

Stimulated diffusion of an adsorbed dimer

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The mobility and the diffusivity of a dimer (two atoms coupled by an elastic spring) in a periodic substrate potential under the action of the dc and ac external forces are studied. It is shown that the dimer diffusivity may be strongly enhanced due to driving.

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I. INTRODUCTION

The manipulation of atoms adsorbed on crystal surfaces, namely, the possibility to operate and control their mobility or diffusivity by applying deterministic forces, is one of the most important issues in nanotechnology [1,2]. A direct manipulation method consists in applying locally a constant (“direct current,” or dc) electric field with the help of the scanning tunnel microscope (STM) tip. The selected adatom will move in the direction of the electrical force (if the adatom has a nonzero charge as is typical for adsorbed atoms due to broken symmetry at the surface) or, for neutral adatoms or admolecules, they will be forced into a region of a stronger field due to induced polarization.

Theoretically this problem can be reduced in the simplest case to motion of a particle in the inclined periodic (substrate) potential. The atomic mobility in this model had been studied in detail in a series of papers as summarized in the monograph by Risken [3]. A less studied question is about effective diffusivity of atoms in the tilted potential. In the *overdamped* limit this problem was solved in closed analytical form by Reimann *et al.* [4], and a giant increase of diffusivity has been found at a critical value of the dc force, when the creeping-to-running transition takes place so that the motion becomes bistable.

Another approach may be based on applying an “alternating current” (ac) force to adsorbed atoms. Gang *et al.* [5] have studied numerically the *overdamped* diffusion of a single particle in the periodic substrate potential under ac driving. The authors found that the diffusivity D may be strongly enhanced and even exceed the free (Brownian) diffusivity $D_f = k_B T / m \eta$ (here k_B is Boltzmann’s constant, T is the temperature, m is the atomic mass, and η is the viscous damping coefficient) for an optimal matching of the frequency Ω of the ac force, its amplitude A , and the external temperature T (through the present paper we use the dimensionless system of units, where the atomic mass is $m = 1$, the height of the external periodic potential is $\varepsilon_s = 2$ and its period is $a_s = 2\pi$). In particular, for the driving frequency Ω

$= 2\pi/10 \approx 0.63$ Gang *et al.* [5] have found that the optimum is achieved at temperatures $T \sim 0.1$ – 0.2 and driving amplitudes $1 < A < 5$ with the maximal effect $D/D_f \approx 3.5$ at $A \approx 1.5$. When the driving frequency Ω is varying with other parameters being fixed, the optimum is also observed at $\Omega \approx 0.63$. They emphasize that in the overdamped case, the enhancement was observed only at very large amplitudes of the driving force, which exceeds the amplitude of periodic potential.

This effect was believed to be connected with the phenomenon of stochastic resonance (SR) [6]. Recall that an external noise may essentially increase the probability of ac stimulated transitions between two stable states of a bistable system, when the rate $R = 1/\tau$ of noise-induced jumps matches with the frequency Ω of the external ac driving according to the relationship $\tau_\Omega = 2\tau$, where $\tau_\Omega = 2\pi/\Omega$ is the driving period. Therefore, the stochastic resonance is expected to occur at

$$\Omega_{\text{SR}} = \pi R. \quad (1)$$

In the *underdamped* system the SR was studied by Evstigneev *et al.* [7]. Because the rate R depends on the damping η [namely, $R \propto \eta$ in the $\eta \rightarrow 0$ limit, $R \propto \eta^{-1}$ in the overdamped limit $\eta \rightarrow \infty$, and $R(\eta)$ reaches its maximum at $\eta \approx 0.6$ [3,8]], one may also tune the matching condition for the SR by changing the damping coefficient η . Indeed, for the double-well potential with the parameters $\varepsilon_b = 1/4$ (the height of the barrier), $\omega_0 = \sqrt{2}$ (the frequency of oscillations at the potential minima), and $T = 0.2$ the authors of Ref. [7] observed that the system’s response as a function of the damping η exhibits a maximum at low driving frequencies $\Omega < 0.3$ at $\eta \sim 0.4$ – 0.6 , i.e., when the rate R is maximal and may be compared with (still larger) frequency Ω .

However, the diffusivity enhancement observed by Gang *et al.* [5] is not connected with the SR effect as shown later by Kim and Sung [9] and Kallunki *et al.* [10]. The SR does exist in bounded (e.g., bistable) systems, but it does not appear in unbounded multistable systems with an infinite number of stable minima as it is for diffusion in the periodic potential. In fact, due to unbound motion, the transition probability decays algebraically, so that there is no persistent synchronized hopping (for details see Ref. [9]). The effect observed by Gang *et al.* [5] in the high-damping limit

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corresponds, as was shown by Kallunki *et al.* [10], to the so-called resonant enhancement of the escape rate R , which takes place when the driving frequency Ω is close to the frequency ω_0 of small oscillations of the particle at the minimum of the external potential. Then, the diffusion coefficient is determined by $D=Rl^2$, where l is the average length of atomic jumps ($l=a_s$ in the overdamped case). On the contrary, in the underdamped limit, when long jumps with $l \gg a_s$ essentially contribute to the diffusion [11], the enhancement of the diffusivity may be achieved because of a broadening of the jump length distribution due to ac driving [10]. This mechanism should operate for low driving frequencies only, when τ_Ω is larger than a typical duration of a jump τ_l ($\tau_l \propto \eta^{-1}$ in the underdamped case).

