Yoshiaki Itoh¹ and Larry Shepp²

Received January 11, 1999

The car parking problem is a one-dimensional model of random packing. Cars arrive to park on a block of length x, sequentially. Each car has, independently, spin up or spin down, w.p. 0 , for spin up and <math>q = 1 - p for spin down, respectively. Each car tries to park at a uniformly distributed random point $t \in [0, x]$. If t is within distance 1 of the location of a previously parked car of the same spin, or within distance a of the location of a previously parked car of the opposite spin, then the new car leaves without parking and the next car arrives, until saturation. We study the problem analytically as well as numerically. The expected number of up spins c(p, a) per unit length for sufficiently large x is neither monotonic in p for fixed a, nor is it monotone in a for fixed p, in general. An intuitive explanation is given for this nonmonotonicity.

KEY WORDS: Parking; probability model; Laplace transform; vector differential equation; explicit solution.

1. INTRODUCTION

Three-dimensional random sequential packing was applied to discuss the geometric strucure of a liquid by Bernal.⁽¹⁾ Car parking problems are onedimensional models for random sequential packing. In the most common version of the problem cars are parked sequentially at random on a street until saturation when no more cars can be parked. Using an interesting analytical method, Renyi⁽¹¹⁾ obtained the packing density (parking constant) $c_R \doteq 0.748$ for the model, which is now well known in the field of probability theory. Other fields use different but similar models.

Lattice models have played a central role in the development of equilibrium statistical mechanics. In the standard lattice-gas representation, the

209

¹ The Institute of Statistical Mathematics, 4-6-7 Minami-Azabu Minato-ku, Tokyo 106-8569, Japan.

² Statistics Department, Rutgers University, Hill Center, Piscataway, New Jersey 08903.

Itoh and Shepp

sites of the lattice have one of two states, empty/vacant, "o", or filled/ occupied, "x". The kinetics of equilibration has also been studied for these models. The car parking problem on a discrete street is equivalent to a lattice-gas model which involves *sequential adsorption* where the state of sites is assumed to change *irreversibly* from empty to fille, $o \rightarrow x$. In the simplest case, adsorption sites are chosen randomly. Such processes are termed *random sequential adsorption* (RSA). The related field has an enormous ammount of activity and was reviewed by Evans.⁽⁴⁾

Renyi's exact analysis for the random parking of unit length cars is based on the observation that after the first car parks on a finite interval, one is left with car parking problems on two smaller intervals. This idea is also used in Flory's combinatorial argument⁽⁶⁾ for random sequential dimer filling. He gave the coverage rate $1 - e^{-2} \doteq 0.865$. Cohen and Reiss⁽²⁾ studied its kinetics by using the rate equation analysis, extending the idea by Flory. Renyi's method to get the parking constant is based on the Laplace transform of the expected number of cars and can be applied to various situation of random space filling. The parking constant is obtained by a direct physical method based on a statistical independence without taking the Laplace transform (Hemmer⁽⁷⁾ and Krapivsky⁽⁹⁾).

Assuming the very strong nearest-neighbor repulsive interactions (NN exclusions) which effectively block the occupation of adjacent adsorption sites, where longer range interactions can be ignored, RSA of monomers with NN exclusion is isomorphic to one-dimensional random dimer filling. Each monomer corresponds to a dimer on the dual lattice. More generally 1D *M*-mer filling is isomorphic to 1D monomer filling with range M-1 blocking.

The car parking problem has applications in biological or sociological problems (Tanemura and Hasegawa⁽¹²⁾ and Itoh⁽⁸⁾) as is reviewed by Evans.⁽⁴⁾ Unfriendly seating arrangement by Freedman and Shepp⁽⁵⁾ is equivalent to RSA of monomer with NN exclusion. We extend their problem to the car parking problem with spins, assuming that a car is friendly with a car of different spin and unfriendly with a car of the same spin. Each car has, independently, spin up or spin down, w.p. 0 , for spin up, and <math>q = 1 - p, for spin down, respectively. A car is not allowed to be parked within distance 1 of the location of a previously parked car of the same spin, or within distance a of the location of a previously parked car of the neighboring spins, and does not assume the length of cars. Our model is a generalization of the 1D monmer filling range M-1 blocking, which is a dual of 1D M-mer filling.

Our model may be applied to RSA in the Widom–Rowlinson binary gas model (Widom and Rowlinson⁽¹³⁾) in which there are two kinds of

particles, with different distance requirements depending on whether two particles are the same type or different. Their model also assumes the distance between like species is shorter than the distance between unlike species, and we focus also on this case, but the other case is also interesting.

The car parking problems without spins have been considered and solved by Renyi,⁽¹¹⁾ Ney,⁽¹⁰⁾ and Dvoretsky and Robbins,⁽³⁾ who obtained explicit expressions for the constant, c, in their versions, in terms of integrals, by solving a first order ordinary differential equation for the Laplace transform, $\phi(\lambda)$, of f, and calculating the limit at $\lambda = 0$, using the fact that $c = \lim_{x \to \infty} (f(x)/x) = \lim_{\lambda \to 0} \lambda^2 \phi(\lambda)$. Let the expected number of up cars in saturation be c(p, a) for our car problem with spin. The c = c(p, a), apparently *cannot* be written in closed form in general. Despite this, we give an algorithm for calculating c(p, a) to arbitrary numerical precision in Section 4. Our solution is perhaps not really so different from an explicit determination of c since evaluation of the integrals involved in the earlier determinations must also be performed by a numerical algorithm. The difference is that one now cannot even solve the differential equation directly in closed form, since it is no longer first order. A direct attack by numerical methods on the differential equation seems difficult because the Laplace transform is singular at zero, and the limit is taken at zero, as discussed. Instead, we give a new technique for the non-commuting matrices which arise in the differential equation for the Laplace transform. which we hope can be generalized to other problems in applied probabilistical physics of similar type involving non-commutativity of matrices.

