Vacancy localization in the square dimer model, statistics of geodesics in large quadrangulations

Jérémie Bouttier

Institut de Physique Théorique, CEA Saclay

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Part I

Vacancy localization in the square dimer model

Joint work with M. Bowick\textsuperscript{1,2}, E. Guitter\textsuperscript{1} and M. Jeng\textsuperscript{2}
\textsuperscript{1} IPhT, CEA Saclay
\textsuperscript{2} Physics Department, Syracuse University

A vacancy in a sea of dimers

The dimer model is a venerable subject in statistical mechanics and combinatorics [Kasteleyn, Fisher, Temperley...]. Here we consider the square lattice, fully covered with dimers except for a few possible vacancies.
A vacancy in a sea of dimers

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The dimer model is a venerable subject in statistical mechanics and combinatorics [Kasteleyn, Fisher, Temperley...]. Here we consider the square lattice, fully covered with dimers except for one vacancy.

Dimers can naturally “slide” onto the vacancy (similarly to the Rush Hour™ game).
Starting from an initial configuration of dimers/vacancy, can we characterize the set of attainable configurations?

What if the initial configuration is drawn (uniformly) at random? (toy model for a glassy system)

For simplicity we consider the case of a rectangular grid of finite size (to be taken later to infinity).

Obvious remarks:

- with one vacancy, the number of sites must be odd: $(2L + 1) \times (2M + 1)$
- coloring every other site in white and black (with white corners), the vacancy must be on the “white” grid
- the vacancy can reach at most every other site of the white grid (“even/odd” white subgrids, corner: even)
Consider first the case where the vacancy is initially in a corner. We have the following:

**Theorem [Temperley]**

There is a bijection between dimer configurations on a \((2L + 1) \times (2M + 1)\) grid with a given corner removed, and spanning trees on a \((L + 1) \times (M + 1)\) grid.
Vacancy in a corner: Temperley’s bijection revisited
Consider first the case where the vacancy is initially in a corner. We have the following:

**Theorem [Temperley]**

There is a bijection between dimer configurations on a $(2L + 1) \times (2M + 1)$ grid with a given corner removed, and spanning trees on a $(L + 1) \times (M + 1)$ grid.

For a given initial configuration with vacancy on the corner (or anywhere on the boundary), the associated spanning tree can be seen as the graph of attainable configurations. The vacancy is **fully delocalized**.
Now for an initial configuration with vacancy in the bulk, the vacancy can be localized.
Vacancy in the bulk: webs

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Now for an initial configuration with vacancy in the bulk, the vacancy can be localized.

**Definition**

A web on a grid is a spanning subgraph with a distinguished vertex (the root), and whose connected components consist of:

- a tree containing the root
- graphs containing exactly one cycle, that moreover winds around the root.

A dimer configuration on a \((2L + 1) \times (2M + 1)\), with vacancy on the even white grid, yields a web on a \((L + 1) \times (M + 1)\) grid. A web with \(n\) cycles has exactly \(4^n\) corresponding dimer configurations.
Vacancy in the bulk: webs
The graph of attainable configurations now corresponds to the central tree component of the web (sites accessible to the vacancy). We have to characterize how big it is ($s$ number of sites).
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**Findings**

- In the thermodynamic limit, $s$ remains finite (localization), with probability distribution $p(s)$.
- However localization is weak in the sense that $p(s) \sim s^{-\delta}$ for $s \to \infty$, with $\delta = 9/8 < 2$
Starting from a random initial state, and applying random moves (according to some natural dynamics), how far does the vacancy go?

