Comment on "Parity–breaking Ising–like model with Spin-Exchange dynamics" [Physica A 677 (2025) 130938]

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Abstract

In this Comment, we discuss some of the conclusions that have been drawn in the paper "Parity–breaking Ising–like model with Spin–Exchange dynamics" [Physica A 677 (2025) 130938], where a one–dimensional Ising–like model with a parity–breaking interaction and a spin–exchange (Kawasaki) dynamics has been investigated by means of Wang–Landau Monte Carlo simulations. We use both Wang–Landau Monte Carlo simulations and, for small system size, exact results. Firstly, we address the issue of the existence of a finite–temperature phase transition, showing that this is not supported by results for the specific heat. Then, we show that the ground state energy at low density is slightly smaller than the value reported in the commented paper. Finally, we address the issue of the existence of a non–vanishing equilibrium current, and we (i) show that in the pure Ising case the equilibrium current vanishes and (ii) argue that in presence of the parity–breaking interaction the reason why this current is non–zero is that the model is simulated using the Wang–Landau algorithm or, more generally, an algorithm whose stationary state is not in detailed balance with the Boltzmann equilibrium distribution.

Keywords:
Ising model, Parity breaking interaction, Spin–exchange dynamics, Wang–Landau algorithm, Particle transport

In a recent paper [1] the equilibrium properties (both thermodynamic and transport) of a one–dimensional Ising–like model with a parity–breaking interaction and a spin–exchange (Kawasaki) dynamics have been investigated by means of Wang–Landau (WL) Monte Carlo simulations. The model is described by the Hamiltonian

$$H(S) = -U_2 \sum_{k=1}^{L} S_k S_{k+1} - U_3 \sum_{k=1}^{L} S_k S_{k+1} S_{k+3}, \tag{1}$$

where L is the lattice size, the boundary conditions are periodic, $S_k = \pm 1$ are Ising spins, with state $+1$ (respectively -1) representing a particle (resp. vacancy), and $S = \{S_k, k = 1, \ldots, L\}$. $N = \sum_{k=1}^{L}(1 + S_k)/2$ denotes the number of particles and $\rho = N/L$ the particle density. In the following we comment on some of the conclusions that have been drawn in [1], regarding in particular the existence of a finite–temperature phase transition and of a non–vanishing equilibrium current, in particular in the pure Ising case ($U_3 = 0$).

The conclusion, drawn in [1], of the existence of a finite temperature phase transition in a one–dimensional model with short range interactions (including a three–spin interaction, which besides breaking parity also breaks the spin–flip symmetry), needs further investigation. In support of this conclusion, various thermodynamic quantities have been computed in [1]. In particular, in their Fig. 5(b) the authors plot a quantity which they call "specific heat capacity" in both the figure caption and the main text, and denote by C_V in the axis label, as a function of temperature T (in units such that Boltzmann's constant $k_B = 1$), for $U_2 = U_3 = 1$, $\rho = 0.5$ and N from 20 to 80. In the main text they write "As number of particles increases, the specific heat peaks become sharper and increase its height.". In the figure, however, the peak width seems independent of N and its height seems proportional to N, suggesting the plotted quantity, C_V, is actually the heat capacity, an extensive quantity. In Fig. 1 (left panel) we report our own WL simulations for the specific heat, C_V/N, which clearly show that it tends to a well–defined, regular shape, with peak height and width which tend to finite, non–zero values in the large size limit. The behaviour of the specific heat as a function of temperature is qualitatively analogous to that of the pure ($U_3 = 0$) one–dimensional Ising model, without any evidence of the singular behaviour which would characterize a phase transition. We have also validated our WL simulation results at relatively small sizes, by comparing them to the exact solution, with perfect agreement, see Fig. 1 (right panel) for an illustration. We can therefore confidently rule out the possibility of a true finite temperature phase transition in this model.

