Probability of dimer reassociation in two dimensions

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We study the problem of dimer dissociation and reassociation in two dimensions through a random-walk-like calculation. In order to find the probability of dimer reassociation after a given number of hops, we give the exact analytical solution for the probability of a first return into a given region (rhombus) for a two-dimensional random walker on a squared lattice.

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The role of dissociation-reassociation processes in dimer surface diffusion has recently attracted interest. Indeed it has been shown that for $Si_2/Si(110)$ [1–3], and for many metal dimers [4,5] diffusing on fcc (110) surfaces, this piecewise diffusion mechanism can be dominant, thus giving the main contribution to dimers mobility. In piecewise diffusion, the dimer dissociates in a position *A* and the two adatoms diffuse over the surface until they meet again in a new position *B*. In many systems dimer mobility is much slower than adatom mobility. Therefore, in a typical experiment, it is very likely to observe only associated dimers. Thus, the dimer will be observed first in *A* and subsequently in *B*, and dissociation reassociation acts as an effective dimer diffusion mechanism. In all the above mentioned references the investigated surface geometry presents a well-defined preferential direction for diffusion, and dimers essentially move in one dimension. The present authors reported a complete analytical treatment of the one-dimensional piecewise diffusion in Ref. [5]. Here we consider dissociation reassociation in two dimensions, and we give an exact analytical result for the probability of reassociation after a given number of hops. It may be worth emphasizing that the study of the two-dimensional problem is interesting since there are many real systems where dimers effectively move in two dimensions: fcc (111) and (100) surfaces, are among the possible examples. As discussed with more details in Sec. V, real dimer dynamics on such surfaces is somewhat more complex than the one described by the model here below reported. Nevertheless, the exact analytical solution that we find can be used as a reference result to be compared with experiments and simulations. More, the random-walk problem we solve could be important for other applications. The paper is organized as follows: in Sec. I we briefly recall some results for dimer reassociation in 1D. In Sec. II we analyze the relation between dimer reassociation and first return to the origin in 2D. An exact recursion formula for the reassociation probability in a given number of steps is found in Sec. III. In Sec. IV we investigate the asymptotic behavior of such probability, and we give an explicit formula for its generating function. The last section contains a final discussion of the results.

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I. REASSOCIATION AND FIRST RETURN TO THE ORIGIN IN ONE DIMENSION

In the following we shall consider a dimer which dissociates at step 1, i.e., one of the two atoms makes a one-site move. Any further step will be characterized by a hop of one of the two atoms. If at a given step the two atoms meet each other again (i.e., if they become first neighbors), we consider this situation stable: the two adatoms remain fixed in such position. We ask which is the probability $Q_{\mathrm{dim}}(m)$ for the dimer to reassociate again exactly after m steps. In one dimension, the probability $Q_{\mathrm{dim}}^{1\mathrm{D}}(m)$ is easily found, since the relative coordinate $x_r = x_2 - x_1 - 1$ (x_1 and x_2 are the two atoms coordinates, $x_2 > x_1$) of the dimer performs a simple unbiased one-dimensional random walk; the probability of dimer reassociation after m steps is nothing but the probability $Q_0^{1\mathrm{D}}(m)$ of a first return to the origin for x_r. As it is well known (for example, see Refs. [6,7]), such probability reads

$$Q_0^{1\mathrm{D}}(2m) = Q_{\mathrm{dim}}^{1\mathrm{D}}(2m) = \binom{2m}{m}\left(\frac{1}{4}\right)^m \frac{1}{(2m-1)}. \qquad (1)$$

II. REASSOCIATION AND FIRST RETURN TO THE STAR IN TWO DIMENSIONS

Let us now consider a two-dimensional square lattice. While in 1D reassociation simply happens when $x_r = 0$, on a square lattice there are four configurations where the dimer is bound. They are shown in Fig. 1.