For the case of very low damping $\eta \ll \omega_0$ the escape rate R in the presence of the ac driving was calculated by Linkwitz and Grabert [12] (see also the review paper by Jung [13], where the numerical results are presented as well, and references therein). It was shown that the function $R(\Omega)$ exhibits a maximum at $\Omega = \Omega_r \approx \omega_0$ for small damping coefficients $\eta \ll 1$. The rate R smoothly increases with increasing frequency for $\Omega < \Omega_r$ (approximately as $R \propto A^2 \Omega^2$), but quickly decreases above the resonance Ω_r , because the system cannot absorb energy from the ac driving when Ω is larger than the largest characteristic frequency (which is $\omega_0 = 1$ in our case). The ratio $G_R \equiv R(\Omega_r)/R(0)$ increases with decreasing of the damping η [e.g., at $T=0.5$ and the driving amplitude $A=0.1$, the maximum of $R(\Omega)$ is observed at $\Omega_r \approx 0.7$ and the enhancement takes a value $G_R \approx 2.5$ for $\eta = 0.1$, but only $G_R \approx 1.15$ for $\eta = 0.5$ according to Fig. 40 of Ref. [13]]. For the overdamped case the escape rate R under weak ac driving and weak noise was calculated analytically by Smelyanskiy *et al.* [14]. The resonant effect at $\Omega \sim \omega_0$ is negligible for small driving amplitudes [15], but may be essential in the strong driving case ($A \geq 1$) and low temperatures ($k_B T \ll \varepsilon_s$) as was shown by Pankratov and Salerno [16]. This explains the enhancement of diffusivity observed by Gang *et al.* [5] at $A \approx 1.5$.

The particle mobility in a periodic potential in the *underdamped* limit was also studied by Marchesoni [17] and Borromeo *et al.* [18]. Close to the critical dc force $f_2 \approx 3.36\eta$, when the sharp creeping-to-running transition takes place at low but nonzero temperatures, the particle mobility exhibits a nontrivial SR-like behavior due to interplay of the noise, which determines the rate of transitions between the two stable states (the locked, or creeping state and the running stationary state) and the oscillation of the particle velocity when it moves in the periodic (washboard) potential. In particular, the mobility may depend nonmonotonically on the temperature, exhibiting a maximum at some T [17]. With the simultaneous action of the dc and ac forces, the system response may be controlled by the driving frequency Ω due to modulation of the switches between the two stable states, and the hysteresis of the mobility as a function of f_{dc} exists even at nonzero temperatures [18].

The goal of the present paper is to study the mobility and diffusivity of a dimer, i.e., two atoms coupled by a spring, in the external periodic potential under the action of dc and ac

driving. This problem is very important for, e.g., dynamics of the Si(100) surface, where Si adatoms are coupled into dimers and move along channels created by the $p(2 \times 1)$ reconstructed Si(100) surface, so that their motion may be approximately considered as one dimensional. The adiabatic motion of the dimer in the sinusoidal potential was described in detail in our previous paper [19]. It was shown that the activation barrier for the dimer motion strongly depends on the relation between the period of the external potential a_s and the natural length of the dimer a . Contrary to a single atom, the dimer has two degrees of freedom, and this fact essentially modifies its diffusional dynamics due to the existence of the so-called entropy barriers [20]. As a result, the diffusivity D may depend nonmonotonically on the dimer's parameters and exhibit peculiarities when the adiabatic trajectory changes qualitatively. Note also that Newtonian motion of the dimer was recently studied by Kovalev and Landau [21] and Fusco *et al.* [22]. It was shown that the nonlinear coupling between the center-of-mass motion and the internal oscillations of the dimer may lead to a complex dynamical behavior with the occurrence of resonant instabilities and stochastic ("quasi-diffusive") motion. At $T > 0$, Fusco and Fasolino [23] have shown that the activation barrier for the diffusive motion of the dimer depends crucially on the dimer length.

The paper is organized as follows. The model is described in Sec. II. The simulation results for the dc and ac driven dimers are presented in Sec. III, both for the commensurate and incommensurate dimers. Finally, Sec. IV concludes the paper.

II. MODEL

Our motion equations have the following standard forms:

$$\begin{aligned} \ddot{x}_1 + \eta \dot{x}_1 + g(x_1 - x_2 + a) + \sin x_1 \\ = \delta F_1(t) + f_{dc} + A_1 \sin(\Omega t - \phi/2), \\ \ddot{x}_2 + \eta \dot{x}_2 + g(x_2 - x_1 - a) + \sin x_2 \\ = \delta F_2(t) + f_{dc} + A_2 \sin(\Omega t + \phi/2), \end{aligned} \quad (2)$$

where $x_{1,2}$ are the coordinates of two atoms of the dimer, g is the elastic constant of the spring connecting the atoms, and a is the natural length of the dimer. The dimer moves under the action of the dc force f_{dc} and the ac force with the amplitude A and frequency Ω . [We included also the parameter ϕ which describes the phase shift between forces acting on the two atoms, and assumed that the forces on the atoms may have different amplitudes if, e.g., the dimer is buckled as on the Si(100) surface. However, in most of the simulation results presented below we used $\phi=0$ and $A_1=A_2=A$.] The stochastic force δF describes the thermal bath and is determined by the fluctuation-dissipation theorem, $\langle \delta F_i(t) \delta F_j(t') \rangle = 2\eta T \delta_{ij} \delta(t-t')$. Typically in simulation we use the damping $\eta=0.1$, which is a realistic value for adsorbed molecules [24], and temperatures $T \leq 0.5$ which lead to activated atomic motion at zero driving (recall that the activation barrier is $\varepsilon_b=4$ for the commensurate rigid

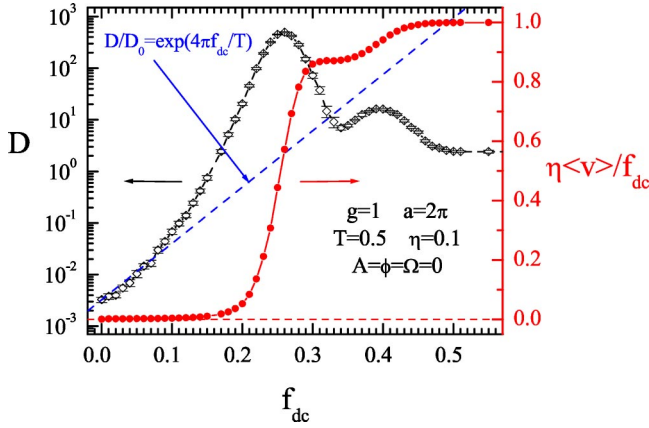


FIG. 1. (Color online) The effective diffusivity D [left axes, (black) open diamonds and dash curve] and the normalized mobility $\eta\langle v\rangle/f_{dc}$ [right axes, (red) circles and solid curve] as functions of the dc force f_{dc} for the commensurate dimer ($a=2\pi$, $g=1$, $\eta=0.1$, and $T=0.5$). The dashed (blue) line shows the dependence $D/D_0=\exp(4\pi f_{dc}/T)$.

dimer). In the following we study the behavior of the center-of-mass displacement and velocity x and v of the dimer.

