can be transformed into a stationary one. While deriving the nondecay probability of the system, we demonstrate that the appropriate technique to use is the less well known method of scattering states. This method is illustrated through two examples, namely, a moving δ-function potential and a moving barrier potential. For expanding potentials, one finds that a small but finite nondecay probability persists at large times. Generalization to scaling potentials of arbitrary shape is briefly outlined.

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I. INTRODUCTION

An interesting issue in cosmology is the evolution of metastable states in the early universe in the original version and its variants in the inflationary models [1,2]. In these models inflation of the early universe is governed by a Higgs field trapped in a metastable state. Inflation ends when the metastable state decays to the true ground state of the universe. During inflation the universe expands exponentially. It is thus obvious that the metastable state of the Higgs field is trapped in a rapidly varying potential. The problem is therefore a truly time-dependent one. However, owing to the inherent difficulties of the problem, more often than not one considers the decay of the Higgs field in a quasistationary approximation, in which the decay is studied by assuming a static potential [3]. Certainly this approximation is hard to justify, but for the present one has to be content with it. Ultimately one hopes to be able to tackle the nonstationary case. To this end, it is desirable to gain some insights first by studying metastability in time-dependent potentials in simple quantum-mechanical models.

Time-dependent potentials can be broadly divided into three classes. Potentials in the first class are of time-dependent strength. When the strength is small, the Schrödinger equation can be solved by time-dependent perturbation theory. Almost all pedagogical examples belong to this type. When the strength of the potential is not small, other methods of solution must be sought. For example, solutions of time-dependent harmonic oscillator [4] and time-dependent linear [5] potentials can be obtained by the method of invariants. We note that the interesting phenomenon of quantum tunneling induced by an externally driven field has also been examined experimentally and theoretically [6–8]. The second class of potentials involves time-dependent boundaries. Unlike the first class, this class of potentials has attracted much less attention, and almost all previous work in this area concerned only the simplest of all cases, namely, an infinite potential well with a moving wall [9,10]. The last class is a combination of the previous two classes.

We believe that the barrier potential in an inflationary universe is nonstationary; not only the barrier height but also the barrier width should be changing as time elapses. However, it will be extremely difficult to study metastability in such a time-dependent potential in full generality. Thus it would be helpful if the quantum tunneling effect could be studied in any class of moving potential, special though it may be, as a step toward understand the decay of a nonstationary metastable system.

In this paper we consider quantum metastability in a class of scaling potentials that allows one to apply techniques used in the corresponding problem with stationary potentials. This class of potentials was introduced by Berry and Klein [11]. These potentials have heights and widths scaled in a specific way so that one can transform the potential into a stationary one.

The organization of the paper is as follows. In Sec. II we give a general discussion of the solutions of the Schrödinger equation with the scaling form of the time-dependent potential introduced in [11]. It is argued that the most suitable technique for studying quantum metastability in such a potential is the less well known method of scattering states. Two simple examples of such metastable systems, a moving δ-function potential and a moving square barrier, are investigated in Secs. III and IV, respectively. A generalization to an arbitrary barrier is briefly discussed in Sec. V. Section VI concludes the paper.

II. SCHRÖDINGER EQUATION WITH A SCALING POTENTIAL

We consider the problem of quantum metastability of a particle of mass m trapped in a moving potential $V(x,t)$ which has the scaling form proposed by Berry and Klein [11], namely, $V(x,t)=\bar{V}(x/L(t))/L^2(t)$, where $L(t)$ is a time-dependent scaling factor. The Schrödinger equation is

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{L^2(t)}\bar{V}\left(\frac{x}{L(t)}\right)\right]\Psi(x,t). \quad (1)$$

So far solution of Eq. (1) is restricted mostly to the special case in which $\bar{V}$ has the functional form of an infinite potential well, i.e., $V(x,t)$ is an infinite well with a moving wall [9,10]. In this case, the scaling factor $L^2(t)$ in front of $\bar{V}$ is immaterial.

We assume $\bar{V}$ to have the generic shape of a potential well that is impenetrable to the left and has a finite barrier to the right, much like that usually employed in the discussion of α decay. The scaling factor $L(t)$ is assumed to be a linear function of time:

$$L(t)=L_0+vt, \quad v=\text{const.} \tag{2}$$

Of course, for $v<0$, the problem is meaningful only for time duration $0<t<L_0/|v|$. Equation (1) cannot be solved by separating the time and spatial coordinates. However, for the scaling form of $V(x,t)$ in Eq. (1) and the linear form of $L(t)$, separation of variables can be achieved through a series of transformations introduced in [12,11] (see also [9,10]). One first transforms the coordinate frame into a rescaled frame with a rescaled coordinate $\bar{x}$ defined by

$$\bar{x}(t)\equiv\frac{x}{L(t)}. \tag{3}$$

In this frame the Schrödinger equation becomes

$$i\hbar\frac{\partial}{\partial t}\Psi(\bar{x},t)=\left[-\frac{\hbar^2}{2mL^2}\frac{\partial^2}{\partial x^2}+i\hbar\frac{v}{L}\bar{x}\frac{\partial}{\partial\bar{x}}+\bar{V}(\bar{x})\right]\Psi(\bar{x},t). \tag{4}$$

Equation (4) can be further simplified by the transformation

$$\Psi(\bar{x},t)=\frac{1}{\sqrt{L(t)}}e^{(im/2\hbar)Lv\bar{x}^2}\Phi(\bar{x},t), \tag{5}$$

and the introduction of a new time variable τ:

$$\tau=\int_0^t\frac{ds}{L^2(s)}=\frac{t}{L_0L(t)}. \tag{6}$$

After substituting Eqs. (5) and (6) into Eq. (4), one obtains the equation

$$i\hbar\frac{\partial}{\partial\tau}\Phi(\bar{x},\tau)=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial\bar{x}^2}\Phi(\bar{x},\tau)+\bar{V}(\bar{x})\Phi(\bar{x},\tau), \tag{7}$$

which resembles the Schrödinger equation with a stationary potential. Equation (7) can be solved by separation of variables:

$$\Phi(\bar{x},\tau)=\Phi(\bar{x})e^{-(i/\hbar)\bar{E}\tau}, \tag{8}$$

where $\Phi(\bar{x})$ satisfies the eigenvalue equation

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\bar{V}(\bar{x})\right]\Phi_k(\bar{x})=\bar{E}_k\Phi_k(\bar{x}). \tag{9}$$

