Array-induced collective transport in the Brownian motion of coupled nonlinear oscillator systems

Zhigang Zheng,[1,2] Bambi Hu,[1,3] and Gang Hu[4,2]
[1]*Department of Physics and Center for Nonlinear Studies, Hong Kong Baptist University, Kowloon Tong, Hong Kong, China*
[2]*Department of Physics, Beijing Normal University, Beijing 100875, China*
[3]*Department of Physics, University of Houston, Houston Texas 77204*
[4]*Center of Theoretical Physics, Chinese Center of Advanced Science and Technology (World Laboratory), Beijing 8730, China*
(Received 20 July 1998)

Brownian motion of an array of harmonically coupled particles subject to a periodic substrate potential, and driven by an external bias, is investigated. In the linear response limit (small bias), coupling between particles may enhance the diffusion process, depending on the competition between the harmonic chain and the substrate potential. An analytical formula of the diffusion rate for the single-particle case is also obtained. In the nonlinear response regime, the moving kink may become phase locked to its radiated phonon waves; hence the mobility of the chain may decrease as one increases the external force. [S1063-651X(98)07712-5]

PACS number(s): 05.40.+j, 05.45.+b

I. INTRODUCTION

Brownian motion of particles subject to periodic substrate potentials and external forces gained great interest due to its wide applications and practical importance in connection with transport processes in many fields including damped pendula, superionic conductor, Josephson tunneling junction, vortex motion in high-T_c oxide superconductors, phase-locked loops, rotation of dipoles, charge-density wave, dislocation, and so on [1–7]. Although the collective transport of coupled nonlinear oscillators has been studied recently for the two-dimensional case in relation to studies on adsorbate islands and monolayer films on surfaces [8], explorations of collective behaviors for the one-dimensional (1D) coupled nonlinear oscillators are still fundamentally important in understanding many physical systems. In dimensionless form, the Langevin equation in describing the 1D case might be written as

$$\ddot{x}_j+\gamma\dot{x}_j+d\sin\left(\frac{2\pi x_j}{b}\right)=\sum_{i=1}^{N}\frac{\partial V(x_j,x_i)}{\partial x_j}+F_j(t)+\xi_j(t), \tag{1}$$

where x_j represents the coordinate of the ith particle and $\dot{x}_j=dx_j/dt$ its corresponding velocity, γ is the friction coefficient, d is the height of the periodic potential, and b denotes the period of the substrate potential. $V(x_j,x_i)$ reflects the interaction between the jth and ith particles. $F_j(t)$ and $\xi_j(t)$ denote the external driving force and the thermal fluctuation induced random force on the jth particle, respectively. In this paper we focus on the case when the external driving is uniformly constant, i.e., $F_j(t)=F$. The thermal noise is frequently assumed to be a both spatially and temporally uncorrelated Gaussian-type one,

$$\langle\xi_j(t)\rangle=0,\quad \langle\xi_i(t)\xi_j(t')\rangle=2\gamma k_B T\delta_{i,j}\delta(t-t'), \tag{2}$$

where k_B is the Boltzmann constant, and T is the environmental temperature. When the interaction among particles is very weak, in many cases one may approximately treat the above problem in terms of Brownian motion of a single particle under a biased periodic potential. The corresponding Fokker-Planck equation then reads [1]

$$\frac{\partial W}{\partial t}=-\dot{x}\frac{\partial W}{\partial x}+\gamma\frac{\partial}{\partial\dot{x}}\left(\dot{x}W+k_BT\frac{\partial W}{\partial\dot{x}}\right). \tag{3}$$

Here $W(x,\dot{x},t)$ denotes the probability distribution of the particle, where the indices of particles are omitted. This equation is sufficiently complicated to solve analytically, so that a closed analytical solution in describing the diffusion process is far from obtainable. Based on the inverse-friction expansion method, we recently gave an analytical perturbative solution of the mobility for the single-particle case valid for arbitrary friction cases [9]. When the interaction among particles can no longer be ignored, one has to treat the coupled case [Eq. (1)]. Interactions between particles introduce new time scales, which leads to more complicated phenomena, and furthermore an analytical treatment of the corresponding Fokker-Planck equation is almost impossible [3]. One of the simplest models in describing the competition between the coupling and the substrate potential is the well-known Frenkel-Kontorova (FK) system [10], which describes a chain of particles with nearest-neighboring harmonic couplings subject to a periodic potential, where the interaction is reduced to

