CHINESE JOURNAL OF PHYSICS VOL. 36, NO. 3 JUNE 1998

Calculation of Numerical Microcanonical Ensemble Method on 2D Statistical Models

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(Received February 11, 1998)

In our earlier work, we proposed a new microcanonical ensemble method and showed that the numerical results of this method are correct in 1D models. In this paper, the numerical data in 2D models are presented. One of our calculations is concentrated on fermionic models, because fermionic models behave quite differently from bosonic models when the dimension is larger than two (there may be boson-fermion duality in 1D). Our results come out to be consistent with exact values. To our knowledge, there is no other numerical methods which can present reliable calculation on fermionic models with large lattice, especially when the temperature is low. In addition to the test on fermionic models, we also show our results on quantum 2D XY model. We calculate longitudinal spin-spin correlation, specific heat, vortex density and vortex pair density. These results agree with the calculations by other methods. The data of vortex density and vortex pair density seem to display directly the unbinding of vortices and antivortices.

PACS. 05.30.Ch – Quantum ensemble theory.
PACS. 65.50.+m – Thermodynamic properties and entropy.

I. Introduction

This paper is a subsequent work of our earlier work [1] where we proposed a new microcanonical canonical ensemble method and showed that its application in calculations in 1D models seems successful. The anti-commutation relation problem in fermionic models has been a unsolved difficulty in computational physics. So, a successful numerical method for fermionic models processes very important meanings. The success of our method in 1D fermionic models is a starting point in developing a convincing tool for fermionic and bosonic models. The primary concept in our method is based on the proof: Expectation values of the energies, rather than the eigenenergies, of quantum states can be used to evaluate the ensemble average of the energy in the standard microcanonical theory. If the energy and the related entropy, which are defined in our method, are well evaluated to their extreme values, our method will produce the same statistical properties as in the standard microcanonical theory in the thermodynamic limit. One important point, which is implied in our proof, is that the entropy calculated in our method should be no larger than the value from the standard theory. This fact promises the stability in our method. That is if we can control the numerical error in calculations, the calculated entropy in our method will converge to the true value from the lower side and the numerical error of each datum will be of the same order. In the present work we extend our calculations to 2D models. In later sections, we will demonstrate that our numerical results are also consistent with exact values of solvable 2D fermionic models. But for other numerical methods, the numerical calculations for fermionic models with large lattice size still encounter difficulty in treating the anticommutation relation of fermion operators. The consistency of our 2D results with exact values indicates that our numerical method provides a way to resolve that issue.

In this paper we also compute quantum 2D XY model. Since the work of Kosterlitz and Thouless(KT)[2], 2D XY model, either classical or quantum, has been of interest to statistical physicists [3-9]. There are still debates [8,9] on whether the KT type phase transition exists in this quantum model. Our computation on quantum 2D XY model is not only to test our method on bosonic model but also to hope to obtain results of interests. We calculate the specific heat, spin-spin correlation, vortex density and vortex pair density of 2D XY model. The data of vortex density and vortex pair density seem to show directly the unbinding of vortices and antivortices. However, as we mentioned in Ref. 1, the accuracy of the 2D data are not good enough at the speed of our computer facility. We do not expect to obtain very precise numerical data.

In our computations, the speed of computer is about 40 mflops. The cpu time is from 20 to 50 cpu days and the disk memory needed is 1 to 3 Gbytes.

The rest of the paper is organized as: In sec. II, we will show the numerical data on 2D spinless fermionic models for testing our method. In sec. III, we present our results for quantum 2D XY model. In sec. IV, we draw our conclusions.