Once Eq. (9) is solved exactly in the rescaled frame, the exact wave function in the original frame is then given by

$$\Psi_k(x,t)=\frac{1}{\sqrt{L(t)}}e^{(im/2\hbar)(v/L)x^2}e^{-(i/\hbar)(1/L_0L)\bar{E}_kt}\Phi_k\left(\frac{x}{L}\right). \tag{10}$$

The set of solutions (10) is complete and orthonormal:

$$\langle\Psi_k(x,t)|\Psi_l(x,t)\rangle=\langle\Phi_k(\bar{x})|\Phi_l(\bar{x})\rangle=\delta_{kl}, \tag{11}$$

so using this set of solutions we can find a solution satisfying any initial condition. Furthermore, if an initial state $\Psi(x,0)$ is expressible in the basis $\{\Psi_k\}$ as

$$\Psi(x,0)=\sum_k c_k\Psi_k(x,0), \quad c_k=\langle\Psi_k(x,0)|\Psi(x,0)\rangle, \tag{12}$$

then at a later time t the state is

$$\Psi(x,t)=\sum_k c_k\Psi_k(x,t). \tag{13}$$

We have now succeeded in transforming the original time-dependent Schrödinger equation into a time-independent one. The problem of calculating the decay probability of a particle confined in $V(x,t)$ at time t is reduced to the corresponding problem with a static potential $\bar{V}(\bar{x})$. Hence techniques used in the time-independent potential for calculating decay rate can be borrowed.

However, there are some subtleties. Naively, one is tempted to employ the best-known method, namely, the complex eigenvalue method, proposed by Gamow in his studies of α decay [13]. In this approach an "outgoing wave boundary condition" is imposed on the solutions of the Schrödinger equation for the particle trapped in the well. That means incoming plane wave solutions outside the potential well are discarded right from the beginning. This procedure naturally leads to an eigenvalue problem with complex energy eigenvalues. One then relates the imaginary parts of the energy to the decay rate. While the complex eigenvalue method is straightforward and physically reasonable, it suffers from some conceptual difficulties [14]. For example, how can energy eigenvalues be complex as we are dealing with a Hermitian Hamiltonian? Also, the eigenfunctions are not normalizable, a difficulty directly related to the eigenvalues being complex. Furthermore, the particle trapped in the well cannot be in an eigenstate of the system in the first place, since such states are not completely confined at $t=0$.

Apart from the difficulties mentioned above, the complex eigenvalue method cannot be employed in the present case for other reasons. First, the problem we are interested in is an intrinsically time-dependent one, with a nonconservative Hamiltonian. Hence energy eigenvalues and eigenstates lose their meanings altogether [$\bar{E}$ in Eq. (9) is not an energy eigenvalue]. Second, the "outgoing wave boundary condition," essential to Gamow's method, cannot be imposed in our case. The reason is as follows. As discussed before, in order to fix a moving potential we need to transform our problem to a corresponding static one in a rescaled frame. But in this frame the meaning of an incoming or outgoing

plane wave is rather obscure. In fact, it can be checked that an outgoing plane wave in the original x-t (rescaled $\bar{x}$-τ) frame contains both "incoming" and "outgoing" components in the rescaled $\bar{x}$-τ (original x-t) frame.

The instanton method is another technique commonly used in the calculation of the decay rate of a metastable state [15]. This semiclassical method amounts essentially to finding the imaginary part of the ground state energy of the system. Since it is based on the idea of eigenvalues of the Hamiltonian, it is therefore not suitable here.

One more method that can be useful in tackling the problem is the complex scaling method [16]. The general idea of this method is to consider a complex rotated Hamiltonian obtained from the usual Hamiltonian by making the position and momentum complex. This resolves the paradox that the eigenenergies are complex, since now the complex rotated Hamiltonian is no longer Hermitian. A pleasant merit of the method is that the eigenfunctions associated with these complex resonant eigenvalues are square integrable, and thus various approximation methods developed for bound states can be applied to the scattering processes. However, this method, while elegant in many respects, is not useful in our present case, since it also requires the idea of eigenenergy.

Since these common methods fail to suit our purpose, we have to look for alternatives. Fortunately, a different method exists, namely, the scattering state method (or virtual level method, as Fermi called it) [17]. This method is much less well known and seldom used in the literature [18]. However, it is conceptually the most satisfying of all the methods. In this method, one first constructs the initial confining state, which is not viewed as an eigenstate, but rather as a linear superposition of scattering states with real energies, and follows its evolution in time. In the course of this evolution, no energy will become complex. Unlike the Gamow states, the scattering states contain both incoming and outgoing components in the region into which the particle escapes. It is this feature of the method that makes it most suitable in the present problem. The method is easily adapted to Eq. (7) by taking the scattering states as the states (8) with real values of $\bar{E}$.

In the next two sections, the scattering state method is applied to two simple examples of the class of scaling potentials. As the scattering state method is not so well known in the literature, we think it appropriate to give some details in order to make this work self-contained. The procedures given in [14] are slightly adapted to our needs.

III. MOVING δ-FUNCTION POTENTIAL

The first example is a uniformly moving δ-function potential

$$V(x,t)=\begin{cases}\infty, & x\leqslant 0,\\ \dfrac{\bar{V}_0}{L(t)}\delta(x-a(t))=\dfrac{\bar{V}_0}{L^2(t)}\delta\left(\dfrac{x}{L(t)}-\bar{a}\right), & x>0,\end{cases} \tag{14}$$

where $a(t)=\bar{a}L(t)>0$ gives the location of the δ-function potential. This class of potentials was defined in the last section and corresponds in the rescaled frame to $\bar{V}(\bar{x})=\infty$ for $\bar{x}<0$ and $\bar{V}(\bar{x})=\bar{V}_0\delta(\bar{x}-\bar{a})$. One has $\Phi(\bar{x})=0$ in the region $\bar{x}<0$. For $\bar{x}>0$, Eq. (9) is

$$-\frac{\hbar^2}{2m}\frac{d^2\Phi(\bar{x})}{d\bar{x}^2}+\bar{V}_0\delta(\bar{x}-\bar{a})\Phi(\bar{x})=\bar{E}\Phi(\bar{x}). \tag{15}$$