$$V(x_j,x_{j-1})=\tfrac{1}{2}K(x_j-x_{j-1}-a)^2, \tag{4}$$

where K and a are the coupling strength and the static length of the spring, respectively. Now there are two competing lengths: a and b. The winding number (or the frustration) is defined as $\delta=a/b$, which may strongly affect the spatial configuration of the system. During the past few years, the FK model was applied to investigations of the ground state of competing systems, and commensurate-incommensurate phase transitions were found and theoretically explored [11]. The theory developed by Aubry stands as one of the deepest achievements in theoretical comprehension of the physics of modulated phases [12]. Dynamics of the FK chain was also explored in relating to many fields, such as the charge-density wave, nanotribology and surface problems, self-organized criticality, and Josephson-junction arrays and ladders [13,14]. In the following investigations, we simply set b to be 2π. Then the Langevin equation connected to the FK chain can be followed from Eq. (1):

$$\ddot{x}_j+\gamma\dot{x}_j+d\sin x_j=K(x_{j+1}-2x_j+x_{j-1})+F+\xi_j(t). \tag{5}$$

One may notice that the static length of the spring a does not enter Eq. (5), but it may play a very significant role in describing the motion of the coupled systems. The corresponding Fokker-Planck equation reads

$$\frac{\partial W}{\partial t}=\sum_j\left[-\dot{x}_j\frac{\partial W}{\partial x_j}+\frac{\partial U}{\partial x_j}\frac{\partial W}{\partial \dot{x}_j}+\gamma\frac{\partial}{\partial \dot{x}_j}\left(\dot{x}_jW+k_BT\frac{\partial W}{\partial \dot{x}_j}\right)\right], \tag{6}$$

where $W=W(\{x_j\},\{\dot{x}_j\},t)$ is the joint probability distribution function, and here we use the total potential $U(\{x_j\})$, and for the case of the FK model $U(\{x_j\})=\Sigma_j[d(1-\cos x_j)+\frac{1}{2}K(x_{j+1}-x_j-a)^2]$. In the high-friction limit one may obtain the Smoluchowski equation by averaging velocities, which can be written as

$$\frac{\partial P}{\partial t}=\frac{1}{\gamma}\sum_j\frac{\partial}{\partial x_j}\left(\frac{\partial U}{\partial x_j}P+k_BT\frac{\partial P}{\partial x_j}\right), \tag{7}$$

where $P(\{x_j\},t)=\int W(\{x_j\},\{\dot{x}_j\},t)\Pi_j d\dot{x}_j$ is the reduced probability distribution for only spatial variables. In many cases one is interested in the mobility of the chain:

$$\mu=\frac{\langle v\rangle}{F}, \tag{8}$$

where $\langle\cdot\rangle$ includes both time and particle averages. This definition was introduced in discussions of Brownian motion of a single particle in the biased periodic potential. We will give a unified solution for the single particle case in the following discussion. Analytical investigations of the coupled case may be more difficult; therefore we will discuss this problem mainly in terms of numerical simulations. The *collective diffusion coefficient*, which is relevant for studying commensurability effects [15], is given by the linear part of the mean-square displacement:

$$D=\lim_{t\to\infty}\frac{1}{2Nt}\sum_{i,j}\langle[x_i(t)-x_j(0)]^2\rangle. \tag{9}$$

This coefficient is connected to the mobility in the small force limit (*linear response*) [1] by

