Influence of moving breathers on vacancies migration

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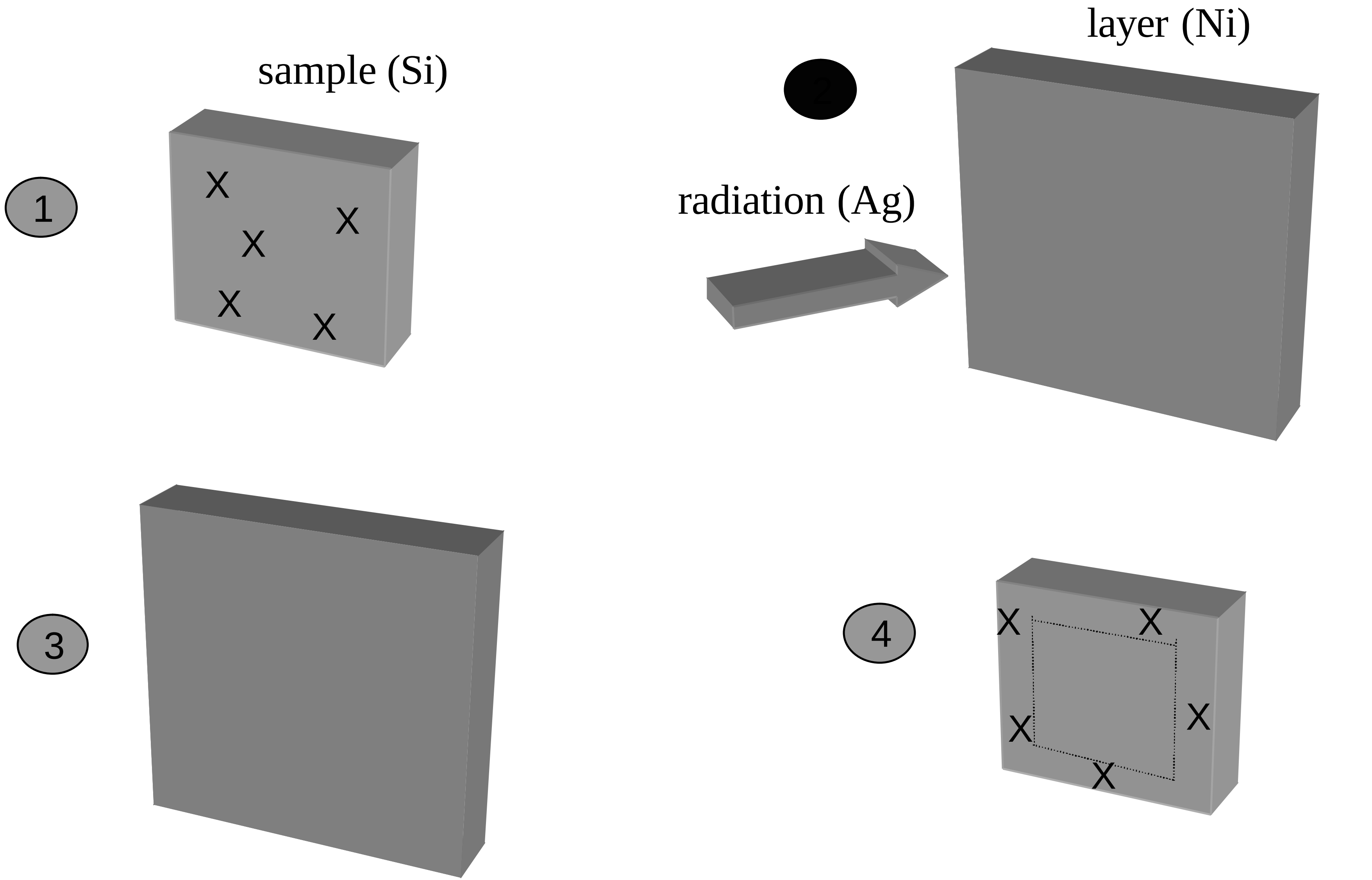
Outline

- Previous: Experimental evidence
- Model
- Vacancy
- MB & vacancy
- Results

Experimental evidence: *defects migrate*

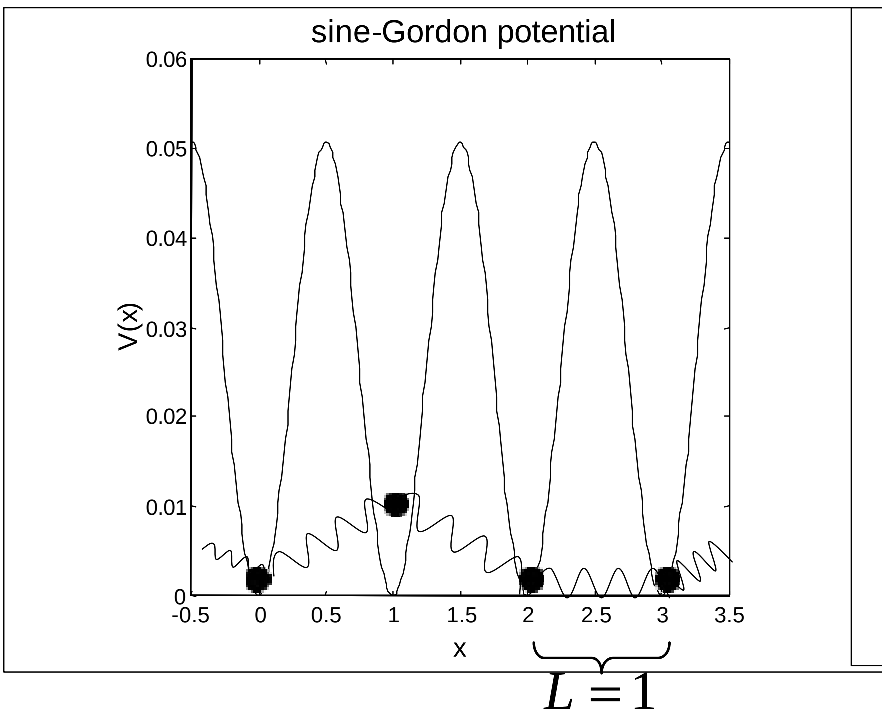


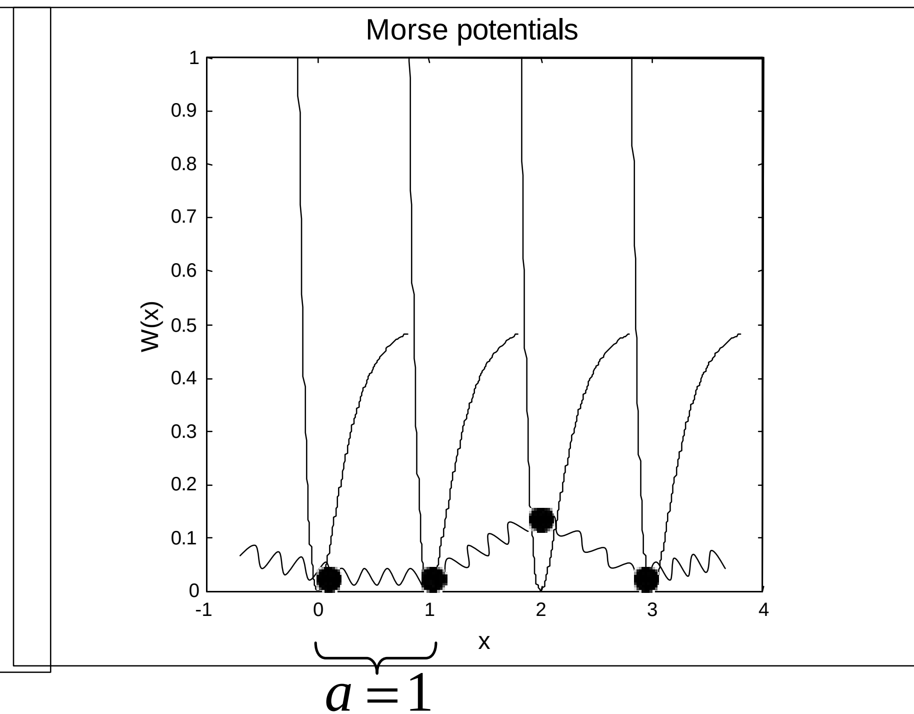
The model

Frenkel-Kontorova + anharmonic interaction

$$V(x) = \frac{L^2}{4p^2}\left[1 - \cos\left(\frac{2px}{L}\right)\right]$$

$$W(x) = \frac{1}{2}\left[\exp\left(-b(x-a)\right) - 1\right]^2$$





The Hamiltonian:

$$H = \sum_n \frac{1}{2}\dot{x}_n^2 + V(x_n) + C' W(x_n - x_{n+1})$$

$$= \sum_n \frac{1}{2}\dot{x}_n^2 + \frac{L^2}{4p^2}\left[1-\cos\left(\frac{2px_n}{L}\right)\right] + C'\left[\frac{1}{2}[\exp(-b(x_{n+1}-x_n-a))-1]^2 + \frac{1}{2}[\exp(-b(x_n-x_{n-1}-a))-1]\right.$$