III. SIMULATION RESULTS

A. Commensurate dimer

First let us present the simulation results for the commensurate dimer, $a=2\pi$. In the case of a relatively strong spring, $g\geq g_s=1/2$, the activation barrier for dimer's diffusion at zero driving is $\varepsilon_{b0}=4$, and the frequencies of characteristic vibrations are $\omega_1=1$ for “in-phase” and $\omega_2=(1+2g)^{1/2}$ for “antiphase” oscillations, respectively [19,20]. Figure 1 shows the dependencies of the average dimer's velocity $\langle v\rangle$ and the effective diffusivity $D=\lim_{t\rightarrow\infty}\langle[x-\langle v\rangle t]^2\rangle/2t$ as functions of the dc force f_{dc} for the $g=1$ case. These dependencies are qualitatively similar to those known for the case of a single particle [3,4]. The creep-to-running transition takes place at $f_{dc}\approx 0.26$ (note that this value is smaller than $f_2\approx 0.336$ expected for the single-particle case [3]), and at the transition we see a giant increase of D similar to what was found by Reimann *et al.* [4] in the overdamped single-atom case. The characteristic trajectories of both atoms of the dimer at different values of the dc force are shown in Figs. 2 and 3.

The increase of mobility with f_{dc} is trivially connected with the decrease of the height of the barrier due to the driving force, $\varepsilon_b\approx\varepsilon_{b0}-2f_{dc}a_s$, where the factor 2 appears because the force is applied to both atoms of the dimer. At small driving, when the diffusion is still activated, $\varepsilon_b\gg k_B T$, the diffusion coefficient grows exponentially with the force as $D/D_0\approx\exp(4\pi f_{dc}/T)$ demonstrated by (blue) dashed line in Fig. 1 (recall that $a_s=2\pi$ in our system of units). At the transitions we observe a strong increase of D (up to two orders of magnitude with respect to the *free* diffusion coefficient $D_f=T/2\eta=2.5$), then the diffusivity decreases, and finally reaches the value $D\approx D_f$ at $f\geq 0.5$.

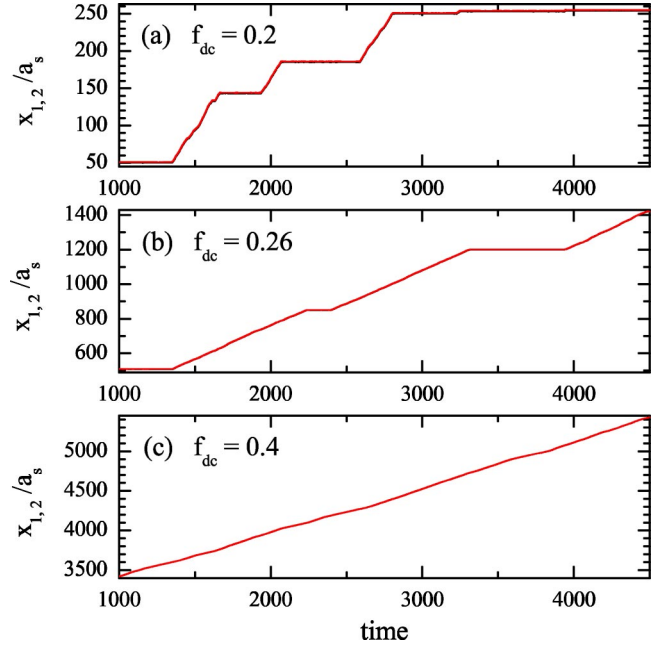


FIG. 2. (Color online) Atomic trajectories of both atoms for the parameters of Fig. 1 for three values of the dc force: (a) $f_{dc}=0.2$ (before the transition), (b) $f_{dc}=0.26$ (at the transition), and (c) $f_{dc}=0.4$ (close to the end of the transition to the sliding state).

Contrary to the single-atom case, now the transition takes place in two steps. At the first step of increase of mobility and diffusivity, the dimer's atoms move “in phase” as one can see from the trajectories presented in Figs. 3(a) and 3(b). The second increase of the mobility and the local maximum of D , observed at $f_{dc}\approx 0.4$, is due to intrinsic structure of the dimer. As we see from Fig. 3(c), at the second transition an antiphase vibration of the dimer's atoms is excited, and this takes energy away from the translational

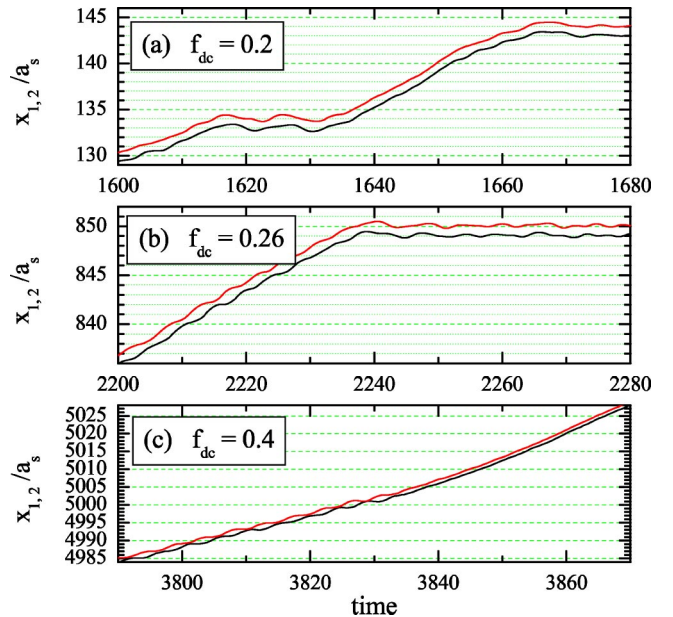


FIG. 3. (Color online) Same as Fig. 2 but for a shorter time scale.

