RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 31, NUMBER 1 1 JANUARY 1985

Disorder softening of the long-time tail in correlated particle diffusion in one dimension

R. A. Tahir-Kheli*
Department of Theoretical Physics, 1 Keble Road, Oxford 0X1 3NP, England
(Received 28 September 1984)

For the asymptotic limit $t \to \infty$, a precision Monte Carlo evaluation of correlated classical particle diffusion in one dimension with quenched bond disorder is reported. The results are accurately described by the coherent potential approximation.

The transport of noninteracting classical particles in bond disordered linear chains has been studied actively in recent years (see Alexander, Bernasconi, Schneider, and Orbach[1] for a comprehensive discussion). A useful analysis in terms of continuous-time random walk (CTRW) representation was given by Klafter and Silbey.[2] This was followed by some exact discussions[3,4] and numerous applications of the coherent potential approximation (CPA) relevant to random bond systems.[5-7] Representative works along these lines are those of Odagaki and Lax,[8] Webman,[9] Webman and Klafter,[10] Haus, Kehr, and Kitahara,[11] and that of Haley.[12] From our point of view the interesting thing about these works is that the random-bond CPA predictions, which are known to be reasonable when the effective coordination number of the system is large compared to unity,[5] are of comparable accuracy to those that follow from usually more reliable procedures (compare, for example, the renormalization-group analysis of Machta[13]). Indeed, some aspects of the CPA predictions are found to be exact,[10,14,15] even though the coordination number is far from being large[5] in one dimension.

In actual physical systems the neglect of interactions is rarely justified. The best realization of a noninteracting fluid, therefore, is the limiting case of a system with a vanishingly small particle concentration, i.e., $c \to 0$. For finite concentrations, interactions have to be taken into account. At the very least, the hard-core repulsion cannot be ignored.

Even in its disordered state, the long-time dynamics of the interacting classical lattice gas in one dimension is known to be qualitatively different from that of the corresponding noninteracting system.[16-20] Here, even the presence of a hard core of zero range, which forbids multiple occupancy but otherwise leaves the gas noninteracting, dramatically slows down the long-time wanderings of labeled particles. Classical diffusion ceases to obtain and the particle wanderings are seriously curtailed. In particular, the mean-square displacement $\Delta(t)$ acquires a non-Brownian form

$$\Delta(t) = \frac{2(1-c)}{c} a^2 \left(\frac{\Gamma t}{\pi} \right)^{1/2} \text{ in the limit of } \Gamma t \gg 1 \ . \qquad (1)$$

(a is the lattice constant and Γ is the particle-hopping rate.)

Despite the relevance of the interacting system, particle dynamics in the presence of lattice disorder has seemingly been studied[1-15] only for the uncorrelated, noninteracting case. In this Rapid Communication we report what appears to be the first attempt at examining correlated particle hopping in a bond disordered system. To keep the analysis simple, we include only the hard-core repulsion at the origin. However, in order to extract quantitatively precise information, we have considered "large" effective system sizes and have proceeded for "long" effective times. The particle concentration is chosen to be ~ 0.5. This concentration lies outside the scope of perturbative schemes which are valid either at small particle concentration or at small vacancy concentration. Thus, the results provide a "real" test for possible theories.

A set of five different "macro" samples was prepared. (For convenience, these samples will be referred to as I, . . . , V, respectively.) All macros were, in turn, made up of 10 intermediate sized systems, i (referred to as $i = 1, \ldots, 10$) each of which totaled 120 000 bonds (links). Nine of the i systems were again broken up into five equal chains of 24 000 links each. In contrast, the $i = 10$ system comprised 120 "mini" chains of 1000 links each. Periodic boundary conditions were used throughout. The objective here was to test for any possible size dependence. The average results for each of the 10 i systems were combined to form a grand average for the relevant macro sample. Fluctuations from the grand average were then tabulated for each of the five constituent chains of the i systems ($i = 1, \ldots, 9$) and also for each of the five groups of 24 mini chains in the $i = 10$ system. We were prepared to throw out of consideration any effective constituent chain of system i for which the deviation from the grand average was 20 times, or more, of the corresponding average root-mean-square deviation (AMSD). [The AMSD was determined for each macro sample for $10\,000 \geq t \geq 100$ MCS/P (Monte Carlo steps per particle) measured in intervals of 25 MSC/P.] We found that for macros I–IV (see below) the overall performance of the different i's (including $i = 10$) was similar. Moreover, it was not necessary to reject any of the constituent chains.[21]

$\Delta(t)$ was measured for samples I–V as a function of t for $t \leq 10\,000$ MCS/P. The large effective sizes (1.2×10^6 bonds, 0.6×10^6 particles) helped reduce the natural fluctuation of the data to 1–3 parts in 10^3. Similarly, the availability of data over an extended time range enabled us to *definitively* rule out any possibility that bond disorder might restore some measure of classical diffusion and/or cause additional structure in $\Delta(t)$ (e.g., terms of the form t^n, $\frac{1}{2} > n > 0$) to appear. Thus, the representation

$$\Delta(t) = \frac{2(1-c)}{c} a^2 \left(\frac{\tilde{\Gamma} t}{\pi} \right)^{1/2} + \text{const, in the limit of } \Gamma t \gg 1 \qquad (2)$$

was established to a high degree of confidence.