$$D(T,K,\delta)=k_BT\lim_{F\to 0}\mu(F,T,K,\delta). \tag{10}$$

One may notice that the diffusion coefficient relates to the temperature, the coupling strength, and the frustration. In particular, the dependence on the coupling strength and the frustration does not happen for the single-particle case. Studies of their dependences are very interesting and significant. In the following discussions, we will investigate both the linear and nonlinear response regimes. We find that in the limit of linear response, the coupling between particles can greatly increase the diffusion rate, which may be important in realistic experiments and technologies. Additionally, we shall investigate the commensurability effects. In the vicinity of the golden mean $\delta=\delta_G=(\sqrt{5}-1)/2$, the chain possesses the maximum diffusion coefficient. In the nonlinear response regime, the transport is dominated by the strong resonant behavior due to the competitive phase locking between the traveling wave and its radiated linear phonons. This resonance may lead to the suppression of the mobility. In the following investigations, we mainly perform numerical simulations for the coupled case. The fourth-order Runge-Kutta integration algorithm is applied and the time step is adjusted according to the numerical accuracy. Periodic boundary conditions are applied, i.e., $x_{j+N}(t)=x_j(t)+2\pi M$, where M is an integer that counts the net number of kinks trapped in the ring, therefore the frustration is $\delta=M/N$ and the spring constant will be $a=2\pi\delta$. Throughout the paper $\gamma=0.1$, and d is set to be 1.

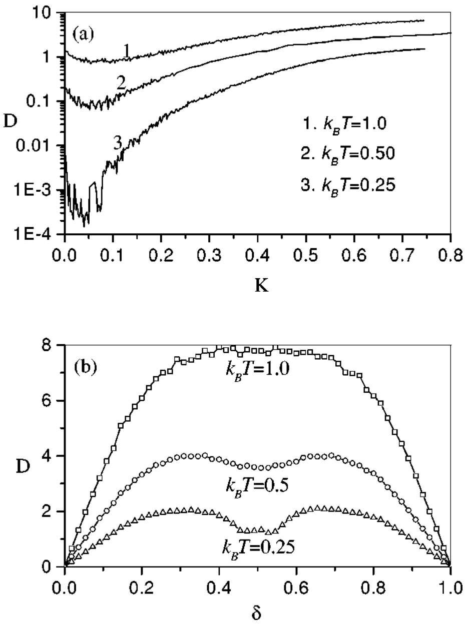

FIG. 1. (a) The diffusion coefficient D of the FK chain vs the coupling strength K for different temperatures $k_BT=0.25$, 0.5, and 1.0. The vertical coordinate is shown by using a logarithm scale. The diffusion coefficient first decreases against the coupling and then increases and exceeds the value for the uncoupled case, indicating a competition between order and disorder. For moderate coupling, the D-K relation is a power type. (b) The diffusion rate D against the winding number (frustration) δ of the chain for different temperatures $k_BT=0.25$, 0.5, and 1.0. The diffusion indicates a strong commensurability effect.

II. LINEAR RESPONSE: ENHANCEMENT OF THE DIFFUSION

In Fig. 1(a), we give the relation between the diffusion coefficient D and the coupling strength K for the incommensurate case (e.g., the gold mean case $\delta=\delta_G$) and for different temperatures. The first phenomenon we observe is that the relation between the diffusion coefficient and the coupling strength is not monotonic. For weak coupling strengths, the diffusion process is suppressed. When $K > K_{c1}$ (*the first threshold*), the diffusion coefficient begins to increase as one increases the coupling strength. Near this critical value, the diffusion coefficient D is found to obey the relation

$$D = D_0(T)|K - K_{c1}|^{\alpha(T)}, \tag{11}$$

where the scaling exponent $\alpha(T)$ decreases with increasing the temperature T. At a *second threshold* K_{c2}, D begins exceeding the single-particle value ($K=0$, the noninteracting case), exhibiting an *array-enhanced diffusion process*. For the moderate coupling strength, we find that the D-K relation obeys the power law:

$$D \propto K^{\beta(T)}, \tag{12}$$

where the scaling exponent scales with the temperature as $\beta(T) \sim T^{-1/2}$, i.e., it decreases with increasing the temperature. At the high coupling constant, the diffusion coefficient may saturate to a value much higher than the single-particle case. This behavior is very interesting, because one must overcome a *threshold coupling* before one can obtain a higher diffusion rate. Additionally, K_{c1} and K_{c2} increase with the temperature; i.e., for higher temperatures, one must overcome stronger coupling thresholds to obtain higher diffusion rates. The result indicates that if one introduces some coupling between the particles (elements), then a higher diffusion rate than uncoupled systems can be achieved. In many realistic applications one hopes that the diffusion process can be improved as quickly as possible. Our exploration indicates that for the incommensurate case the coupling between particles may enhance the diffusion process.