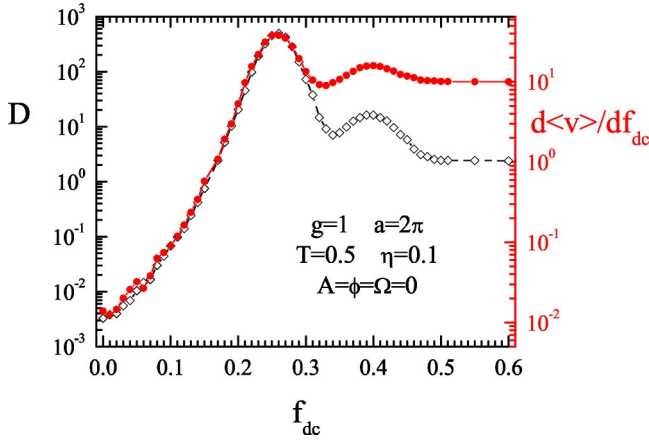


FIG. 4. (Color online) Comparison of D and $d\langle v \rangle/df_{dc}$ for the data presented in Fig. 1.

motion. The excitation of antiphase vibrations is observed when the “washboard” frequency $\omega_{\text{wash}} = (a_s/2\pi)\langle v \rangle$ becomes close to the second harmonic of the antiphase characteristic frequency $\omega_2 = \sqrt{3} \approx 1.73$.

From the fluctuation-dissipation relation it follows that at zero dc driving the diffusion coefficient can be calculated as $D = k_B T d\langle v \rangle/df_{dc}|_{f_{dc}=0}$. Figure 4 demonstrates that the proportionality relation $D \propto d\langle v \rangle/df_{dc}$ remains qualitatively correct at nonzero driving as well.

Now let us consider the dimer motion under the ac driving (in what follows we concentrate on the simulation results for the symmetric case only, $A_1 = A_2 = A$ and $\phi = 0$). The diffusion coefficient D as a function of the driving frequency Ω is presented in Fig. 5 for a small driving amplitude $A = 0.1$ and in Fig. 6 for the strong driving with $A = 0.6$.

Assuming that the diffusion occurs by single jumps with the rate R over a distance of one lattice constant, the diffusion coefficient is equal to $D \approx R a_s^2$ for one-dimensional motion, so that the characteristic SR frequency defined by Eq.

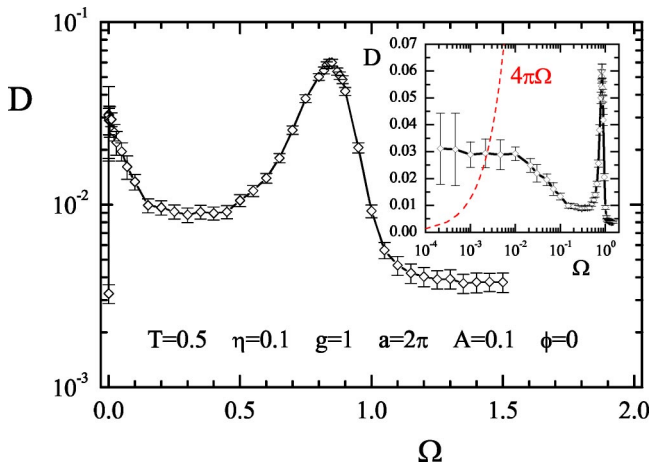


FIG. 5. (Color online) Dependence of the diffusivity D on the frequency Ω of the external driving with a small amplitude $A = 0.1$ for the commensurate dimer ($T = 0.5$, $\eta = 0.1$, $g = 1$, $a = 2\pi$, and $\phi = 0$). The dashed (red) curve corresponds to the SR frequency given by Eq. (1).

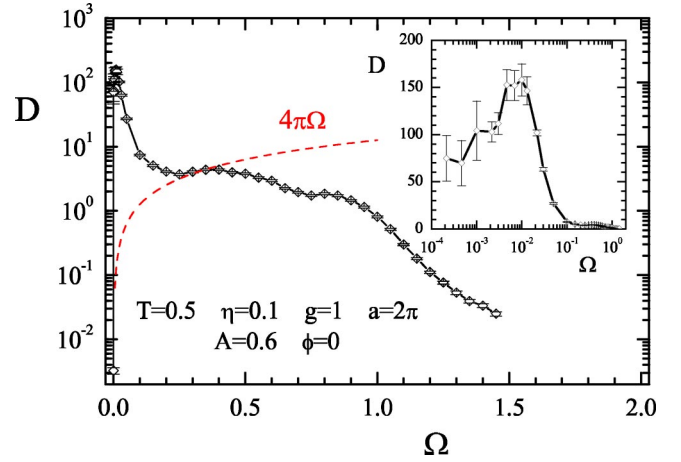


FIG. 6. (Color online) The same as in Fig. 5 for a large driving amplitude $A = 0.6$ ($T = 0.5$, $\eta = 0.1$, $g = 1$, $a = 2\pi$, and $\phi = 0$).