Its general solutions are

$$\Phi(\bar{x})=\begin{cases}\sin(\bar{k}\bar{x}), & 0<\bar{x}<\bar{a},\\ C\cos(\bar{k}\bar{x}+\theta), & \bar{a}<\bar{x},\end{cases} \tag{16}$$

where $\bar{k}=\sqrt{2m\bar{E}}/\hbar$, C is a real constant, and θ is a phase angle. Note that the wave function is real, and includes an incoming wave component in the region $\bar{x}>\bar{a}$. This ensures that $\bar{k}$, and hence $\bar{E}$, is always real. The wave function and its first derivative satisfy the following boundary conditions at $\bar{x}=\bar{a}$:

$$\Phi(\bar{x}=\bar{a}^+)=\Phi(\bar{x}=\bar{a}^-) \tag{17}$$

and

$$\left.\frac{d\Phi(\bar{x})}{d\bar{x}}\right|_{\bar{x}=\bar{a}^+}-\left.\frac{d\Phi(\bar{x})}{d\bar{x}}\right|_{\bar{x}=\bar{a}^-}=\frac{2m}{\hbar^2}\bar{V}_0\Phi(\bar{x}=\bar{a}). \tag{18}$$

From these relations the coefficient C can be determined as a function of $\bar{k}$:

$$C^2(\bar{k})=\sin^2(\bar{k}\bar{a})+\left(\cos(\bar{k}\bar{a})+\frac{2m\bar{V}_0}{\hbar^2\bar{k}\bar{a}}\sin(\bar{k}\bar{a})\right)^2. \tag{19}$$

Physically, the value of $C^2(\bar{k})$ can be interpreted as the ratio of the probability of finding particles in the region $\bar{x}>\bar{a}$ to the probability of finding them within the confined region $0<\bar{x}<\bar{a}$ for a particular $\bar{k}$. The general shape of $C^2(\bar{k})$ is shown in Fig. 1, from which we can assert that the particle can be trapped within the confined region only when C^2 assumes one of its minima, which occur only in the neighborhood of some specific values of $\bar{k}$. In these regions the values of $C^2(\bar{k})$ are extremely small. From Eq. (19) it is obvious that these minima will be centered around $\bar{k}_n=n\pi/\bar{a}$ $(n=1,2,\ldots)$ [i.e., $\sin(\bar{k}_n\bar{a})=0$] as long as $\bar{V}_0$ is large enough so that $2m\bar{V}_0/\hbar^2\gg n\pi$.

For large $\bar{V}_0$ approximate analytic expressions can be obtained and compared with the corresponding results in the time-independent case [19]. According to the scattering state method, one constructs confining states in the potential well by taking a suitable superposition of the scattering states with $\bar{k}$ in the neighborhood of $\bar{k}_n$. To this end, let us first expand C^2 about $\bar{E}_n=\hbar^2\bar{k}_n^2/2m$ (we revert to the variable $\bar{E}$ below):

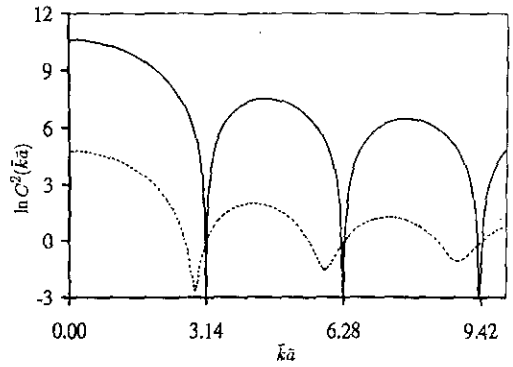

FIG. 1. The shape of $\ln C^2(\bar{k}\bar{a})$ in Eq. (19) as a function of $\bar{k}\bar{a}$ for $2m\bar{V}_0/\hbar^2=10$ (dotted line) and 200 (solid line). The minima of $\ln C^2(\bar{k}\bar{a})$ will be centered around $\bar{k}_n\bar{a}=n\pi$ $(n=1,2,\ldots)$ for large values of $2m\bar{V}_0/\hbar^2$.

$$C^2(\bar{E})\approx\left(\frac{m\bar{a}}{\hbar^2\bar{k}_n}\right)^2\left[1+\left(\frac{2m\bar{V}_0}{\hbar^2\bar{k}_n}\right)^2\right](\bar{E}-\bar{E}_n+\delta)^2+\left[1+\left(\frac{2m\bar{V}_0}{\hbar^2\bar{k}_n}\right)^2\right]^{-1} \tag{20}$$

$$\equiv G^2(\Delta+\delta)^2+F^2, \tag{21}$$

where $\Delta=\bar{E}-\bar{E}_n$ and the constants

$$\delta=\frac{2\bar{V}_0}{\bar{a}}\left[1+\left(\frac{2m\bar{V}_0}{\hbar^2\bar{k}_n}\right)^2\right]^{-1}, \tag{22}$$

$$G^2=\left(\frac{m\bar{a}}{\hbar^2\bar{k}_n}\right)^2\left[1+\left(\frac{2m\bar{V}_0}{\hbar^2\bar{k}_n}\right)^2\right], \tag{23}$$

$$F^2=\left[1+\left(\frac{2m\bar{V}_0}{\hbar^2\bar{k}_n}\right)^2\right]^{-1}. \tag{24}$$

The scattering states with $\bar{E}$ in the neighborhood of $\bar{E}_n$ can then be written as

$$\psi_\Delta(\bar{x})=\begin{cases}\sqrt{\frac{2}{R}}\frac{1}{\sqrt{G^2(\Delta+\delta)^2+F^2}}\sin(\bar{k}\bar{x}), & 0<\bar{x}<\bar{a},\\ \sqrt{\frac{2}{R}}\cos(\bar{k}\bar{x}+\theta), & \bar{a}<\bar{x}.\end{cases} \tag{25}$$

This system is quantized in the interval $[0,R]$, where $R\gg\bar{a}$, which at the end of the calculation will be set to infinity. With these scattering states, an initial state is constructed that is completely confined within the well by taking a linear combination of the scattering states with different Δ but the same value of $\bar{E}_n$,

$$\Phi(\bar{x},\tau=0)=\sum_\Delta c_\Delta\psi_\Delta(\bar{x})=\begin{cases}\phi_n(\bar{x}), & \bar{x}<\bar{a},\\ 0, & \bar{x}>\bar{a}.\end{cases} \tag{26}$$