In the special case, p = 1/2, the matrices do commute and the usual methods for differential equations for systems with commuting matrices can be used to solve the differential equations explicitly, and we obtain an explicit expression for $c(\frac{1}{2}, a)$ involving an integral, similar to those in the earlier works, in Section 3.

It is surprising (see Figures 2–4) that c(p, a) is neither monotonic in a for fixed p, nor is it (see Figures 5–7) monotone in p for fixed a, in general. A post-facto intuitive explanation is given in Section 5.

2. VECTOR RECURRENCE

Cars arrive to park on a block of length x, sequentially. Each car has a spin up or down, w.p. 0 , for spin up, independendently, and each $chooses to park at a uniformly distributed random point <math>t \in [0, x]$. If t is within distance 1 of the location of a previously parked car of the *same* spin, or within distance a of the location of a previously parked car of the opposite spin then the new car leaves without parking and the next car arrives, until saturation, when no more cars can park on [0, x]. It's easy to see (using sub-additivity arguments) that, asymptotically as $x \to \infty$, the expected number of spin up cars in saturation is $\sim c(p, a) x$. We give a formula for c(p, a) usable for numerical calculation when $\frac{1}{2} \le a \le 1$ which will suffice to demonstrate the method. The cases $a < \frac{1}{2}$, and a > 1 can be treated by the same method, but the calculations are more tedious, and we have not carried them out. The expected number of cars for a block of length x can be written as an integral equation/recurrence which in turn gives rise to non-commuting matrices, and a new technique is found to deal with these. In the special case, p = 1/2, the matrices do commute and the usual methods for commuting matrices, can be used to give a more conventionally explicit value for $c(\frac{1}{2}, a)$, which we give.

The method could be extended (but we have not done it) for the case of many spin types, i = 1,..., n and with arbitrary probabilities, p_i , for cars of each spin type, *i*, and for an arbitrary matrix of allowed distances, $a_{i,j}$ between cars of spin *i*, *j*. We anticipate that there will be other problems in physics involving non-commutative matrices where our new technique will be useful to obtain numerical answers where explicit formulas in terms of elementary functions may be impossible.

The case a = 1 is equivalent to a problem posed and solved by Renyi^(11, 3) when cars have no spin but length, and cars are not allowed to overlap. Renyi⁽¹¹⁾ shows that the expected number of cars of length one that park in saturation on a block of length x is asymptotic to $c_R x$, as $x \to \infty$, where $c_R = \int_0^\infty e^{-2\int_0^u [(1-e^{-v})/v] dv} du = 0.7475798$. Renyi's results were sharpened by Dvoretzky and Robbins,⁽³⁾ and generalized by Ney⁽¹⁰⁾ to the case where cars have a *random* length. The Renyi case is common to both the problem of length and the problem of spin. Another version of the problem, where cars do not leave but always park *in the available space, if space is available*, would be closer in spirit to the Ney extension, but we do not treat this case. It should not be hard to extend our method to handle this case as well, but we have not done it. It is also possible to generalize our results to more than two spins, as discussed above, but we have not done this either.

The reason that "spin problems" are more difficult than "length problems" is that in a spin problem the recurrence is a *vector* recurrence while in a length problem it is a scalar or one-dimensional recurrence. Thus the real contribution of this paper is to develop methodology for problems involving recurrences which deal with multi-dimensional arrays when the matrices involved do not commute. Renyi⁽¹¹⁾ emphasizes the *one-dimensional* character of the problem. In a sense, the spin problems are not one dimensional, but we show they can also be solved in a "numerically explicit" sense.

It is not hard to obtain the following recurrence for the expected number of cars in equilibrium, *conditional on having cars already parked at the endpoints, with specified spins*, in the following way.

After the first car with a spin parks on a finite interval, we have car parking problems on two smaller intervals. Let $f_{\uparrow\uparrow}(x)$ denote the expected number of *up-cars* in saturation in a block of length x with two up-cars at the endpoints, and let $f_{\downarrow\downarrow}(x)$ and $f_{\uparrow\downarrow}(x)$ be defined similarly, again, keeping track only of up-cars.

Then, clearly, for x > 2,

$$f_{\uparrow\uparrow}(x) = p \int_{1}^{x-1} (f_{\uparrow\uparrow}(u) + f_{\uparrow\uparrow}(x-u) + 1) \frac{du}{x} + q \int_{a}^{x-a} (f_{\uparrow\downarrow}(u) + f_{\uparrow\downarrow}(x-u)) \frac{du}{x} + \left(p \frac{2}{x} + q \frac{2a}{x}\right) f_{\uparrow\uparrow}(x)$$
(1)

$$f_{\downarrow\downarrow}(x) = p \int_{a}^{x-a} (f_{\uparrow\downarrow}(u) + f_{\uparrow\downarrow}(x-u) + 1) \frac{du}{x} + q \int_{1}^{x-1} (f_{\downarrow\downarrow}(u) + f_{\downarrow\downarrow}(x-u)) \frac{du}{x} + \left(p \frac{2a}{x} + q \frac{2}{x}\right) f_{\downarrow\downarrow}(x)$$
(2)

$$f_{\uparrow\downarrow}(x) = p \int_{1}^{x-a} (f_{\uparrow\uparrow}(u) + f_{\uparrow\downarrow}(x-u) + 1) \frac{du}{x} + q \int_{a}^{x-1} (f_{\uparrow\downarrow}(u) + f_{\downarrow\downarrow}(x-u)) \frac{du}{x} + \left(p \frac{1+a}{x} + q \frac{1+a}{x}\right) f_{\uparrow\downarrow}(x) \quad (3)$$

where we have used $f_{\uparrow\downarrow}(x) = f_{\downarrow\uparrow}(x)$ which holds by symmetry (Fig. 1), and we have the term $(p(2/x) + q(2a/x)) f_{\uparrow\uparrow}(x)$ for the case that the first car can not park in the equation (1), similarly for other equations (2) and (3).