TABLE I. CPA predictions of the long time effective hopping rate, $\tilde{\Gamma}_{\mathrm{CPA}}$, are compared with the corresponding Monte Carlo results, $\tilde{\Gamma}_{\text{Monte Carlo}}$. In samples I–IV, $\Gamma^A=\frac{1}{2}$, $\Gamma^B=\frac{1}{20}$, and Γ^C is $\frac{1}{50}$. The relative concentrations, x^A, x^B, x^C of the corresponding bonds as well as the average particle concentration, c, are recorded. For sample V, the bond distribution is a rectangle for bond strengths Γ lying in the range $\frac{1}{20}\leq\Gamma\leq\frac{1}{2}$.

No.	c	x^A	x^B	x^C	$\tilde{\Gamma}_{\mathrm{CPA}}$	$\tilde{\Gamma}_{\text{Monte Carlo}}$
I	0.500 625	0.749 729	0.250 271	0	0.153 731	0.1535 ± 0.0005
II	0.500 667	0.499 750	0.500 250	0	0.090 872	0.0907 ± 0.0003
III	0.500 375	0.249 604	0.750 396	0	0.064 486	0.0645 ± 0.0002
IV	0.500 667	0.334 167	0.333 041	0.332 792	0.041 721	0.0418 ± 0.0002
V					0.195 433	0.1935 ± 0.0020
		Rectangular between $\Gamma_{\max}=\frac{1}{2}$ and $\Gamma_{\min}=\frac{1}{20}$.				

For an accurate determination of the effective particle hopping rate, $\tilde{\Gamma}$, it was found best to proceed as follows: Choose a starting time t_0 (which should be long compared to π, e.g., 100) and find

$$\alpha(t-t_0)=\Delta(t)-\Delta(t_0) \quad . \tag{3}$$

This eliminates any constant term in Eq. (2). Now the best fit to the single parameter, $S(t_0)$,

$$S(t_0)=[\Delta(t)-\Delta(t_0)]/(t^{1/2}-t_0^{1/2}) \quad , \tag{4}$$

is determined. The procedure is then repeated for the next higher starting point, i.e., for $t_0'=t_0+25$ MCS/P, until $t_0'=9475$ MCS/P is reached.

In the thermodynamic limit, and for $\Gamma t_0\rightarrow\infty$, the slope $S(t_0)$ should be independent of t_0. In practice we get a distribution of such slopes. The average of the distribution, $\bar{s}$, consisting of 235 values of $S(t_0')$, is determined for each macro system and the mean-square deviation from $\bar{s}$ is computed. In order to get a confidence level of $\sim 90\%$ or so, we take our estimated error to be three times such root-mean-square deviation. However, since $\tilde{\Gamma}$ is proportional to the square of the slope $\bar{s}$, the error estimates displayed in Table I are proportionally double those for the corresponding slopes, $\bar{s}$.

Samples I, II, and III consisted of random mixtures of only two types of bonds with hopping rates $\Gamma^A=\frac{1}{2}$ and $\Gamma^B=\frac{1}{20}$ (in units of inverse MCS/P). The relevant concentration of these bonds (see Table I) was approximately $\frac{3}{4}$, $\frac{1}{4}$, for sample I, $\frac{1}{2}$ and $\frac{1}{2}$ for sample II, and $\frac{1}{4}$ and $\frac{3}{4}$ for sample III. In sample IV, three sets of hopping rates were included. Here, Γ^A and Γ^B were, as before, $\frac{1}{2}$ and $\frac{1}{20}$ and $\Gamma^C=\frac{1}{50}$. These bonds were mixed randomly in roughly equal proportions. Sample V was prepared differently, wherein a rectangular distribution of bonds ranging between the limits $\Gamma_{\max}=\frac{1}{2}$ and $\Gamma_{\min}=\frac{1}{20}$ was used.