The above behavior can be heuristically interpreted, which is a typical consequence of *the competition between order and disorder*. The mechanism of order comes from the coupling among particles, where the coupling tends to organize the chain to move in a collective way; the mechanism of disorder is the thermal fluctuation, which tends to destruct the ordered motion. For very weak couplings, thermal noise may dominate; thus particles cannot organize themselves very well to diffuse collectively. In this case interactions between elements introduce another resource of the dissipation that leads to higher friction [18]. When the coupling between particles increases and exceeds a threshold, then the role of disorder may be supressed, and particles can gradually move collectively, leading to high diffusion rates. At higher temperatures, the noise produces much more disorder, hence the chain needs a stronger coupling to organize the collective diffusion.

All the above discussions are valid for the incommensurate case. In Fig. 1(b), we give the numerical result of the diffusion coefficient against the winding number (frustration) δ for different temperatures, and the coupling strength $K = 1.0$, which is strong enough for the chain to diffuse. It can be found that, for high temperatures, the commensurability effect is not very significant. Because the curve is symmetric about $\frac{1}{2}$, we only discuss the range $\delta \in [0, \frac{1}{2}]$. For small winding numbers, the relation is a linear one [see Fig. 1(b)],

$$D = D_0 T \delta, \tag{13}$$

where the slope is proportional to the temperature. This indicates that for small frustrations, the diffusion is suppressed by introducing the coupling among particles. The curve becomes flat when δ further increases. This result indicates that although the particles are coupled, for small frustrations, the diffusion process is still very slow. In this case couplings between particles act as an additional source of dissipation [18]. This suppression of the diffusion is because the Peierls-Nabarro (PN) barrier is high (for the coupled case the motion of the chain is dominated by the moving kink, as pointed out below. The Peierls-Nabarro barrier corresponds to the barrier for the kink translation along the chain. It is also the minimum energy necessary to move the kink along the chain.), and the collision of particles with the substrate potential plays a more significant role, thus one needs a higher activated energy to overcome the PN barrier. A commensurate effect is clearly shown when the temperature decreases. For the case $k_BT = 0.25$, we observe that the diffusion rate reaches a maximum value at approximately $\delta = \frac{1}{3}$ and $\frac{2}{3}$. These two values are very close to the golden mean value $\delta_G = (\sqrt{5}-1)/2$ and $1-\delta_G$. In order to obtain a higher diffusion, one should choose winding numbers near the golden mean. This result can be applied to the dynamics of Josephson-junction arrays, where the frustration can be altered by changing the magnetic field strength [19].

The relation between D and T is not trivial. We first discuss the noninteracting case. For the very small damping constant and high enough temperature case, the diffusion coefficient was approximately obtained as [1]

$$D = \frac{\pi k_B T}{2\gamma} \exp\left(-\frac{2d}{k_B T}\right), \tag{14}$$

i.e., the diffusion rate increases with the temperature. In the high damping and low temperature limit, the diffusion is dominated by thermally activated hoppings; then one has the formula [1]

$$D = \frac{k_B T}{\gamma}\left[I_0\left(\frac{d}{k_B T}\right)\right]^{-2} \rightarrow \frac{2\pi d}{\gamma} \exp\left(-\frac{2d}{k_B T}\right), \tag{15}$$

where $I_n(x)$ is the modified Bessel function. One may find the same Boltzmann factor (Arrhenius form) $\exp(-2d/k_BT)$ as in the low damping case, except the prefactor. The common factor comes from the thermal-fluctuation-induced hopping effect. In general cases, we are still able to derive a unified formula of the diffusion rate. We investigated the mobility and obtained a successively perturbative solution of the mobility [9]. By using the relation between the mobility and the diffusion coefficient (10), in the linear response limit, $F \rightarrow 0$, we have the formula

$$D = \frac{(2\pi)^2 k_B T}{\gamma[\Omega(d,T,0)\Delta(d,T,0) - \Lambda(\gamma,T,d,0)]}, \tag{16}$$