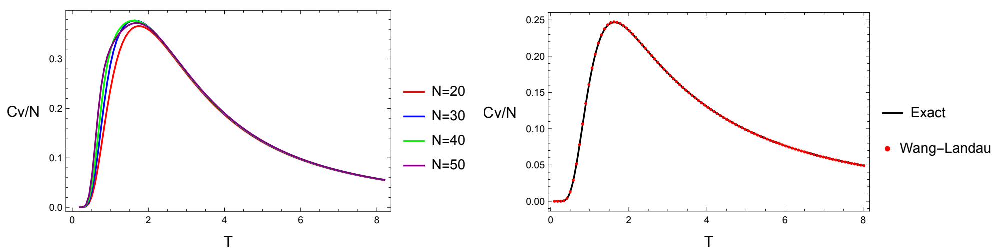

Figure 1: Specific heat as a function of temperature for $U_2 = U_3 = 1$ and $\rho = 0.5$. Left panel: WL simulations, $N = 20, 30, 40$ and 50. Right panel: $N = 5$, WL simulations (red dots) and exact results (black line).

An additional minor remark on thermodynamic properties regards the ground state energy. In their Fig. 1(a) the authors of [1] report the average energy per particle as a function of temperature, for $U_2 = U_3 = 1$, $N = 30$ and ρ from 0.1 to 0.9. As they say in the main text, all curves converge, in the low temperature limit, to the same ground state energy (per particle), which is slightly larger than -2. We argue instead that this is the case only for sufficiently high density. In the case $U_2 = U_3 = 1$, and (for simplicity) even lattice size L, sample ground state configurations and their energies are easily determined. For $\rho > \rho_* = 3/7$ the ground state energy is $E_{GS} = -2N + 4$ (provided $N \leq L - 3$, but this is a tiny detail which does not affect the following discussion). See Tab. C.3 in [1] for examples of ground state configurations. The corresponding energy density is $E_{GS}/N = -2 + 4/N$, which for $N = 30$ takes the value $-56/30 \simeq -1.8667$ to which the curves in Fig. 1(a) in [1] converge. At low densities, $\rho \leq \rho_*$, configurations with a lower energy exist: the ground state is made of pairs of adjacent particles and isolated particles. Different pairs or isolated particles must be separated by at least three vacancies, with the exception of an isolated particle on the right of a pair, in which case the separation must be at least one vacancy. These ground states have energy $E_{GS} = -2N$ and energy density $E_{GS}/N = -2$. An example of a ground state configuration, for $L = 10$ and $N = 4$, is $++---++---$. Another example, for $L = 12$ and $N = 5$, is $++---++-+---$. The difference in the values of E_{GS}/N is not negligible at $N = 30$ and should be appreciated on the scale of Fig. 1(a) in [1]. Our own simulations are reported in Fig. 2 (left panel) and are consistent with the above picture. Again, we have validated them at relatively small sizes by comparison with exact results, finding perfect agreement, as shown in Fig. 2 (right panel). The different behaviour found in [1], namely a ground state energy independent of ρ, may be the signal of an insufficient sampling of the low density ground state configurations and/or a consequence of binning the energy spectrum (which we have not done) in the simulation (we thank an anonymous referee for pointing out binning as a possible issue).

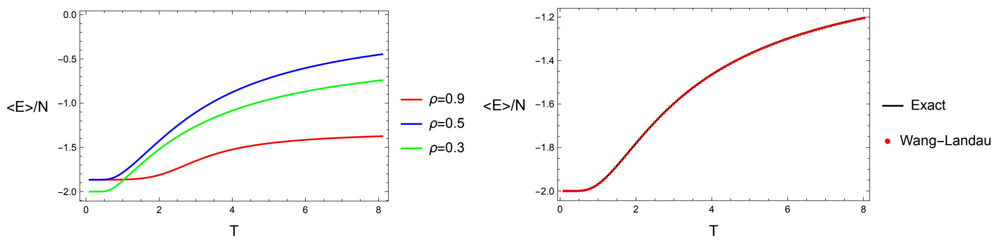

Figure 2: Average energy per particle as a function of temperature for $U_2 = U_3 = 1$. Left panel: WL simulations, $N = 30$, $\rho = 0.3, 0.5$ and 0.9. Right panel: $N = 8$, $\rho = 0.4$, WL simulations (red dots) and exact results (black line).

Notice that the behaviour of the specific heat shown in Fig. 1 (left panel) for $\rho = 0.5 > \rho_*$ is qualitatively independent of the density. See Fig. 3 for an example in the low–density regime, $\rho = 2/7 < \rho_*$. Since these results confirm that the model does not exhibit a finite temperature phase transition at any density, the ground state phase transition at density $\rho = \rho_*$ must be replaced by a smooth crossover at finite temperature. Moreover, given the different nature of the low– and high–density ground states, the dynamical picture proposed in [1], where particles are weakly (respectively strongly) localized in the low- (resp. high-) density regime is likely to be correct. A more quantitative analysis would certainly be interesting, but this is beyond the scope of the present comment.