II. Two-dimensional fermionic models

II-1. Description of models

Two Hamiltonians of 2D spinless fermionic models are considered in this paper. They are

$$H_1 = \sum_{ij} t_1 C_i^+ C_j \tag{1}$$

and

$$H_2 = \sum_{ij} t_1 C_i^+ C_j + \sum_{ik} t_2 C_i^+ C_k \tag{2}$$

where i, j are nearest neighbor sites and i, k are next nearest neighbor sites of a square lattice. The t_1 is set to be -1 eV and the t_2 is set to be **-0.5** eV. C_i^+, C_j and C_k are fermionic operators. Our calculation are done on 64 x 64 lattices and the exact statistical values are evaluated on 400 x 400 lattices by canonical ensemble method. Open boundary condition is used, because it is easier in our numerical method.

II-2. Results and discussion

Our numerical results and the corresponding exact values are shown in Fig. 1 to Fig. 4. Figs. **1** and 2 are for H_1, and Figs. 3 and 4 are for Hz. The low temperature C_v data of Figs. 1 and 2 are better than those in the 1D cases [1]. We think it may result from the smaller quantum fluctuation in 2D. But the low temperature C_v data of Figs. 3 and 4 are not very satisfactory. This may be due to two factors. First, the energy band width for H_2 is wider than for Hr. This means that at the same temperature the accuracy of C_v data for H_2 is worse. Second, we use open boundary in our computation. When the lattice is small the fluctuation of particle density is large. Thus, this will introduce larger particle density deviation when we combine energy states into bundles. But whether the second factor introduces larger deviation for Hamiltonian H_2 than for H_1 is not clear to us. It needs more accurate calculations and more extensive tests on other models to clarify the reason. The numerical program for periodic boundary condition is more complicated. We must evaluate the state energies under periodic boundary condition, and then get rid of the contribution from boundary when calculate the hopping and interacting matrix elements, which are used to merge lattices at the next step of computation. These surveys are planed to finish in future.