It is clear from the fact that $f_{\sigma}(x)$ is sub-additive, that the limit $c_{\sigma} = \lim_{x \to \infty} f_{\sigma}(x)/x$ exists. It follows easily from the above recurrence that c_{σ} does not depend on σ (just substitute the asymptotic forms and one gets equations among c_{σ} , which easily imply that c_{σ} is independent of σ), i.e., that end effects can be neglected. But it is false that one can erase the σ 's from the above recurrence and still get the right limit.

Note that for 0 < x < 2 we can write down $f_{\sigma}(x)$ explicitly for 1/2 < a < 1, (this gets somewhat more complicated for other values of *a*). Indeed, for x < 2, and $1/2 \le a \le 1$, it is clear that

$$\begin{split} f_{\uparrow\uparrow}(x) &= 0, & 0 < x < 2; \\ f_{\downarrow\downarrow}(x) &= 0, & 0 < x < 2a, & f_{\downarrow\downarrow}(x) = 1, & 2a < x < 2, \\ f_{\uparrow\downarrow}(x) &= 0, & 0 < x < 1 + a, & f_{\uparrow\downarrow}(x) = p, & 1 + a < x < 2 \end{split}$$



 $f_{\uparrow\uparrow}(\cdot)$: expected number of up-cars in saturation in a block of length x with two up cars at the endpoints.

 $f_{\uparrow\downarrow}(\cdot)$: expected number of up-cars in saturation in a block of length x with one up-car and one down-car at the endpoints.

Fig. 1. Parking cars with spin in a block of length x with two up-cars at the end points.

Now take Laplace transforms ϕ (with lower limit at x = 2) of f defined for $\lambda > 0$, and use the starting relations in x < 2, above to calculate

$$\phi_{\sigma}(\lambda) = \int_{2}^{\infty} e^{-\lambda x} f_{\sigma}(x) \, dx \tag{4}$$

where σ can be any one of the pairs, $\uparrow\uparrow$, $\downarrow\downarrow$, and $\uparrow\downarrow$.

3. COMMUTATIVE CASE

It is easy to verify that, $c(p = 1, a) \equiv c_R$ for any *a*, because when p = 1, only up cars appear and cars of opposite spins do not arise. It's also clear that $c(p, a = 1) = pc_R$, because if a = 1 then spin is irrelevant since all distances between cars must be > 1, and we are as well in the situation where

cars have length, and if we count *only* up cars we get p times Renyi's constant. Finally we note that c(p, a) is not continuous at p = 0, because c(p = 0, a) = 0 because there are no up cars at all, but if p is small but positive, then, essentially, only down cars arrive until these become saturated, and then *exactly* one up car can park in those spaces between adjacent down cars, of length 2a < x < 2. Thus the mean number of spaces in saturation having a length >a, in Renyi's problem, is asymptotically, $c(p = 0^+, a) x$ for an initial block of length x. We can give the number, $c(0^+, a)$, explicitly since in this case, the problem separates (because $A(\lambda)$ has two zeros in its middle row when p = 0) and so the recurrence for $\phi_{\downarrow\downarrow}$ does not involve the other variables. The answer is $c(0^+, a) = \int_0^{\infty} (e^{-(2a-1)u} - e^{-u}) e^{-2\int_0^u [(1-e^{-v})/v] dv} du$. In cases other than p = 0, p = 1/2, p = 1, or a = 1, explicit representation of c(p, a) appears to be impossible in terms of elementary functions, although we succeed in giving an algorithm for determing c(p, a).

One obtains, after a calculation, the column-vector equations,

$$\mathbf{\Phi}'(\lambda) + \mathbf{A}(\lambda) \mathbf{\Phi}(\lambda) + \mathbf{g}(\lambda) = 0$$
(5)

where $\Phi(\lambda) = (\phi_{\uparrow\uparrow}(\lambda), \phi_{\downarrow\downarrow}(\lambda), \phi_{\uparrow\downarrow}(\lambda))^T$ and where A(u) is the matrix,

$$\begin{pmatrix} 2p + 2aq + \frac{2pe^{-u}}{u} & 0 & \frac{2qe^{-au}}{u} \\ 0 & 2ap + 2q + \frac{2qe^{-u}}{u} & \frac{2pe^{-au}}{u} \\ \frac{pe^{-au}}{u} & \frac{qe^{-au}}{u} & 1 + a + \frac{e^{-u}}{u} \end{pmatrix}$$

and $\mathbf{g}(\lambda) = (g_{\uparrow\uparrow}(\lambda), g_{\downarrow\downarrow}(\lambda), g_{\uparrow\downarrow}(\lambda))^T$, where

$$\begin{split} g_{\uparrow\uparrow}(\lambda) &= \frac{pe^{-2\lambda}}{\lambda^2} + \frac{2pqe^{-a\lambda}}{\lambda^2} \left(e^{-(1+a)\lambda} - e^{-2\lambda} \right) \\ g_{\downarrow\downarrow}(\lambda) &= \frac{pe^{-2\lambda}}{\lambda^2} + \frac{2p(1-a)e^{-2\lambda}}{\lambda} + \frac{2p^2e^{-a\lambda}}{\lambda^2} \left(e^{-(1+a)\lambda} - e^{-2\lambda} \right) \\ &+ \frac{2qe^{-\lambda}}{\lambda^2} \left(e^{-2a\lambda} - e^{-2\lambda} \right) \end{split}$$

$$g_{\uparrow\downarrow}(\lambda) = \frac{pe^{-2\lambda}}{\lambda^2} + \frac{p(1-a)e^{-2\lambda}}{\lambda} + p \frac{e^{-\lambda}}{\lambda^2} (e^{-(1+a)\lambda} - e^{-2\lambda})$$
$$+ \chi \left(a \ge \frac{2}{3}\right) q \frac{e^{-a\lambda}}{\lambda^2} (e^{-2a\lambda} - e^{-2\lambda})$$
$$+ \chi \left(a < \frac{2}{3}\right) \frac{q}{\lambda} \left((2-3a)e^{-2\lambda} + \frac{(e^{-2\lambda} - e^{-(2+a)\lambda})}{\lambda}\right)$$