The linearized equations:

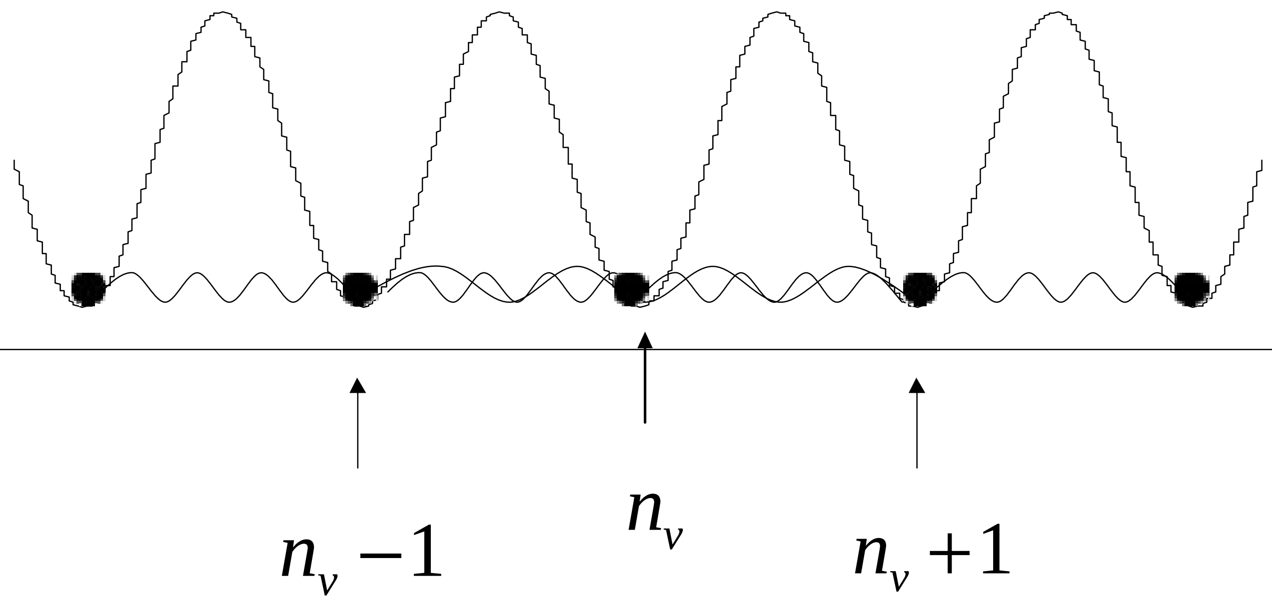
$$\ddot{x}_n + x_n + b^2 C'(2x_n - x_{n-1} - x_{n+1}) = 0$$

Plane waves (phonons) ⟶ $x_n(t) = x_0 e^{i(qn - w_{ph}t)}$

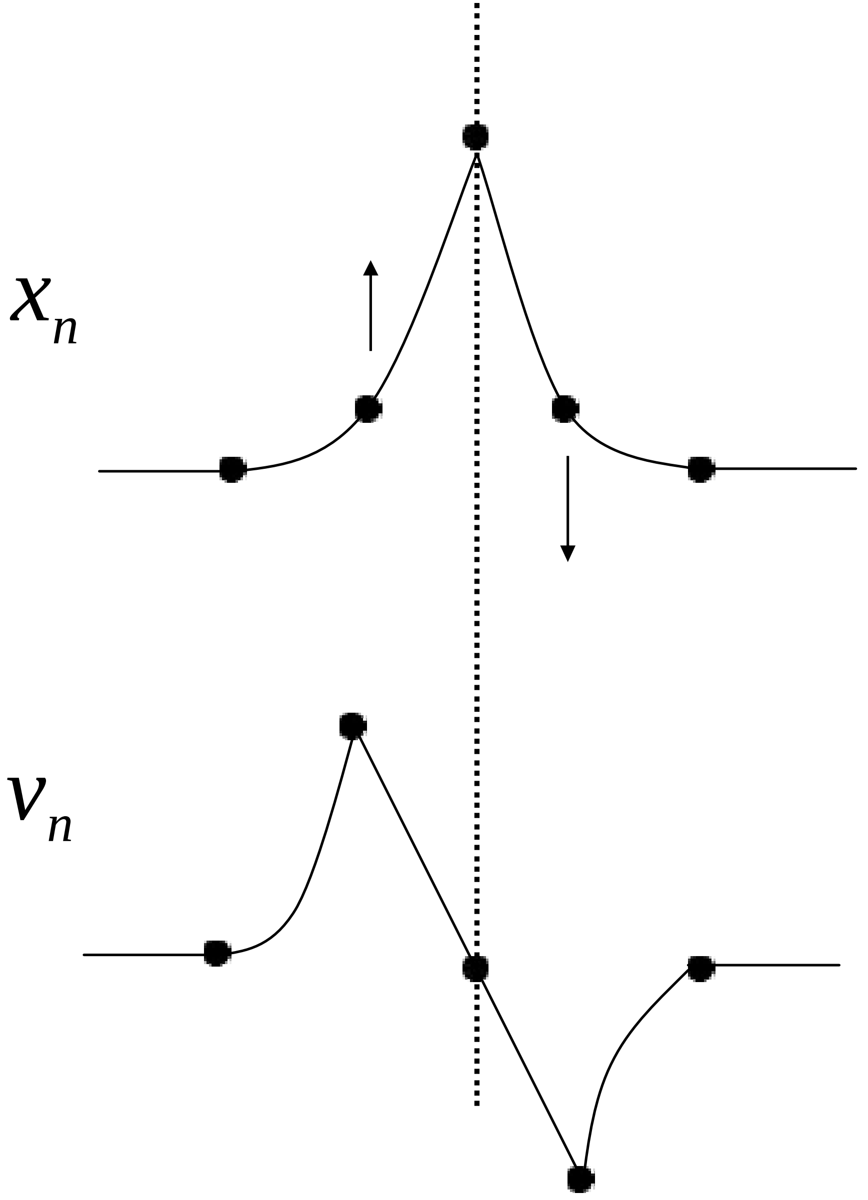
Dispersion relation ⟶ $w_{ph}^2 = w_0^2 + 4C\sin^2\left(\frac{q}{2}\right)$,, $C \equiv b^2 C'$