The second conclusion drawn in [1] which we want to discuss here regards the existence of a non–vanishing equilibrium current, in particular in the pure Ising case $U_3 = 0$ (see Fig. 4(c) in [1]). This would imply that a non–vanishing equilibrium current is produced by the spin–exchange dynamics and the WL algorithm alone, without the need of the parity–breaking term in the Hamiltonian. We have investigated the equilibrium current using our own WL simulations and, for system sizes up to $L = 24$, exact solutions of the stochastic process which defines the WL algorithm. To this end we write

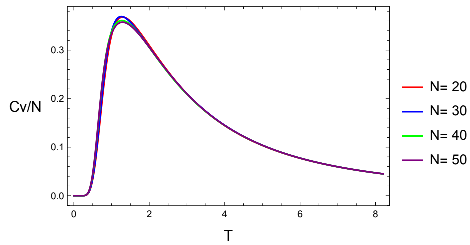

Figure 3: Specific heat as a function of temperature for $U_2 = U_3 = 1$, $\rho = 2/7 < \rho_*$.

the current as

$$\begin{aligned} J &= \sum_S \sum_{S'} P(H(S)) W(S \to S') J(S \to S') \\ &= \sum_E P(E) \sum_{S:H(S)=E} \sum_{S'} W(S \to S') J(S \to S') \\ &= \sum_E P(E) J(E). \end{aligned} \tag{2}$$

Here $P(E) = \exp(-E/T)/Z$ is, according to the Boltzmann distribution (with $k_B = 1$), the probability of a state of energy E, $Z = \sum_E g(E) \exp(-E/T)$ is the partition function and $g(E)$ is the number of states with energy $H(S) = E$ (the "density of states"), which can be computed exactly at small sizes. $W(S \to S')$ denotes the WL transition probability from configuration S to S', that is $W(S \to S') = \min(1, g(H(S))/g(H(S')))/L$ if S and S' differ only by the exchange of 2 neighbouring spins, and 0 otherwise. $J(S \to S')$ denotes the contribution of the transition to the particle current, that is $+1$ for the transition $+- \to -+$ and -1 for the transition $-+ \to +-$. In the second line of Eq. 2, the summation $\sum_{S:H(S)=E}$ denotes a sum over all states whose energy is E, and in the third line we have introduced the "microcanonical" current

$$J(E) = \sum_{S:H(S)=E} \sum_{S'} W(S \to S') J(S \to S') = \sum_{S:H(S)=E} J(S), \tag{3}$$

that is the contribution to the total current due to the transitions which leave from a state of energy E (notice that this definition differs by a factor $g(E)$ from the corresponding definition in [1]). Similarly,

$$J(S) = \sum_{S'} W(S \to S') J(S \to S') \tag{4}$$

is the contribution due to the transitions leaving from a given state.

For $U_3 = 0$ our exact solutions for $L \leq 24$ always yield a vanishing current, for all possible values of the number of particles N. The "microcanonical" current $J(E)$ also vanishes for all possible energy values, while $J(S) \neq 0$ for many states S. Results of our WL simulations are reported in Fig. 4 (left panel), where cases with different values of U_3, including $U_3 = 0$, are reported. One can see that the current values for $U_3 = 0$ are negligible with respect to those for $U_3 > 0$, suggesting that they vanish, in agreement with our exact results at small size. We therefore conclude that in the pure Ising case $U_3 = 0$ the equilibrium current vanishes. We stress here that this conclusion is drawn on the basis of exact results at small sizes, and WL simulations are consistent with these exact results.

