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Exact calculation of the phase properties of one dimensional finite lattice gas systems

T.C. King[1] and Y.K. Kuo[2,a]

[1] Department of Physics and Earth Science, National Pingtung Teachers College, Pingtung, 900 Taiwan, P.R. China
[2] Department of Physics, National Dong Hwa University, Shou-Feng, Hualien, 974 Taiwan, P.R. China

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Abstract. The small-size partially filled one-dimensional (1D) lattice gas system with $1/r^{\delta}$ repulsive interactions is numerically studied. Our results indicate that phase change with vacancy ordering involved exists in the partially filled 1D lattice gas systems, and the phase properties of the studied system strongly depend on the occupancy n_{av} and the interaction strength δ. Most interestingly, it is found that the phase change still exists in the 1D finite-size lattice gas systems even with nearest neighbor interactions, i.e. δ is infinite. These results provide valuable information about the phase properties of 1D confined systems, such as molecules inside the carbon nanotubes, with long-range interactions between particles.

PACS. 64.60.Cn Order-disorder transformations; statistical mechanics of model systems – 05.10.-a Computational methods in statistical physics and nonlinear dynamics – 45.50.Jf Few- and many-body systems

1 Introduction

In early years the phase properties of one-dimensional (1D) systems were studied mostly by mathematical physicists. These works up to 1965 were summarized by Lieb and Mattis [1], and later reviewed by Griffiths on the studies of phase transitions in one-dimensional systems with finite and infinite-range interactions [2]. It was generally found that 1D systems with short-range interactions do not exhibit phase transitions at finite temperature. For example, Buar, Nosanow, and Araki predicted that the lattice systems with finite-range interactions do not exhibit phase transitions [3,4]. Ruelle found that the classical lattice gas with interactions that fall off faster than r^{-2} do not exhibit first-order phase transitions, but that higher-order transitions are possible [5]. Dyson has showed that 1D Ising ferromagnets with interactions that decrease as $r^{-\alpha}$ will exhibit phase transitions when $1 < \alpha < 2$ [6]. The appearance of quasi-one-dimensional (Q1D) materials provides the opportunity to test these 1D models. Recent measurements on the Q1D sulfide $KCu_{7-x}S_4$ have shown that phase transitions with drastic changes in the transport and thermodynamic properties occur at low temperatures [7–9]. It was suggested that the phase transitions found in $KCu_{7-x}S_4$ were due to vacancy ordering involving Cu^+ ion diffusion along the zigzag chains. King et al. introduced a Long Range Mean Field (LRMF) method to study vacancy ordering in a one-dimensional chain with $1/r$ Coulomb interactions [10–12]. These numerical calculations gave a satisfactory explanation for the unusual phase properties found in these Q1D materials and provided a possible method to examine the properties of partially occupied 1D lattice gas system in detail.

Recently, nanotechnology including fabrication and characterization of reduced dimension and small sized structures have attracted tremendous attention. In particular, the discovery of a variety of nanotubes such as carbon [13], BN [14,15], $BC_3$and BC_2N [16] makes a small-size one-dimensional model system available. These nanotubes have long narrow cylindrical structure with closed or open ends. Experimentally Smith et al. observed that the C_{60} molecules can be contained within the carbon nanotubes [17]. Teizer et al. experimentally measured ^{4}He desorption from single wall carbon nanotube bundles, and approximately described the adsorbate by one-dimensional adsorption with a binding energy [18,19]. Kuznetsova and Yates experimentally measured Xe adsorption on single wall carbon nanotubes [20]. Calbi et al. summarized the theory of the various phases predicted to occur when gases are absorbed within the carbon-nanotube bundle [21]. Hodak and Girifalco further considered the clustering of C_{60} molecules as a function of temperature for different linear densities of the internal molecules [22]. They applied the lattice gas model with nearest-neighbor attractive interactions to describe the behavior of the C_{60} molecules inside the carbon nanotubes, and used Monte Carlo simulations to study the C_{60} molecules in the carbon nanotubes with different diameters [22,23]. It was found that

[a] e-mail: ykkuo@mail.ndhu.edu.tw

the C_{60} molecules form an almost perfect 1D solid at room temperature and exhibit quasimelting when the temperature is increased, and the small-diameter nanotubes can be well described by a 1D model. The heat-capacity curve of the larger diameter carbon nanotube has an extra peak, which is due to the transformation of a zigzag structure existing at low temperatures to a disordered one [23]. Xia et al. theoretically studied hydrogen molecules confined in single-walled carbon nanotubes with the many-body Brenner potential and van der Waals intermolecular interactions [24]. The Brenner potential only counts the nearest neighbor pair interactions, which are dependent on the distance between the two molecules [25]. Their results predicted that H_2 molecules confined in carbon nanotubes with high density could be condensed and exhibit a solid-liquid phase transition.