Frecuency breather: $w_b = 0.9 \longrightarrow T_b = \frac{2p}{w_b}$,, $w_0 = 1$

The vacancy



The moving breather



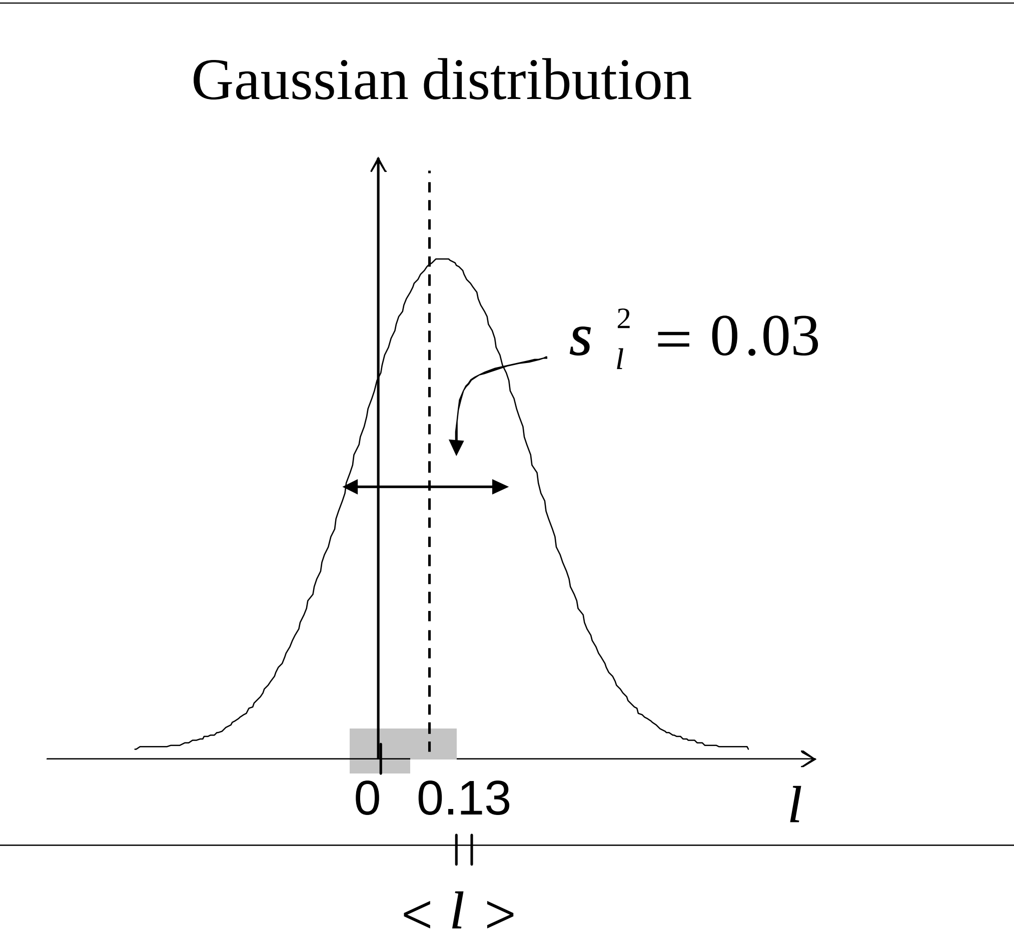
$$\vec{v}_0 = \left(0,\cdots,0,-\frac{1}{\sqrt{2}},0,\frac{1}{\sqrt{2}},0,\cdots,0\right)$$

$$\vec{v} = l\,\vec{v}_0$$

Energy added to the breather:

$$K = \frac{1}{2}\left(l\,\vec{v}\right)^2 = \frac{1}{2}\,l^2$$

The moving breather



Analysis:

- b (Morse potential)
- l

K Forinash, T Cretegny and M Peyrard.

Local modes and localization in a multicomponent nonlinear lattices. *Phys. Rev. E*, 55:4740, 1997.

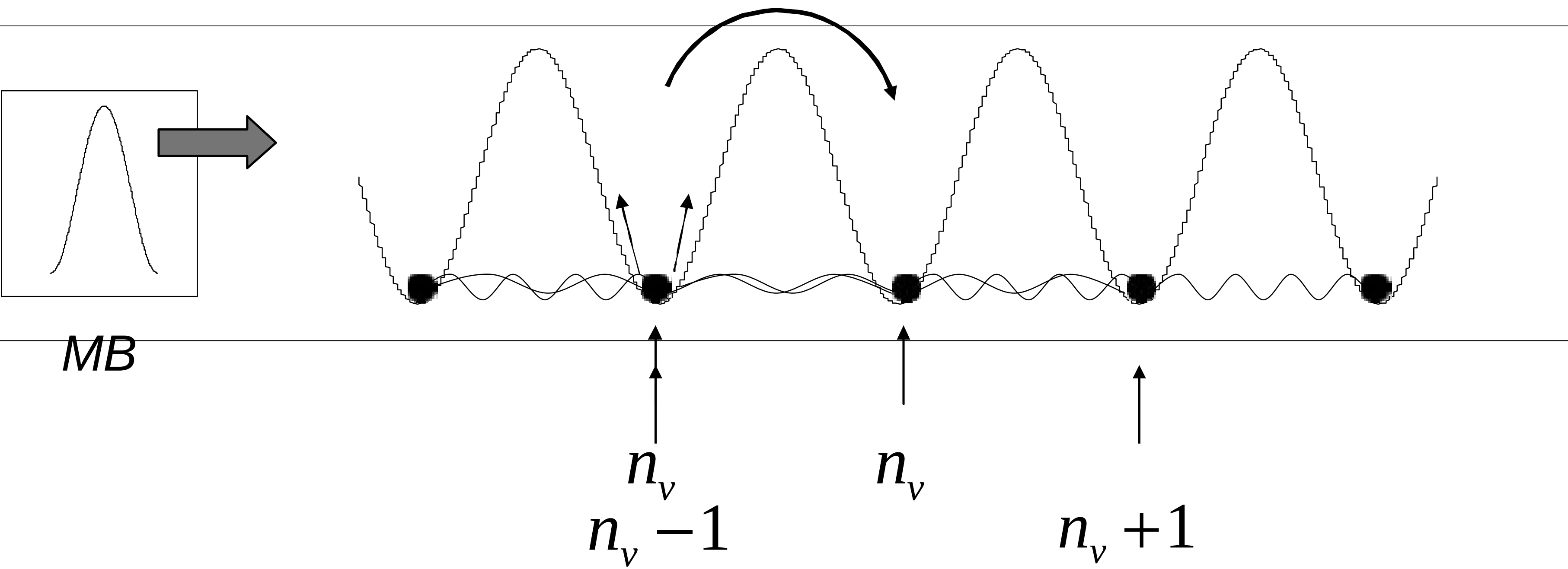
Three types of phenomena

i) The vacancy moves backwards.

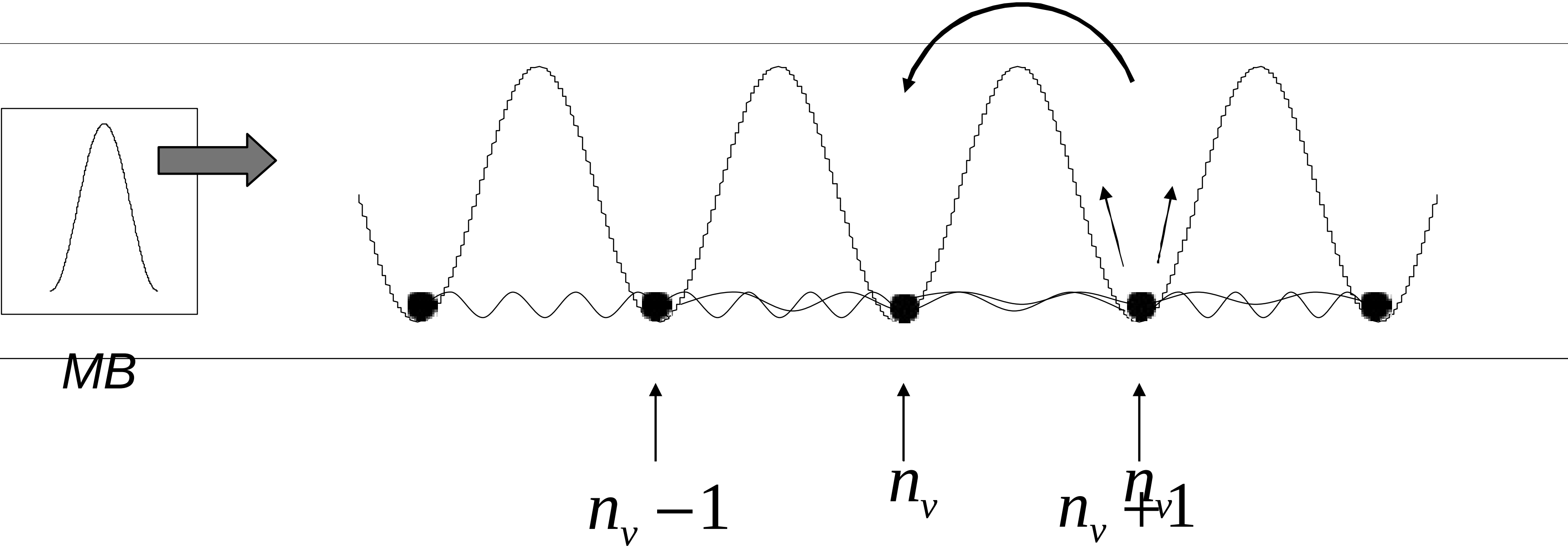
ii) The vacancy moves forwards.

iii) The vacancy remains at its site.