In the case of Renyi, and all the cases considered by Ney, the equation above is a scalar one, $\phi'(\lambda) + A(\lambda) \phi(\lambda) + g(\lambda) = 0$ with $A(\lambda) = 1 + 2e^{-\lambda}/\lambda$, $g(\lambda) = e^{-\lambda}/\lambda^2$ and one can use the familiar differential equation trick of the *variation-of-constants formula* to solve for ϕ in closed form, as Renyi did:

$$\phi(\lambda) = \int_{\lambda}^{\infty} g(u) \, e^{\int_{\lambda}^{u} A(v) \, dv} \, du$$

or, more explicitly,

$$\phi(\lambda) = \int_{\lambda}^{\infty} \frac{e^{-\lambda}}{u^2} e^{\int_{\lambda}^{u} (2e^{-v/v}) dv} du$$

Now it is a simple matter to find the limiting fraction of the expected number of cars of length one in the Renyi case, since, we can write,

$$\lambda^2 \phi(\lambda) = \int_{\lambda}^{\infty} e^{-\lambda} e^{-2 \int_{\lambda}^{u} \left[(1 - e^{-v})/v \right] dv} du$$

and by the Abelian theorem for Laplace transforms,

$$c_{R} = \lim_{x \to \infty} f(x)/x = \lim_{\lambda \to 0} \lambda^{2} \phi(\lambda) = \int_{0}^{\infty} e^{-2 \int_{0}^{u} [(1 - e^{-v})/v] \, dv} \, du$$

This method does not extend to the case where $A(\lambda)$ is a matrix *unless* the matrices, $A(\lambda)$, all *commute*, as in the scalar, or Renyi, case, because explicit solution of the differential equation is possible only in the commutative case. For parking with spins, commutativity holds only in the case when p = 1/2. We have to find a new way to carry the result further for $p \neq 1/2$. Note that if F(x) is the expected *time* until saturation, then F(x) > 1/(x-1), for 1 < x < 2, which is not integrable and so it follows from the integral equation for F, similar to the one for f, that for x > 2, $F(x) \equiv \infty$, i.e., small intervals arise and these lead to (many) refused cars, and long waits.

One may write, an exact solution for the vector $\mathbf{\Phi}$, valid even in the non-commutative case,

$$\mathbf{\Phi}(\lambda) = \sum_{n=1}^{\infty} \int_{\lambda < u_1 < u_2 \cdots < u_n} \mathbf{A}(u_1) \mathbf{A}(u_2) \cdots \mathbf{A}(u_{n-1}) \mathbf{g}(u_n) du_1 \cdots du_n$$
(6)

which can be verified by formal differentiation. However this formula seems quite useless for obtaining the constant c(p, a). If the A's commute, then the *n*th term of the series can be written as

$$\int_{\lambda}^{\infty} \mathbf{g}(u) \, \frac{\int_{\lambda}^{u} \mathbf{A}(v) \, dv^{n-1}}{(n-1)!} \, du \tag{7}$$

and then the series can be summed to give

$$\mathbf{\Phi}(\lambda) = \int_{\lambda}^{\infty} \mathbf{g}(u) \ e^{\int_{\lambda}^{u} \mathbf{A}(v) \ dv} \ du \tag{8}$$

It is easy to verify that, when p = 1/2,

$$\mathbf{A}(u) = \left(1 + a + \frac{e^{-u}}{u}\right)\mathbf{I} + \frac{e^{-au}}{u}\mathbf{B}$$
(9)

where **B** does not depend on *u*. Hence the matrices, A(u) commute. This allows us to carry out the explicit solution for Φ above. We get,

$$\mathbf{\Phi}(\lambda) = \int_{\lambda}^{\infty} \mathbf{g}(u) \ e^{\int_{\lambda}^{u} \mathbf{A}(v) \ dv} \ du \tag{10}$$

and it's a simple calculation, representing g(u) as a linear combination of the (common) eigenvectors of A(u) to obtain the constant. The answer is easiest to give using the methods of the non-commutative case, however, as we do at the end of the next section.

4. $p \neq 1/2$; THE NON-COMMUTATIVE CASE

We proceed instead, for $p \neq 1/2$ to seek a matrix, $\Psi(\lambda)$ satisfying

$$\Psi'(\lambda) = \Psi(\lambda) \mathbf{B}(\lambda) \tag{11}$$

where

$$\mathbf{B}(\lambda) = \mathbf{A}(\lambda) - \left(2 + \frac{2}{\lambda}\right)\mathbf{I}$$

Although existence theory for differential equations guarantees the existence of Ψ , it is not clear how to find Ψ explicitly. If we can do this, then we can write

$$(\lambda^{2}e^{2\lambda}\Psi(\lambda) \Phi(\lambda))' = \lambda^{2}e^{2\lambda}\left(\left(\frac{2}{\lambda}+2\right)\Psi(\lambda) \Phi(\lambda)+\Psi'(\lambda) \Phi(\lambda)+\Psi(\lambda) \Phi'(\lambda)\right)$$
$$=\lambda^{2}e^{2\lambda}\left(\frac{2}{\lambda}+2\right)\Psi(\lambda) \Phi(\lambda)+\Psi(\lambda) B(\lambda) \Phi(\lambda)$$
$$+\Psi(\lambda)(-A(\lambda) \Phi(\lambda)-g(\lambda))$$
$$=-\Psi(\lambda) \lambda^{2}e^{2\lambda}g(\lambda)$$
(12)

where we have used the equation (5).