where $\Omega(d,T,F)$, $\Delta(d,T,F)$, and $\Lambda(\gamma,T,d,F)$ are given by

$$\Omega(d,T,F)=\int_0^{2\pi}\exp\{[f(x)-Fx]/k_BT\}dx,$$

$$\Delta(d,T,F)=\int_0^{2\pi}\exp\{[-f(x)+Fx]/k_BT\}dx,$$

$$\Lambda(\gamma,T,d,F)=\int_0^{2\pi}dx\,\exp\{[-f(x)+Fx]/k_BT\}\times\int_0^{x}q(\xi)\exp\{[f(\xi)-F\xi]/k_BT\}d\xi, \tag{17}$$

where $f(x)=-d\cos x$. The kernel function $q(x)$ can be obtained from the operation (see Ref. [9] for a detailed discussion)

$$q(x)=\frac{1}{c}\gamma\hat{\mathcal{H}}c, \tag{18}$$

where c is a constant, and $\hat{\mathcal{H}}$ is a continued-fraction operator acting on the constant c:

$$\hat{\mathcal{H}}=\hat{I}-\frac{1}{\gamma^2}\hat{K}^+\frac{1}{\hat{I}-\frac{1}{2\gamma^2}\hat{K}^+\cdots\hat{K}^-}\hat{K}^-, \tag{19}$$

where $\hat{I}$ is the unit operator, and $\hat{K}^+$ and $\hat{K}^-$ are given as

$$\hat{K}^+=\sqrt{k_BT}\frac{\partial}{\partial x},\quad \hat{K}^-=\hat{K}^++\frac{1}{\sqrt{k_BT}}\left[\frac{df(x)}{dx}-F\right]. \tag{20}$$

This is a unified formula of the diffusion coefficient valid for arbitrary damping and temperature cases.

When the particles are coupled in an array way, they will move collectively, leading to the wave motion. In this case, the diffusion is mainly related to the kink motion (traveling wave) [14,16]. The kink describes the minimally possible, topologically stable, compression of the commensurate structure. The kink is a quasiparticle, characterized by an effective mass, rest energy and the PN amplitude $E_{\rm PN}$. In the low temperature case, the diffusion rate can be given as [17]

$$D=D_0\exp\left(-\frac{E_{\rm PN}}{k_BT}\right), \tag{21}$$

where D_0 is the prefactor that scales with $E_{\rm PN}$ as $D_0\propto E_{\rm PN}^{1/2}$ for the low damping case and $D_0\propto E_{\rm PN}$ for the high damping case. In the strong coupling case, one may have

$$D\approx Ck_BT\left[1-\frac{1}{8}\left(\frac{E_{\rm PN}}{k_BT}\right)^2\right]. \tag{22}$$

Equation (22) indicates that there are two competing terms. For very high temperatures, the diffusion rate may be dominated by D_0. In the low temperature regime, the two terms may compete and the exponential term plays an important role. Because the PN barrier closely relates to the commensurability effect, the diffusion rate will be strongly affected by the commensurability of the system. It may be easily found that, for both single-particle and coupled-particle systems, an Arrhenius factor always exists, except that *for the single-particle case the factor relates to the potential barrier, but for the chain it relates to the PN barrier.*

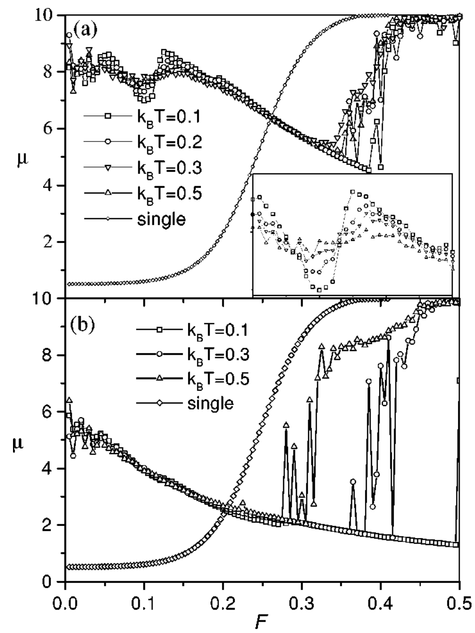

FIG. 2. The mobility of the chain μ varying with the external driving force F for cases (a) $N=8$ and $M=3$ and (b) $N=8$ and $M=1$ for different temperatures. The comparison line corresponds to the case of a single particle at the temperature $k_BT=0.5$. The inset of (a) is plotted for $F=0.05-0.2$ to make a clearer observation. In many regions the mobility decreases when increasing the external force for the coupled case. This anomalous behavior is a consequence of the competition between the moving kink (traveling wave) and the phonons radiated by the collision between the harmonic chain and the periodic potential.