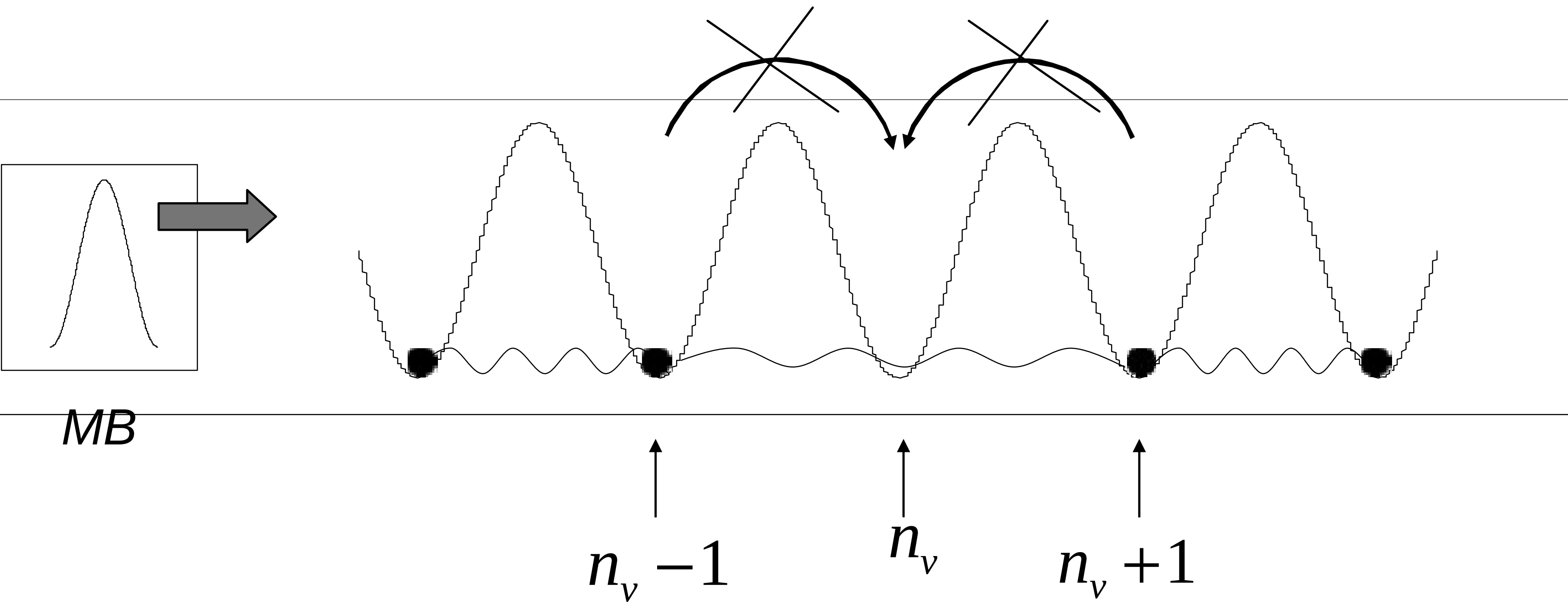
i) The most probably is that the vacancy moves backwards