This causes a noticeable complication by respect to the 1D case, since $Q_{\mathrm{dim}}^{2\mathrm{D}}(m)$ cannot be obtained directly by computing the probability $Q_0^{2\mathrm{D}}(m)$ for the first return to the origin in m steps of a simple two-dimensional random walker ($\vec{x}_r$). Nevertheless, $Q_0^{2\mathrm{D}}(m)$ will be useful, so that we briefly outline how to evaluate it. For a two-dimensional simple random walker starting from the origin, the probability $T_0^{2\mathrm{D}}(2m)$ to be at the origin (not necessarily for the first time) after $2m$ steps (only at even steps the walker can reach the origin) is given by [7]

$$T_0^{2\mathrm{D}}(2m) = \frac{(2m!)^2}{4^{2m}(m!)^4}. \qquad (2)$$

In our opinion, the easiest way to find $Q_0^{2\mathrm{D}}(2m)$ once $T_0^{2\mathrm{D}}(2m)$ is known, is to introduce the *generating functions*

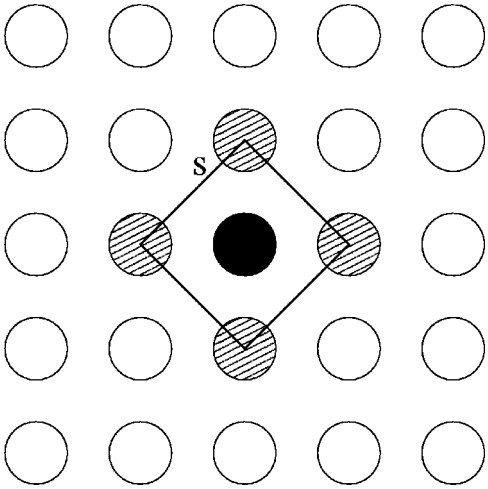

FIG. 1. The dimer is associated in each of the four configurations displayed in the figure. One adatom is represented by a black full circle, the other by a striped circle.

$$\hat{T}_0^{2D}(\xi)=\sum_{m=0}^{\infty} T_0^{2D}(2m)\xi^{2m},$$

$$\hat{Q}_0^{2D}(\xi)=\sum_{m=0}^{\infty} Q_0^{2D}(2m)\xi^{2m}. \tag{3}$$

Indeed, it can be easily shown (for example, see Ref. [6]) that the two generating functions satisfy the simple relation

$$\hat{Q}_0^{2D}(\xi)=1-\frac{1}{\hat{T}_0^{2D}(\xi)}. \tag{4}$$

So, $Q_0^{2D}(0)=1-1/T_0^{2D}(0)$, while for $m>0$ the recursion relation

$$Q_0^{2D}(2m)=-\sum_{i=0}^{m-1} T_0^{2D}(2m-2i)Q_0^{2D}(2i), \tag{5}$$

together with Eq. (2) gives $Q_0^{2D}(2m)$. While numerically computing $Q_0^{2D}(2m)$ for large m's, in order to avoid to handle with large factorials, it may be useful the recursion relation

$$T_0^{2D}(2m+2)=T_0^{2D}(2m)\frac{[(2m+2)(2m+1)]^2}{16(m+1)^4}. \tag{6}$$

Indeed, by using Eqs.(5),(6) together, the probabilities $Q^{2D}(2m)$ up to $m\sim 10^5$ are quickly obtained. The two probabilities display the asymptotic behaviors [7,8]

$$Q_0^{1D}(2m)\sim(2m)^{-3/2}$$

$$Q_0^{2D}(2m)\sim\frac{1}{2m\ln^2(2m)}. \tag{7}$$

Now we can go back to our original problem: the two-dimensional dimer diffusion. Once again, we want to get information about the dimer by considering the two-dimensional walker represented by the relative coordinate