- number of distinct sites visited: $\langle \tilde{N}(t) \rangle \sim t^\eta$, $\eta = 0.54 \pm 0.03$
- mean square displacement: $\langle \tilde{r}^2(t) \rangle \sim t^\theta$, $\theta = 0.56 \pm 0.01$

This is for the vacancy initially in the bulk. If we start with the vacancy on the boundary, we find different exponents characteristic of diffusion on spanning trees:

- $\eta_0 = 0.61 \pm 0.02$
- $\theta_0 = 0.62 \pm 0.02$
Our methods

- finite-size scaling (via efficient counting)
- numerical simulations (some via perfect algorithms)
- few rigorous/exact results
The number of spanning trees rooted at a site $i_0$ on a graph is $\det (\Delta_{i,j})_{i,j \neq i_0}$ where $\Delta$ is the Laplacian matrix:

$$\Delta_{i,j} = \begin{cases} 
  d_i \equiv - \sum_{j \neq i} \Delta_{ij} & \text{for } i = j \\
  -1 & \text{for } i, j \text{ neighbours} \\
  0 & \text{otherwise}
\end{cases}$$
Counting via matrix-tree theorem
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Webs can be counted by introducing a defect line (seam).

\(\det (\Delta(a)_{i,j})_{i,j} \neq i_0\) counts webs rooted at \(i_0\) and a weight \(y = 2 - a - a^{-1}\) per cycle, where:

\[
\Delta(a)_{i,j} = \begin{cases} 
    d_i \equiv - \sum_{j \neq i} \Delta_{ij} & \text{for } i = j \\
    -1 & \text{for a normal edge } i, j \\
    -a & \text{for a seam edge } i \to j \\
    -a^{-1} & \text{for a seam edge } j \to j \\
    0 & \text{otherwise.}
\end{cases}
\]
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The number of dimer configurations with a fixed vacancy corresponds to $y = 4$ and $a = -1$. 
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We consider dimers on a $(4L + 1) \times (4L + 1)$ grid with the vacancy at the center, corresponding to webs on a $(2L + 1) \times (2L + 1)$ grid with root at the center. Due to the fourfold rotational symmetry, the determinant factorizes into:

$$Z_L(y) = P_L(\alpha)P_L(-\alpha)P_L(i\alpha)P_L(-i\alpha)$$

with $y = 2 - \alpha^4 - \alpha^{-4}$. $P_L(\alpha)$ counts webs symmetric under rotation.
Applications

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with \( y = 2 - \alpha^4 - \alpha^{-4} \). \( P_L(\alpha) \) counts webs symmetric under rotation.
We have computed \( P_L(\alpha) \) up to \( L = 60 \). Amusing conjecture: \( P_L(i) \) counts the number of dimer configurations on a cylinder of height \( 2L \) and width \( 2L + 1 \).
Applications

\begin{align*}
\text{(a)} & \quad \log_{10}(\pi L, i) \\
\text{(b)} & \quad \frac{\log_{10}(\pi L, i)}{\log_{10}(\pi L, 0)}
\end{align*}
Asymptotic behaviour

We expect:

\[ P_L(\alpha) \sim \tilde{c}(\alpha) \frac{\mu^{L(L+1)} \lambda^L}{L^{\tilde{\gamma}(\alpha)}} \]

\( \mu \) and \( \lambda \) are known from spanning trees [Duplantier-David] :

\[ \mu = \exp \left( \frac{4G}{\pi} \right) = 3.209912300728158 \cdots \]

\[ \lambda = \sqrt{2} - 1 \quad G = \sum_{i=0}^{\infty} \frac{(-1)^i}{(2i+1)^2} \quad (\text{Catalan’s constant}) \]
Asymptotic behaviour

Estimate for $\mu$

$L$

$\alpha = -1$

$\alpha = 1$

$\alpha = -1$

$\alpha = 1$
Asymptotic behaviour

For the critical exponent $\tilde{\gamma}(\alpha)$ we find:

$$\tilde{\gamma}(1) = 0.749999(1)$$
$$\tilde{\gamma}(-1) = -0.249999(1)$$
$$\tilde{\gamma}(i) = \tilde{\gamma}(-i) = 0.000000(1)$$
$$\tilde{\gamma}(e^{i\pi/4}) = \tilde{\gamma}(e^{-i\pi/4}) = 0.3125002(2)$$
$$\tilde{\gamma}(e^{3i\pi/4}) = \tilde{\gamma}(e^{-3i\pi/4}) = -0.187499(1)$$
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$$\tilde{\gamma}(1) = 0.749999(1) = \frac{3}{4}$$
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$$\tilde{\gamma}(i) = \tilde{\gamma}(-i) = 0.000000(1) = 0$$
$$\tilde{\gamma}(e^{i\pi/4}) = \tilde{\gamma}(e^{-i\pi/4}) = 0.3125002(2) = \frac{5}{16}$$
$$\tilde{\gamma}(e^{3i\pi/4}) = \tilde{\gamma}(e^{-3i\pi/4}) = -0.187499(1) = -\frac{3}{16}$$
Asymptotic behaviour

Estimate for \( \tilde{\gamma} \)

- \( 0 \)
- \( -0.2 \)
- \( -0.4 \)
- \( 0 \)
- \( 0.2 \)
- \( 0.4 \)
- \( 0.6 \)
- \( 0.8 \)

\( L \)

range from 0 to 60
Asymptotic behaviour

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$\tilde{\gamma}(e^{3i\pi/4}) = \tilde{\gamma}(e^{-3i\pi/4}) = -0.187499(1)$

This is consistent with the analytic expression:

$\tilde{\gamma}(\alpha) = \frac{3}{4} - e(2 - e)$

$\alpha = e^{i\pi e}$

$0 \leq e \leq 2$
Asymptotic behaviour

\[ \tilde{\gamma}(\alpha = \exp(i\pi e)) \]

\[ \frac{3}{4} - e(2 - e) \]
Asymptotic behaviour

Back to $Z_L$ we find:

$$Z_L(y) \sim c(y) \frac{\mu^{(2L+1)^2} \lambda^{4L}}{L \gamma(y)}$$

$$\gamma(y) = \tilde{\gamma}(\alpha) + \tilde{\gamma}(-\alpha) + \tilde{\gamma}(i\alpha) + \tilde{\gamma}(-i\alpha) \quad y = 2 - \alpha^4 - \alpha^{-4}$$
Asymptotic behaviour

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The ratio $Z_L(0)/Z_L(4) \sim L^{-1/4}$ can be interpreted as the vacancy delocalization probability on the finite grid.
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The ratio $Z_L(0)/Z_L(4) \sim L^{-1/4}$ can be interpreted as the vacancy delocalization probability on the finite grid. This indicates that the vacancy remains localized as $L \to \infty$. Another indication: at $y = 4$ the average number of cycles in a web grows as $\frac{1}{\pi^2} \ln L$. 
For an infinite lattice, the “tree component” accessible to the vacancy is almost surely finite. It has a size probability distribution $p(s)$ with $\sum_{s=1}^{\infty} p(s) = 1$. Using Monte-Carlo simulations we have estimated this probability distribution on dimer grids up to size 401 (simulating webs with a perfect sampling algorithm) or 1001 (periodic b.c. and pivot algorithm). $p(s) \sim s^{-\delta}$ with $\delta = 1.122 \pm 0.008$. We conjecture the exact value $\delta = 9/8$, also in agreement with the scaling relation $\gamma(0) - \gamma(4) = 1/4 = 2(1 - \delta)$. 

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Size distribution

Fit on $s < 200$

Free b.c.

Periodic b.c.

$\log_{10}(s)$

$\log_{10}(p(s))$
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p(2) = 0.055905353801942(1) = \frac{1}{32}(72817\sqrt{2} - 102977)
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These quantities (and some critical exponents) have been derived recently by V.S. Poghosyan, V.B. Priezzhev and P. Ruelle in the Toeplitz matrix formalism.
By Monte-Carlo simulations we studied the diffusion on spanning trees and webs (i.e. vacancy moving from the boundary/bulk).