(1) is now determined by the relationship $\Omega_{\text{SR}} \approx \pi R \approx D/4\pi$. For low driving frequencies, $\Omega \lesssim \Omega_{\text{SR}}$, the jump rate should follow adiabatically the changes of the barrier height, $\varepsilon_b(t) \approx \varepsilon_{b0} - 2a_s A \sin(\Omega t)$, and for small amplitudes, when the jumps remain activated, we may expect an increase of the averaged rate of jumps by the factor

$$\frac{R}{R_0} \approx \frac{1}{\tau_\Omega} \int_0^{\tau_\Omega} dt e^{(2a_s A/T) \sin(\Omega t)} = I_0(4\pi A/T), \quad (3)$$

where I_0 is the modified Bessel function of order zero. For the parameters $T = 0.5$ and $A = 0.1$ this gives the factor of $I_0(4\pi/5) \approx 3.32$ only, and the same should be true for the diffusion coefficient in the overdamped case, $\eta \gtrsim 1$, when the jumps are over one lattice constant only, $l = a_s$. In the underdamped case shown in Figs. 5 and 6 we see, on the contrary, a giant increase of the diffusivity at low driving frequencies $0 < \Omega \lesssim \Omega_l \sim \Omega_{\text{SR}}$. For example, for $\Omega = 0.01$ the diffusion coefficient increases ten times for the small amplitude $A = 0.1$ and more than four order of magnitude for $A = 0.65$ (the whole dependence of D on the amplitude A is shown in Fig. 7). The increase of diffusivity in the low-frequency case is connected with an increase of jump lengths. As clearly seen from Fig. 8, even a small-amplitude driving leads to the increase of jump length of about three times, while the jump rate remains approximately unchanged.

With further increase of the amplitude A in the case of low-frequency driving, the average jump length l and, therefore, the diffusion coefficient D increase too (see Fig. 7). At a high amplitude A such as, e.g., the $A = 0.6$ case shown in Fig. 9, the jumps become strongly correlated with the driving force, so that $\tau = \tau_\Omega$ and $R = \Omega/2\pi$. The average jump length in this case reaches large values, e.g., $l \approx 50 a_s$ for $\Omega = 0.01$. Note that now the jump length should be determined as a difference between the lengths of the forward (l_+) and backward (l_-) jumps during one period of the ac force, $l^2 = \langle (l_+ - l_-)^2 \rangle$, while lengths of individual jumps are much larger, $l_+ \sim l_- \sim v \tau_\Omega$ ($l_\pm/a_s \sim A/4\eta\Omega \sim 150$ for $\Omega = 0.01$ according to Fig. 9).

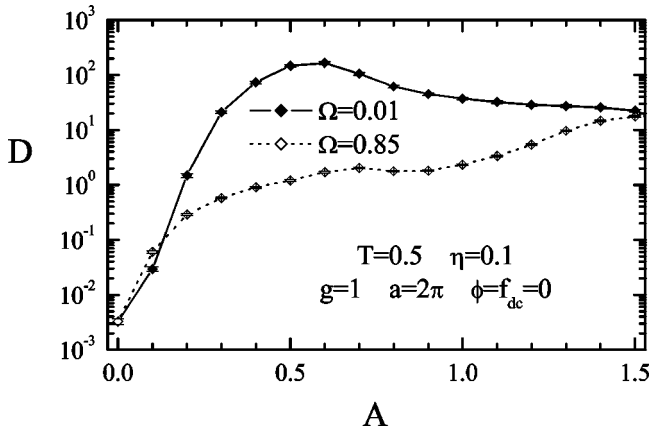


FIG. 7. Dependencies of the diffusivity D on the amplitude of the external driving A for two frequencies of driving: $\Omega=0.01$ (solid symbols and curve) and $\Omega=0.85$ (open symbols and dotted curve) for the commensurate dimer ($T=0.5$, $\eta=0.1$, $g=1$, $a=2\pi$, and $\phi=f_{dc}=0$).

It is interesting that the diffusion coefficient D as a function of frequency Ω exhibits a “resonant” behavior at large driving amplitudes. As shown in inset of Fig. 6, $D(\Omega)$ reaches a maximum at $\Omega=\Omega'_r\approx 0.01$. Such a behavior may be explained qualitatively as an interplay between the increasing of the jump rate $R\propto\Omega$ at $\Omega<\Omega'_r$ and decreasing of the jump length $l\propto\Omega^{-1}$ at $\Omega>\Omega'_r\sim\Omega'_r$.

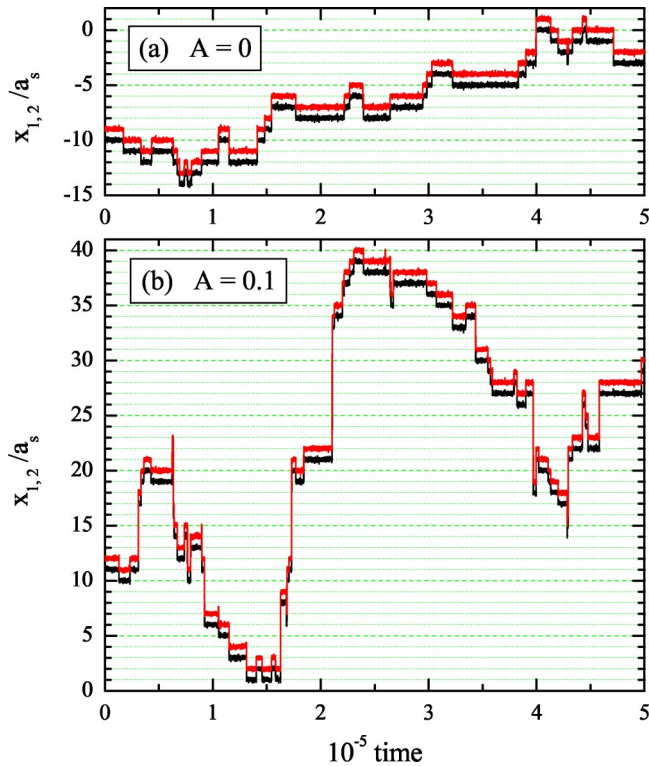


FIG. 8. (Color online) Atomic trajectories of both atoms for the parameters of Fig. 5 ($T=0.5$, $\eta=0.1$, $g=1$, and $a=2\pi$) for the low driving frequency $\Omega=0.01$ and two values of the driving amplitude: (a) $A=0$ (without driving) and (b) $A=0.1$ (low-amplitude driving).

