Dimer diffusion in a washboard potential

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Introduction: examples and possible applications

- An example of Brownian motion in periodic substrate is in the crystal growth of many elements, such as Si and Ge, e.g. in surface coating and thin-film growth since. First individual atoms diffusing on the crystal surface meet and form dimers (or trimers), which then recombine and contribute to the crystal growth.

- In condensed matter physics, the Frenkel-Kontorova model is known to exhibit a peculiar behavior is observed as the ratio between the equilibrium monomer-monomer distance and the potential period is varied. The case of a dimer is helpful to explore the basic mechanism with a minimal model.

- In fcc crystal, (screw or edge) dislocations preferably dissociate into two partials. In the Volterra model of a dissociated dislocation the two partial dislocations are modeled as two coupled particles in a washboard potential. They can translate if the stress is parallel to the Burgers vector, they change the equilibrium distance if it is parallel. The mobility of the dislocation depend in a crucial way on the the ratio between equilibrium distance and lattice constant (G. Schoek).

- A most important problem in nanotechnology is how to manipulate small particles, e.g. applying a constant dc or ac local electric field by means of a scanning tunnel microscope tip. This problem can be modeled as a Brownian motion on a tilted periodic 2D substrate and effectively reduced to 1D systems. In these cases the mobility and diffusivity of atoms adsorbed onto crystal surfaces can be controlled by applying deterministic forces.

Model

monomer = 1 Brownian particle:

$$\ddot{x} = -\gamma\dot{x} + \sin x + F + \xi(t)$$

ξ – Gaussian white noise with zero average and autocorrelation function

$$\langle \xi(t)\, \xi(t') \rangle = 2\,\gamma T\, \delta(t - t')$$

dimer = 2 harmonically interacting Brownian particles:

$$\begin{aligned} \ddot{x}_1 &= -\gamma\dot{x}_1 + \sin x_1 + F + K(x_2 - x_1 - a_0) + \xi_1(t) \\ \ddot{x}_2 &= -\gamma\dot{x}_2 + \sin x_2 + F - K(x_2 - x_1 - a_0) + \xi_2(t) \end{aligned}$$

$\xi_{1,2}$ – 2 independent Gaussian white noises with autocorrelation function

$$\langle \xi_i(t)\, \xi_j(t') \rangle = 2\,\gamma T\, \delta_{ij}\delta(t - t')$$

γ – damping constant

K – coupling constant

a_0 – equilibrium distance

F – constant bias

T – temperature

Quantities of interest

center of mass coordinate: $X = \frac{1}{2}(x_1 + x_2)$

the asymptotic velocity: $v = \lim_{t\to\infty} \frac{\langle X(t)\rangle}{t}$

mobility: $\mu = v/F$

diffusion coefficient: $D = \lim_{t\to\infty} \frac{\langle \delta X^2(t)\rangle}{2t}$

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relative coordinate: $Y = x_2 - x_1$

– By introducing *X* and *Y* it is possible to perform some approximate calculations and map the 1D dimer problem into the problem of a monomer on a 2D potential surface