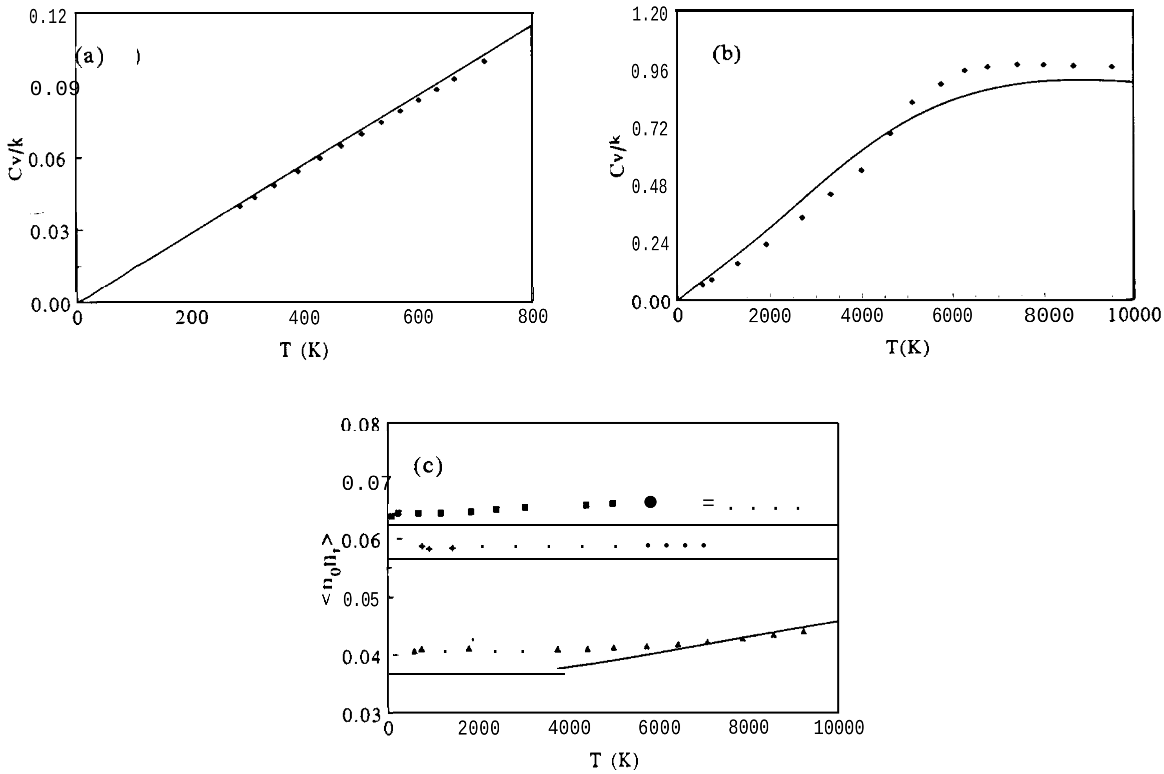

FIG. 1. Data for Hamiltonian H_1, when the particle density $< n >$ is $1/4$. (a) Specific heat over k as a function of temperature (in unit of Kelvin); the line shows the exact value and the squares show our data. (b) Same as (a) except that the temperature is higher. (c) Density correlation $< n_0 n_r >$ for r = 1, $\sqrt{2}$, 2 as a