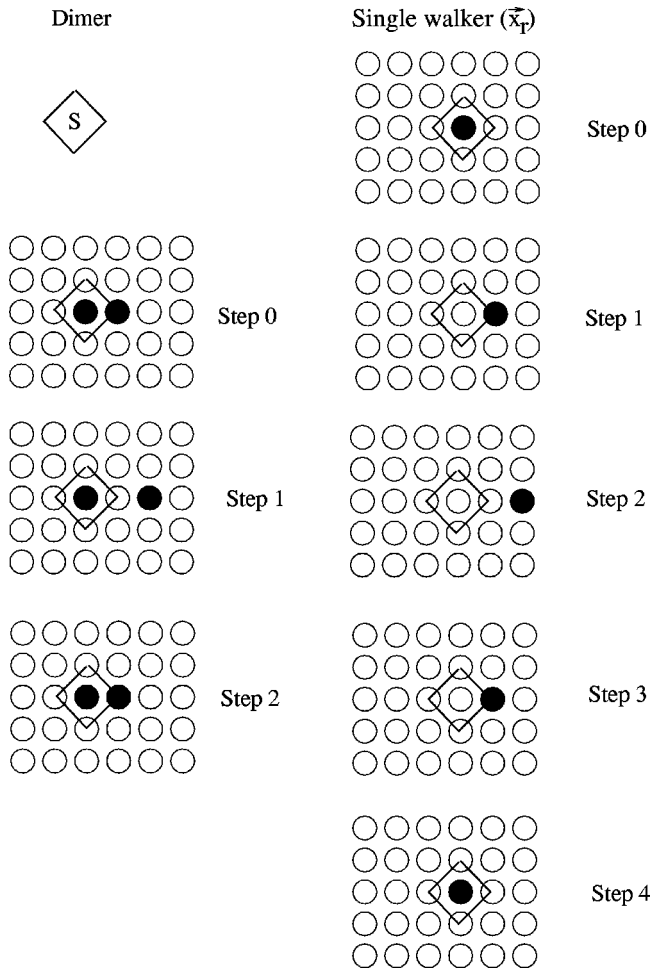

FIG. 2. Left: dimer random walk, showing a dissociation-reassociation event in two steps. Right: corresponding random walk for the relative coordinate $\vec{x}_r$. In order to extract the probability for the first return to S (starting from S) from the probability for the first return to the origin (starting from 0), a four-step random walk must be considered.

$\vec{x}_r=(x_2-x_1,y_2-y_1)$. Dimer and induced-$\vec{x}_r$ random walks are schematically represented in Fig. 2. The dimer is initially bound, so that $\vec{x}_r$ occupies one of the four points of the *star* S (rhombus) displayed in Fig. 1. In the following we shall remember that when $\vec{x}_r\in S$, the dimer is associated. At the subsequent step, we impose its dissociation, i.e., there are six possible configurations, since the two adatoms are not allowed to occupy the same position: this means that $\vec{x}_r$ must move outside the star. After this step, $\vec{x}_r$ moves as a simple unbiased 2D-random walker. We want to find $Q_S^{2D}(m)$, i.e., the probability it has, *starting from S*, to reach again *one of the four star points* for the first time in a given number of steps m, knowing the probability, *starting from the origin* to reach again the *origin* for the first time in m steps $[Q_0^{2D}(m)]$. Obviously, $Q_{\rm dim}^{2D}(m)\equiv Q_S^{2D}(m)$. We note that if $\vec{x}_r$ reaches the origin for the first time at the mth step, it was in S at step $m-1$: this may suggest to look for a relation between $Q_0^{2D}(2m+2)$ and $Q_S^{2D}(2m)$ [the number of steps is always even, and two extra steps are needed to the random walker $\vec{x}_r$ by respect to the dimer: the first, is required to move from

the origin to S, and the last is required to go back to the origin after the walker is in S at the $(2m+1)$th step]. We notice that, once the unbiased two-dimensional walker is in S, it can move again out of the star. Therefore if it reaches the origin at the mth step for the first time, we know it was in S at the $(m-1)$th step, but not necessarily for the first time.

III. SOLUTION OF THE TWO-DIMENSIONAL PROBLEM

Let us introduce $\mathcal{U}^0_{2m+2}$, the set of all distinct random walks leading to a first return to the origin for the first time after $2m+2$ steps. Now we introduce $\mathcal{U}^S_{(2m+2);(2m+1)}$, i.e., the set of distinct random walks leading to a first return to the origin in $2m+2$ steps where the walker is in S for the first time (after the first step) at step $2m+1$. By definition,

$$\mathcal{U}^S_{(2m+2);(2m+1)} \subset \mathcal{U}^0_{2m+2}.$$

The key observation is that

$$\mathcal{U}^0_{2m+2} = \cup_{k=0}^{m-1} \mathcal{U}^S_{(2m+2);(2m+1-2k)}. \tag{8}$$

So, we are making a partition of the set of all possible random walks leading to a first return to the origin in $2m+2$ steps, by creating subsets of such random walks whose elements are characterized by a first return to S at a given step. Of course, such subsets are disjoints, and we can calculate $Q_0^{2D}(2m+2)$ as

$$Q_0^{2D}(2m+2) = \sum_{k=0}^{m-1} \tilde{Q}_0^{2D}[\mathcal{U}^S_{(2m+2);(2m+1-2k)}], \tag{9}$$

where $\tilde{Q}_0^{2D}[\mathcal{U}^S_{(2m+2);(2m+1-2k)}]$ is the contribution given to $Q_0^{2D}(2m+2)$ only from the random walks of $\mathcal{U}^S_{(2m+2;2m+1-2k)}$.