Note: in our simulations $Y > 0$ always

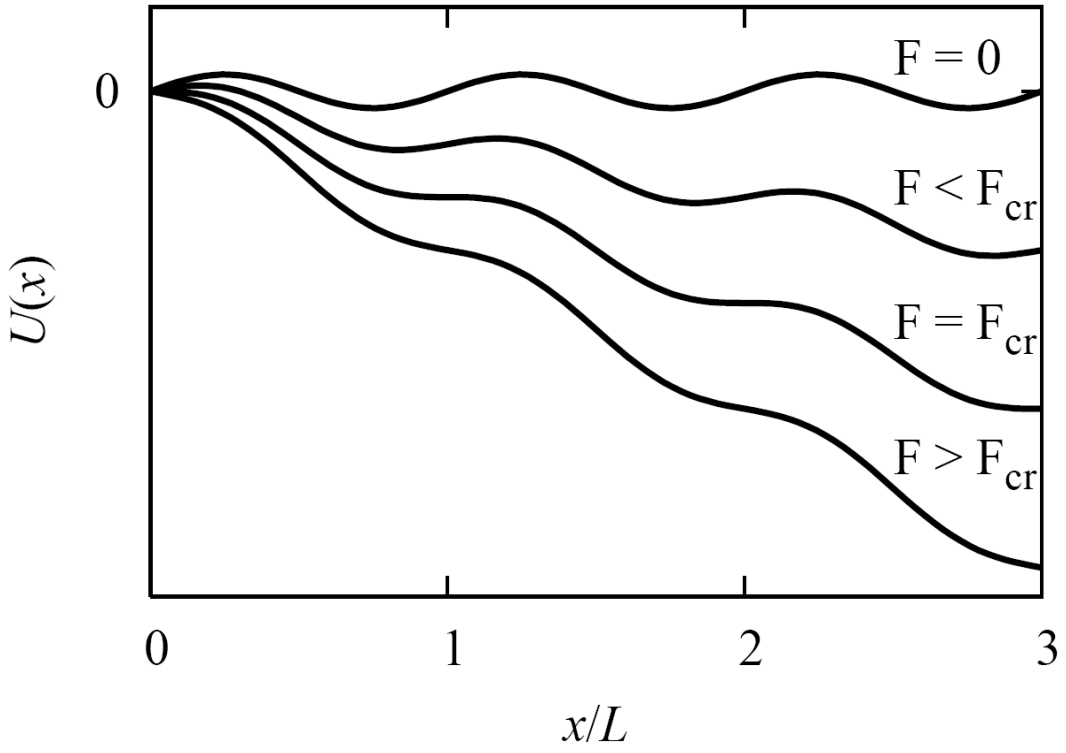
General considerations

free mobility for the monomer as well as the dimer: $\mu_0 = 1/\gamma$

free diffusion coefficient for a monomer: $D_0(T) \equiv T/\gamma$

free dimer diffusion coefficient: $D_\infty = D_0(T/2)$

a washboard potential and the definition of the critical bias F_{cr}:

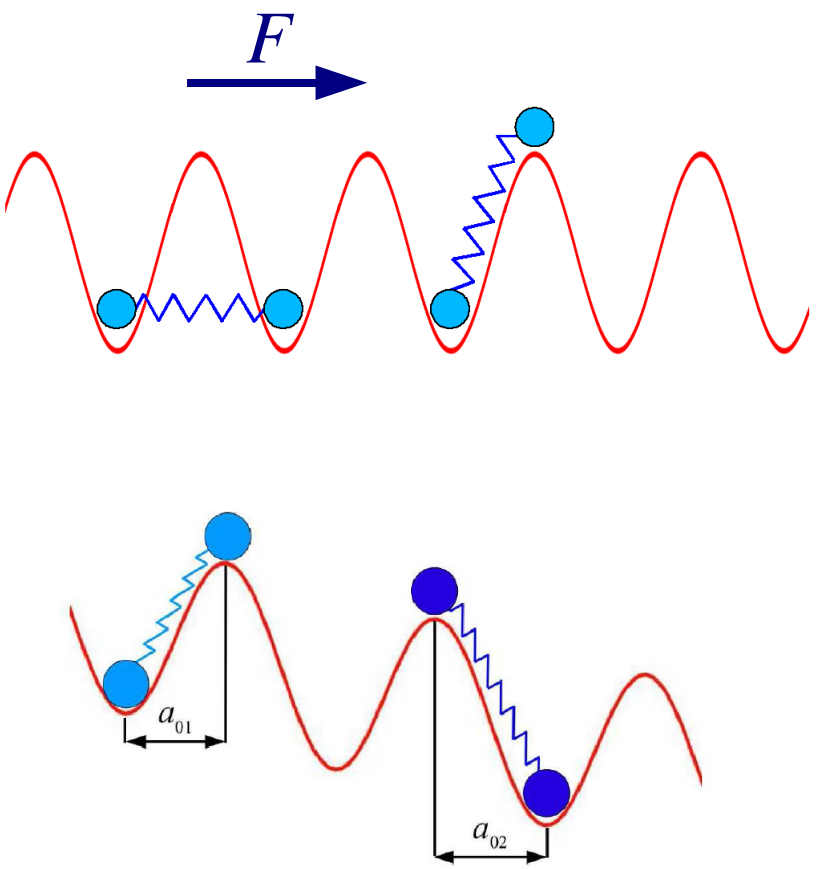


for a monomer the depinning threshold is:

$$F_d \approx 3.36\,\gamma\sqrt{F_{cr}} \quad \text{for} \quad \gamma \to 0$$

$$F_d \approx F_{cr} \quad \text{for} \quad \gamma \geqslant \sqrt{F_{cr}}$$

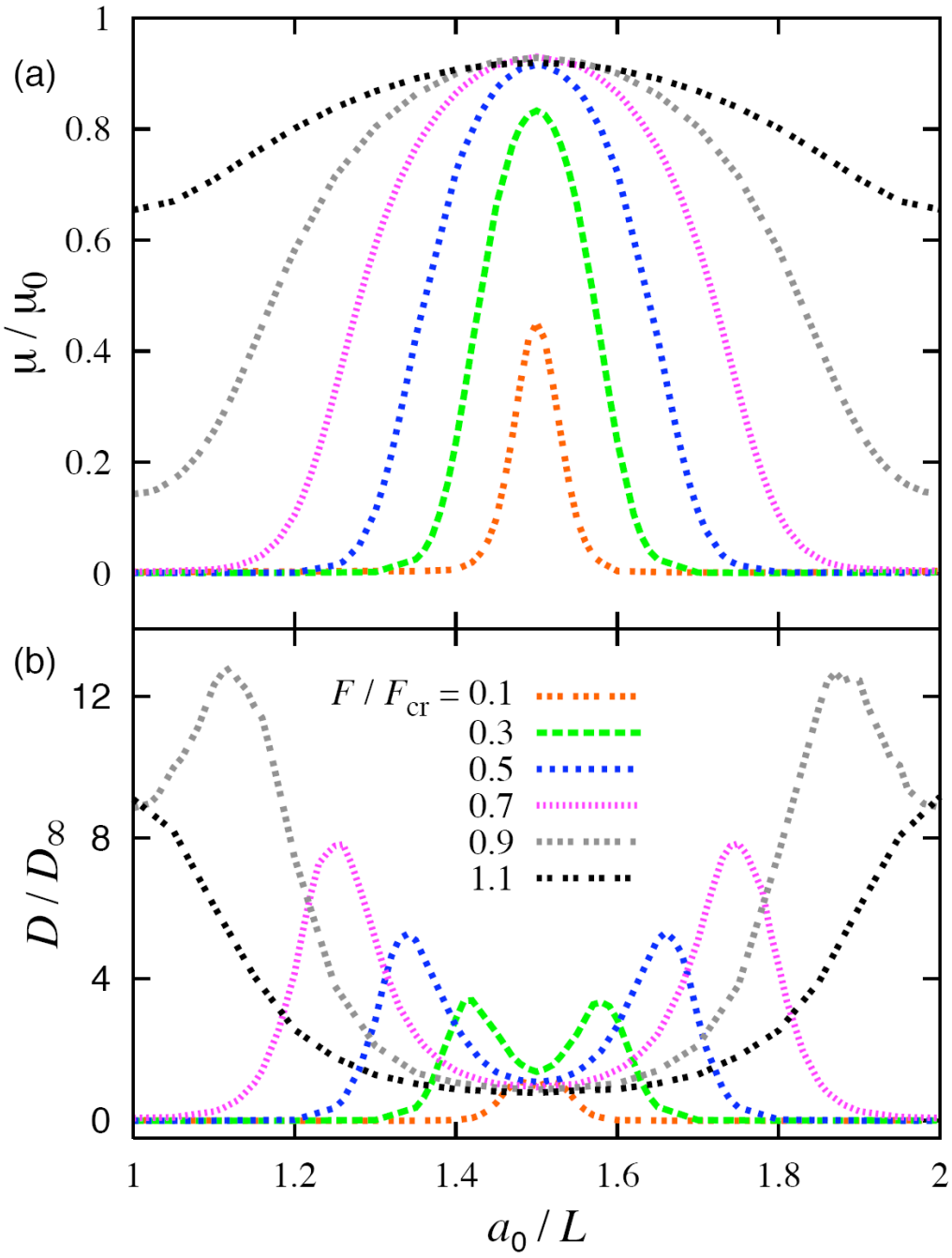
Dependence on the dimer length



simulation parameters:

- coupling constant $K = 1.5$
- temperature $T = 0.1$
- damping coefficient $\gamma = 1$