Up to now, studies of molecules in the carbon nanotubes mostly focused on rare gases, hydrogen, and C_{60}, with which the interactions are treated as short-range interactions. Based on the groundwork we previously developed on 1D systems with long-range interactions between particles [10–12], it is of physical interest to study small-size one-dimensional lattice gas systems with various interaction strengths. With the rapid development of nanotechnology, we believe that the physical properties of 1D confined systems with long-range interactions between particles will be experimentally measurable soon. In this article, we exactly studied the phase properties of a small-size partially filled 1D lattice gas system with $1/r^{\delta}$ interactions up to the cluster size of 37 sites, where δ is between zero (long range interaction) and infinity (nearest neighbor interaction). Monte Carlo simulations were also performed on the large-size (more than 12000 sites) lattice gas systems to examine the possible finite size effect to our model system. In addition, we numerically calculated the thermodynamic average site particle numbers $\{\langle n_i\rangle\}$ and specific heat C of the model system. It is found that the partially filled finite-size 1D lattice gas system could exhibit a phase change between order and disorder states, depending on the value of the interaction strength δ. It has to be pointed out that the suggestive conclusions of our results are based on studies of small-sized systems with strong influence of the finite size effects. These findings would not warrant the general statement on the existence of phase transformations in the thermodynamic limit. However, we believe our results will provide valuable information about the phase properties of 1D confined systems with long-range interactions between particles.

2 Hamiltonian

The Hamiltonian of a 1D lattice gas with $1/r^{\delta}$ interactions is expressed by

$$\mathbf{H} = \sum_{i=1}^{N_S} \sum_{j>i} \frac{J}{|i-j|^{\delta}} n_i n_j, \tag{1}$$

where J is the coupling energy between two nearest neighbor particles, n_i ($n_i = 0$ or 1) is the particle number at site i, and N_S is the number of total sites in the 1D lattice gas system. We assume the lattice gas system has N_P particles where $N_P < N_S$ for a partially filled chain. In this study, we focus on the order-disorder properties of particle distributions as a function of temperature, while the order parameters of the model system can be defined from the average particle numbers which are given by $\langle n_i\rangle$ at the site i, and can be described as following

$$\langle n_i\rangle = \frac{\sum_{\{n_j\}} [n_i \exp(-\mathbf{H}/kT)]}{\sum_{\{n_j\}} [\exp(-\mathbf{H}/kT)]}, \tag{2}$$

where k is the Boltzmann constant, and $\sum_{\{n_j\}}$ sums over all configurations of the 1D lattice gas system. Since X-ray diffraction patterns are determined by the average particle number distributions, the ensemble of $\langle n_i\rangle$ is certainly a reasonable set of order parameters. For convenience we also adopt the order index q, which was defined in a previous article [10] and is expressed by

$$q = \frac{\sum_{\{i\}} (\langle n_i\rangle - n_a)^2}{N_P(1-n_a)^2 + (N_S - N_P)n_a^2}, \tag{3}$$

where $\sum_{\{i\}}$ sums over all sites except the sites near the two ends, and $n_a = N_P/N_S$ is the average particle number for all the counted sites. Since we use open boundary conditions in our calculations, the average site numbers of the two end sites are always equal to 1 at any temperature. Thus we eliminate those sites near the two ends in evaluating the order index q to avoid boundary effect. It is easy to show that the values of q range from 0 to 1. When $q = 0$, all the $\langle n_i\rangle$ are equal to n_a, and the lattice gas system is completely disordered. When $q = 1$, $\langle n_i\rangle$ is equal to either 0 or 1, and the system is completely ordered. The energy of the 1D lattice gas system is expressed by

$$E = \frac{\sum_{\{n_j\}} [\mathbf{H} \exp(-\mathbf{H}/kT)]}{\sum_{\{n_j\}} [\exp(-\mathbf{H}/kT)]}, \tag{4}$$

where $\sum_{\{n_j\}}$ also sums over all configurations, and the specific heat of the system can be calculated as $C = dE/dT$.

3 Results and discussions

To compare with our previous mean-field and Monte Carlo results [10,11], we first calculate the ground-state particle distribution of small-size 1D lattice gas systems with $1/r$ ($\delta = 1$) Coulomb repulsive interactions. When T approaches absolute zero, the particle distribution will be the average of the lowest potential configurations. It is found that the ground states of the lattice gas systems with an odd number of sites are different from those with an even number of sites, which is reasonable due to the symmetry properties. In Table 1, we tabulate the ground-state average site numbers $\{\langle n_i\rangle\}$ of the lattice gas systems with $1/r$ repulsive interactions with both even ($N_S = 20$,

Table 1. The ground state configurations of the small size 1D lattice gas systems with $1/r$ Coulomb repulsive interactions with various values of N_S and N_P.