The coefficient c_Δ can be calculated from orthogonality of the states $\psi_\Delta(\bar{x})$,

$$c_\Delta=\int_0^R d\bar{x}\,\psi_\Delta(\bar{x})\Phi(\bar{x},0)=\sqrt{\frac{2}{R}}\frac{1}{\sqrt{G^2(\Delta+\delta)^2+F^2}}\int_0^{\bar{a}}d\bar{x}\sin(\bar{k}\bar{x})\phi_n(\bar{x}). \tag{27}$$

Choosing

$$\phi_n(\bar{x})\approx\sqrt{\frac{2}{\bar{a}}}\sin\left(\frac{n\pi\bar{x}}{\bar{a}}\right), \quad n=1,2,3,\ldots, \tag{28}$$

we get

$$c_\Delta\approx\frac{1}{\sqrt{R\bar{a}}}\frac{2}{\sqrt{G^2(\Delta+\delta)^2+F^2}}\int_0^{\bar{a}}d\bar{x}\sin(\bar{k}\bar{x})\sin\left(\frac{n\pi\bar{x}}{\bar{a}}\right) \tag{29}$$

$$\approx\sqrt{\frac{\bar{a}}{R}}\frac{1}{\sqrt{G^2(\Delta+\delta)^2+F^2}}. \tag{30}$$

The initial state is then given by

$$\Phi(\bar{x},\tau=0)\approx\sqrt{\frac{\bar{a}}{R}}\sum_\Delta\frac{1}{\sqrt{G^2(\Delta+\delta)^2+F^2}}\psi_\Delta(\bar{x}). \tag{31}$$

From Eqs. (10), (12), and (13), the solution at a later time τ is

$$\Phi(\bar{x},\tau)\approx\sqrt{\frac{\bar{a}}{R}}\sum_\Delta\frac{1}{\sqrt{G^2(\Delta+\delta)^2+F^2}}\psi_\Delta(\bar{x})e^{-(i/\hbar)(\bar{E}_n+\Delta)\tau}. \tag{32}$$

As the system is quantized in the interval $[0,R]$, we have $\bar{k}R=n'\pi/2$, where n' is a very large integer $(n'\gg n)$. After replacing the sum by an integral

$$\sum_\Delta\rightarrow\int d\Delta\frac{R}{\pi\hbar}\sqrt{\frac{2m}{\bar{E}_n}}, \tag{33}$$

Eq. (32) becomes

$$\Phi(\bar{x},\tau)\approx\frac{R}{\pi\hbar}\sqrt{\frac{2m}{\bar{E}_n}}\sqrt{\frac{\bar{a}}{R}}\int_{-\infty}^{\infty}d\Delta\times\frac{1}{\sqrt{G^2(\Delta+\delta)^2+F^2}}\psi_\Delta(\bar{x})e^{-(i/\hbar)(\bar{E}_n+\Delta)\tau}. \tag{34}$$

Substituting $\psi_\Delta(\bar{x})$ from Eq. (25), we obtain the approximate wave function of the state confined in the well $(0<\bar{x}<\bar{a})$ as

$$\Phi(\bar{x},\tau)\approx\frac{2}{\pi\hbar}\sqrt{\frac{m\bar{a}}{\bar{E}_n}}\sin(\bar{k}_n\bar{x})e^{-(i/\hbar)\bar{E}_n\tau}\times\int_{-\infty}^{\infty}d\Delta\frac{e^{-(i/\hbar)\Delta\tau}}{G^2(\Delta+\delta)^2+F^2}=\frac{2}{\hbar}\sqrt{\frac{m\bar{a}}{\bar{E}_n}}\frac{\sin(\bar{k}_n\bar{x})}{|FG|}e^{-(i/\hbar)\bar{E}_n\tau}e^{-(1/\hbar)|FG|\tau}. \tag{35}$$

For metastable systems an important quantity is the nondecay probability $P(t)$ that the particle is still in the well at time t if it is initially confined in the well at $t=0$ [$P(t=0)=1$]. In our case $P(t)$ is defined as

$$P(t)=\frac{\int_0^{a(t)}|\Psi(x,t)|^2dx}{\int_0^{a(0)}|\Psi(x,0)|^2dx}=\frac{\int_0^{\bar{a}}|\Phi(\bar{x},\tau)|^2d\bar{x}}{\int_0^{\bar{a}}|\Phi(\bar{x},0)|^2d\bar{x}}. \tag{36}$$

From Eq. (35) we find

$$P(t)\sim\exp[-\gamma_n(t)], \tag{37}$$

where

$$\gamma_n(t)=2\left|\frac{F}{G}\right|\frac{t}{L_0L(t)} \tag{38}$$

$$=2\left(\frac{\hbar^2\bar{k}_n}{m\bar{a}}\right)\left[1+\left(\frac{2m\bar{V}_0}{\hbar^2\bar{k}_n}\right)^2\right]^{-1}\frac{t}{L_0L(t)}. \tag{39}$$

We have used Eqs. (6), (23), and (24) to obtain the result (39). We note that for an expanding potential $(v>0)$

$$\gamma_n(t)\to2\left|\frac{F}{G}\right|\frac{1}{L_0v} \tag{40}$$

as $t\to\infty$. Unlike the stationary case $(v=0)$, there is a small but finite probability that the particle does not tunnel out of the well. This result is reasonable, since as the barrier moves away from $x=0$ it leaves more room for the particle to stay within the well.

For $\bar{V}_0$ much larger than the characteristic value of $\bar{k}_n$ of the escaping particles, $\gamma(t)$ becomes

$$\gamma_n(t)\to\left[\frac{(\hbar^2\bar{k}_n)^3}{2m^3\bar{a}\bar{V}_0^2}\right]\frac{t}{L_0L(t)}=\left[\frac{\hbar^6(n\pi)^3}{2m^3\bar{a}^4\bar{V}_0^2}\right]\frac{t}{L_0L(t)}, \tag{41}$$

where $\bar{k}_n=n\pi/\bar{a}$ has been substituted. It is proper to compare Eq. (41) with the corresponding result in the stationary case $(v=0)$. In the limit $v\to0$, we have $L(t)\to L_0$, $\bar{a}\to a/L_0$, $\bar{E}_n\to E_nL_0^2$, and $\bar{k}_n\to k_nL_0$, where E_n is the corresponding energy in the static frame, and $k_n=\sqrt{2mE_n}/\hbar$. In this limit $\gamma(v=0)$ is directly proportional to the time t. We can therefore define a decay rate by $\Gamma_n\equiv\gamma_n(v=0)/t$, which in this case is

$$\Gamma_n=\frac{\hbar^6k_n^3}{2m^3a(\bar{V}_0/L_0)^2}=\frac{\hbar^6(n\pi)^3}{2m^3a^4(\bar{V}_0/L_0)^2}. \tag{42}$$

Equation (42) is consistent with the result obtained by the complex eigenvalue method in [19] for a static δ-function potential located at $x=a$ with strength $\bar{V}_0/L_0$.