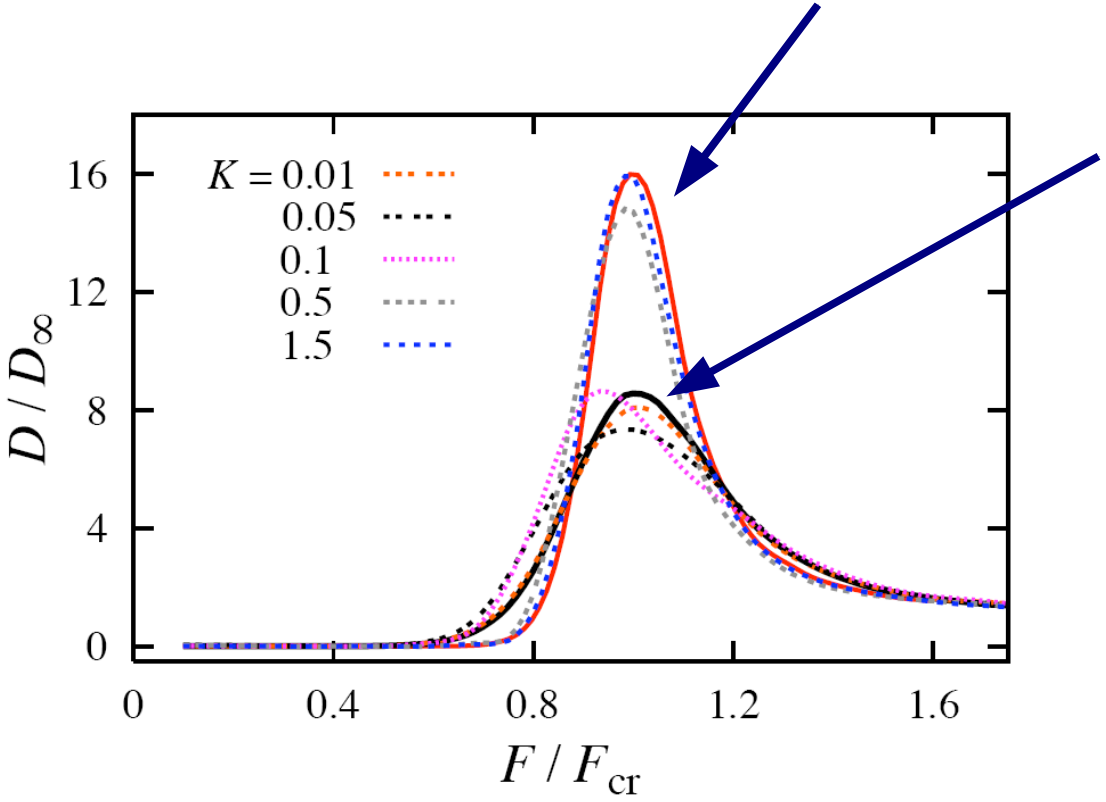
The dependences are given mod(L).