N_S, N_P	$\{\langle n_i\rangle\}$
$N_S = 20$, $N_P = 10$	$\{1,0,1,0,1,0,1,0,1,0,0,1,0,1,0,1,0,1,0,1\}$
$N_S = 21$, $N_P = 11$	$\{1,0,1,0,1,0,1,0,1,0,1,0,1,0,1,0,1,0,1,0,1\}$
$N_S = 21$, $N_P = 12$	$\{1,1,0,1,0,1,0,1,0,1,0,1,0,1,0,1,0,1,0,1,1\}$
$N_S = 21$, $N_P = 13$	$\{1,1,2/3,1/3,1,0,1,0,1,0,1,0,1,0,1,0,1,1/3,2/3,1,1\}$

$N_P = 10$) and odd ($N_S = 21$, $N_P = 11$, 12, and 13, respectively) total lattice sites. It is seen that the ground-state configuration for the even-site 1D lattice gas systems has two possible configurations which are mirror symmetry to each other, while the odd-site systems has an unique ground-state configuration. Since the even-site systems can be viewed as the combination of two odd-site systems, in this article we will focus our calculations on the odd-site systems with particle number nearly half-filled. As shown in Table 1, the ground-state particle distributions of the 1D lattice gas systems with $1/r$ interaction have average particle numbers repeating themselves every two sites except at the two ends, i.e., the period of $\{\langle n_i\rangle\}$ is 2. When temperature increases from absolute zero, the particle distributions $\langle n_i\rangle$ (except at the two ends) change their values continuously from $\{\langle n_i\rangle\} = \{1,0,1,0,...\}$ to $\{\langle n_i\rangle\} = \{n_a, n_a, n_a, n_a, ...\}$ at a phase change temperature t_C ($= kT_C/J$), i.e., the systems transform from the completely ordered state to a disordered state with increasing temperature. In Figure 1a, we show the results of q versus t ($t = kT/J$) for some small-size 1D lattice gas systems with $1/r$ repulsive interactions for various N_S and $N_P = \frac{N_S+1}{2}$. At low temperatures, $q = 1$ and the lattice gas systems are completely ordered with a two-site period, as shown in Table 1. At high temperatures, $q \approx 0$ and the average site particle numbers are almost the same except for the sites near the two ends, and the lattice gas systems are disordered. Apparently, the phase property of this system changes from the ordered state to the disordered state at about t_C with increasing temperature. It is also seen that the phase change temperature t_C decreases with increasing cluster size. These observations are in excellent agreement with our previous studies [10,11]. In Figure 1b, we illustrate the temperature dependence of the order index for $N_P = \frac{N_S+3}{2}$ with $\delta = 1$. An obvious difference between the $N_P = \frac{N_S+1}{2}$ case (upper panel of Fig. 1) and the $N_P = \frac{N_S+3}{2}$ case (lower panel of Fig. 1) is that the latter shows a weaker dependence of t_C on the cluster size.

The parameter δ in equation (1) could be viewed as an index of the interaction strength. The interactions are nearest-neighbor-like when δ is infinite, and the interactions of all particle pairs are the same when δ is 0. Figures 2 and 3 show the results of q versus t for $N_S = 17$, $N_P = 10$ ($N_P = \frac{N_S+3}{2}$) and $N_S = 17$, $N_P = 9$ ($N_P = \frac{N_S+1}{2}$) with various δ's. In these figures, the upper panels show the results of $\delta \leq 1$, and the lower panels show the results of $\delta \geq 1$. As shown in Figure 2 and Figure 3, there is no phase change when $\delta \lesssim 0.1$ or $\delta \gtrsim 8$ for the $N_P = \frac{N_S+3}{2}$ system, while the phase change is absent only if $\delta \lesssim 0.6$ for the $N_P = \frac{N_S+1}{2}$ system. That is, the

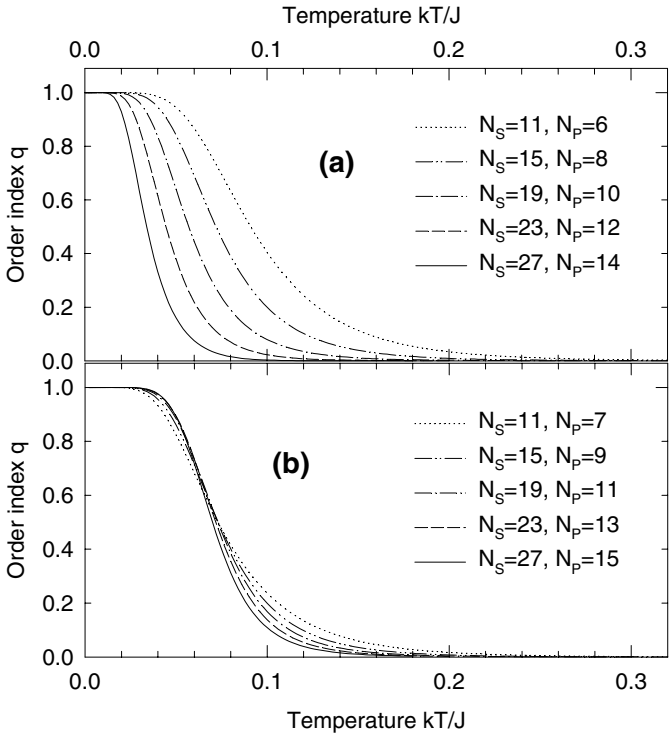

Fig. 1. The order indexes q versus temperature t of the small size 1D lattice gas systems with $1/r$ Coulomb repulsive interactions. The upper panel shows the results of systems with $N_P = \frac{N_S+1}{2}$, and the lower panel shows the results of systems with $N_P = \frac{N_S+3}{2}$.