function of temperature; the lines show exact values and our data are marked by triangles $(r = 1)$, crosses $(r = \sqrt{2})$ and squares $(r = 2)$.

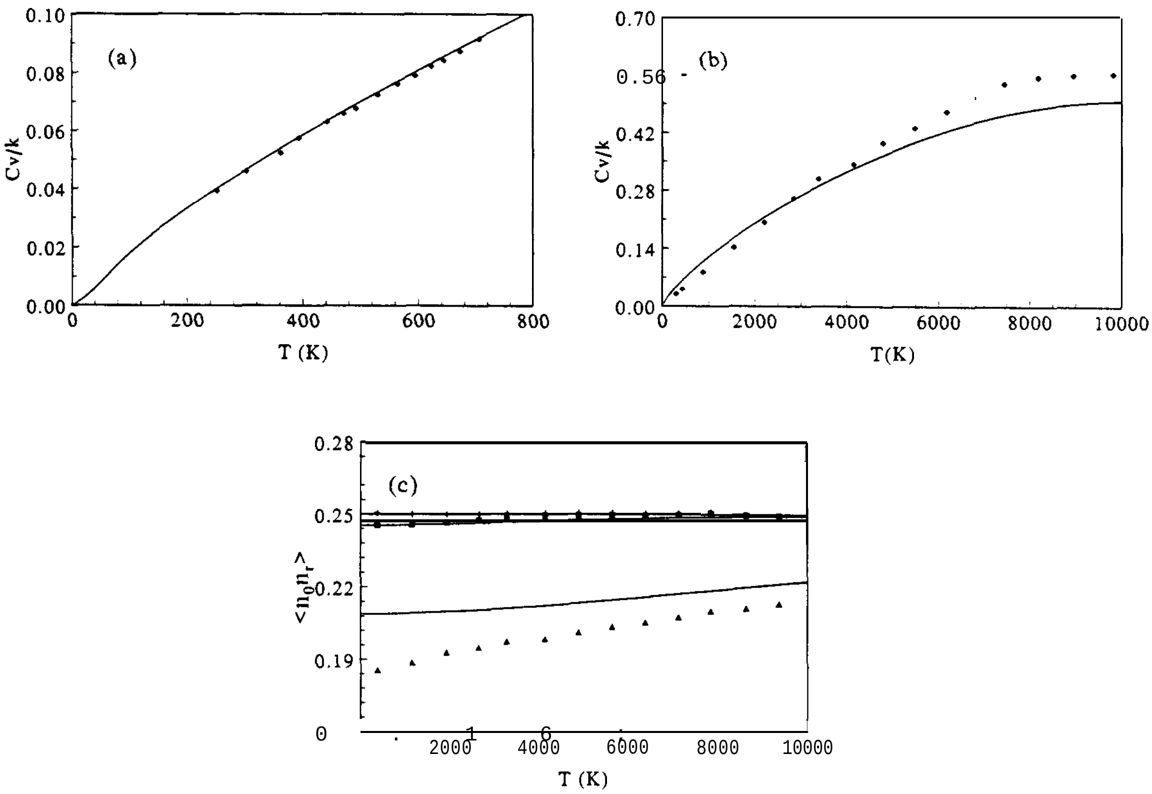

FIG. 2. Same as Fig. 1 except that the particle density $< n >= 1/2$ and in (c) $r = 1, \sqrt{2}, \sqrt{5}$. We do not show r = 2 data, because they are almost the same as $r = \sqrt{2}$ data.