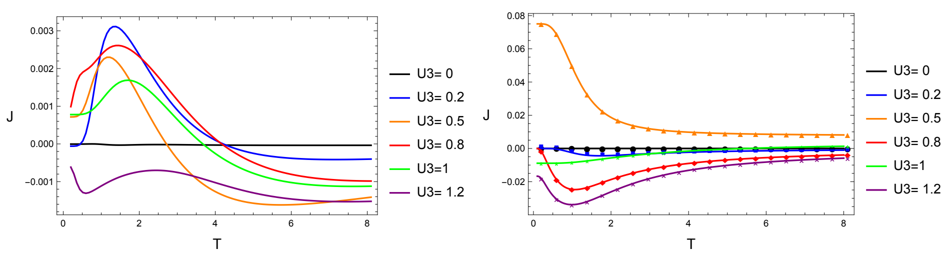

Figure 4: Equilibrium current as a function of temperature for $U_2 = 1$ and $\rho = 0.5$. Left panel: WL simulations, $N = 20$. Right panel: $N = 5$, WL simulations (symbols) and exact results (lines).

For $U_3 > 0$ we confirm that a non–vanishing equilibrium current exists, although the numerical values we obtain differ from those in [1]. See the curves in the left panel of Fig. 4 and, for a validation, the right panel of the same figure, where we compare our WL simulations and exact results. It is non–trivial to explain this non–vanishing equilibrium current in the WL algorithm. One possible explanation could be a bias in the sampling of configurations within an energy level. Such a bias should be in principle detectable by comparing the simulated "microcanonical" current $J(E)$ with the exact one (we thank an anonymous referee for suggesting the possibility of this bias and the test). We have compared exact and simulated "microcanonical" currents in Fig. 5, which shows a very good agreement, confirming the correctness of the intra–level sampling in the WL algorithm. We argue however that, in addition to the parity–breaking term in the Hamiltonian, another condition required in order to observe a non–vanishing equilibrium current is that the model is simulated using the WL algorithm or, more generally, an algorithm whose stationary state is not in detailed balance with the Boltzmann equilibrium distribution. Indeed, in the first line of Eq. 2, detailed balance with the Boltzmann distribution implies $P(H(S))W(S \to S') = P(H(S'))W(S' \to S)$ and due to the antisymmetry $J(S' \to S) = -J(S \to S')$ the total current must vanish. This is numerically confirmed by our simulations of the same model, with spin–exchange (Kawasaki) dynamics and a Metropolis algorithm (whose stationary state is indeed in detailed balance with the Boltzmann equilibrium distribution), which yield a vanishing equilibrium current (see Fig. 6 for an example of numerical results, which turn out to be fluctuating around zero for the Metropolis algorithm and clearly non–vanishing, with a well–defined temperature dependence, for the WL algorithm). Another argument in favor of our claim comes from the work by Cornu and Hilhorst [2]. In the cited paper, the authors have considered a similar problem, with the same Hamiltonian and spin–exchange dynamics, the temperature of the thermal bath fluctuating between 2 values T_1 (with probability $1 - \lambda$) and T_2 (with probability λ), and a heat bath simulation algorithm (again in detailed balance with the Boltzmann distribution) instead of a WL one. They have shown that the equilibrium current vanishes when $\lambda = 0$ (or 1), that is in a constant temperature case like the one under investigation.

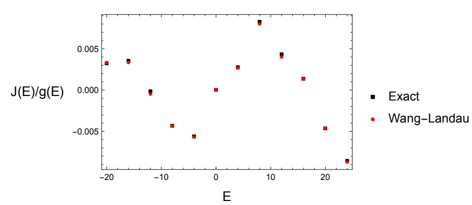

Figure 5: Equilibrium "microcanonical" current $J(E)/g(E)$ (normalized by density of states for rendering reasons) as a function of energy E for $U_2 = U_3 = 1$, $\rho = 0.5$ and $N = 12$. Black squares: exact results; red circles: WL simulation results.

We conclude by observing that the fact that the very existence of this equilibrium current depends on the simulation algorithm raises doubts on its physical meaning. We do not have a definitive explanation for this difference in the equilibrium current predicted by different algorithms, and further research in this direction would certainly be welcome.

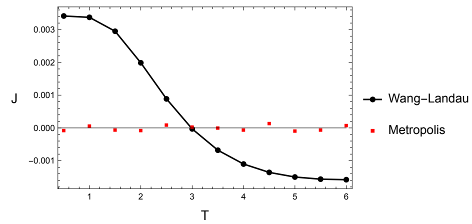

Figure 6: Equilibrium current J, simulated using the Metropolis (red squares) and the WL (black circles and solid line) algorithms, as a function of temperature T, for $U_2 = U_3 = 1$, $\rho = 0.5$ and $N = 12$.

References

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