Monomer-like regimes

equilibrium distance = **integer multiple of the period**

rigid dimer limit = monomer at temperature $T/2$



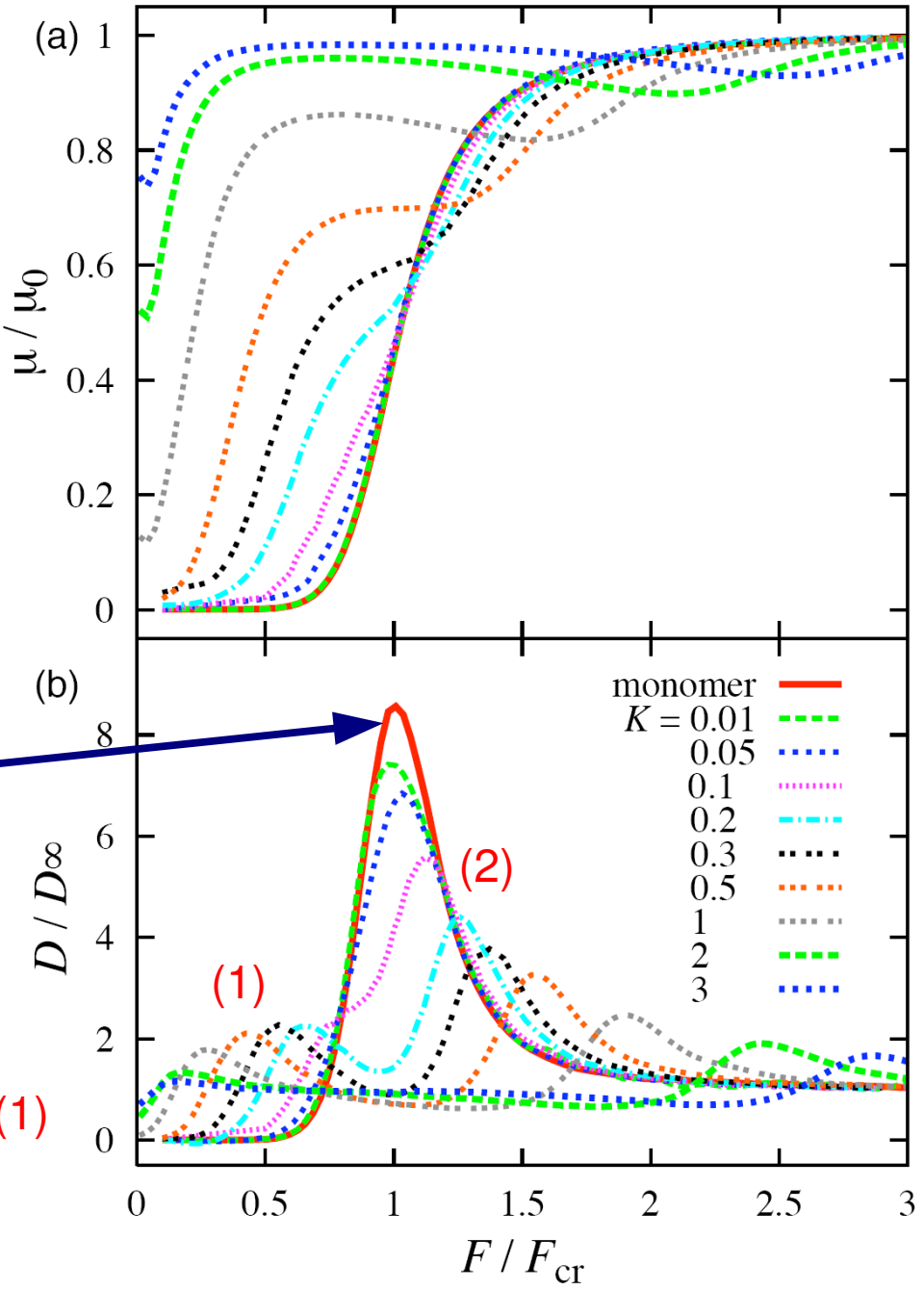
uncoupled dimer limit = monomer at temperature T

simulation parameters:
- dimer length $a_0 = 1$
- temperature $T = 0.1$
- damping coefficient $\gamma = 1$

Dependence on the coupling strength

here equilibrium distance =
half-integer multiple of the period

simulation parameters:
- dimer length $a_0 = 1.5$
- temperature $T = 0.1$
- damping coefficient $\gamma = 1$



- uncoupled dimer limit = monomer at temperature T
- rigid dimer limit = free diffusion
- the two maxima of D vs F are located at:

$$F_1 \approx [(2/\pi)\langle\psi^2(t)\rangle]^{1/2} = \sqrt{2T/\pi K} \quad (1)$$

$$F_2 \approx \frac{1}{2} + \gamma\sqrt{2K - \frac{\gamma^2}{2}} \quad (2)$$

Dependence on dimer length

simulation parameters:
- coupling constant $K = 1.5$
- temperature $T = 0.1$
- damping coefficient $\gamma = 1$

relatively rigid dimer !