It now follows easily that we have explicitly,

$$\Psi(\lambda) \ \lambda^2 \Phi(\lambda) = \int_{\lambda}^{\infty} \Psi(u) \ \mathbf{h}(u) \ du \tag{13}$$

where $\mathbf{h}(u) = u^2 e^{2u} \mathbf{g}(u)$. Explicitly,

$$\begin{split} h_{\uparrow\uparrow}(u) &= p + 2pq(e^{-(2a-1)u} - e^{-au}) \\ h_{\downarrow\downarrow}(u) &= p + 2p(1-a)u + 2p^2(e^{-(2a-1)u} - e^{-au}) + 2q(e^{-(2a-1)u} - e^{-u}) \\ h_{\uparrow\downarrow}(u) &= p + p(1-a)u + p(e^{-au} - e^{-u}) + \chi(a \ge \frac{2}{3})q(e^{-(3a-2)u} - e^{-au}) \\ &+ \chi(a < \frac{2}{3})q((2-3a)u + 1 - e^{-au}) \end{split}$$

Now we would like to write a solution for Ψ that would enable us to calculate the limit

$$(c, c, c)^T = \lim_{\lambda \to 0} \lambda^2 \Phi(\lambda)$$

We have not yet specified the initial condition on Ψ . One might choose $\Psi(0) = \mathbf{I}$ so that we have a formula for $\lambda^2 \Phi(\lambda)$, but this is not a good idea because then $\Psi(\lambda)$ will not be analytic at $\lambda = 0$. Instead, we will choose

 $\Psi(0)$, as a degenerate matrix of 3 identical rows. The reason is that we seek a power-series solution in the form

$$\Psi(\lambda) = \sum_{n=0}^{\infty} \Psi_n \lambda^n$$
(14)

and we will not be able to satisfy this if $\Psi(0) = I$. For a power series expansion of $\Psi(\lambda)$, we find that the equation (11) becomes

$$\sum_{n>0} n \Psi_n \lambda^{n-1} = \sum_{n\ge 0} \Psi_n \lambda^n \sum_{n\ge -1} \mathbf{B}_n \lambda^n$$
(15)

which gives the condition, that $\Psi_0 \mathbf{B}_{-1} = 0$. Now, \mathbf{B}_{-1} is the matrix,

/-	-2q	0	2q
	0	-2p	2 <i>p</i>
(р	q	-1/

and the equation, $\Psi_0 \mathbf{B}_{-1} = 0$ says that each row of $\Psi(0)$ must be a member of the nullspace of \mathbf{B}_{-1} . It turns out that we may as well take $\Psi(0)$ to have identical rows, each $(p^2, q^2, 2pq)$, which is a left eigenvector of \mathbf{B}_{-1} , with eigenvalue zero, as may be verified. This specifies Ψ_0 . For $n \ge 0$, we have the recurrence,

$$\Psi_{n+1}((n+1) \mathbf{I} - \mathbf{B}_{-1}) = \sum_{k=0}^{n} \Psi_{n-k} \mathbf{B}_{k}$$
(16)

or

$$\Psi_{n+1} = \left(\sum_{k=0}^{n} \Psi_{n-k} \mathbf{B}_{k}\right) ((n+1) \mathbf{I} - \mathbf{B}_{-1})^{-1}$$
(17)

and we see that for each n, Ψ_n is a matrix with identical rows, each of which we will also denote by Ψ_n .

 \mathbf{B}_0 is the matrix

$$\begin{pmatrix} 2aq-2 & 0 & -2aq \\ 0 & 2ap-2 & -2ap \\ -ap & -aq & -1 \end{pmatrix}$$

and for $k \ge 1$, \mathbf{B}_k is the matrix,

$$\begin{pmatrix} 2p \ \frac{(-1)^{k+1}}{(k+1)!} & 0 & -2q \ \frac{(-a)^{k+1}}{(k+1)!} \\ 0 & -2p \ \frac{(-1)^{k+1}}{(k+1)!} & 2p \ \frac{(-a)^{k+1}}{(k+1)!} \\ p \ \frac{(-a)^{k+1}}{(k+1)!} & q \ \frac{(-a)^{k+1}}{(k+1)!} & \frac{(-1)^{k+1}}{(k+1)!} \end{pmatrix}$$

This specifies Ψ_n for all $n \ge 0$, recursively, because the matrix $(n+1)\mathbf{I} - \mathbf{B}_{-1}$ is never singular since its eigenvalues are n+1, n+2, n+3 and hence non-zero. Thus we can write the formula for the filling constant, c = c(p, a), as

$$c(p, a) = \int_0^\infty \Psi(u) \mathbf{h}(u) \, du \tag{18}$$

or

$$c(p, a) = \int_0^\infty \sum_{n \ge 0} \Psi_n u^n \mathbf{h}(u) \, du \tag{19}$$

where $\mathbf{h}(u) = u^2 e^{2u} \mathbf{g}(u)$, and **g** is given in Section 1. We have used the fact that the sum of the components of Ψ_0 is unity.