IV. MOVING SQUARE BARRIER POTENTIAL

For the next example, consider a moving barrier potential

$$V(x,t)=\begin{cases}\infty, & x\leq0,\\ \dfrac{1}{L^2(t)}\bar{V}_0, & a(t)<x<b(t),\\ 0, & x>b(t),\end{cases} \tag{43}$$

with $a(t)=\bar{a}L(t)$ and $b(t)=\bar{b}L(t)$ ($\bar{a}$ and $\bar{b}$ are two positive constants). When the problem is transformed to the rescaled frame, it is equivalent to solving Eq. (9) with a stationary potential

$$\bar{V}(\bar{x})=\begin{cases}\infty, & \bar{x}\leq0,\\ \bar{V}_0, & \bar{a}<\bar{x}<\bar{b},\\ 0, & \bar{x}>\bar{b}.\end{cases} \tag{44}$$

The general solutions are

$$\Phi(\bar{x})=\begin{cases}\sin(\bar{k}\bar{x}), & 0<\bar{x}<\bar{a},\quad \bar{k}=\sqrt{2m\bar{E}/\hbar^2},\\ Ae^{\bar{k}'\bar{x}}+Be^{-\bar{k}'\bar{x}}, & \bar{a}<\bar{x}<\bar{b},\quad \bar{k}'=\sqrt{2m(\bar{V}_0-\bar{E})/\hbar^2},\\ C\cos(\bar{k}\bar{x}+\theta), & \bar{a}<\bar{x}.\end{cases} \tag{45}$$

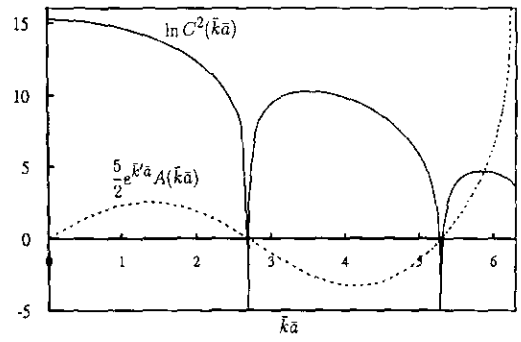

FIG. 2. The shapes of $\ln C^2(\bar{k}\bar{a})$ (solid line) in Eq. (48) and $5e^{\bar{k}'\bar{a}}A(\bar{k}\bar{a})/2$ (dotted line) in Eq. (46) as functions of $\bar{k}\bar{a}$ for $\bar{b}=2\bar{a}$ and $2m\bar{V}_0\bar{a}^2/\hbar^2=40$ showing that the minima of $\ln C^2(\bar{k}\bar{a})$ occur only in a finite number of neighborhoods of $\bar{k}_n$ ($n=1,2,\ldots$) such that $A(\bar{k}_n\bar{a})=0$.

Here A, B, and C are real constants, and θ is a phase angle. As before, one can set the solutions real in the whole region to ensure that $\bar{k}$ is always real. The solutions and their derivatives need to be continuous at the boundaries $\bar{x}=\bar{a}$ and $\bar{b}$. These boundary conditions determine the values of the coefficients A, B, and C as functions of $\bar{k}$:

$$A(\bar{k})=\frac{1}{2}e^{-\bar{k}'\bar{a}}\left[\sin(\bar{k}\bar{a})+\frac{\bar{k}}{\bar{k}'}\cos(\bar{k}\bar{a})\right], \tag{46}$$

$$B(\bar{k})=\frac{1}{2}e^{\bar{k}'\bar{a}}\left[\sin(\bar{k}\bar{a})-\frac{\bar{k}}{\bar{k}'}\cos(\bar{k}\bar{a})\right], \tag{47}$$

$$C^2(\bar{k})=\left(1+\frac{\bar{k}'^2}{\bar{k}^2}\right)e^{2\bar{k}'\bar{b}}A^2+2\left(1-\frac{\bar{k}'^2}{\bar{k}^2}\right)AB+\left(1+\frac{\bar{k}'^2}{\bar{k}^2}\right)e^{-2\bar{k}'\bar{b}}B^2. \tag{48}$$

The general shapes of $A(\bar{k})$ and $C^2(\bar{k})$ are shown in Fig. 2. Note that metastable states of the system will occur only in a finite number of neighborhoods of $\bar{k}_n$ ($n=1,2,\ldots$) such that $A(\bar{k}_n)=0$. The roots $\bar{k}_n$ satisfy

$$\sin(\bar{k}_n\bar{a})+\frac{\bar{k}_n}{\bar{k}'_n}\cos(\bar{k}_n\bar{a})=0. \tag{49}$$

Equation (48) implies that $C^2(\bar{k})$ is minimal at $\bar{k}_n$. For a given $\bar{V}_0$, the number of roots $\bar{k}_n$ is restricted by the condition that $\bar{k}'_n$ in Eq. (45),

$$\bar{k}'_n=\sqrt{\frac{2m\bar{V}_0}{\hbar^2}-\bar{k}_n^2}, \tag{50}$$

must be real. Hence the possible values of $\bar{k}_n$ can lie only in the interval $(0,\sqrt{2m\bar{V}_0/\hbar^2})$. For instance, there are only two roots for the parameters assumed in Fig. 2.