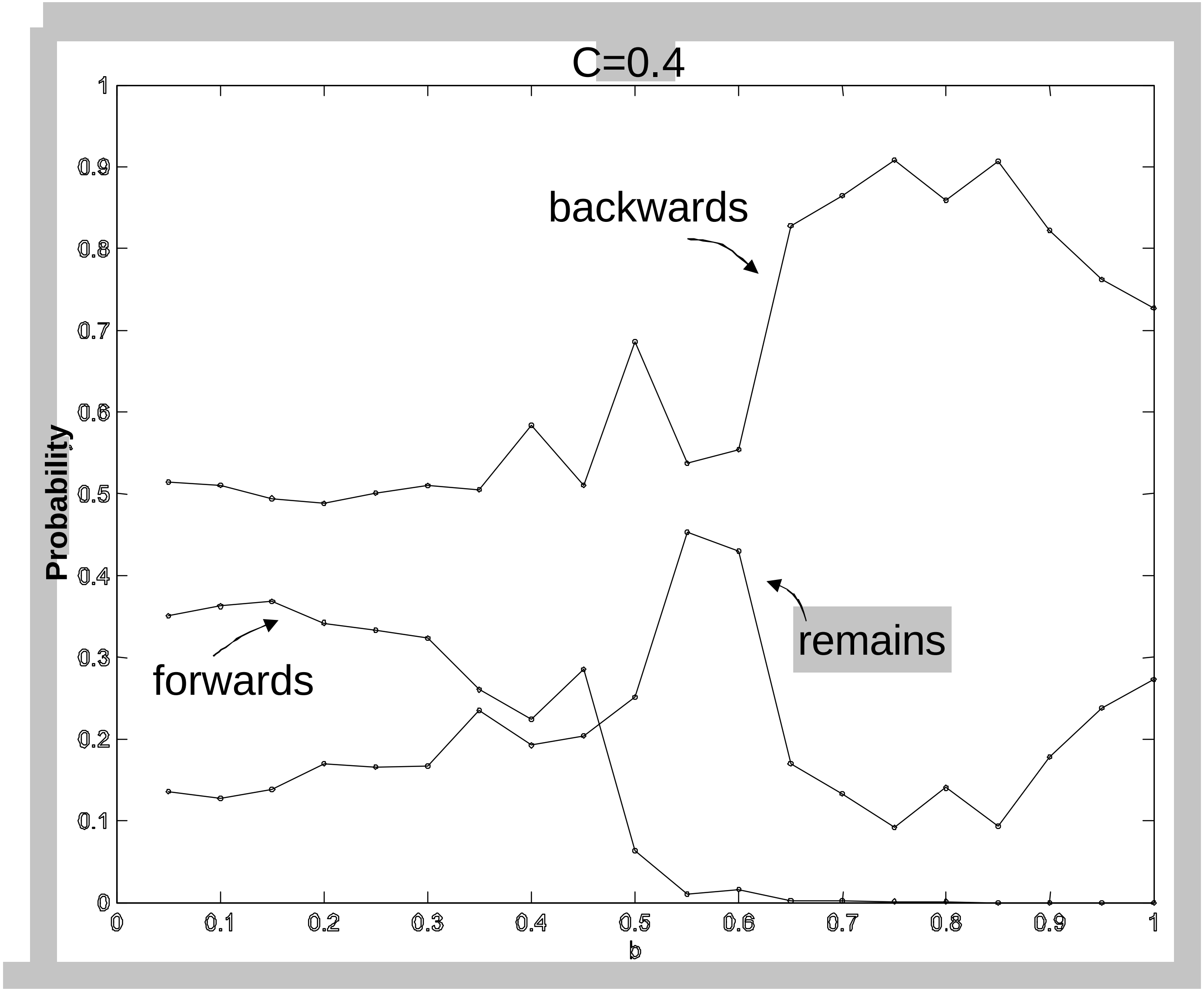
ii) But the vacancy can move forwards



iii) And the vacancy can stay motion-less



Probability of the vacancy’s movement



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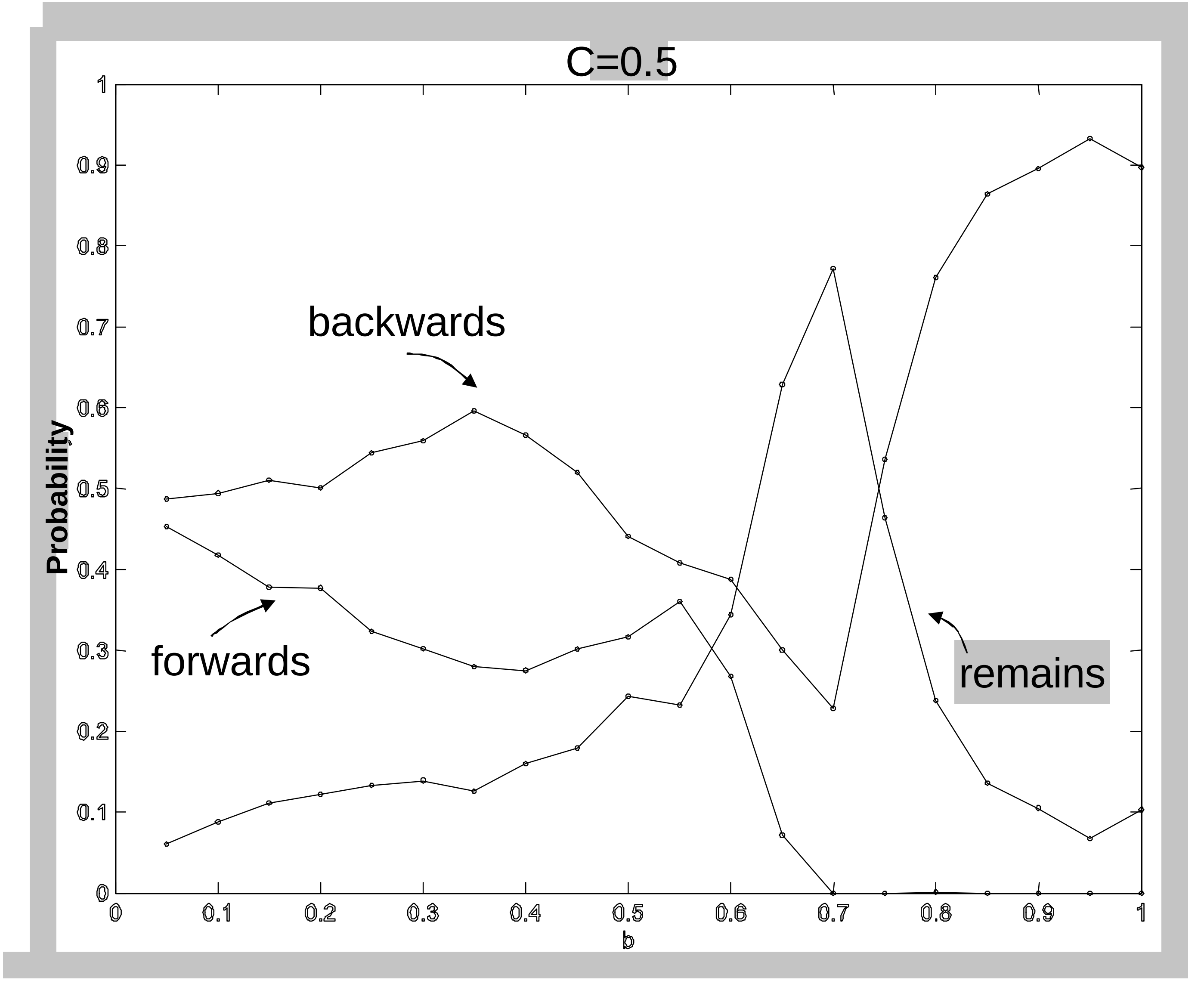
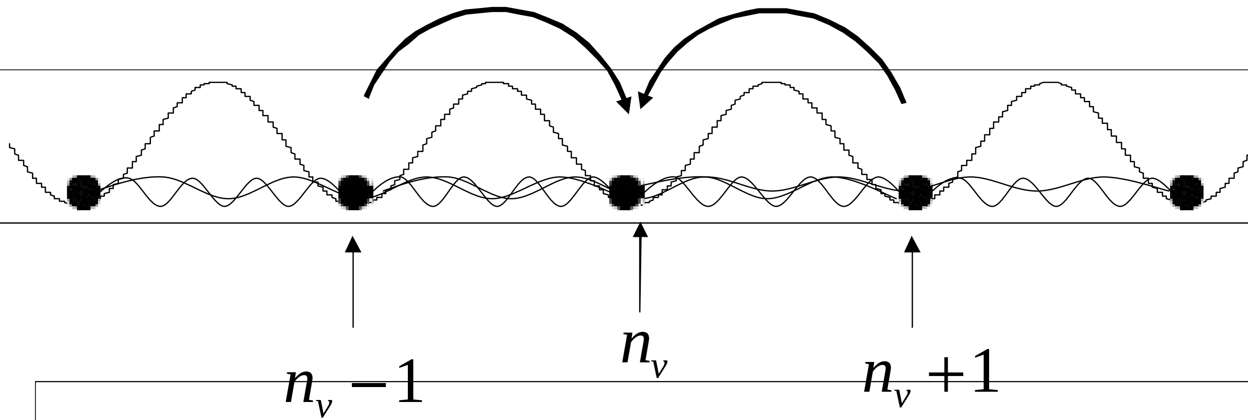
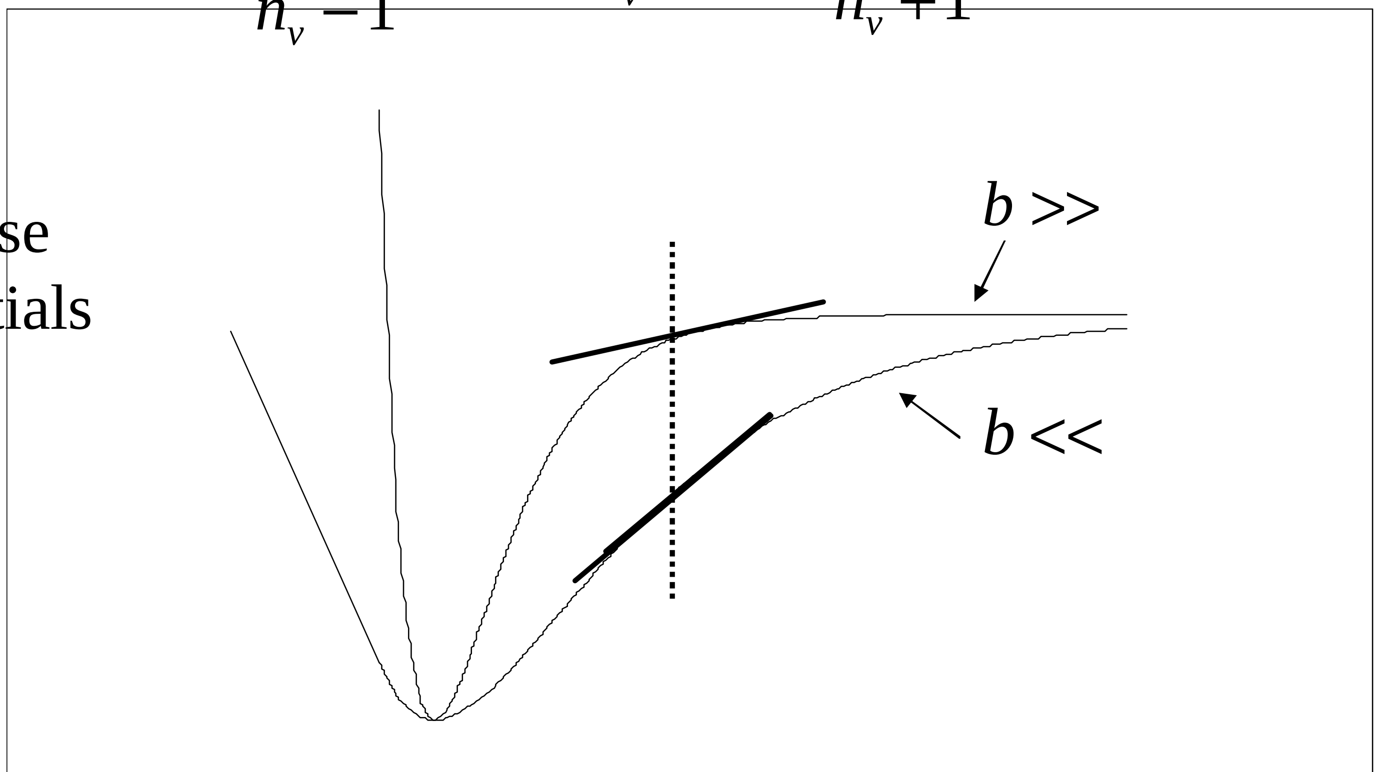