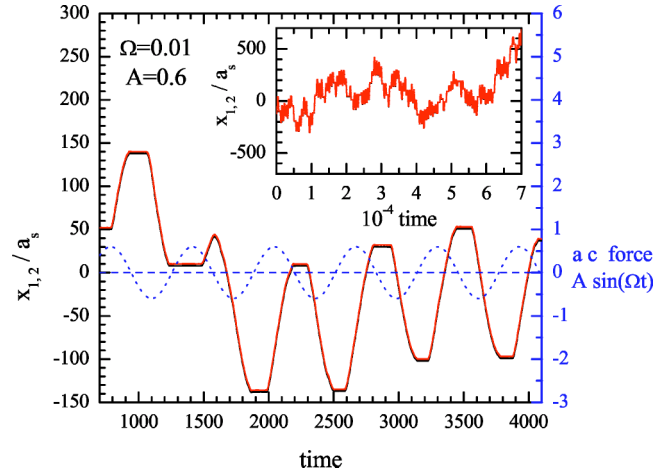


FIG. 9. (Color online) Atomic trajectories for the parameters of Fig. 5 for low driving frequency $\Omega=0.01$ and high driving amplitude $A=0.6$ [(blue) sinusoidal curve and right axes show the driving force $A\sin(\Omega t)$]. Inset shows a long-time trajectory.

However, as we see in Fig. 7, after reaching a maximum at $A\approx 0.6$, the low-frequency diffusivity begins to decrease. Indeed, the low-frequency case in some aspects is similar to the static one, where we observed that the maximum of D is reached at the dc driving force $f=f_{dc}\approx 0.26$ (see Fig. 1). Thus, for the low-frequency ac driving one may expect a maximum of D for the driving amplitude $A=2f\approx 0.52$.

The above described enhancement of the diffusivity disappears with increasing Ω above the value $\Omega_l=2\pi/\tau_l$ because of the destruction of very long jumps, when the period τ_Ω becomes smaller than the flight time τ_l . In agreement with Refs. [9,10] discussed in the Introduction, we do not observe any stochastic resonance at *small* driving amplitudes. However, with further increase of Ω at $\Omega\gg\Omega_l$ we again see the increase of diffusivity according to the law $D\propto\Omega^2$ approximately, and at $\Omega=\Omega'_r\approx 0.85$ the diffusion coef-

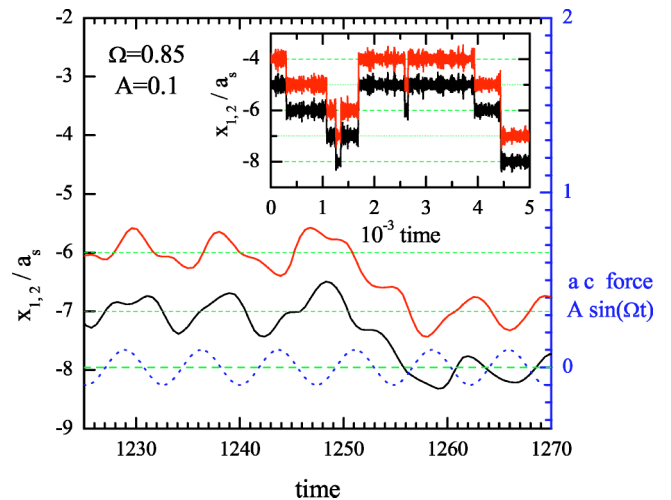


FIG. 10. (Color online) Atomic trajectories for the parameters of Fig. 5 for high driving frequency $\Omega=0.85$ but small driving amplitude $A=0.1$ [(blue) sinusoidal curve and right axes show the driving force $A\sin(\Omega t)$]. Inset shows a long-time trajectory.

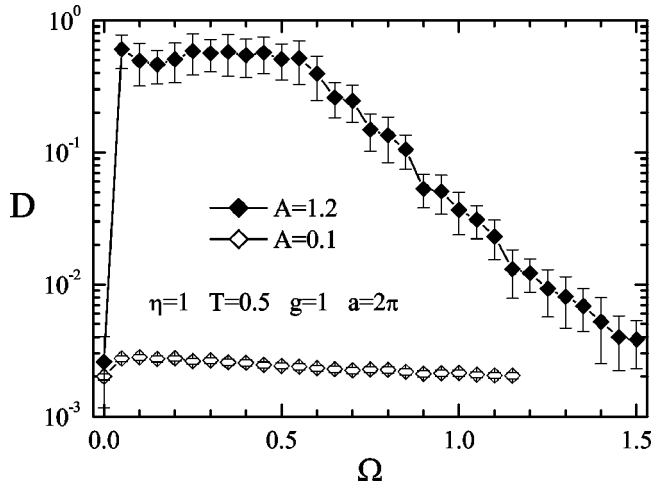


FIG. 11. Dependence of the diffusivity D on the frequency Ω of the external driving with a small amplitude $A = 0.1$ (open diamonds) and the large amplitude $A = 1.2$ (solid symbols) for the commensurate dimer in the case of large damping ($\eta = 1$, $T = 0.5$, $g = 1$, and $a = 2\pi$).

ficient reaches a large maximum in the case of low-amplitude driving (see Fig. 5). This effect is connected with the resonant increase of the escape rate $R(\Omega)$ at $\Omega = \Omega_r$, while the average jump length is again of the order of one lattice constant (see trajectories in Fig. 10 for this case). Note that for a high driving amplitude, e.g., for $A = 0.6$ shown in Fig. 6, the diffusivity decreases monotonically with the increase of frequency in the region $\Omega > \Omega_l$, and no resonant effects are observed. Notice also that for a high driving frequency, e.g. for $\Omega = 0.85$ shown in Fig. 7, the diffusivity increases monotonically with the increase of the amplitude A , and no resonant effects have been observed as well.