Let us now consider $m=1$, where things are particularly simple, since all random walkers coming back to the origin for the first time at step 4 were back in S for the first time at step 3. Thus,

$$\mathcal{U}^S_{4;3} \equiv \mathcal{U}^0_4. \tag{10}$$

This means that there is a one by one correspondence between random walks of four steps leading to a first return to the origin and the two-step random walk of $\vec{x}_r$ which starts from S and reaches back S in exactly two steps, moving out of S at the first step (see Fig. 2). Nevertheless, while computing the probabilities of such random walks, one should take into account that in the four-step random walk, the second step, i.e., the move from S outside S has a probability 3/4, while in the $\vec{x}_r$ two-step random walk this moves is imposed, i.e., has unit probability. More, the last move from S to the origin in the four-step random walk occurs with probability 1/4. So,

$$Q_0^{2D}(4) = \frac{3}{4}\frac{1}{4} Q_S^{2D}(2). \tag{11}$$

Before giving the general formula for $Q_S^{2D}(2m)$, it may be instructive to analyze the case $m=2$ too. Now we must consider that

$$\mathcal{U}^0_6 = \mathcal{U}^S_{6;5} \cup \mathcal{U}^S_{6;3}, \tag{12}$$

and from Eq. (9) follows

$$Q_0^{2D}(6) = \tilde{Q}_0^{2D}[\mathcal{U}^S_{6;5}] + \tilde{Q}_0^{2D}[\mathcal{U}^S_{6;3}]. \tag{13}$$

The first addendum can be evaluated as in the $m=1$ case, and it gives a contribution to $Q_0^{2D}(6)$:

$$\tilde{Q}_0^{2D}[\mathcal{U}^S_{6;5}] = \frac{3}{16} Q_S^{2D}(4). \tag{14}$$

For the second addendum a small additional effort is needed: All random walks $\in \mathcal{U}^S_{6;3}$ are first back to S at step 3, then are back in S after two further steps, and finally reach the origin. By separating such intermediate two steps return to S from the other four steps, we find

$$\tilde{Q}_0^{2D}[\mathcal{U}^S_{6;3}] = \frac{3}{4} Q_S^{2D}(2) Q_0^{2D}(4), \tag{15}$$

and

$$Q_0^{2D}(6) = \frac{3}{4}\frac{1}{4} Q_S^{2D}(4) + \frac{3}{4} Q_S^{2D}(2) Q_0^{2D}(4). \tag{16}$$

Note that, as in the $m=1$ case, a factor 3/4 must be considered for each move where the walker moves from S outside S, while the factor 1/4 weights the last step from S to the origin. We can now summarize the procedure and give the final result. For a given number of steps $2m+2$, one can group the set of random walks leading to a first return to the origin at the final step, into the disjoint subsets where the first return to the star happens at a given step $2m+1-2k$ $(k=0,1,2,\ldots,m-1)$. The total probability $Q_0^{2D}(2m+2)$ can be written as the sum over such subsets. The one corresponding to $k=0$ simply gives a contribution $(3/16)Q_S^{2D}(2m)$; for $k=1$ one finds $(3/4)Q_S^{2D}(2m-2)Q_0^{2D}(4)$; for $k=2$ we have $(3/4)Q_S^{2D}(2m-4)Q_0^{2D}(6)$, and so on. The final result for $Q_S^{2D}(2m)(m \geqslant 2)$, reads

$$Q_S^{2D}(2m) = \frac{16}{3} Q_0^{2D}(2m+2) - 4\sum_{k=1}^{m-1} Q_0^{2D}(2m+2-2k) Q_S^{2D}(2k) \tag{17}$$

which can be easily solved iteratively.

In order to check that $Q_S^{2D}(2m)$ given by Eq. (17) is right, we run a set of Monte Carlo simulations. In such simulations, we considered a dimer associated at step 0; at each step one of the two adatoms was left free to increase or to decrease one of the two coordinates. Of course at the first step, the two adatoms were not allowed to have the same coordinates. Simulations were stopped at the reassociation step. After 10^7 simulations, we found the results reported in Fig. 3, in perfect agreement with Eq. (17).