The natural fluctuation of the $\Delta(t)$ data in I–IV followed the $\sqrt{N}$ law. For a system with a total of $N\sim 10^6$ bonds (and $N'\sim 5\times 10^5$ particles), the relative size of the fluctuations was between 1 and 3 parts per thousand. For sample V, the fluctuations were approximately three times larger. A plausible explanation for this lies in the fact that the limiting factor in the determination of $\Delta(t)$ is always the slowest set of hopping rates.[20] Thus, for the given rectangular distribution, $\Delta(t)$ was most affected by a narrow range of bonds near $\Gamma_{\min}$. The effective width of this range is only about $\frac{1}{10}$ that of the entire rectangle. Hence, an additional factor of three in the overall size of the fluctuation.

The CPA formula for $\tilde{\Gamma}$, which is the zero frequency (infinite time) effective hopping rate[5] in the presence of a random distribution of bonds (of strength Γ^λ and concentration x^λ, such that $\sum_\lambda x^\lambda=1$) is the following

$$\sum_\lambda x^\lambda(\Gamma^\lambda-\tilde{\Gamma})/[(z-2)\tilde{\Gamma}+\Gamma^\lambda]=0 \quad , \tag{5}$$

where z is the coordination number of the lattice. In one dimension $z=2$, and accordingly we get

$$\tilde{\Gamma}_{\mathrm{CPA}}=\left(\sum_\lambda x^\lambda/\Gamma^\lambda\right)^{-1} \quad . \tag{6a}$$

For the rectangular distribution lying between $\Gamma_{\max}=\frac{1}{2}$ and $\Gamma_{\min}=\frac{1}{20}$, Eq. (6a) becomes

$$\Gamma_{\mathrm{CPA}}=0.45/\ln(10) \quad . \tag{6b}$$

Implicit in the use of the CPA is the statement that disorder does not affect the asymptotic form of the mean-square deviation. This fact is corroborated to a high degree of accuracy by these simulations. Moreover, as we also observe from Table I, the Monte Carlo results for $\tilde{\Gamma}$ are accurately reproduced by the CPA formulas given in Eqs. (6a) and (6b). This happenstance, nevertheless, leaves open the deeper question as to why the CPA theory is seemingly exact in this particular instance.

This work has been supported by a grant from the National Science Foundation. Helpful discussions with R. J. Elliott, J. D. Gunton, R. B. Stinchcombe, and P. Beale are gratefully acknowledged. My thanks are also due to the Royal Society for financial support and the Department of Theoretical Physics, Oxford University, for its gracious hospitality.

*Permanent address: Department of Physics, Temple University, Philadelphia, PA 19122.

[1]S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, Rev. Mod. Phys. **53**, 175 (1981).
[2]J. Klafter and R. Silbey, Phys. Rev. Lett. **44**, 55 (1980).
[3]T. Odagaki and M. Lax, Phys. Rev. Lett. **45**, 847 (1980).
[4]H. van Beijeren, Rev. Mod. Phys. **54**, 195 (1982).
[5]R. A. Tahir-Kheli, Phys. Rev. B **6**, 2808 (1972).
[6]R. J. Elliott and D. E. Pepper, Phys. Rev. B **8**, 2374 (1973).
[7]R. J. Elliott, J. A. Krumhansl, and P. Leath, Rev. Mod. Phys. **46**, 465 (1974).
[8]T. Odagaki and M. Lax, Phys. Rev. B **24**, 5284 (1981).
[9]I. Webman, Phys. Rev. Lett. **47**, 1496 (1981).
[10]I. Webman and J. Klafter, Phys. Rev. B **26**, 5950 (1982).
[11]J. W. Haus, K. W. Kehr, and K. Kitahara, Phys. Rev. B **25**, 4918 (1982).
[12]S. B. Haley, Phys. Rev. B **25**, 5824 (1982).
[13]J. Machta, Phys. Rev. B **24**, 5260 (1982).
[14]R. Zwanzig, J. Stat. Phys. **28**, 127 (1982).
[15]J. W. Haus, K. W. Kehr, and K. Kitahara, Z. Phys. B **50**, 161 (1983).
[16]D. G. Levitt, Phys. Rev. A **8**, 3050 (1973).
[17]P. M. Richards, Phys. Rev. B **16**, 1393 (1977); P. A. Fedders, *ibid.* **17**, 40 (1978).
[18]S. Alexander and P. Pincus, Phys. Rev. B **18**, 2011 (1978).
[19]H. van Beijern, K. W. Kehr, and R. Kutner, Phys. Rev. B **28**, 5711 (1983).
[20]R. A. Tahir-Kheli, Phys. Rev. B **28**, 2257 (1983).
[21]It should be mentioned that initially we also experimented with micro chains of only 100 links each. Here, two of the five effective 24 000 link chains (each formed by combining results for 240 micro chains) failed our acceptance test. Moreover, the overall average for the corresponding *i* sample, made up of 1200 micro chains, was also choppier than that of the others. We, therefore, decided not to do any further computations on chains shorter than 1000 links each.