$N_P = \frac{N_S+1}{2}$ systems will exhibit a phase change even with nearest neighbor interactions ($\delta = \infty$), while the $N_P = \frac{N_S+3}{2}$ systems show no phase change with nearest neighbor interactions. It is quite surprising that adding one particle to the $N_P = \frac{N_S+1}{2}$ systems would cause such a drastic difference in the phase properties. In order to resolve the subtleties between the two systems, we examined the ground-state particle distribution for systems with the same N_S but various N_P's with nearest neighbor interactions. It is found that the $N_P = \frac{N_S+1}{2}$ systems with nearest neighbor interactions have an unique ground-state configuration, while the $N_P > \frac{N_S+1}{2}$ systems have many possible ground-state configurations. In the following we thus classify the lattice gas systems into two kinds: the special system, with $N_P = \frac{N_S+1}{2}$; and the general system, with $N_P > \frac{N_S+1}{2}$ for descriptive convenience.

Figure 4 shows the results of q versus t for the special system with nearest neighbor interactions for lattice sites up to $N_S = 37$, the largest size feasible in this study

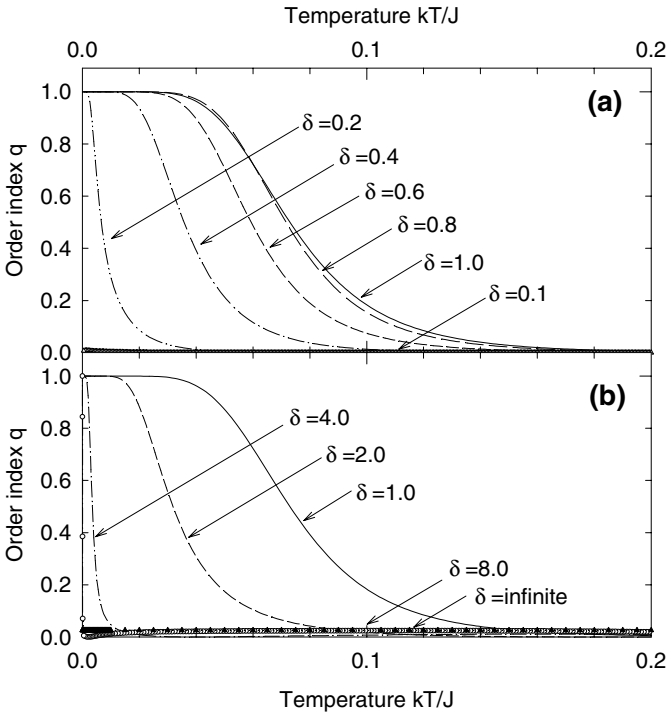

Fig. 2. The order indexes q versus temperature t of the general 1D lattice gas systems with various δ's with $N_S = 17$, $N_P = 10$. The upper panel shows the results of $\delta \leq 1$, and lower panel shows the results of $\delta \geq 1$. The systems exhibit phase transition with $0.1 < \delta \leq 8$. Note that the plots for $\delta = 0.1$ in (a) and $\delta = 8.0$ and infinity in (b) are nearly coincident with the axes.

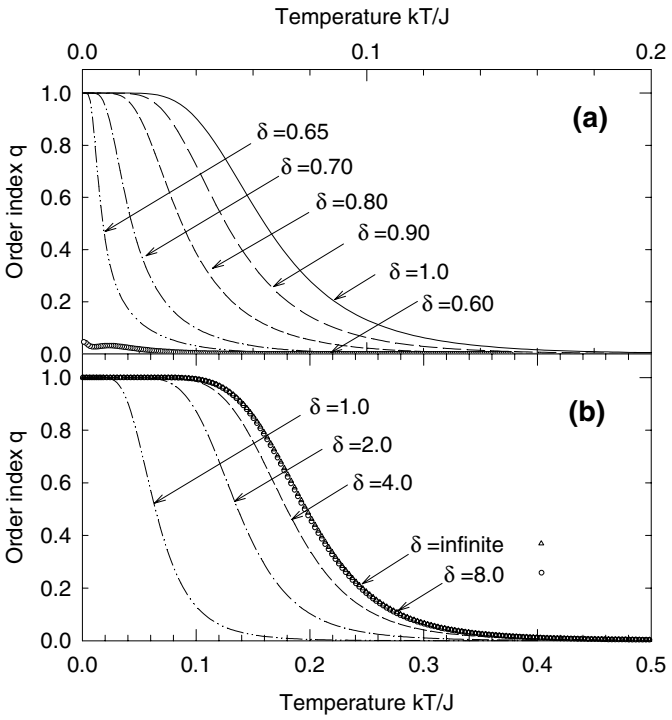

Fig. 3. The order indexes q versus temperature t of the special 1D lattice gas systems with various δ's with $N_S = 17$ and $N_P = 9$. The upper panel shows the results of $\delta \leq 1$, and the lower panel shows the results of $\delta \geq 1$. The system will exhibit phase transition as long as $\delta > 0.6$.