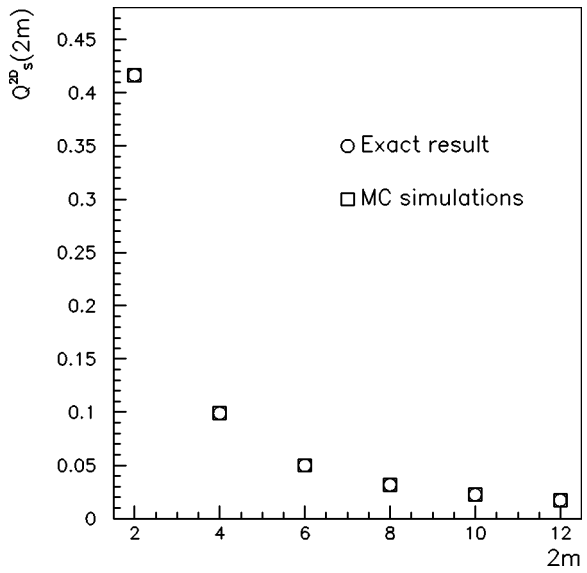

FIG. 3. Comparison between Monte Carlo simulations (circles) and the exact result for $Q_S^{2D}(2m)$ (squares): the perfect agreement confirms that our procedure in finding Eq. (17) was correct.

IV. EXPLICIT SOLUTION FOR THE GENERATING FUNCTION AND ASYMPTOTIC BEHAVIOR

Multiplying both sides of Eq. (17) by ξ^{2m} and summing over $m>1$, we obtain

$$\sum_{m=2}^{\infty} Q_S^{2D}(2m)\xi^{2m}=\frac{16}{3}\sum_{m=2}^{\infty} Q_0^{2D}(2m+2)\xi^{2m}-4 \times\sum_{m=2}^{\infty}\xi^{2m}\sum_{k=1}^{m-1} Q_0^{2D} \times(2m+2-2k)Q_S^{2D}(2k). \quad (18)$$

By introducing the generating functions

$$\hat{Q}_S^{2D}(\xi)=\sum_{m=0}^{\infty} Q_S^{2D}(2m)\xi^{2m},$$

$$\hat{Q}_0^{2D}(\xi)=\sum_{m=0}^{\infty} Q_0^{2D}(2m)\xi^{2m}, \quad (19)$$

after some calculations Eq. (18) gives

$$\hat{Q}_S^{2D}(\xi)-Q_S^{2D}(2)\xi^2=\frac{16}{3\xi^2}[\hat{Q}_0^{2D}(\xi)-\xi^2Q_0^{2D}(2)-\xi^4Q_0^{2D}(4)] -\frac{4}{\xi^2}\hat{Q}_0^{2D}(\xi)\hat{Q}_S^{2D}(\xi) +4Q_0^{2D}(2)\hat{Q}_S^{2D}(\xi). \quad (20)$$

By recalling that $Q_0^{2D}(2)=1/4$, and that $Q_S^{2D}(2)=(16/3)Q_0^{2D}(4)$, from Eq. (20) one easily obtains

$$\hat{Q}_S^{2D}(\xi)=\frac{4}{3}-\frac{\xi^2}{3\hat{Q}_0^{2D}(\xi)}, \quad (21)$$

which gives the explicit solution for the generating function of dimer reassociation probability. Equation (21) may be also put in the form

$$\hat{Q}_S^{2D}(\xi)=\frac{4}{3}-\frac{2\xi^2K[\xi^2]}{6K[\xi^2]-3\pi}, \quad (22)$$

where

$$K[m]=\int_0^{\pi/2}\frac{1}{\sqrt{1-m\sin^2\alpha}}d\alpha, \quad (23)$$

is the complete elliptic integral. Equation (22) follows from Eqs. (21),(4) and from [9]

$$\hat{T}_0^{2D}(\xi)=\frac{2}{\pi}K[\xi^2]. \quad (24)$$

Once the generating function is known, one can try to infer the asymptotic behavior of the associated power series coefficients by using the discrete Tauberian theorem [6]. Indeed, if

$$\hat{f}(\xi)=\sum_{n=0}^{\infty} f_n\xi^n, \quad (25)$$

the conditions

$$\hat{f}(\xi)\sim(1-\xi)^{-p}L\left(\frac{1}{1-\xi}\right) \text{ if } \xi\to1^- \quad (26)$$

and

$$f_n\sim n^{p-1}L(n) \text{ if } n\to\infty, \quad (27)$$

are equivalent provided that f_n is monotonic, $p>0$, and $\lim_{x\to\infty}[L(\lambda x)/L(x)]\to1\ \forall\lambda$. Of course, such theorem cannot be applied to the generating function of a normalized probability, since $\lim_{\xi\to1^-}\hat{f}(\xi)=1$. A possible trick is to consider the associated power series having partial sums for coefficients, in our case $\hat{Q}_S^{sum}(\xi)$ defined by

$$\hat{Q}_S^{sum}(\xi)=\sum_{m=0}^{\infty}\xi^{2m}\left(\sum_{m=k}^{\infty} Q_S^{2D}(2k)\right). \quad (28)$$