equilibrium distance =
integer multiple of the period

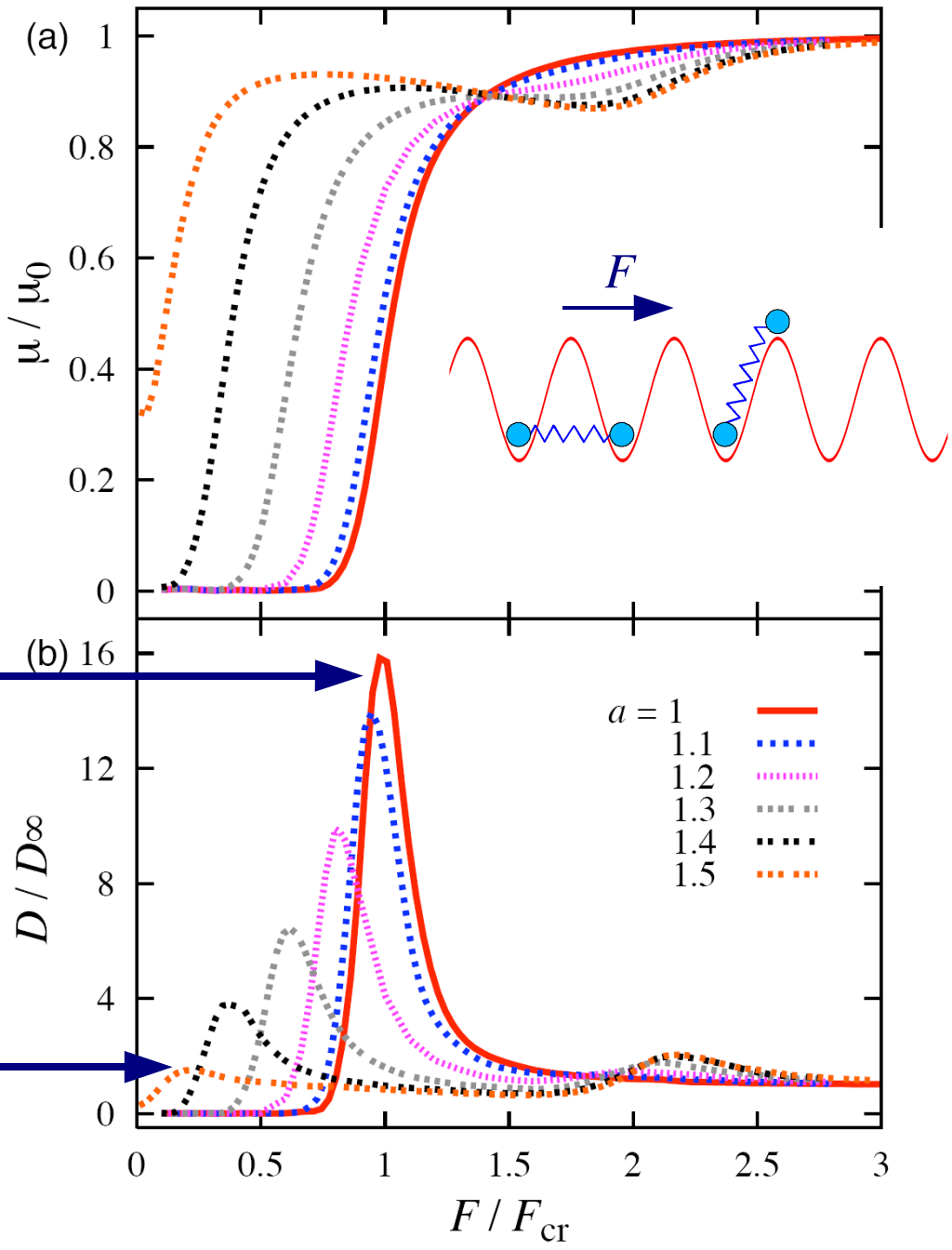
↓

rigid dimer limit =
monomer at temperature $T/2$

equilibrium distance =
half-integer multiple of the period

↓

rigid dimer limit = free diffusion



Dependence on damping constant

Here equilibrium distance = **half-integer multiple of the period**

relatively non-rigid dimer

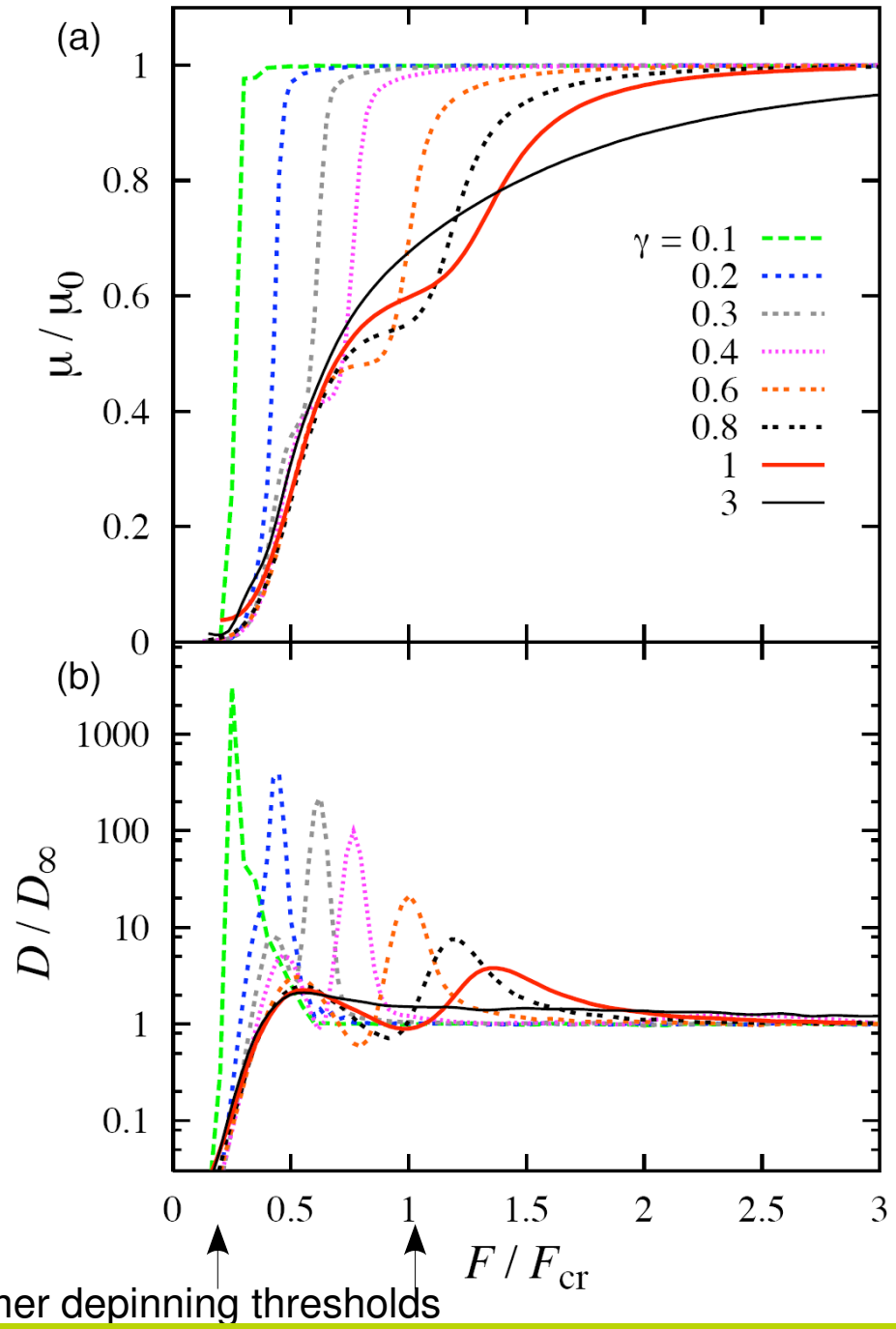
In the overdamped regime ($\gamma > 1$) only one peak is present for the diffusion coefficient D.

In the underdamped regime ($\gamma \leq 1$) the two peaked diffusion curves are clearly distinguishable.

For very small values of γ the two peaks of D merge.

simulation parameters:

- dimer length $a_0 = 1.5$
- temperature $T = 0.1$
- coupling constant $K = 0.3$



Conclusion

- We have studied a system consisting of two harmonically interacting Brownian particles diffusing in a 1D washboard potential.

- We have found that the average current and the diffusion coefficient of such a dimer exhibit a complicated non-monotonous behavior as a function of the driving force and the ratio of the dimer length to substrate constant.

- We studied in detail the dimer transport for different coupling strengths and damping constants. We have concluded that the appearance of the second resonant peak of the diffusion coefficient versus the driving force is not related to the dimer length-to-substrate constant ratio, but rather to the damping-to-coupling constant ratio; The diffusion coefficient $D(F)$ possesses two peaks only for relatively low damping values.

Collaborators and Sponsors

Collaboration

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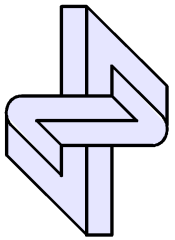

Additional information

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