Why does this technique work to give a usable algorithm to determine c(p, a), when a direct technique based on the differential equation for Φ fails to work? There seem to be two reasons: (1) the initial condition for Φ is non-existent, since the value of $\Phi(0) = \infty$, and (2) the technique above with Ψ separates **g** out of the problem and allows $\Psi(0)$ to have a finite value.

In the commutative case, p = 1/2, we can use the above formula to obtain a completely classically explicit expression for the answer in terms quite similar to Renyi's case. Indeed now we have inside the one dimensional subspace generated by $(p^2, q^2, 2pq) = (1/4, 1/4, 1/2)$ in the case p = 1/2 we can write $\Psi(u) = vf(u)$, where v = (1/4, 1/4, 1/2), because of the commutativity of the A(u). We find that $f'(u) = f(u)(a - 1 + (e^{-u} + e^{-au} - 2)/u)$ and so we get easily that

$$c(p=1/2,a) = \int_0^\infty e^{(a-1)u - \int_0^u \left[(1-e^{-v})/v + (1-e^{-av})/v \right] dv} \left(\frac{1}{4}, \frac{1}{4}, \frac{1}{2}\right) \mathbf{h}(u) du$$
(20)

where $\mathbf{h}(u)$ is given explicitly above, for p = 1/2, by

$$\begin{split} h_{\uparrow\uparrow}(u) &= \frac{1}{2} + \frac{1}{2}(e^{-(2a-1)u} - e^{-au}) \\ h_{\downarrow\downarrow}(u) &= \frac{1}{2} + (1-a)u + \frac{1}{2}(-(2a-1)u - e^{-au}) + (e^{-(2a-1)} - e^{-u}) \\ h_{\uparrow\downarrow}(u) &= \frac{1}{2} + \frac{1}{2}(1-a)u + \frac{1}{2}(e^{-au} - e^{-u}) + \chi(a \ge \frac{2}{3})\frac{1}{2}(e^{-(3a-2)u} - e^{-au}) \\ &+ \chi(a < \frac{2}{3})\frac{1}{2}((2-3a)u + 1 - e^{-au}) \end{split}$$

Remark 1. In the general non-commutative case, one could, in principle, interchange the sum and integral and integrate, term-by-term, to obtain,

$$c = \sum_{n \ge 0} \Psi_n \int_0^\infty u^n \mathbf{h}(u) \, du$$

but this sum does not converge even in the Renyi case. To see this, note that this would mean in the Renyi case where $g(u) = e^{-u}/u^2$, that

$$c = \sum_{n \ge 0} \Psi_n n! = \int_0^\infty \Psi(u) \ e^{-u} \ du$$

where $\Psi_0 = 1$, and for $n \ge 0$,

$$(n+1) \Psi_n = \sum_{k=0}^n \Psi_{n-k} b_k$$

But if the above series converged, then the function, Ψ , would be of exponential type 1, since $\Psi_n n!$ must tend to zero. But in the Renyi case we know that $\Psi(u) = e^{u-2\int_0^u [(1-e^{-v})/v] dv} du$ and this is not entire of type 1 as we see by letting *u* be large negative. However, we can still use the integral for numerical evaluation of c(p, a). The formula obtained gives an algorithm, at least in principle, to find it.

Remark 2. We can simplify the recurrence for the Ψ_n by noting that the inverse of (n+1) **I** - **B**₋₁ can be written as

$$((n+1) \mathbf{I} - \mathbf{B}_{-1})^{-1} = \frac{1}{n+1} \mathbf{A}_0 + \frac{1}{n+2} \mathbf{A}_1 + \frac{1}{n+3} \mathbf{A}_2$$

where \mathbf{A}_i , i = 0, 1, 2 are given as $\mathbf{A}_i = r_i \times l_i$, where r_i, l_i are the right and left eigenvectors of \mathbf{B}_{-1} . This is obtained by noting that the eigenvalues of

 $((n+1) \mathbf{I} - \mathbf{B}_{-1})^{-1}$ are $(n+1)^{-1}$, $(n+2)^{-1}$, $(n+3)^{-1}$ and that the left eigenvectors of \mathbf{B}_{-1} corresponding to the eigenvalues, 0, -1, -2 of \mathbf{B}_{-1} are $l_0 = (p^2, q^2, 2pq), \ l_1 = (-p, q, p-q), \ l_2 = (1, 1, -2).$ Similarly the right eigenvectors of \mathbf{B}_{-1} are $r_0 = (1, 1, 1)^T$, $r_1 = (-2q, 2p, p-q)^T$, $r_2 = (q^2, p^2, -pq)^T$. Thus,

$$\mathbf{A}_{0} = \begin{pmatrix} p^{2} & q^{2} & 2pq \\ p^{2} & q^{2} & 2pq \\ p^{2} & q^{2} & 2pq \end{pmatrix}$$
$$\mathbf{A}_{1} = \begin{pmatrix} 2pq & -2q^{2} & -2pq + 2q^{2} \\ -2p^{2} & 2pq & 2p^{2} - 2pq \\ -p^{2} + pq & pq - q^{2} & (p-q)^{2} \end{pmatrix}$$
$$\mathbf{A}_{2} = \begin{pmatrix} q^{2} & q^{2} & -2q^{2} \\ p^{2} & p^{2} & -2p^{2} \\ -pq & -pq & 2pq \end{pmatrix}$$

5. NUMERICS

The new approach may shed light even in the commutative case. Thus suppose that we did not know the exact solution for $\lambda^2 \phi(\lambda)$ in the form of the exponential of an integral in the Renyi case. We could try to proceed via the power series. Which method would give better numerical performance?

In calculating $c_R = \int_0^\infty e^{-2\int_0^u [(1-e^{-v})/v] dv} du$, it is preferable to use the alternative expression, $c_R = 2\int_0^\infty e^{-u-2\int_0^u [(1-e^{-v})/v] dv} du$, obtained by integration by parts from the first expression, choosing u = u, in the usual v du notation for integrating by parts.