Rearranging the terms in the double sum, after few calculations one obtains

$$\hat{Q}_S^{sum}(\xi)=\frac{1}{1-\xi^2}[1-\xi^2\hat{Q}_S^{2D}(\xi)]. \quad (29)$$

Now, since [9]

$$K[\xi^2]\sim\frac{1}{2}\ln\frac{16}{(1-\xi^2)} \text{ if } \xi\to1^-, \quad (30)$$

then

$$\hat{Q}_S^{sum}(\xi)\sim-\frac{1}{1-\xi}\frac{1}{\ln(1-\xi)} \text{ if } \xi\to1^-. \quad (31)$$

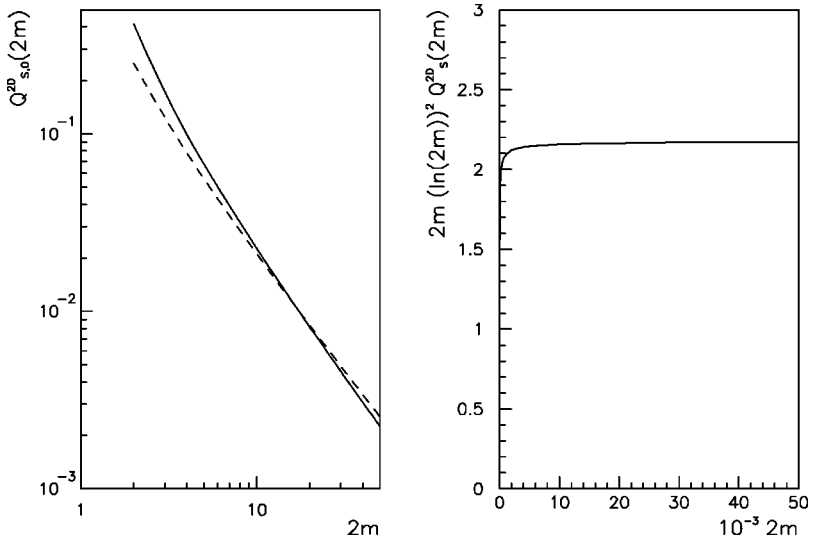

FIG. 4. Left: double logarithmic plot for $Q_S^{2D}(2m)$ (full line) and $Q_0^{2D}(2m)$ (dashed line). Right: for $2m\to\infty, Q_S^{2D}(2m)\sim 1/[2m\ln^2(2m)]$.

We thus can apply the Tauberian theorem, finding

$$\sum_{k=m}^{\infty} Q_S^{2D}(2k)\sim\frac{1}{\ln 2m}\quad\text{if}\quad m\to\infty, \tag{32}$$

and finally

$$Q_S^{2D}(2m)\sim\frac{1}{2m\ln^2(2m)},\quad m\to\infty. \tag{33}$$

So, $Q_S^{2D}(2m)$ and $Q_0^{2D}(2m)$ follow the same asymptotic behavior. In Fig. 4 we compare $Q_S^{2D}(2m)$ and $Q_0^{2D}(2m)$ for small values of m, and we show $Q_S^{2D}(2m)$ multiplied by its asymptotic limit $(2m)\ln^2(2m)$. For very small m, $Q_S^{2D}(2m) > Q_0^{2D}(2m)$, since as soon as the walker is closed to its original position, the probability of falling into a finite region around the origin is of course larger than the probability of reaching the origin. We can think that in order to avoid S in the first steps, the walker necessarily moves, on average, far away from its initial position. That is why the probability to reach S in $2m$ steps for large values of m is smaller than $Q_0^{2D}(2m)$. The same asymptotic behavior can be justified by thinking that for very large m's, the walker goes so far from the origin that the whole S is seen as a single point.