The higher temperature C_v data, except for Fig. 4(b), are quite consistent with exact values when the temperature is not very high (when T is lower than 5000 K). For very high temperature, the C_v value is higher than the exact value, because the calculated energies are larger than exact values by 6 to 7%. Therefore, the curvature of the calculated energy vs. entropy data will be larger than exact values at high temperature.

The data of density correlation are basically consistent with exact values. As we mentioned above, due to the open boundary condition the density fluctuation is larger at smaller lattice. This fact also reflects in correlation data. The truncation effect, which results from the finite number of bundles of states and the finite matrix dimension, is more apparent in 2D than in 1D.

III. Two-dimensional XY model

III-l. Description of the model

The following quantum 2D spin Hamiltonian is considered.

$$H = 2J \sum_{ij} (S_i^x S_j^x + S_i^y S_j^y) \tag{3}$$

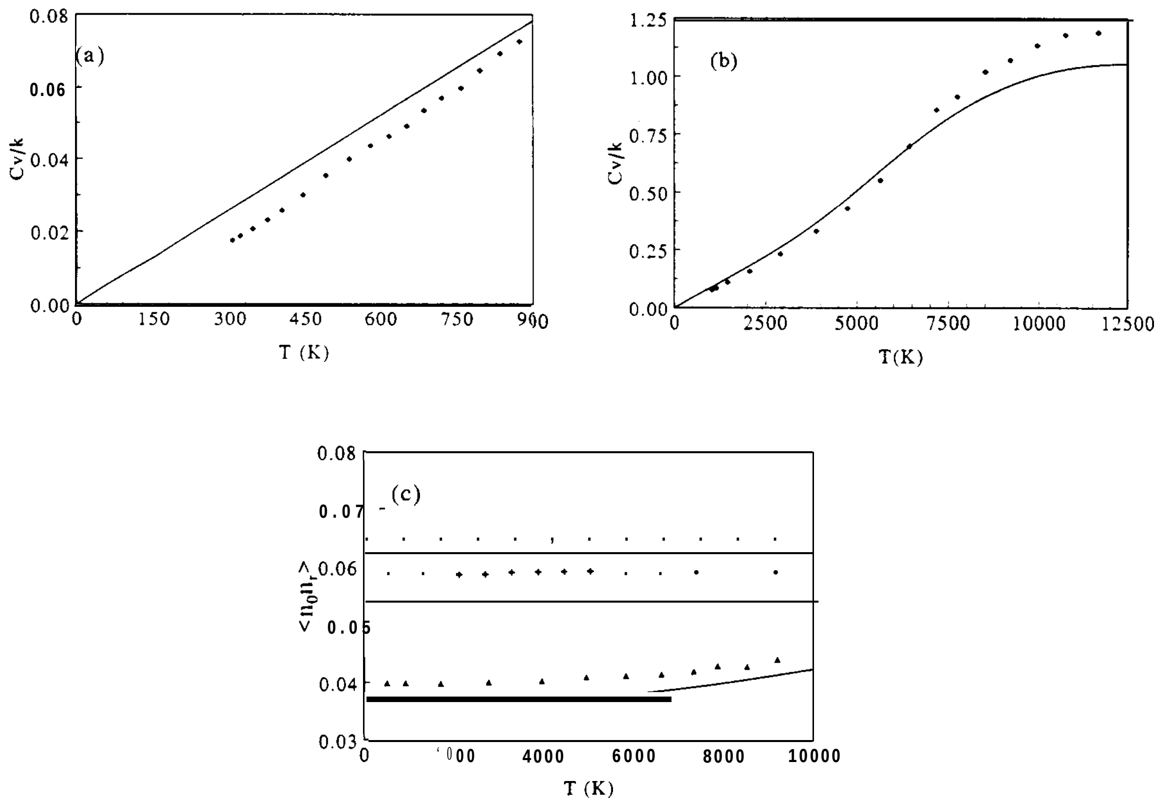

Fig. 3. Same as Fig. 1 except that the Hamiltonian is H_2.

where the S_i^x, S_j^x, S_i^y and S_j^y are spin $1/2$ operators and i, j are nearest neighbor sites of a square lattice. We map this spin model to the hard core boson model with Hamiltonian

$$H = J \sum_{ij} C_i^{+} C_j \tag{4}$$

where C_i^{+} and C_j are hard core boson operators (that is $[C_i^{+}, C_j] = [C_i, C_j] = [C_i^{+}, C_j^{+}] = 0$ for $i \neq j, [C_i, C_i^{+}] = 1$ and $C_i^{+} C_i^{+} = C_i C_i = 0$). Square 64 x 64 lattice is used in computation.

111-P. Results and discussion

In Fig. 5 we show the specific heat, spin-spin correlation, vortex density and vortex pair density data. The vortex density and vortex pair density are defined by Betts et al. [3]. The total density of vortices is

$$< V^2 >= (1 - 2 < \sigma_1^x \sigma_3^x - \sigma_1^x \sigma_2^y \sigma_3^x \sigma_4^y >)/4. \tag{5}$$