III. NONLINEAR RESPONSE: SUPPRESSION OF THE MOBILITY

When one increases the external driving force, the transport behavior becomes a drift one. In this case one usually uses the mobility $\mu=\langle v\rangle/F$ to describe the transport process of the system. In Figs. 2(a) and 2(b), we give the the numerical μ-F relation for $\delta=\frac{3}{8}$ and $\frac{1}{8}$, respectively. The mobility of the single particle for $k_BT=0.50$ is also plotted to make a clearer comparison. The first result one may clearly observe is that when the driving force is small, the mobility of the chain is much higher than that of the single-particle case. As one increases the force, the mobility decreases. These two phenomena are much different from the single-particle case (see the single-particle line in Fig. 2). Another behavior different from the single-particle case is that at the left side of the decreasing lines [e.g., different lines between 0.15 and 0.4 in Fig. 2(a) corresponding to different temperatures, see the left side $F=0.15$], the mobility decreases when one increases the temperature [see, for example, $F=0.15$ in the inset of Fig. 2(a); the mobilities corresponding to higher temperatures are smaller]. In the middle of the decreasing lines

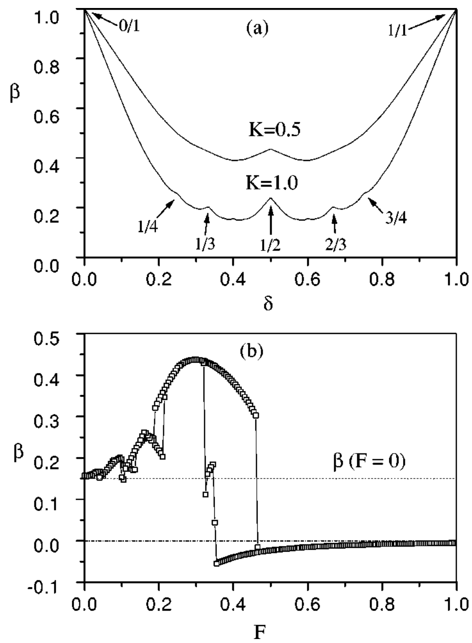

FIG. 3. (a) The contraction factor β varies with the frustration δ with $F=0$ for $K=0.5$ and 1.0. Peaks at the rational $\delta=0,1,\frac{1}{2},\ldots$ shows the commensurate effect. (b) β against the external force F with $\delta=\frac{3}{8}$. The dashed horizontal line corresponds to the value of β at $F=0$. The hysteresis loop can be observed due to the bistability of the system.

[e.g., $F=0.25$ in Fig. 2(a)], the mobility is almost unaffected by the increasing temperature. At the right hand side of the decreasing lines, the mobility increases with increasing the temperature, which is a natural consequence (similar phenomenon could also occur at approximately $F=0.1$). The above anomalous phenomena are consequences of the interaction among particles. In fact, one may study the noiseless case to find this intrinsic cause. In this case it is found [20–22] that the motion of the chain is dominated by the moving localized kink, i.e., a distorted traveling wave that is composed of a moving kink and the oscillating linear wave around it. In the underdamped case, the moving kink may become phase locked to its radiated phonons [14]. We have obtained a mean-field formula of the resonance-velocity spectrum (see Ref. [21] for a detailed derivation):

$$v(m_1,m_2)=\frac{m_2}{m_1}\sqrt{\beta+4K\sin^2\left(\frac{m_2\delta\pi}{m_1}\right)}. \tag{23}$$