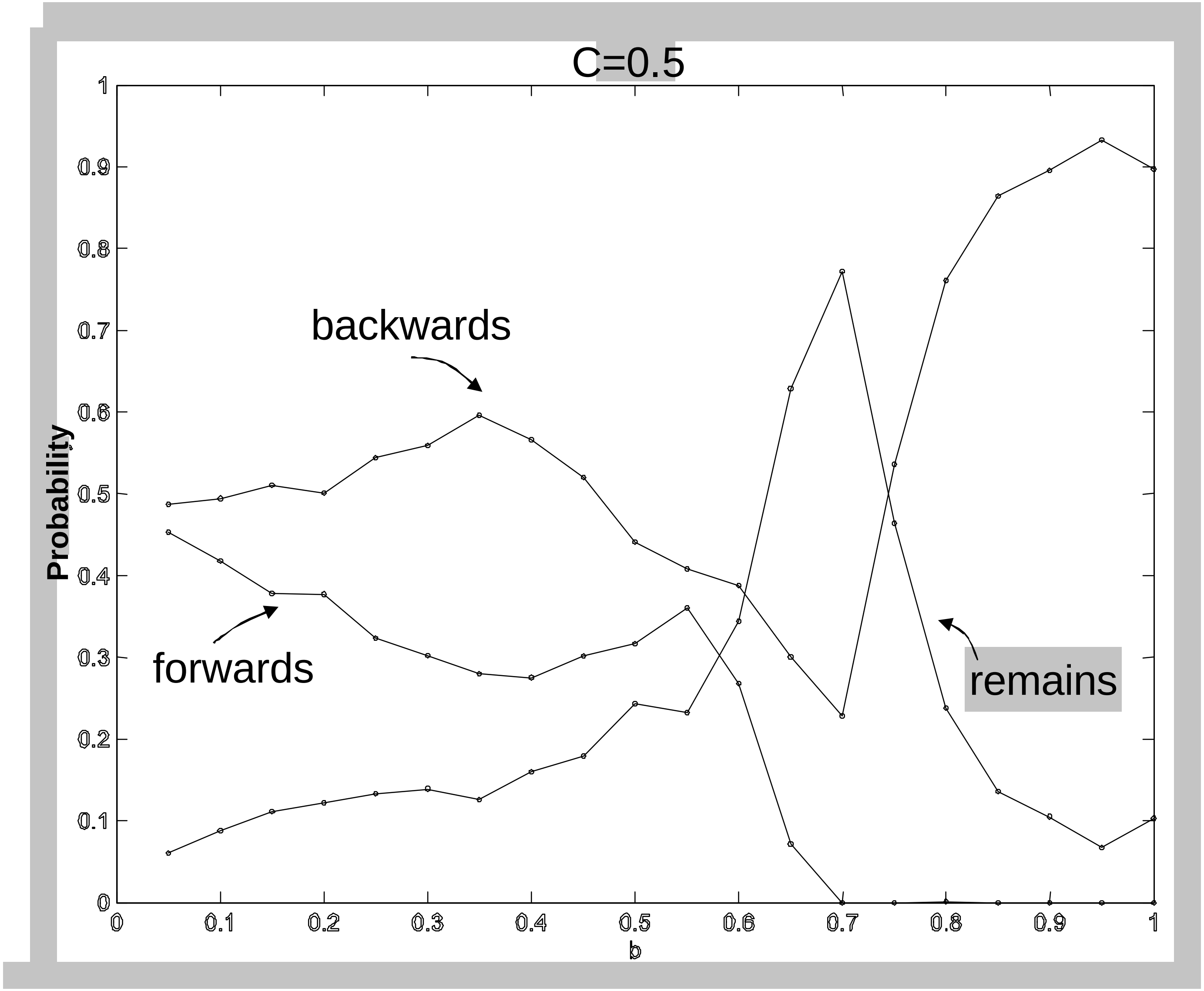
The coupling forces



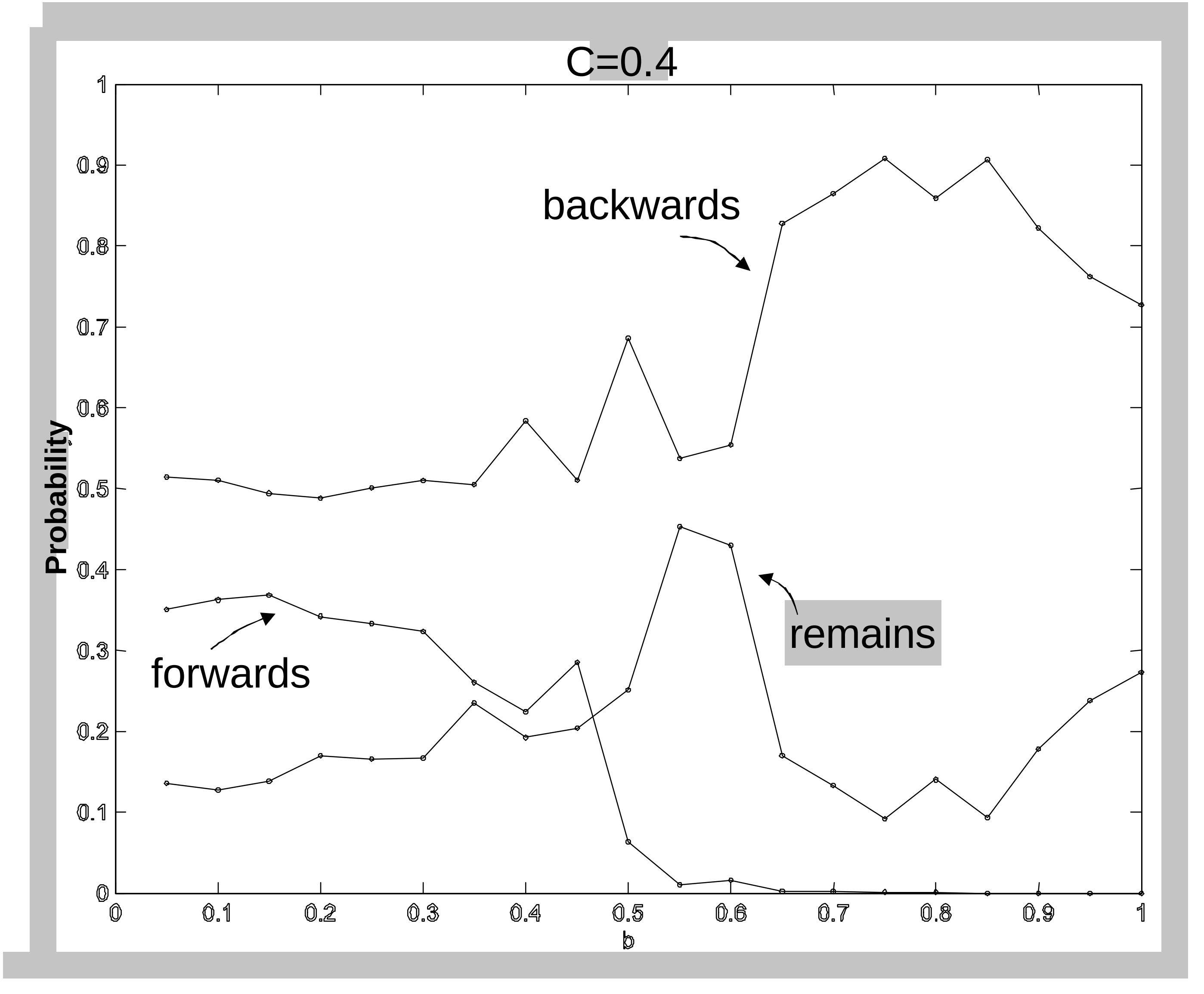
Morse potentials



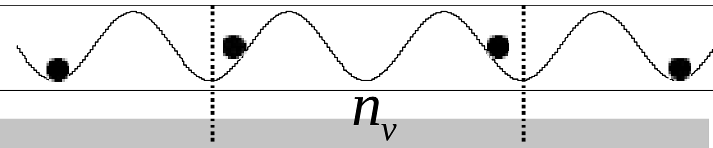
Probability of the vacancy's movement

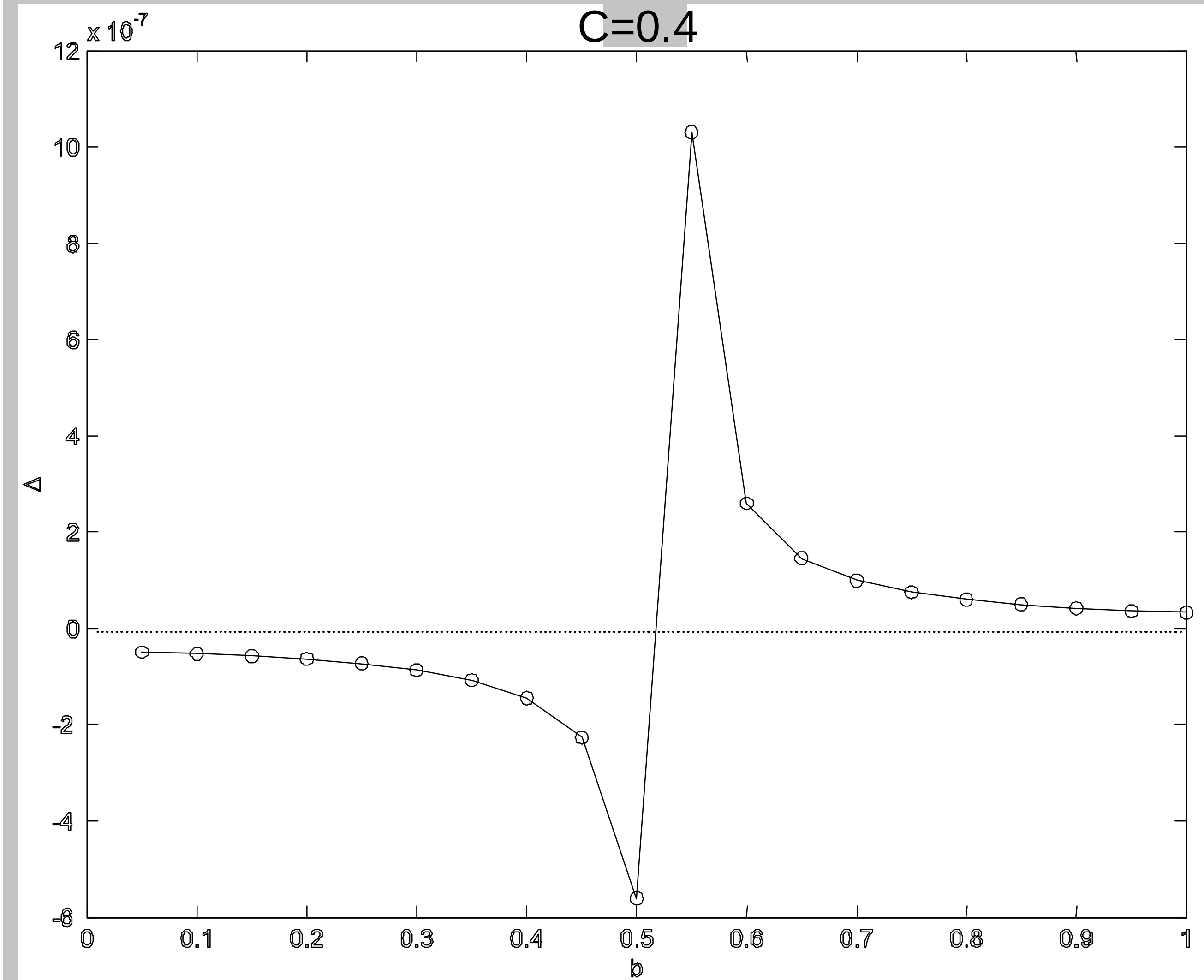