We now expand the coefficients $A(\bar{k})$ and $B(\bar{k})$ about $\bar{E}_n$ $(=\hbar^2\bar{k}_n^2/2m)$:

$$A(\bar{E})\approx\left[\frac{dA}{d\bar{E}}\right]_{\bar{E}=\bar{E}_n}(\bar{E}-\bar{E}_n), \tag{51}$$

$$B(\bar{E})\approx B(\bar{E}_n). \tag{52}$$

Inserting Eqs. (51) and (52) into Eq. (48), after some tedious calculations we find that $C^2(\bar{E})$ behaves in the neighborhood of $\bar{E}_n$ as

$$C^2(\bar{E})=G^2(\Delta+\delta)^2+F^2, \tag{53}$$

where $\Delta=\bar{E}-\bar{E}_n$ as in the previous example, and the constants in the present case are

$$G^2=\frac{1}{4}\left(\frac{m\bar{a}}{\hbar^2\bar{k}_n}\right)^2\left(1+\frac{\bar{k}'^2_n}{\bar{k}_n^2}\right)\left[\cos(\bar{k}_n\bar{a})-\frac{\bar{k}_n}{\bar{k}'_n}\sin(\bar{k}_n\bar{a})\right]^2\times e^{2\bar{k}'_n(\bar{b}-\bar{a})}, \tag{54}$$

$$F^2=\left(1+\frac{\bar{k}_n^2}{\bar{k}'^2_n}\right)^{-1}\left[\sin(\bar{k}_n\bar{a})-\frac{\bar{k}_n}{\bar{k}'_n}\cos(\bar{k}_n\bar{a})\right]^2 e^{-2\bar{k}'_n(\bar{b}-\bar{a})}, \tag{55}$$

and

$$\delta=\left(\frac{\hbar^2\bar{k}_n}{m\bar{a}}\right)\left(\frac{\bar{k}_n^2-\bar{k}'^2_n}{\bar{k}_n^2+\bar{k}'^2_n}\right)\times\left(\frac{\bar{k}'_n\sin(\bar{k}_n\bar{a})-\bar{k}_n\cos(\bar{k}_n\bar{a})}{\bar{k}'_n\cos(\bar{k}_n\bar{a})-\bar{k}_n\sin(\bar{k}_n\bar{a})}\right)e^{-2\bar{k}'_n(\bar{b}-\bar{a})}. \tag{56}$$

From the relation (53), the scattering states relevant to this metastable system can be constructed by following exactly the same procedures as in the previous section. The nondecay probability $P(t)$ of finding the particle within the confined region $(0<\bar{x}<\bar{a})$ at time t is again of the form $P(t)\sim\exp(-\gamma_n(t))$, where $\gamma_n(t)$ is now given by

$$\gamma_n(t)=2\left|\frac{F}{G}\right|\frac{t}{L_0L(t)}=\frac{8\hbar^2\bar{k}_n^3}{m\bar{a}}\left(\frac{\bar{k}'_n}{\bar{k}_n^2+\bar{k}'^2_n}\right)^2 e^{-2\bar{k}'_n(\bar{b}-\bar{a})}\frac{t}{L_0L(t)}, \tag{57}$$

where we have used Eqs. (54), (55), and (49). When the barrier height is much larger than the characteristic "energy" of the escaping particles ($\bar{V}_0\gg\bar{E}_n$), which is equivalent to the relation $\bar{k}'_n\gg\bar{k}_n$, $\gamma_n(t)$ becomes

$$\gamma_n(t)\to\frac{8\hbar^2}{m\bar{a}}\frac{\bar{k}_n^3}{\bar{k}'^2_n}e^{-2\bar{k}'_n(\bar{b}-\bar{a})}\frac{t}{L_0L(t)}. \tag{58}$$

As in the previous example, for positive $v>0$ (the expanding case) one finds a small but finite probability that the particle does not tunnel out of the well at large time. In this case not only does the barrier leave more room for the particle to stay within the well as it moves away from $x=0$, but its width also becomes thicker, thus making tunneling difficult.

In order to transform the result (58) to the stationary one, we simply apply the same substitutions as given at the end of the last section, with the addition of $\bar{b}\to b/L_0$ and $\bar{k}'_n\to k'_nL_0$, where $k'_n=\sqrt{2m[(\bar{V}_0/L_0^2)-E_n]}/\hbar$. Once again $\gamma_n(v=0)$ is directly proportional to the time t, in which case a decay rate can be defined: $\Gamma_n\equiv\gamma_n(v=0)/t$. For the present example,

$$\Gamma_n(v=0)=\frac{8\hbar^2}{ma}\frac{k_n^3}{k'^2_n}e^{-2k'_n(b-a)}, \tag{59}$$

which is the same as the result obtained by the complex eigenvalue method for a square barrier with width $(b-a)$ and height $\bar{V}_0/L_0^2$ [20].

V. GENERAL SCALING POTENTIALS

We have calculated the nondecay probabilities of two nonstationary metastable systems explicitly. The potential barriers in the rescaled frame considered in these systems assumed the form of a δ function and a square barrier. These calculations can be immediately generalized to barriers with more general shapes. Without giving further examples, we only discuss briefly the close connection between the nondecay probability $P(t)$ of a particle in a metastable scaling potential $V(x,t)=\bar{V}(x/L(t))/L^2(t)$ and the decay rate Γ of the same particle if it were instead confined in a static potential well $V(x)=\bar{V}(x)$.

From the previous examples, we know that the calculation of $P(t)$ is reduced to the corresponding computation in a static potential $\bar{V}(\bar{x})$ in the rescaled frame. Now this last task would be exactly the same as that carried out in the potential $V(x)=\bar{V}(x)$ in ordinary coordinates. The only difference, as seen from the previous two examples, is that all ordinary parameters, such as E, k, k', t, a, etc., are replaced by the corresponding rescaled ones, i.e., $\bar{E}$, $\bar{k}$, $\bar{k}'$, τ, $\bar{a}$, etc. Application of the scattering state method to the general α decay type of potential $V(x)$ in normal coordinates was given in [14], and can be carried over directly. Following [14] the important step is to determine the discrete values E_n (or equivalently k_n) that minimize the amplitude C of the wave function in the region outside the well. Consider a confining state constructed with E centered around a specific E_n. Minimization of C then gives the two functions $F(E_n)$ and $G(E_n)$ (other parameters in F and G are not indicated). The nondecay probability in $V(x)$ is then given by $\exp(-\Gamma_nt)$, where the decay rate Γ_n is

$$\Gamma_n(E_n)=2\left|\frac{F(E_n)}{G(E_n)}\right|. \tag{60}$$

Suppose all these computations have been done in ordinary coordinates. Then one can immediately write down the expression of the nondecay probability $P(t)\sim\exp[-\gamma_n(t)]$ for the scaling potential $V(x,t)$ as

$$\gamma_n(t)=2\left|\frac{F(\bar{E}_n)}{G(\bar{E}_n)}\right|\frac{t}{L_0L(t)}=\Gamma_n(\bar{E}_n)\frac{t}{L_0L(t)}. \tag{61}$$

Here the functional form of the decay rate Γ_n is taken over directly, but with all the parameters replaced by the corresponding rescaled ones. Equation (61) gives the connection between the nondecay probability in $V(x,t)=\bar{V}(x/L(t))/L^2(t)$ and the decay rate in $V(x)=\bar{V}(x)$. Finally, in the nonmoving limit $v=0$, $V(x,t)$ becomes $V(x)=\bar{V}(x/L_0)/L_0^2$. Setting $v=0$ in Eq. (61) then gives the decay rate in this potential, $\Gamma_n(E_n)/L_0^2$, as seen in the previous cases.