The vortex pair density is

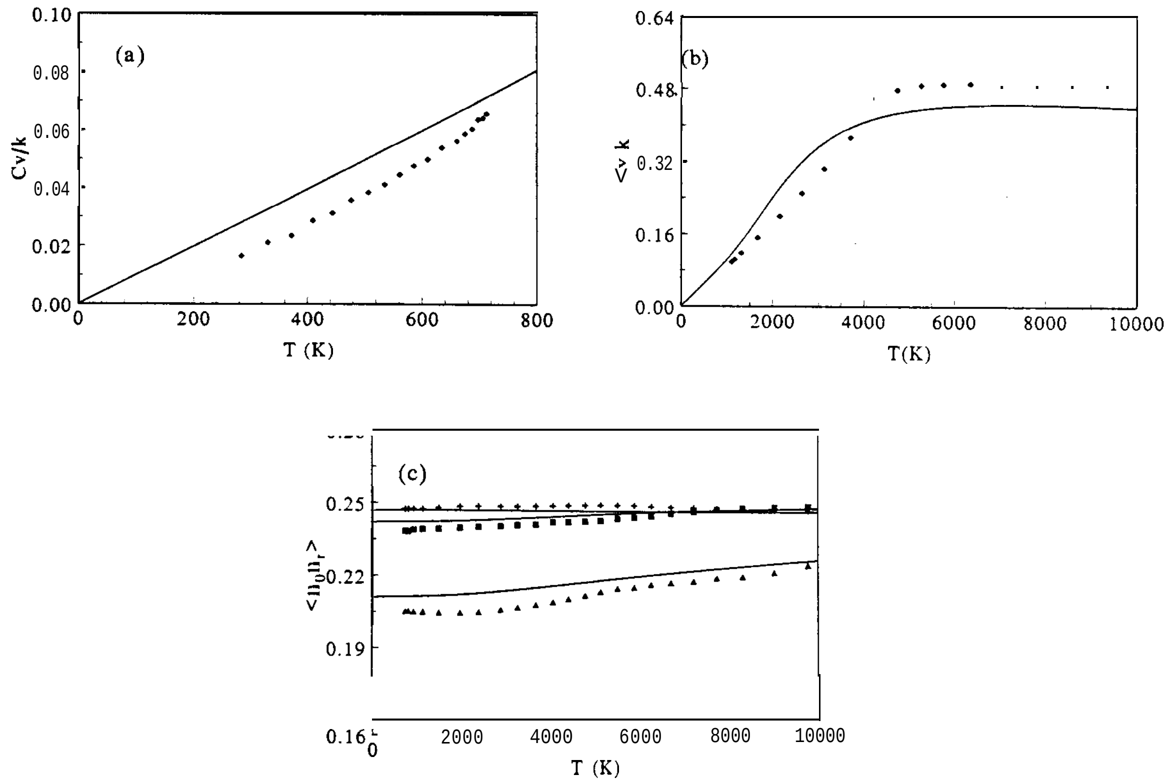

FIG. 4. Same as Fig. 1 except that the Hamiltonian is H_2 and the particle density $< n >= 1/2$.

$$
\begin{aligned}
< P >= & \ (1 - 4 < \sigma_1^x \sigma_3^x > +2 < \sigma_1^x \sigma_5^x > + < \sigma_1^x \sigma_4^y \sigma_5^x \sigma_6^y > +2 < \sigma_1^x \sigma_2^y \sigma_3^x \sigma_4^y > \\
& +2 < \sigma_1^x \sigma_2^y \sigma_3^x \sigma_6^y > -4 < \sigma_1^x \sigma_4^y \sigma_3^x \sigma_6^y >)/8.
\end{aligned} \tag{6}
$$

The number subscripts are the same as those used by Betts *et al.* [3]. σ are Pauli operators.

In Fig. 5, the temperature is in unit of 2J. These data are consistent with other calculations [3-6]. The ground state energy per site is -0.528 (in unit of $2J$). Our results support that the C_v peak is finite. But our numerical data in the temperature below C_v peak are quantitatively not very accurate. The reason is that the state energies change very slightly in this range of temperature. So, we must use larger number of bundles of states and larger matrix dimension to overcome the deviation introduced by numerical computation. On the other hand, we think that if we use periodic boundary condition, the accuracy will also be improved. Because the state energies converge to final values much faster. As shown in the estimate of the ground state energy by Oitmaa *et al.* [7], even when the lattice is 8 x 8 the state energies are very close to final energies in large lattice.

In Fig. 5(b) it is interesting to note that the data seem to display directly the unbinding of vortices and antivortices. At low temperature the vortex density is almost two times of vortex pair density. The vortex density begins to grow larger than two times of