- number of distinct sites visited: $\langle \tilde{N}(t) \rangle \sim t^{\eta}$
  
  \[ \eta_0 = 0.61 \pm 0.02 \text{ (trees)} \quad \eta_4 = 0.54 \pm 0.03 \text{ (webs)} \]

- mean square displacement: $\langle \tilde{r}^2(t) \rangle \sim t^{\theta}$
  
  \[ \theta_0 = 0.62 \pm 0.02 \text{ (trees)} \quad \theta_4 = 0.56 \pm 0.01 \text{ (webs)} \]
Diffusion exponents

Fit for $10^2 < t < 10^7$
Num. data ($L = 200$)

$\log_{10}(t)$
$\log_{10}(\langle \tilde{S}(t) \rangle)$

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Predictions: $\eta = \theta$, $\eta_4 = (2 - \delta) \eta_0 = 7/8 \eta_0$

(as seen by a scaling argument: $t^{\eta_4} \sim \int \max(t^{\eta_0}, s) \rho(s) ds$)
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(as seen by a scaling argument: $t^{\eta_4} \sim \int \max(t^{\eta_0}, s) \rho(s) ds$)

In a less conclusive manner, our results would be consistent with the simple values: $\eta_0 = 5/8$ and $\eta_4 = 35/64$. 
We find a weak localization for the vacancy, leading to a non-trivial diffusive behaviour.

(Still) many open questions, especially regarding rigorous results (domino tilings of the “holey square”).

Further directions:

- how about the possible interactions between several vacancies
- other lattices, e.g. the triangular lattice where a completely different behaviour is expected (strong localization) [see recent numerical results by Jeng et al.]
Part II

Statistics of geodesics in large quadrangulations

Joint work with E. Guitter

arXiv:0712.2160, IOP Select
We consider random planar quadrangulations as introduced in the talk of J.-F. Le Gall. We consider the “uniform” measure over all quadrangulations with a finite number $n$ of faces (possibly with multiple edges, etc), and will be especially interested in the $n \to \infty$ limit. The general framework: viewing a quadrangulation as a discrete random surface (metric space), what can be said about its statistical properties?
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Though quadrangulations have been much studied since the 60s (in combinatorics) and 80s (in physics), the seminal step came during G. Schaeffer’s PhD (1998) in what is known as Schaeffer’s bijection [Marcus-Schaeffer, Chassaing-Schaeffer...] between rooted planar quadrangulations and well-labeled trees (different from Cori-Vauquelin’s bijection).
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Our approach is “complementary” to the continuous approach of J.-F. Le Gall: we first delve into the discrete side, derive exact discrete data, then take the continuous limit.
We start from a rooted planar quadrangulation, and label every vertex by its (graph) distance from the origin (of the root edge).
Schaeffer’s bijection

We start from a rooted planar quadrangulation, and label every vertex by its (graph) distance from the origin (of the root edge). Due to properties of the graph distance, every planar quadrangulation being bipartite, there exists 2 type of faces (simple and confluent) and we apply the basic rules:

(a) 
- $i 
- i + 1 
- i + 2$

(b) 
- $i 
- i + 1 
- i + 1 
- i + 1$
Schaeffer’s bijection

An example:

(a) (b)

(origin)

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If we mark an entire geodesic instead of an edge, the information about it is “lost” in Schaeffer’s bijection, but the fix is “easy”:

![Diagrams](image)

We obtain a spine tree.
However not all spine trees are obtained this way. The actual bijection involves quadrangulations with a geodesic boundary.
Quadrangulations with a geodesic boundary

However not all spine trees are obtained this way. The actual bijection involves *quadrangulations with a geodesic boundary*. Quadrangulations with a marked geodesic correspond to *irreducible* quadrangulations with a geodesic boundary.
Our basic object is the generating function for well-labeled trees:

\[ R_i = 1 + g R_i(R_{i-1} + R_i + R_{i+1}) \]

where \( g \) is a weight per edge (tree)/face (quadrangulation), \( i \) is the label of the root vertex. Labels are positive so the equation holds for \( i > 0 \) only, with convention \( R_0 = 0 \). NB : “original” well-labeled trees correspond to \( R_1 \).
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**Theorem [B., Di Francesco, Guitter 2003]**