VI. CONCLUSION

The problem of quantum metastability in a class of moving potentials introduced by Berry and Klein is considered. The potential in this class has its height and width scaled in a specific way so that it can be transformed into a stationary one. In deriving the nondecay probability of the system, we employed a method that is less well known but conceptually more satisfactory, namely, the method of scattering states. Nondecay probabilities in a moving δ-function potential and a moving square barrier potential were derived, and a connection between the nondecay probability in a general scaling potential and the decay rate in a related static potential was established.

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訪問日本大阪大學物理系理論組

心得報告

在本計劃之補助下，本人得以在 2002 年 4 月 11 日至 20 日訪問日本大阪大學物理系理論組。

本人此次訪問的主要目的是和細谷裕教授（Prof. Y. Hosotani）討論相關合作研究的課題。在訪問期間，也很高興認識多位教授、博士後研究員及研究生。並作多方面的討論。期間本人也應邀作了一個講演，題目是「準精確可解之物理模型」。

此次訪問讓本人對日本的大學及研究所制度有深一層的了解，對日本人在基礎科學研究的認真與投入，深感敬佩。無怪乎日本人能在最近的 3 年內連得四個諾貝爾物理及化學獎。他們的精神，很值得我們學習。

這次行程中本人得益最多的是在舉各位學者討論中，對準精確可解性此一議題有更進一步的領會。未回國後，本人對此一議題繼續探討，並在暑假期間，與一名印度學者 Pinaki Roy 教授合作有關的研究。目前並已得到一些不錯的成果。

何俊耕

2002. 10. 31

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出席「第廿四屆物理學中群論方法」國際研討會

心得報告

在本計劃補助下，本人於2002年7月15日至20日參加了「第24屆物理學中群論方法」國際研討會。

此會每兩年召開一次之群論方法的重要會議。會議目的是將群論方法在物理學各子領域中的應用及新進展作一階段性的綜合介紹。此次會議約有五、六百名國際學者參與。

本人在會議期間聽了不少知名學者的重要報告，得以了解當前群論方法的重要方向及成果。獲益匪淺。本人也在會上發表了一篇文章，題目是：

Quantum Frenkel-Kontorova Model.

何俊偉

2002.10.31

Quantum Frenkel-Kontorova Model

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Abstract. This paper presents a simple variational approach to the quantum Frenkel-Kontorova model.

1. Introduction

The Frenkel-Kontorova (FK) model [1] is a simple one-dimensional model used to study incommensurate structures appearing in many condensed-matter systems, such as charge-density waves, magnetic spirals, and adsorbed monolayers. These modulated structures arise as a result of the competition between two or more length scales. The FK model describes a chain of atoms connected by harmonic springs subjected to an external sinusoidal potential. In an important development in the study of the classical FK model, Aubry [2] first made use of the connection between the FK model, the so-called "standard map", and the Kolmogorov-Arnold-Moser (KAM) theorem to reveal many interesting features of the FK model. Particularly, he showed that when the mean distance (also called the winding number) between two successive atoms is rational, the system is always pinned. But when the winding number is irrational, there exits a critical external field strength below (above) which the system is unpinned (pinned). This transition is called by Aubry a "transition by breaking of analyticity", and is closely connected with the breakup of a KAM torus. It is very analogous to a phase transition, and various critical exponents and questions of universality have been extensively studied in the past.

Needless to say, quantum effects are very important in the FK model. However, unlike the classical case, study of quantum FK models is rather scanty. It was first considered in a quantum Monte Carlo (QMC) analysis in [3]. Their main observation is that the map appropriate to describe the quantum case is no longer the standard map, but rather a map with a sawtooth shape.

Previous theoretical attempts at obtaining the sawtooth map require one to go beyond the independent-particle approximation. In [4], however, we showed that all the essential features observed in the QMC studies can indeed be obtained from an independent-particle picture of the many-body ground state. Our strategy is to derive an effective Hamiltonian for the quantum FK model by adopting Dirac's time-dependent variational principle together with the Jackiw-Kerman (JK) function [5] as the single particle state. The JK wavefunction can be viewed as the Q-representation of the squeeze state.

2. Effective Hamiltonian

The Hamiltonian of the quantum FK model is given by

$$\mathcal{H} = \sum_i \left[\frac{\hat{p}_i^2}{2m} + \frac{\gamma}{2} (\hat{q}_{i+1} - \hat{q}_i)^2 - V \cos(l_0 \hat{q}_i) \right]. \tag{1}$$

Here $\hat{q}_i$ and $\hat{p}_i$ are the position and momentum operators, respectively, of the ith atom, γ the elastic constant of the spring, V and $2\pi/l_0$ are the strength and the period of the external potential. It is convenient to use the dimensionless variables $\hat{Q}_i = l_0\hat{q}_i$, $\hat{P}_i = l_0\hat{p}_i/\sqrt{m\gamma}$, and $K = Vl_0^2/\gamma$. With these new variables, we obtain the following dimensionless Hamiltonian H

$$H = \sum_i \left[\frac{\hat{P}_i^2}{2} + \frac{1}{2}\left(\hat{Q}_{i+1} - \hat{Q}_i\right)^2 - K\cos(\hat{Q}_i)\right]. \tag{2}$$

We have $\mathcal{H} = \gamma H/l_0^2$. The effective Planck constant is $\tilde{\hbar} = \hbar l_0^2/\sqrt{m\gamma}$. For the classical FK model, the Aubry transition occurs at the critical value $K_c = 0.971635\cdots$.