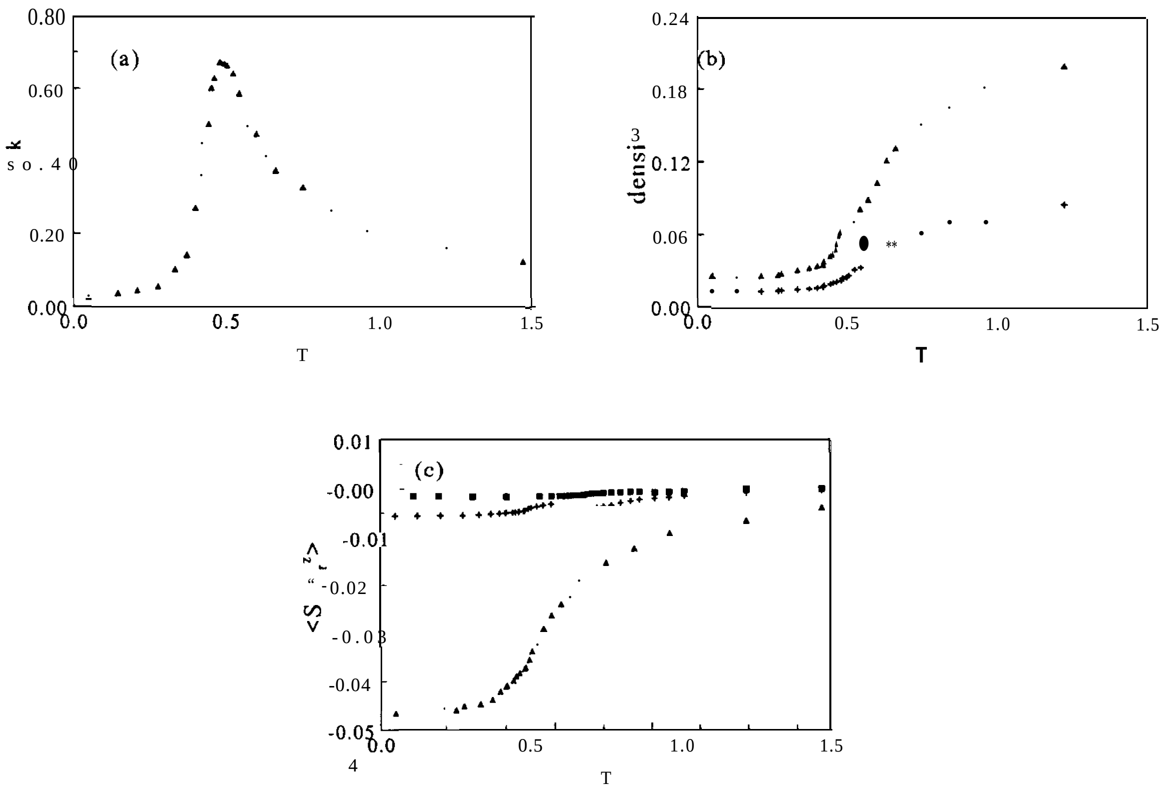

FIG. 5. Data for 2D XY model. (a) Specific heat over k as a function of temperature (in unit of 25). (b) Vortex density, $< V^2 >$, (triangles) and vortex pair density, $< P >$, (crosses) as a function of temperature. (c) Spin-spin correlation $< S_0^z S_r^z >$ for $r = 1, \sqrt{2}, 2$ as a function of temperature; the data are marked by triangles $(r = 1)$, crosses $(r = \sqrt{2})$ and squares $(r = 2)$.

vortex pair density when the temperature is near 0.4. Due to the uncertainty of our data in this temperature range, we are not sure at what temperature when this begins to happen. But it is confirmed that the change is gradual.

In Fig. 5(c), the longitudinal spin-spin correlation is shown. Because of the truncation effect, as we mentioned in Ref. 1, the correlation can not be calculated at a long distance. Therefore, we do not focus on the computation of this part, for example the evaluating of the correlation length. The spin-spin correlation $< S_0^z S_r^z >$ of ground state for $r = 1, \sqrt{2}, 2, \sqrt{5}, 2\sqrt{2}$ are -0.0466, -0.0056, -0.0015, -0.0038 and -0.0004. Except that **some** fluctuations exist when the correlation values are very small, the change of correlation with distance is consistent with other calculations [6, 7].

IV. Conclusions

As a summary of our computations, we may say that the numerical results are reasonable. Although the accuracy of data is not very satisfactory in the 2D models, no strange deviation of the data is found in our calculations. The most important meaning of the present numerical results for fermionic models is that our new numerical method can overcome effectively the difficulty in treating the anti-commutation relation of fermions. The difficulty resulting from anticommutation relation has been a long-time problem. In future work, if we can confirm that our method is applicable for all fermionic models, it will be a very valuable advance in computational physics. The accuracy of the data for 2D XY model in present work are not good enough. To improve the accuracy, at one hand we can use a faster computer in future to perform the calculations, at the other hand we can modify the procedure, like the boundary condition, in calculation. The open boundary, which we use in calculation, seems to introduce not small deviation in numerical data (this is not apparent in 1D). We believe that if the periodic boundary is used, the energy deviation will be improved by 2 to 3% and thereafter the C_v and correlation data be improved.

Acknowledgments

This work is supported by National Science Council of R.O.C. through Grants Nos. NSC 85-2112-M-009-029-PH and NSC 86-2112-M-009-022.

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