Finally, at very high driving frequencies, $\Omega > 1$, the diffusivity decreases to values that it had without driving. (a slightly larger value of D may be attributed to an effective increase of temperature due to driving.)

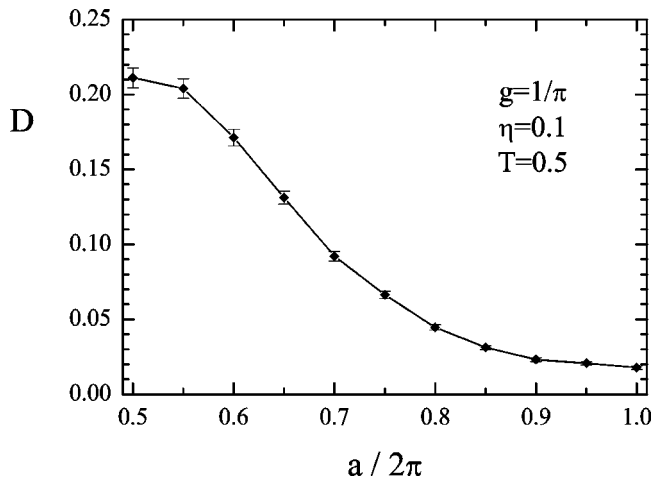


FIG. 12. The diffusion constant D vs the dimer length a for $g = 1/\pi$, $\eta = 0.1$ and $T = 0.5$.

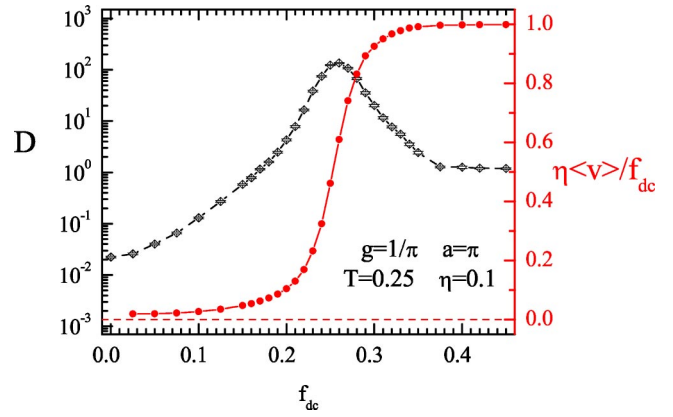


FIG. 13. (Color online) The effective diffusivity D [left axes, (black) open diamonds and dash curve] and the normalized mobility $\eta\langle v \rangle / f_{dc}$ [right axes, (red) circles and solid curve] as functions of the dc force f_{dc} for the incommensurate dimer ($a = \pi$, $g = 1/\pi$, $\eta = 0.1$, and $T = 0.25$).

Above we have described stimulated motion of the commensurate dimer ($a = 2\pi$) for a relatively high value of the elastic constant, $g = 1$. If the interaction strength decreases, then the activation barrier decreases too (approximately linearly with g) from the value $\varepsilon_b = 4$ for the “rigid” dimer with $g \geq 1/2$ down to $\varepsilon_b = 2$ at $g = 0$ as was described in Refs. [19,20], so that the low-temperature mobility and diffusivity should grow when decreases g . Moreover, with decreasing g , a change of the adiabatic trajectory, and as a result a peculiarity in the $D(g)$ dependence, takes place near the points $g = 1/2$ and $g = 1/\pi$, when the saddle frequencies (in-phase and antiphase, respectively) become zero as was described in our previous paper [20]. This may lead to shifts of the positions and strengths of resonances in the $D(\Omega)$ dependence, but qualitatively the behavior is expected to remain unchanged.

Finally, we studied the role of the external damping η . As one can see from Fig. 11, in the overdamped case the effect

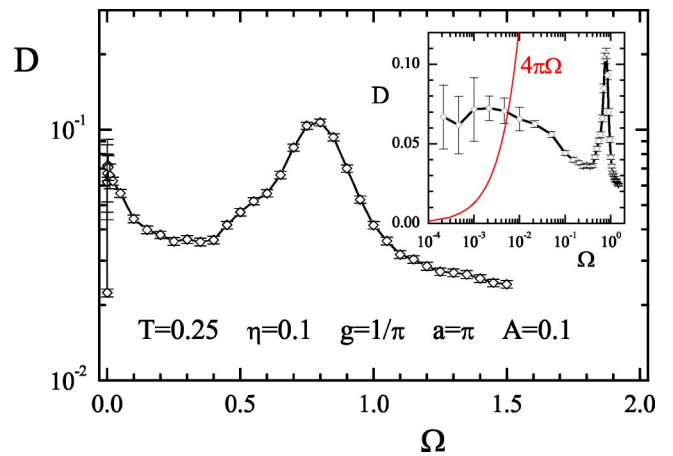


FIG. 14. (Color online) Dependence of the diffusivity D on the frequency Ω of the external driving with a small amplitude $A = 0.1$ for the incommensurate dimer ($T = 0.25$, $\eta = 0.1$, $g = 1/\pi$, $a = \pi$, and $\phi = 0$).