The resonance is denoted by a pair of integers (m_1,m_2). Here $\beta=\langle\Sigma_{j=1}^{N}1/N\cos((x^*(t))\rangle$ is called the *contraction factor*, which describes the collective effect of the chain (kink). Here $x^*(t)$ denotes the steady state of system (5), and $\langle\cdot\rangle$ represents the time average. In Fig. 3(a), we give the relation between β and δ for $F=0$. In this case, a commensurate effect can be clearly observed, where some rational peaks correspond to commensurate cases $\delta=0,1,\frac{1}{2},\frac{1}{3},\frac{2}{3},\ldots$. In Fig. 3(b), we plot the contraction factor β vs the external driving F. The dashed horizontal line is the value for $F=0$. It is clearly illustrated that β varies with F in a nonmonotonic way. The value of β for $F\neq 0$ is higher than that of $F=0$, i.e., the chain is further contracted when one increases F. At $F\approx 0.47$, β suddenly drops off to a negative value. The compressed topology of the chain (kink) becomes extended, indicating a transition to a new state. This transition is also shown in Figs. 2(a) and 2(b), where the mobility jumps to a much higher value. We called this regime with a high mobility the ''high velocity regime.'' This effect will be described in another work, which is beyond our present interest.

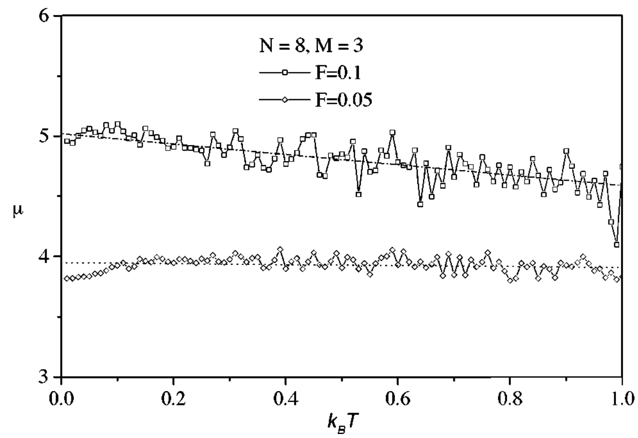

FIG. 4. The mobility of the chain μ varying with the temperature k_BT for the cases $N=8$ and $M=3$ for different external drives $F=0.05$ and 0.1. The mobility remains almost unchanged or decreases, which is much different from the single-particle case.

The resonance behavior between the traveling wave and its radiated phonons remains robust even when finite temperature effect (thermal noise) is considered. The mode locking behavior leads to resonant steps of the averaged velocity of the chain when one adiabatically increases the external force; thus a decrease of the mobility with increasing forces can be expected. When the driving force is increased along a resonant step, the input energy is mainly consumed for amplifying the excited linear phonon and even exciting new linear modes, while the average velocity of the chain remains nearly constant. Thus the coupling between particles here acts as an additional source of dissipation. Due to the amplification of the linear wave, the resonance will be gradually unstable, and will eventually destruct when one increases the external force. As one increases the temperature, the excited linear waves will be further amplified. At the right end of a resonant step these very strong linear waves would destruct the resonances, thus the mobility increases. This is the so-called ''smearing effect.'' At the left hand side of the resonance, the noise can only slightly affect the resonance, hence the coupling between particles may stabilize the resonance. In this case the noise tends to drive the resonance state to a lower resonance state; thus the mobility decreases when the temperature is increased. This interprets the observation reported above. To obtain a deeper understanding, in Fig. 4 we give the relation between the mobility and the temperature for different external forces $F=0.05$ and 0.10 at $\delta=\frac{3}{8}$. $F=0.10$ corresponds approximately to the left hand side of the resonance and $F=0.05$ to the middle of the resonance. It can be clearly shown that, in the middle of the resonance, the mobility keeps nearly constant, while on the left hand side the mobility decreases with increasing temperature.

In conclusion, in this paper we investigated the collective transport behavior of the underdamped Frenkel-Kontorova chain under a constant external driving force and the influence of the environmental noise, and found complicated behaviors. Results reported in this paper should be valuable for applications in many physical cases, such as charge-density waves, Josephson-junction arrays and ladders, and tribology. Some results need a theoretical exploration, and studies along this line are currently in progress.

ACKNOWLEDGMENTS

One of the authors (Z.Z.) thanks all colleagues in the Center for Nonlinear Studies of Hong Kong Baptist University for many valuable discussions. This work was supported in part by the Research Grant Council (RGC) and the Hong Kong Baptist University Faculty Research Grant (FRG). Support by the National Natural Science Foundation of China is acknowledged.

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