Probability of the vacancy's movement



$$\Delta \equiv u_{n_v-1} + u_{n_v+1}$$





bifurcation

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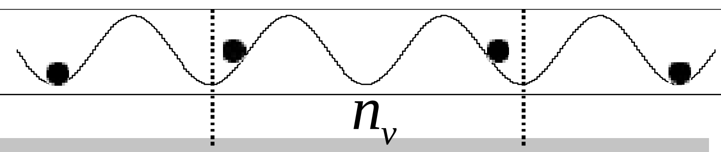
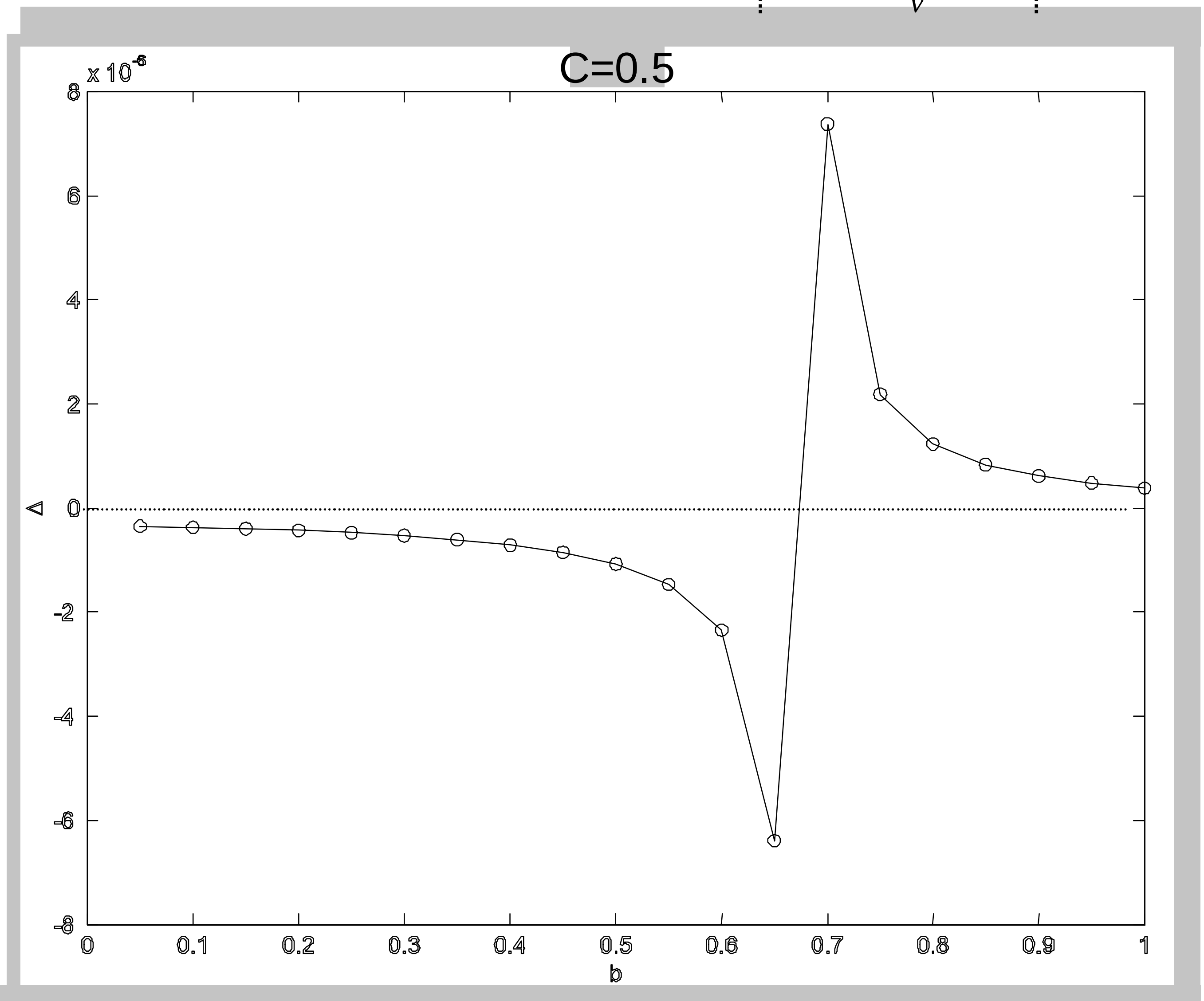
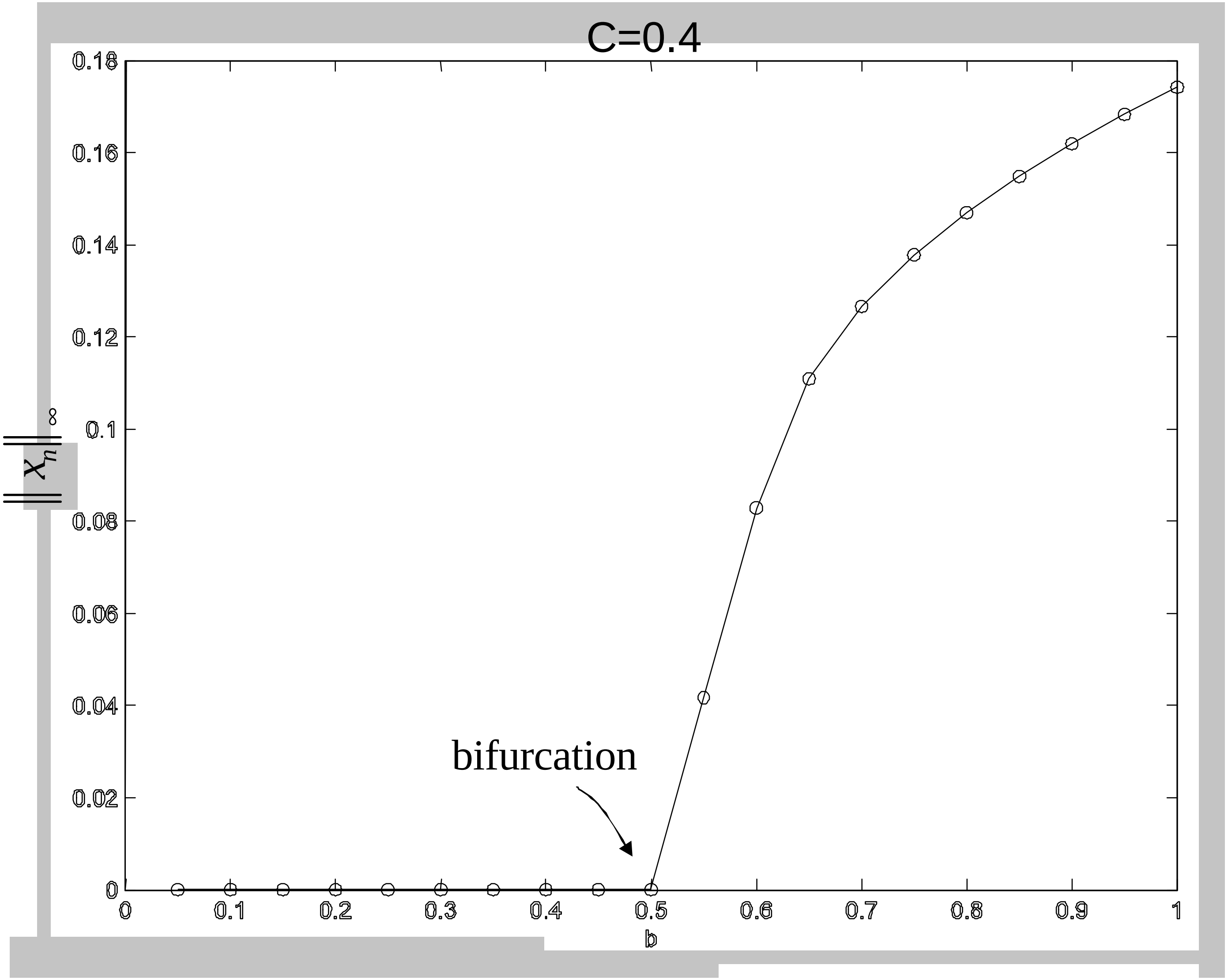