To study the ground state properties of the quantum FK model in (2), we adopt here the time-dependent variational principle pioneered by Dirac. In this approach, one first constructs the effective action $\Gamma = \int dt\ \langle\Psi, t|i\tilde{\hbar}\partial_t - H|\Psi, t\rangle$ for a given system described by H and $|\Psi, t\rangle$. Variation of Γ is then the quantum analogue of the Hamilton's principle. The time-dependent Hartree-Fock approximation emerges when a specific ansatz is made for the state $|\Psi, t\rangle$. We now assume the trial wavefunction of the ground state of our quantum FK system to have the Hartree form $|\Psi, t\rangle = \prod_i |\psi_i, t\rangle$, where the normalized single-particle state $|\psi_i, t\rangle$ is taken to be the JK wavefunction [5]:

$$\begin{aligned}\langle Q_i|\psi_i, t\rangle = {} & \frac{1}{(2\pi\tilde{\hbar}G_i)^{1/4}} \\ & \times \exp\left\{-\frac{1}{2\tilde{\hbar}}\left(Q_i - x_i\right)^2\left[\frac{1}{2}G_i^{-1}\right.\right. \\ & \left.\left. - 2i\Pi_i\right] + \frac{i}{\tilde{\hbar}}p_i\left(Q_i - x_i\right)\right\}.\end{aligned} \tag{3}$$

The real quantities $x_i(t)$, $p_i(t)$, $G_i(t)$ and $\Pi_i(t)$ are variational parameters the variations of which at $t = \pm\infty$ are assumed to vanish. Squeezed state function in the form of the JK wavefunction has the advantage that the physical meanings of the variational parameters contained in the JK wavefunction are most transparent, as we shall show below. Furthermore, the JK form is in the general Gaussian form so that integrations are most easily performed.

It is not hard to check that x_i and p_i are the expectation values of the operators $\hat{Q}_i$ and $\hat{P}_i$: $x_i = \langle\Psi|\hat{Q}_i|\Psi\rangle$, $p_i = \langle\Psi|\hat{P}_i|\Psi\rangle$. Also, one has $\langle\Psi|(\hat{Q}_i - x_i)^2|\Psi\rangle = \tilde{\hbar}G_i$, and $\langle\Psi|i\tilde{\hbar}\partial_t|\Psi\rangle = \sum_i(p_i\dot{x}_i - \tilde{\hbar}G_i\dot{\Pi}_i)$, where the dot represents derivative with respect to time t. It is now clear that $\tilde{\hbar}G_i$ is the mean fluctuation of the position of the i-th atom, and that $G_i > 0$. From the form of the effective action one sees that that p_i and Π_i are the canonical conjugates of x_i and G_i, respectively. The Dirac variational principle leads to the following effective Hamiltonian

$$\begin{aligned}H_{eff} &= \langle\Psi|H|\Psi\rangle \\ &= \sum_i \frac{1}{2}\left[p_i^2 + \tilde{\hbar}\left(\frac{1}{4}G_i^{-1} + 4\Pi_i^2 G_i\right)\right] \\ &+ \sum_i \frac{1}{2}\left(x_{i+1} - x_i\right)^2 \\ &+ \sum_i \frac{\tilde{\hbar}}{2}\left(G_{i+1} + G_i\right) \\ &- \sum_i K\exp\left(-\frac{\tilde{\hbar}}{2}G_i\right)\cos x_i\,.\end{aligned} \tag{4}$$

We can obtain the equations for the equilibrium states in the Hartree-Fock approximation by directly varying the effective Hamiltonian H_{eff} with respect to the variables p_i, Π_i, x_i and G_i, which give, respectively,

$$p_i = 0 \quad , \quad 4\Pi_i G_i = 0 \, , \tag{5}$$

$$x_{i+1} - 2x_i + x_{i-1} = K \exp\left(-\frac{\tilde{\hbar}}{2} G_i\right) \sin x_i \, , \tag{6}$$

$$\frac{1}{4} G_i^{-2} - K \exp\left(-\frac{\tilde{\hbar}}{2} G_i\right) \cos x_i - 2 = 4\Pi_i^2 \, . \tag{7}$$

The second equation in (5) implies $\Pi_i = 0$ as $G_i > 0$. This in turn means that the right hand side of eq.(7) is equal to zero:

$$\frac{1}{4} G_i^{-2} - K \exp\left(-\frac{\tilde{\hbar}}{2} G_i\right) \cos(x_i) - 2 = 0 \, . \tag{8}$$

In the limit $\hbar = 0$, eq.(6) is equivalent to the standard map.

3. Numerical results

We numerically solve for the set of variables x_i and G_i which characterize the ground state using the Newton method. In all our numerical computations the winding number $P/Q = 610/987$, which is an approximation of the golden mean winding number $(\sqrt{5}-1)/2$, is used with the periodic boundary condition $x_{i+Q} = x_i + 2\pi P$. This winding number is much more accurate than those used in previous works to approximate the golden mean number, thus giving us better accuracy in the computations of physical quantities related to the ground state.

Having obtained the values of x_i which give the mean positions of the quantum atoms in the chain, we can compare the results with the classical configuration by plotting the so-called g-function, defined by

$$g_i \equiv K^{-1} \left(x_{i+1} - 2x_i + x_{i-1}\right) \tag{9}$$

versus the actual atomic positions x_i. From (6), we also have

$$g_i = \exp\left(-\frac{\tilde{\hbar}}{2} G_i\right) \sin x_i \, . \tag{10}$$

Here G_i is related to x_i by eq.(8). We see from this equation that quantum fluctuations G_i will modify the shape of the classical *sine*-map.

In Fig. 1 we show the graphs of the g-function for the case $K = 5$. The curve defined by (10) with G_i satisfying (8) are shown here as dashed curves for different $\tilde{\hbar}$. In the classical limit ($\tilde{\hbar} = 0$) this curve is simply the standard map (*sine*-curve). As $\tilde{\hbar}$ increases, the amplitude of the curve decreases. For sufficiently large $\tilde{\hbar}$, the curve resembles more closely a "sawtooth" shape. This is first noted in QMC study in [3]. Here we see that it comes out very naturally from the equation of motion (8) and (10). We have therefore demonstrated that the sawtooth map could be recovered in the independent-particle approximation. In the supercritical case ($K = 5$), when $\tilde{\hbar} < \tilde{\hbar}_c \approx 6.58$, the positions x_i of the atoms cover only a subset of the g-curves. This is in accord with the fact that the atoms are in the pinning phase.

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Figures captions

Fig. 1 g-function plotted against actual atomic positions for $K = 5$ and winding number $P/Q = 610/987$ at $\tilde{\hbar} = 2$ (black dots), 6 (white dots) and 7 (black curve) (the dashed curves represent eq.(10) with G_i satisfying (8).