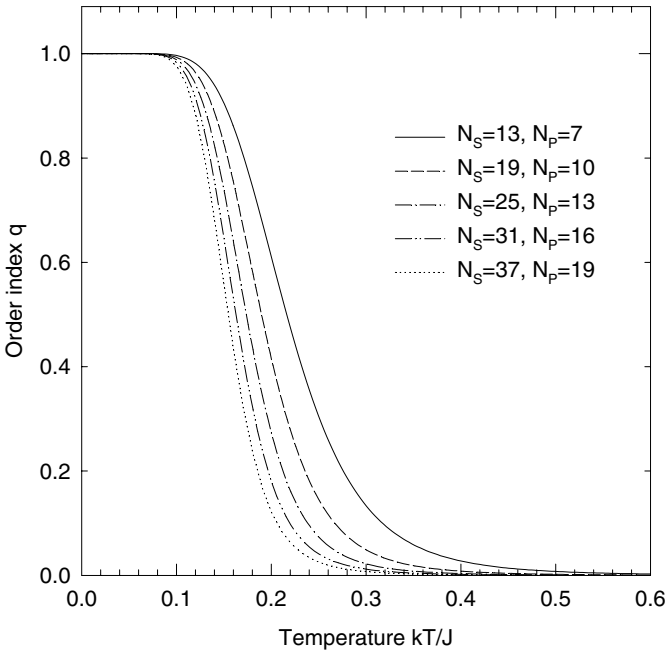

Fig. 4. The order indexes q versus temperature t of the 1D special systems ($N_P = \frac{N_S+1}{2}$) with nearest neighbor interactions ($\delta = \infty$) and various size numbers N_S. All systems with various site numbers exhibit a second order phase transition, however, the transition temperature shifts toward lower temperature with increasing N_S.

due to computer capability. A clear trend seen in this figure is that the phase change temperature shifts toward lower temperature with increasing N_S, similar to that of the $1/r$ interactions shown in Figure 1a. According to these results, one might suspect that the infinite-site system would exhibit no such order-disorder phase change. In order to elucidate the possible size effect to our model system, we thus studied large-size systems up to more than 12000 sites by using the Monte Carlo method introduced in reference [11]. In Figure 5, we show the results of Monte Carlo simulation on t-dependent order index q for the large-size special system with nearest neighbor interactions. It is seen that a phase change at about $t \approx 0.1$ was also observed with Monte Carlo simulations, consistent with the exact calculations. It is worth mentioning that the results of the lattice site $N_S = 25$ are almost identical as shown in Figure 4 (analytical method) and Figure 5 (Monte Carlo method), a confirmation of the validity of the Monte Carlo results. Near the onset of the phase change, the results depend on the size of lattice gas system, as the curves around the phase change are smoother with smaller site number. Such a rounding effect on small-size systems is presumably due to the end effect (or size effect), since this feature is consistently seen in all small-size exact calculations. With increasing site number, while a weaker end effect is expected to the model system, the phase change becomes sharper and the phase change temperature t_C shifts toward lower temperature. If we define the t_C of each site number to be the intersection point of the given $q-$ t curve and a horizontal

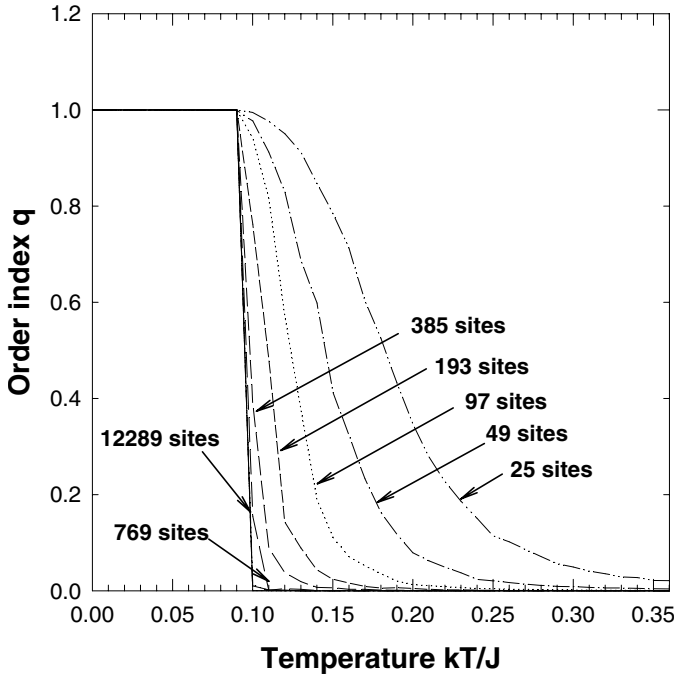

Fig. 5. The Monte Carlo results of order indexes q versus temperature t of large-size special 1D lattice gas systems with nearest neighbor interactions.