\[ R_i = R \frac{(1 - x^i)(1 - x^{i+3})}{(1 - x^{i+1})(1 - x^{i+2})} \]

where \( R, g \) are power series in \( g \) defined by:

\[ R = 1 + 3gR^2 \]

\[ x + \frac{1}{x} + 1 = \frac{1}{gR^2} \]
We deduce the generating function for spine trees of length $i$ (i.e. quadrangulations with a geodesic boundary of length $2i$):

$$Z_i = \prod_{j=1}^{i} R_j = R_i \frac{(1 - x)(1 - x^{i+3})}{(1 - x^3)(1 - x^{i+1})}$$
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Quadrangulations with a marked geodesic are obtained through:

$$U_i = Z_i - \sum_{j=1}^{i-1} U_j Z_{i-j}$$
For “free” we also get quadrangulations with $k$ confluent geodesics.

$$U_i^{(k)} = (Z_i)^k - \sum_{j=1}^{i-1} U_j^{(k)} (Z_{i-j})^k \quad \text{(weakly avoiding)}$$

$$\tilde{U}_i^{(k)} = (U_i)^k \quad \text{(strongly avoiding)}$$
Large \( n \) asymptotics are obtained by expansion around the critical point \( g = 1/12 \). For instance:

\[
Z_i = A_i + C_i \frac{\xi^2}{n} + \frac{2}{3} i D_i \frac{\xi^3}{n^{3/2}} + \cdots
\]

\[
g = \frac{1}{12} \left( 1 + \frac{\xi^2}{n} \right)
\]

\[
A_i = \frac{2^i(i + 3)}{3(i + 1)}
\]

\[
Z_i \bigg|_{g^n} \sim \frac{12^n D_i}{2 \sqrt{\pi} n^{5/2}} = \frac{12^n}{\sqrt{\pi} n^{5/2}} \frac{2^i i(i + 2)(i + 3)(i + 4)(3i^2 + 12i + 13)}{840(i + 1)}
\]

\((i \text{ finite})\)
Large $n$ asymptotics are obtained by expansion around the critical point $g = 1/12$. For instance:

$$Z_i = A_i + C_i \frac{\xi^2}{n} + \frac{2}{3} i D_i \frac{\xi^3}{n^{3/2}} + \cdots$$

$$g = \frac{1}{12} \left( 1 + \frac{\xi^2}{n} \right) \quad A_i = \frac{2^i (i + 3)}{3(i + 1)}$$

$$Z_i \big|_{g^n} \sim \frac{12^n D_i}{2 \sqrt{\pi} n^{5/2}} = \frac{12^n}{\sqrt{\pi} n^{5/2}} \frac{2^i i(i + 2)(i + 3)(i + 4)(3i^2 + 12i + 13)}{840(i + 1)}$$

(i finite)

A natural normalization is to divide by

$$C_{n,i} = \log (R_i/R_{i-1}) \big|_{g^n} \sim \frac{12^n}{\sqrt{\pi} n^{5/2}} \frac{3i^3}{7}, \quad i \to \infty$$

corresponding to quadrangulations with two marked points at distance $i$. 

Jérémie Bouttier
Results

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  \item $\tilde{U}_i^{(k)} |_{g^n/C_{n,i}} \sim k(3 \times 2^i)^k 4^{k-1} i^{3-3k}$ : average number of $k$-tuples of strongly avoiding geodesics
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  - two weakly avoiding geodesics have an extensive number of contacts ($\propto i/3$)
  - they remain “close” in the sense that they delimit two regions, one being always finite (area $\propto i^3$) and the other infinite (area $\propto n$)
  - this is not true for strongly avoiding geodesics: pairs of points linked by distinct geodesics become “rare” in the $i \to \infty$ limit
- results remain mostly true in the scaling limit $i \propto n^{1/4}$
Our discrete approach enables to study the statistics of geodesics in large quadrangulations in a computational manner.

Work in progress: an interesting connection with heaps

Other directions: find other observables, connect with the continuous approach, study more general classes of maps (matter...