bifurcation

Amplitude maxima of a vacancy breather



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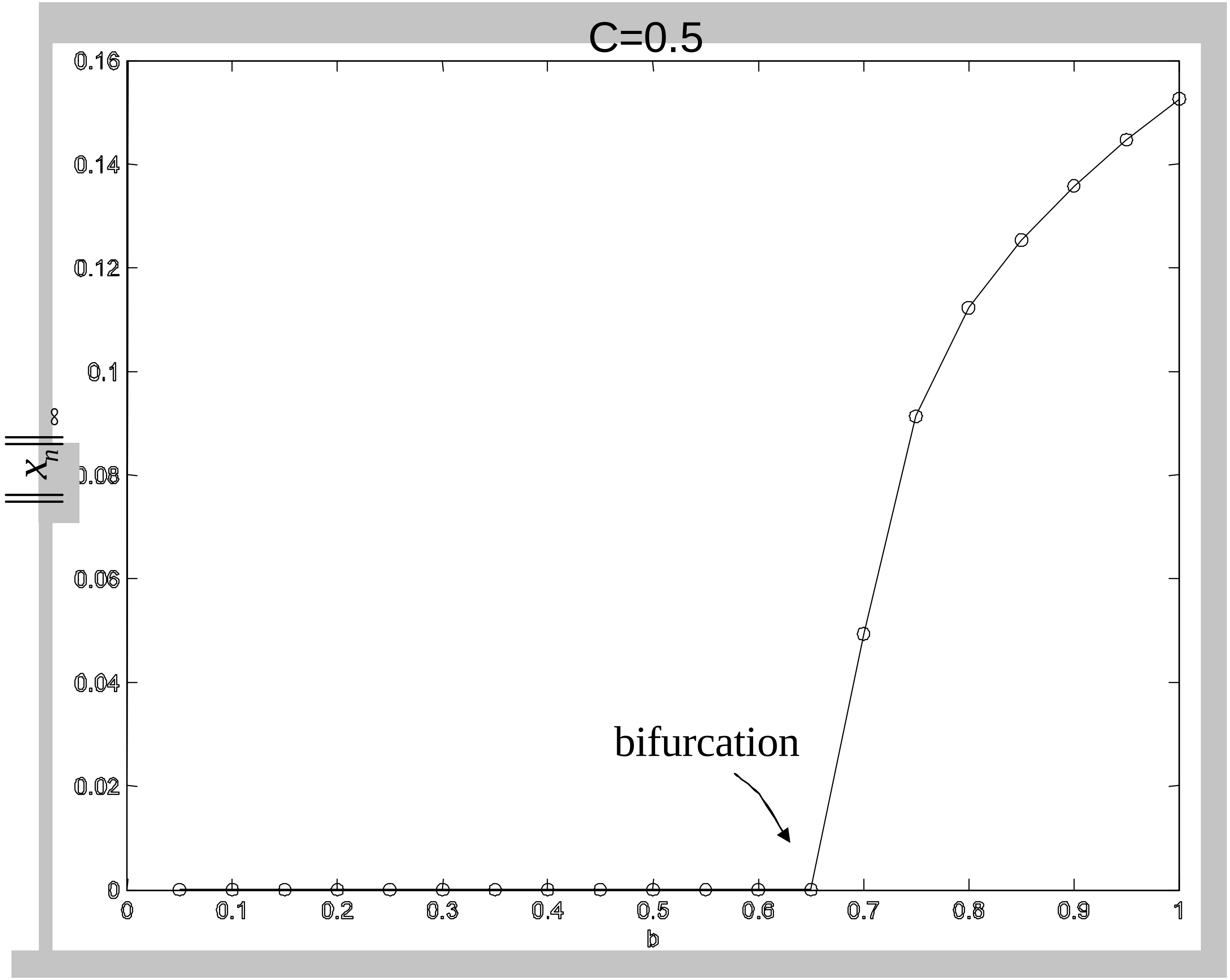

Conclusions

- The moving breathers can move vacancies.

- The behaviour is very complex and it depends of the values of the coupling.

- The changes of the probabilities of the different movements of the vacancies are related with the existence of bifurcations.

- Is there a more rich complexity from 1-dim to 2-dim ?

Thank you very much.