straight line at $q = 0.5$, then a disappearing t_C at a site number of approximately 500 can be determined in the small-size region (25–193). Nevertheless, this scaling picture totally fails in the large-size regions (385–12289), as the t_C gradually approaches to $t = 0.09$. It has to be noticed here that the algorithm for carrying out a Monte Carlo simulation is to perform a random walk through configuration space in which the relative frequency of visitations generate the equilibrium ensemble distribution. As a result, Monte Carlo calculations always involve finite errors and fluctuations. These fluctuations play an important role near the t_C, especially in 1D systems where it is well-known that thermal fluctuations would significantly depress the t_C. In order to resolve this deficiency, we make a simple estimation on how thermal fluctuations would affect the t_C of our model system. At the temperature lower than t_C, the particle number distribution of the special system can be approximately represented by alternating 0 and 1, i.e. $\{\langle n_i \rangle\} = \{1, 0, 1, 0, ..., 1, 0, 1\}$, as shown in Table 1. Due to the existence of thermal fluctuations, the probability p of any particle jumping to its two adjacent sites to form a nearest-neighbor pair can be described by the classical Boltzmann expression $p = 2\exp(-1/t_C)$. In other words, the total number of nearest-neighbor pairs could be found under the influence of thermal fluctuations is $2N_P \exp(-1/t_C)$. Apparently, the formation of such kind of neighboring pairs would destroy the long range order of the 1D chain, thus the order-disorder phase change no longer occurs. According to our results shown in Figure 5, the largest considered system is $N_S = 12289$ ($N_S = 6145$) with $t_C \sim 0.09$, so the number of the possible nearest-neighbor pairs is about 0.18. It is trivial to show that the numbers of the two or more nearest-neighbor pairs found in our model system is even less than that of the a single nearest-neighbor pair. From this simple estimation, we could safely conclude that thermal fluctuations do not strongly affect the phase properties in our considered cases. Therefore, we argue that the rounding effect and the depression of t_C in the small-size region are a consequence of the size effect. Consequently, the end effect plays an essential role of the phase properties in our model system, and our results are only applicable to the mesoscopic systems. Certainly it is expected that such an order-disorder phase change would vanish in the thermodynamic limit, since there will be no telling difference between the special system and general system as the size of the 1D lattice gas system goes to infinite. Besides, thermal fluctuations would also destroy the long range order as the size of the 1D chain becomes sufficiently large.

At this point, we would like to point out that the existence of phase changes is possible in the finite lattice gas system, at least for the system size less than 12000 sites. On the other hand, experimentally the length of the single walled carbon nanotubes is found to be on the order of several hundred nanometers [20], i.e., the number of molecules inside a nanotube is not more than 5000. Therefore, our results of Monte Carlo simulations could qualitatively describe the phase properties of all available 1D confined systems with nearest neighbor interactions. In addition, it is worth mentioning that the 1D lattice gas could be mapped into the 1D Ising system, and that the 1D Ising system is known to have no phase transition at finite temperatures. However, the special system with nearest neighbor interactions was found to have an unique ground state, while the Ising model has two possible ground states (all particles with spin up or spin down). We believe that it is this difference which makes our model system sustain phase change at finite temperatures.

Figures 6 and 7 show C versus t for the general and special systems with various δ's. As illustrated in Figure 6, the specific heat for $\delta = 1$ has a peak at about $t = 0.08$, which corresponds to the order-disorder phase change shown in Figure 2. It is seen in the upper (lower) panel of Figure 6 that the phase change temperature shifts toward lower temperature with decreasing (increasing) δ as $\delta < 1$ ($\delta > 1$), consistent with the results of Figure 2. It is noted that the specific-heat peaks appear to be sharper for larger δ (lower panel of Fig. 6), and the appearance of broad maximums at high temperatures in these cases is not a consequence of phase changes but the heat capacity background. For the special system, specific-heat peaks corresponding to the order-disorder phase change are also observed for $\delta > 0.6$ (see Fig. 7), and the peak positions shift toward higher temperature with increasing δ. These observations are in good agreement with that of the results shown in Figure 3. It should be mentioned that the broad maximums appearing at high temperatures for small δ ($\delta \leq 0.8$) is again due to background contributions.