V. DISCUSSION AND CONCLUSIONS

In the previous sections, we proposed a simple model for dimer dissociation-reassociation in two dimensions. In order to solve the model analytically, rather strong assumptions have been made, so that the description of real systems may appear oversimplified. Our aim was to give a reference model, whose solution can be easily computed and compared, e.g., with Monte Carlo simulations where the real dimer dynamics can be considered. Let us briefly review the basic hypothesis required for our model to hold. First of all, we neglected the atom-atom interaction out of first-neighbor sites. This assumption may be questionable on close-packed surfaces, where the calculation of the atom-steps interactions [10] and of the pair atom-atom interaction [11–13] showed that longer range interactions can play an important role. Nevertheless, the situation may be different on open surfaces. Very recently, indeed, Bogicevic *et al.* [14] showed that metal dimers diffusing on the open fcc (100) surface are effectively dissociated beyond second-neighbor distances. Note that such surfaces are characterized by a square geometry, exactly as the lattice considered in our model. Nevertheless, also the real metal-dimer dynamics on the fcc (100) surfaces is more complex than the one described by our model. Indeed, we did not take into account the complexity of the configuration where the two atoms are placed along the diagonal of the square cell, separated by a distance of $\sqrt{2}$ (assuming that first neigbors are at distance 1). At least for Al_2, Rh_2, and Au_2 [14], and Cu_2 [15] it was shown that from this configuration, the two atoms tend to switch back to the associated configuration (where they are separated by distance 1). Thus, the hypothesis of unbiased random walk does not hold in this configuration. More, also the possibility of dimer dissociation via this metastable diagonal configuration should be taken into account [14]. Therefore, a better description of real dimer dynamics in the above systems would imply the study of more complicated models, whose solution could be achieved by Monte Carlo simulations.

In this paper we have calculated the probability $Q_{\rm dim}^{2D}(2m)$ for dimer reassociation in two dimensions on a square lattice. While in one dimension this probability coincides with the probability for a first return to the origin of the relative coordinate of the two dimer atoms, in two dimensions the reassociation problem is mapped to the first return to a finite region enclosing the origin. By making a suitable subdivision of the random walks into a set of disjoint subwalks, it is still possible to extract $Q_{\rm dim}^{2D}(2m)$ from the probability of a first return to the origin in $[Q_0^{2D}(2m)]$ in two dimensions, even if this requires an iterative procedure. An explicit formula can be given by the generating function of $Q_{\rm dim}^{2D}(2m)$. From the generating function, one can obtain the asymptotic behavior $(\sim 1/[2m\ln^2(2m)])$ of $Q_{\rm dim}^{2D}(2m)$ which turns out to be the same of $Q_0^{2D}(2m)$.

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[1] B. Borovski, M. Krueger, and E. Ganz, Phys. Rev. Lett. **78**, 4229 (1997).
[2] B. Borovski, M. Krueger, and E. Ganz, Phys. Rev. B **59**, 1598 (1999).
[3] C.M. Goringe and D.R. Bowler, Phys. Rev. B **56**, R7073 (1997).
[4] F. Montalenti and R. Ferrando, Surf. Sci. **432**, 27 (1999).
[5] F. Montalenti and R. Ferrando, Phys. Rev. B **60**, 11 102 (1999).
[6] D. Hughes, *Random Walks and Random Environments* (Oxford Science, Oxford, 1995), Vol. 1.
[7] W.P. Pfluegl and R.J. Silbey, Phys. Rev. E **58**, 4128 (1998).
[8] G.H. Weiss, *Aspects and Applications of the Random Walk* (North-Holland, Amsterdam, 1994).
[9] *Handbook of Mathematical Functions*, edited by M. Abramowitz and I.A. Stegun (Dover Publications, New York, 1965).
[10] R. Stumpf and M. Scheffler, Phys. Rev. B **53**, 4958 (1996).
[11] F. Watanabe and G. Ehrlich, J. Chem. Phys. **95**, 6075 (1991).
[12] F. Watanabe and G. Ehrlich, J. Chem. Phys. **96**, 3191 (1992).
[13] S.J. Koh and G. Ehrlich, Phys. Rev. B **60**, 5981 (1999).
[14] A. Bogicevic, S. Ovesson, B.I. Lundqvist, and D.R. Jennison, Phys. Rev. B **61**, R2456 (2000)
[15] G. Boisvert and L.J. Lewis, Phys. Rev. B **56**, 7643 (1997).