A similar technique works for the general case, starting from the main formula (18), and integrating by parts we get,

$$c(p, a) = -\int_0^\infty u(\Psi(u) \mathbf{h}(u))' \, du$$
$$= -\int_0^\infty u\left(\Psi(u) \mathbf{A}(u) - \left(2 + \frac{2}{u}\right)\mathbf{I}\right) \mathbf{h}(u) + \Psi(u) \mathbf{h}'(u)) \, du \qquad (21)$$

Now in making a numerical quadrature of the integral to obtain c(p, a), one could calculate $\Psi(u)$ for each needed value of u either from the



Fig. 2. Plot of c(p, a) for fixed p = 0.5 as functions of 0.5 < a < 1 in steps of 0.01.



Fig. 3. Plot of c(p, a) for fixed p = 0.7 as functions of 0.5 < a < 1 in steps of 0.01.



Fig. 4. Plot c(p, a) for fixed p = 0.9 as functions of 0.5 < a < 1 in steps of 0.01.



Fig. 5. Plot of c(p, a) for fixed a = 0.5 as functions of 0 .

power series representation given in Section 2, or, alternatively, directly from the differential equation. If one used the former method, then if the step size for the quadrature is δ , then the quadrature sum, based on the trapezoid rule, which we will call $J(\delta)$ should have a power series with only even powers of δ , namely $J(\delta) = J(0) + c_2 \delta^2 + \cdots$, where J(0) is the



Fig. 6. Plot of c(p, a) for fixed a = 0.52 as functions of 0 .

actual value of the integral, i.e., c(p, a). If, instead, however, we use the differential equation to update the needed values of $\Psi(u)$, then, because of the inherent error of comuting $\Psi(u_{n+1})$ from the value at u_n , the quadrature sum will have all powers of δ , and a smaller step size must be used in using Simpson's or Romberg's rule. Nevertheless, for ease of programming



Fig. 7. Plot of c(p, a) for fixed a = 0.54 as functions of 0 .

we chose the second method which seems to work quite well. The following simple C program computes the value of c(p, a) for all values of $p \in [0, 1]$ and $a \in [\frac{1}{2}, 1]$ to 5 decimal place accuracy, as was checked by halving the step size and verifying that the results agreed to at least 5 digit accuracy.



Fig. 8. An expansion of the region of the oscillations in Fig. 6 is given.

If the step size is doubled, from that indicated (0.01), then the last decimal place accuracy is lost.

We made direct simulations to make sure the numerical values. In the Renyi case, for the expected number $\mu(x)$ of cars in a street of length x, the form $(\mu(x)+1)/(x+1)$ gives a very good approximation of the parking



Fig. 9. c(p, 0.6), is again monotonic in p.

```
#include <math.h>
 #include <stdio.h>
main()
 ſ
                           double A[3][3], f0[3], f1[3], h[3], h1[3], k[3], a, p, q, del, del0, sum, u, ans, Q;
                           int i, j, n, nmax;
    for(j=0;j<101;j++) {
                           p= .9; a = .5+.5*.01*j; del0 = 2*.01; del = del0;
                           q = 1-p; ans =0;
           for(i=0;i<3;i++) (
                           del = del/2;
                           nmax = 60/del;
                           sum = 0;
                           f1[0] = p*p; f1[1] = q*q; f1[2] = 2*p*q;
                           for(n=1;n<nmax;n++) {</pre>
                                                      f0[0] = f1[0]; f0[1] = f1[1]; f0[2] = f1[2];
                                                      u = (n-1) * del + del/2;
             A[0][0] = 2*p+2*a*q+2*p*exp(-u)/u; A[0][1] = 0; A[0][2] = 2*q*exp(-a*u)/u;
             A[1][0] = 0; A[1][1] = 2*q+2*a*p+2*q*exp(-u)/u; A[1][2] = 2*p*exp(-a*u)/u;
              A[2][0] = p^{exp}(-a^{u})/u; A[2][1] = q^{exp}(-a^{u})/u; A[2][2] = 1+a+exp(-u)/u;
                           h[0] = p+2*p*q*(exp(-(2*a-1)*u)-exp(-a*u));
                           h[1] = p+2*p*u*(1-a)+2*p*p*(exp(-(2*a-1)*u)-exp(-a*u))+2*q*(exp(-(2*a-1)*u)-exp(-u));
                           h[2] = p+p*u*(1-a)+p*(exp(-a*u)-exp(-u))+(a \ge 2/3)*q*(exp(-(3*a-2)*u)-exp(-a*u))+(a \ge 2/3)*q*(exp(-(3*a-2)*u)-exp(-(3*a-2)*u))+(a \ge 2/3)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-2)*q*(a*a-
  (a<2/3)*q*(u*(2-3*a)+1-exp(-a*u));
 /* f(u) = psi(u) e^{-2u}, h(u) = g(u)u^2 e^{+2u} h^1 = h^prime^{-2u}
                                     f1[0] = f0[0] + del*(f0[0]*(A[0][0]-2-2/u)+f0[2]*A[2][0]);
                                     f1[1] = f0[1] + del*(f0[1]*(A[1][1]-2-2/u)+f0[2]*A[2][1]);
                                     f1[2] = f0[2] + de1*(f0[0]*A[0](2]+f0[1]*A[1](2)+f0[2]*(A[2](2)-2-2/u));
                           h1[0] = 2*p*q*((1-2*a)*exp(-(2*a-1)*u)+a*exp(-a*u));
                           h1[1] = 2*p*(1-a) + 2*p*p*((1-2*a)*exp(-(2*a-1)*u)+a*exp(-a*u)) +
 2*q*((1-2*a)*exp(-(2*a-1)*u)+exp(-u));
                           h1[2] = p*(1-a)-p*a*exp(-a*u)+p*exp(-u)+(a \ge 2/3)*q*((2-3*a)*exp(-(3*a-2)*u)+(a \ge 2/3)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*q*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-3*a)*a)*a)*((2-3*a)*a)*((2-3*a)*a)*((2-
 a*exp(-a*u))+(a<2/3)*q*((2-3*a)+a*exp(-a*u));
           k[0] = u*h1[0] +u*((A[0][0]-2)*h[0]+A[0][1]*h[1]+A[0][2]*h[2]);
           k[1] = u*h1[1] +u*(A[1][0]*h[0]+(A[1][1]-2)*h[1]+A[1][2]*h[2]);
          k[2] = u*h1[2] +u*(A[2][0]*h[0]+A[2][1]*h[1]+(A[2][2]-2)*h[2]);
                           Q = f1[0]*k[0]+f1[1]*k[1]+f1[2]*k[2];
                           sum = sum + del*Q;
                                                      if(n+1 == nmax) {
                                                                                 if(i == 0) ans = ans+sum/3.;
                                                                                 if(i == 1) ans = ans-2*sum;
                                                                                 if(i == 2) {
                                                                                                           ans = ans+8*sum/3.;
                                                                                                           printf("%g %g\n",a,ans);
                                                                                 }
                                                       ł
                           ł
          }
     ł
 ł
```