In fact, both the case (1) of the molecules in the closed nanotubes and case (2) of the ions in the one-dimensional chains for the Q1D materials in which the particles are

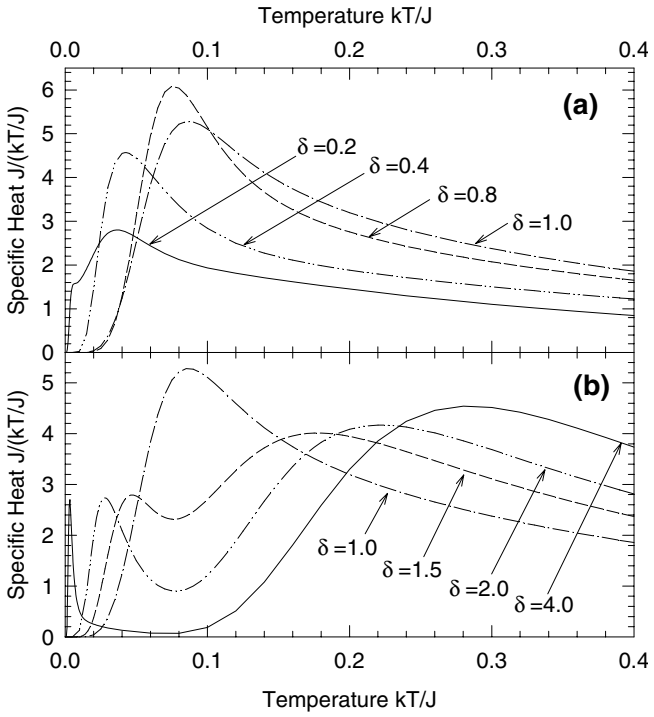

Fig. 6. The specific heats versus temperature t for the general systems. The upper panel shows the results of $\delta \leq 1$, and lower panel shows the results of $\delta \geq 1$. The peaks in specific heat correspond to the phase transitions shown in Figure 2.

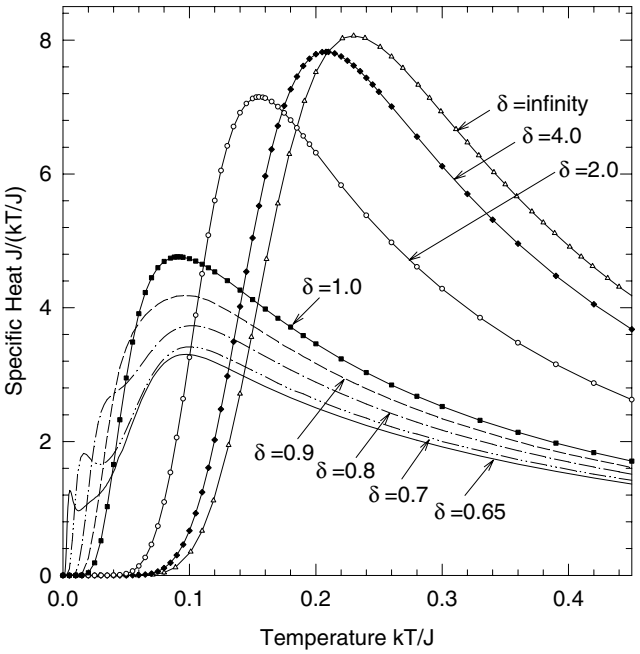

Fig. 7. The specific heats of the special systems. The peaks in specific heat correspond to the phase transitions shown in Figure 3.

free to move in a periodic potential caused by the interactions between particles, can be simplified as partially filled lattice gas systems. Normally, 1D systems with short-range interactions do not exhibit phase transitions. However, in the present study we strikingly found that small-size 1D lattice gas systems with $N_P = \frac{N_S+1}{2}$ (namely the special systems) exhibit a order-disorder phase change even with nearest neighbor interactions ($\delta = \infty$). With the preliminary success in explaining the phase transitions in the $KCu_{7-x}S_4$ system with our mean-field model [10–12], we expect that such kinds of phase changes in mesoscopic systems such as molecules in the long narrow nanotubes may be experimentally observable in the not too distant future. At this point, it would be instructive to compare our results with other works on 1D nanotube systems. In reference [22], Hodak and Girifalco considered the 1D nanotube system as a 1D lattice gas model with nearest-neighbor attractive interactions [22]. They obtained the probability of occurrence of a single cluster, which can be regarded as an order parameter, as a function of temperature plotted in Figure 3, and the heat capacity versus temperature of the studied systems plotted in Figure 6. We notice that our results of the order index q and specific heats C with respect to t are very similar to those shown in their Figures 3 and 6 of reference [22]. We argue that such a result suggests that the 1D lattice gas systems with repulsive interactions versus those with attractive interactions is analogous to the antiferromagnetic systems versus the ferromagnetic systems. On the other hand, the results of the special system with large δ in the present study can be considered as a simplification for Xia's system in extremely narrow carbon nanotubes with high density [24]. The pair ven der Waals interactions between all molecules in Xia's system with high density can be regarded as the special system in our model with $\delta = 12$, plus a nearest neighbor term. Each molecule in Xia's system will be in a fixed position when t is near 0, i.e., there is only one ground state, and the system undergoes an order-disorder phase change. This finding is in accord with our results for the special systems.