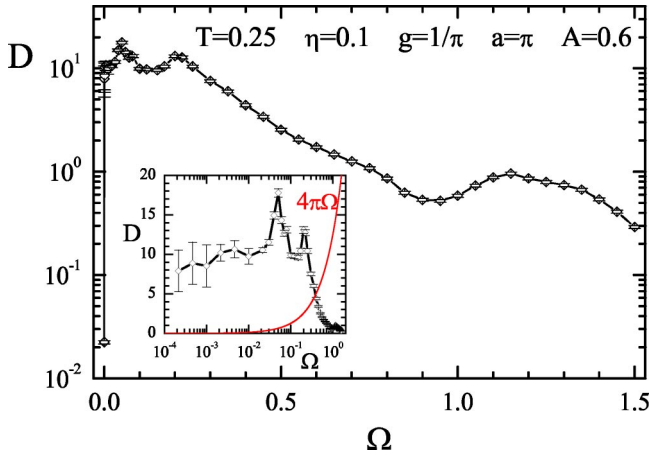


FIG. 15. (Color online) Same as in Fig. 14 but for a large driving amplitude $A=0.6$ ($T=0.25$, $\eta=0.1$, $g=1/\pi$, $a=\pi$, and $\phi=0$).

is strongly suppressed, in particular, the high-frequency resonant peak of $D(\Omega)$ disappears at all.

B. Incommensurate dimer

In the case when the dimer length a is “incommensurate” with the lattice spacing $a_s = 2\pi$, $\pi \leq a < 2\pi$, the activation barrier ε_b for dimer’s motion is smaller than that of the commensurate case [19]. For example, in the limit $g \rightarrow \infty$ the barrier decreases according to the law $\varepsilon_b = 4|\cos(a/2)|$ from $\varepsilon_b = 4$ at $a = 2\pi$ down to $\varepsilon_b = 0$ at $a = \pi$. For a “weak” dimer, $g \ll 1$, the activation barrier varies as $\varepsilon_b \approx 2 + \pi g (a - 3\pi/2)$ according to Ref. [19]. Therefore, the dimer diffusivity should strongly increase when a changes from the commensurate value $a = 2\pi$ to the incommensurate one $a = \pi$ as demonstrated in Fig. 12. Below we present the simulation results for the most incommensurate case of $a = \pi$ only. The dimer mobility and effective diffusivity under the dc driving are presented in Fig. 13 (here we used much lower temperature $T=0.25$, because the activation barrier is much smaller for the incommensurate dimer). Contrary to the case of the commensurate dimer described above, now the transition to the sliding state occurs in one step. However, again the effective diffusivity strongly increases at the transition point and may exceed the free diffusion coefficient by more than two orders of magnitude.

The next two figures show the dependencies of the diffusivity on the frequency of the external driving with a small amplitude $A=0.1$ (Fig. 14) and the large amplitude $A=0.6$ (Fig. 15). Again we see a large increase of D at small frequencies, and a resonant peak at the large frequency $\Omega_r \approx 0.8$ in the case of small-amplitude driving. Because the incommensurate dimer is characterized by a smaller frequency of the in-phase vibrations (e.g., $\omega_1^2 \approx 1 - \pi^2 g^2/2$ for the $g \ll 1$ case [19]), now the resonant frequency Ω_r is also smaller than that for the commensurate dimer. In all other aspects the stimulated behavior of the incommensurate dimer is qualitatively similar to that of the commensurate one.

IV. DISCUSSION AND CONCLUSION

In the previous sections, we have shown that by applying a low-frequency ac driving to the adsorbed dimer, one may achieve a giant increase of its diffusivity, which may exceed the free-diffusion coefficient by several orders of magnitude.

One of the possible applications of the effect described in the present paper may be connected with growth of the Si(100) surface. As is well known (e.g., see Ref. [25] and references therein), the $p(2 \times 1)$ structure of the Si(100) surface is characterized by two types of “channels,” the “on-top channels” which are on top of the substrate dimer rows and the “deep channels” in between the dimer rows. At initial stage of the Si(100) growth, two Si adatoms which diffuse along the on-top channel can easily find each other and form a dimer (ad-dimer). Such a dimer has a length $a \approx 2.44 \text{ \AA}$, i.e., it is approximately commensurate with the periodic substrate potential. The barrier for its diffusion along the channel is $\varepsilon_b \approx 0.94 \text{ eV}$, and the frequency of antiphase vibrations of the dimer’s atoms is $\omega_2 \approx 10^{14} \text{ s}^{-1}$ [26], so that the Si_2 dimer can be considered as the rigid one. To achieve a uniform coverage of the surface by incoming Si atoms (dimers), one should increase their diffusivity, which can be done typically with the help of increase of the substrate temperature. According to the results of the present work, the same goal may be achieved at low temperature by applying a small-frequency ac field to the dimers. Moreover, with the help of STM tip such increase of diffusivity may be done locally, in a given region of the surface.

Finally, we studied also an asymmetric ac driving of the dimer [the asymmetry may be due to nonzero phase shift ϕ or because of a difference in amplitudes of forces acting on the two atoms, $A_1 \neq A_2$, in Eq. (2)] with the aim to find a ratchet effect [27]. A possibility of a directed motion of the dimer in the periodic potential under the asymmetric ac driving in the overdamped zero-temperature system has been demonstrated and studied in detail by Cilla *et al.* [28]. The authors found that the directed motion exists within quite narrow windows of the force parameters only, and the effect (the so-called ratchet efficiency) is rather weak. Although our study on this point has not been systematic, we can sketch the following conclusion. First, we have seen that the inclusion of a phase shift does not lead to qualitative changes in the behavior of the system, the resonant behavior being robust with respect to the phase shift. We also tried to find the directed motion in our model too, because of its important application for, e.g., buckled Si dimers on the Si(100) surface. Unfortunately, we did not find any directed motion of the dimer for the asymmetric ac driving, neither for $\phi \neq 0$ nor for $A_1 \neq A_2$ driving, in the $T > 0$ case, at least for the particular sets of parameters that we studied. Thus, we came to the conclusion that the ratchet effect for the dimer in the sinusoidal potential is so weak that it is completely destroyed by thermal fluctuations.

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