Fig. 10. Program that generated the data for the figures.

constant c_R even for small x. By making numrical studies for our problem for the discrete street, we experimentally found that the form

$$c(p, a, x) = \frac{p^2 f_{\uparrow\uparrow}(x) + q^2 f_{\downarrow\downarrow}(x) + 2pq f_{\uparrow\downarrow}(x) + p}{x}$$
(22)

gives a good approximation to the c(p, a) even for small x. This approximation formula may be verified analytically. We make use of this form for our simulation of seven decimal precision for the continuous street. We make 10,000 trials for each of the three $f, f_{\uparrow\uparrow}(x), f_{\downarrow\downarrow}(x), f_{\uparrow\downarrow}(x)$ and obtained c(p, a, 15) and c(p, a, 20) for every 0.05 of $1/2 \le a \le 1$ for p = 0.5, 0.7, 0.95. The values by our simulations agree with the values obtained by our numerical method by three decimals.

Figures 2–4 plot c(p, a) for fixed p = 0.5, 0.7, 0.9 as functions of 0.5 < a < 1 in steps of 0.01 (we only have considered this range of a). Figures 5–7 plot c(p, a) for fixed a = 0.5, 0.52, 0.54 as functions of 0 .Note that c(p, a) is not monotonic in p in Figs. 5 and 6, which at first was surprising to us. A post-facto and intuitive explanation is that for smaller *p* there will be, as parking nears saturation, more intervals with length, 1 < L < 2 with down spins at each endpoint, than there would be such intervals with up spins at the endpoints, for larger p. In either case, the spin of the last car to park in such an interval is determined and must be the opposite spin to those at the ends. Note also that c(p, a) is neither monotonic in a for fixed p in Fig. 4. Here the explanation is even more subtle and post-facto. We believe it is that for fixed large p, close to 1, an interval, waiting for its last car and of length slightly larger than 2 is likely to have up-spin cars at its endpoints, and then is more likely to be filled by a car with down spin if a is smaller than when a is larger. Thus making asmaller keeps down the number of up-spin cars parking in the last available space. Finally, note the very strange oscillations in c(p, a) in Figs. 6 and 7 for a = 0.52, 0.54, near p = 0. An expansion of this region is given in Fig. 8 for a = 0.52. Figure 9 shows c(p, 0.6), again monotonic in p.

We give in Fig. 10 a listing of the program that generated the data for the figures.

REFERENCES

- 1. J. D. Bernal, A geometrical approach to the structure of liquids, *Nature* 183:141–147 (1959).
- E. R. Cohen and H. Reiss, Kinetics of reactant isolation. I. One-dimensional problems, J. Chem. Phys. 38:680–691 (1963).
- 3. A. Dvoretzky and H. Robbins, On the parking problem, *Publ. Math. Inst. Hungar. Acad. Sci.* **9**:209–225 (1962).

- 4. J. W. Evans, Random and cooperative sequential adsorption, *Rev. Mod. Phys.* 65: 1281–1329 (1993).
- D. Freedman and L. Shepp, An unfriendly seating arrangement, SIAM Review 4:150–150 (1962).
- P. J. Flory, Intramolecular reaction between neighboring substituents of vinyl polymers, J. Am. Chem. Soc. 61:1518–1521 (1939).
- 7. P. C. Hemmer, The random parking problem, J. Stat. Phys. 57:865-869 (1989).
- Y. Itoh, On the minimum of gaps generated by one-dimensional random packing, J. Appl. Prob. 17:134–144 (1980).
- 9. P. L. Krapivsky, Kinetics of random sequential parking on a line, J. Stat. Phys. 69:135–150 (1992).
- 10. P. E. Ney, A random interval filling problem, Ann. Math. Statist. 33:702-718 (1962).
- A. Renyi, On a one-dimensional problem concerning space-filling, Publ. Math. Inst. Hungar. Acad. Sci. 3:109–127 (1958).
- M. Tanemura and M. Hasegawa, Geometrical models of territory I. Models for synchronous and asynchronous settlement of territories, J. Theor. Biol. 82:477–496 (1980).
- B. Widom and J. S. Rowlinson, New model for the study of liquid-vapor phase transition, J. Chem. Phys. 52:1670–1684 (1970).