4 Summary

In this paper, we exactly studied the phase properties of small-size partially filled one-dimensional lattice gas system with $1/r^\delta$ repulsive interactions. The results show that such systems exhibit an order-disorder phase change in a certain range of δ, depending on the filling parameter $n_a = N_P/N_S$. These results are qualitatively consistent with our previous LRMF results with $\delta = 1$ [10]. It is found that the systems for $N_P > \frac{N_S+1}{2}$ (general system) have many possible ground-state configurations with nearest neighbor interactions, while the systems for $N_P = \frac{N_S+1}{2}$ (special system) have an unique ground state. The general system with pair interaction proportional to $1/r^\delta$ will exhibit a phase change if and only if $0.1 < \delta \leq 8$, while the special system will exhibit phase change as long as $\delta > 0.6$. The largest size system which was exactly performed in this study is $N_S = 37$, due to the computer capability. A complementary calculation using the Monte Carlo method up to lattice site more than $N_S = 12000$

on the special system with nearest neighbor interactions was also performed. Even though the phase change is still found in the 1D lattice gas systems even with nearest neighbor interactions, it has to be pointed out that the end effect plays an essential role in the phase properties of our model system. Nevertheless, our present study provides an extensive phase diagram for the 1D finite-size lattice gas system with the full range of interactions between particles. These results would yield valuable information of the phase properties for 1D confined systems. We expect such behaviors may be experimentally observable soon.

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References

1. E.H. Lieb, D. Mattis, "*Mathematical Physics in One Dimension*" (Academic Press, London, New York, 1966)
2. R.B. Griffiths, "*Phase Transition and Critical Phenomena*", edited by C. Domb, M.S. Green (Academic Press, New York, London, 1972), Vol. **I**, p. 89–94
3. M.E. Baur, L.H. Nosanow, J. Chem. Phys. **37**, 153 (1962)
4. H. Araki, Commun. Math. Phys. **14**, 120 (1969)
5. D. Ruelle, Commun. Math. Phys. **9**, 267 (1968)
6. F.J. Dyson, Commnu. Math. Phys. **12**, 91 (1969)
7. S.-J. Hwu, H. Li, R. Mackay, Y.-K. Kuo, M.J. Skove, M. Mahapatro, C.K. Bucher, J.P. Halladay, M.W. Hayes, Chem. Materials **10**, 6 (1998)
8. Y.-K. Kuo, M.J. Skove, D.T. Verebelyi, H. Li, R. Mackay, S.-J. Hwu, M.-H. Whangbo, J.W. Brill, Phys. Rev. B **57**, 3315 (1998)
9. H. Li, R. Mackay, S.-J. Hwu, Y.-K. Kuo, M.J. Skove, Y. Yokota, T. Ohtani, Chem. Materials **10**, 3172 (1998)
10. T.C. King, Y.K. Kuo, M.J. Skove, S.-J. Hwu, Phys. Rev. B **63**, 45405 (2001)
11. T.C. King, Y.K. Kuo, M.J. Skove, Physica A **313/3-4**, 427 (2002)
12. T.C. King, Y.K. Kuo, Phys. Rev. E **68**, 036116 (2003)
13. S. Iijima, Nature (London) **354**, 56 (1991)
14. N.G. Chopra, R.J. Luyken, K. Cherrey, V.H. Crespi, M.L. Cohen, S.G. Louie, A. Zettl, Science **269**, 966 (1995)
15. A. Loiseau, F. Willaime, N. Demoncy, G. Hug, H. Pascard, Phys. Rev. Lett. **76**, 4737 (1996)
16. D. Golberg, Y. Bando, W. Han, K. Kurashima, T. Sato, Chem. Phys. Lett. **308**, 337 (1999)
17. B.W. Smith, M. Monthioux, D.E. Luzzi, Nature (London) **396**, 323 (1998)
18. W. Teizer, R.B. Hallock, E. Dujardin, T.W. Ebbesen, Phys. Rev. Lett. **82**, 5305 (1999)
19. W. Teizer, R.B. Hallock, E. Dujardin, T.W. Ebbesen, Phys. Rev. Lett. **84**, 1844 (2000)
20. A. Kuznetsova, J.T. Yates, J. Liu, R.E. Smalley, J. Chem. Phys. **112**, 9590 (2000)
21. M.M. Calbi, M.W. Cole, S.M. Gatica, M.J. Bojan, G. Stan, Rev. Mod. Phys. **73**, 857 (2001)
22. M. Hodak, L.A. Girifalco, Phys. Rev. B **64**, 035407 (2001)
23. M. Hodak, L.A. Girifalco, Phys. Rev. B **68**, 085405 (2003)
24. Y. Xia, M. Zhao, Y. Ma, X. Liu, M. Ying, L. Mei, Phys. Rev. B **67**, 115117 (2003)
25. D.W. Brenner, Phys. Rev. B **42**, 9458 (1990)