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TITLE QUANTUM MONTE CARLO STUDY OF SYMMETRY BREAKING IN A DOUBLE-WELL CHAIN

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QUANTUM MONTE CARLO STUDY OF SYMMETRY BREAKING IN A DOUBLE-WELL CHAIN

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INTRODUCTION

We report the results of a quantum Monte Carlo simulation of a double-well chain. This chain is a system of particles that move on a lattice of symmetric, double-well potentials which are coupled harmonically to one another. The physical properties of this system are invariant, like those of the the Ising model, under the symmetry operations of the Z_2 group. In this case, changing the sign of the displacement variables leaves the energy unchanged and leads to a doubly-degenerate ground-state. Classically, this symmetry is always broken, and the particles all sit in the left- or the right-hand side of their wells. Quantum mechanically, however, we find that below a critical value of the double-well coupling constant the symmetry is restored by quantum fluctuations.

Our interest in this model was motivated by a series of quantum Monte Carlo simulations we are performing on one dimensional models of conducting polymers and synthetic metals. The properties of these materials are described by a system of interacting electrons coupled to a system of phonons. Several years ago, for similar models, Fradkin and Hirsch[1] investigated how the electron motion can generate an effective double-well potential for the phonons and thereby cause the lattice to dimerize. They also argued, based on continuum renormalization group considerations and quantum Monte Carlo simulations, that for certain models quantum fluctuations at low temperatures restore symmetry (i.e., destroy the dimerization). We were attracted to the quantum double well chain because it is a simpler problem than the electron phonon models on which to test new numerical methods and to study similar issues.

The model, however, is also interesting on its own. It is a discretized version of a 1 + 1 dimensional quantum ϕ^4 field theory. Although considerable numerical work has been done for these models in higher dimensions, little has been done for one spatial dimension. Analytically, some interesting results are known about the continuum version of the one dimensional model.[2] For instance, kink/anti kink pairs

are the elementary excitations above the ground state. One of our objectives was to learn more about the nature and consequence of these excitations.

The model is also relevant to the study of the structural properties of such hydrogen-bonded materials as the hydrogen halides.[3] In many cases, the energy as a function of lattice spacing for these chain-like materials has been obtained by local density approximation calculations of their electronic structure and fitted to the physical parameters in the double-well chain. Thus, with the phase diagram of the model, we can suggest whether these materials exist in the broken symmetry phase.

MODEL HAMILTONIAN

The Hamiltonian we are considering is

$$\hat{H} = : \sum_{n=1}^{N} \left[\frac{\hat{\pi}_n^2}{2m} + \frac{w}{2}(\hat{\phi}_n - \hat{\phi}_{n+1})^2 - \frac{k}{2}\hat{\phi}_n^2 + \frac{g}{4}\hat{\phi}_n^4 \right] : \tag{1}$$

where $\hat{\phi}_n$ and $\hat{\pi}_n$ are the coordinate and momentum operators of a particle with mass m on n^{th} site of a chain of length N. At each site, the particle moves within a potential well whose harmonic and anharmonic parts are characterized by the constants k and g. These wells are coupled to their nearest neighbors with coupling strength w. The constants m, w, k, and g are all non-negative, and the bracketing colons denote normal ordering of the quantum operators. Periodic boundary conditions are assumed. We also assumed that the quantum fluctuations do not cause the neighboring particles to interchange and that the lattice structure does not melt.

The first two terms on the right-hand side of (1) are those of a harmonic oscillator whose quantum of energy is $\hbar\omega = \hbar\sqrt{w/m}$. The remaining two terms are those for the symmetric, on-site double-well potentials. These potentials have two absolute minima displaced $\pm\sqrt{k/g}$ relative to each lattice site and have an energy barrier $E_b = k^2/4g$ between these minima. Using the energy quantum, the harmonic frequency, and the displaced distance of minima to scale energies, time, and lengths, we rewrite (1) in the following dimensionless form

$$\hat{H} = : \epsilon \sum_{n=1}^{N} \left[\frac{\gamma}{2}\hat{\pi}_n^2 + \frac{\gamma}{2}(\hat{\phi}_n - \hat{\phi}_{n+1})^2 + \frac{1}{4}(\hat{\phi}_n^4 - 1)^2 \right] : \tag{2}$$

where $\epsilon = 4E_b/\hbar\omega$ and $\gamma = w/k$, and a constant term has been added. In (1), the parameter γ measures the relative strengths of the on site part of the harmonic potential to the harmonic part implicit in the double well. In (2), it is the harmonic frequency Ω associated with the coupling of the double wells.

We will calculate the ground state properties of (2) by doing quantum Monte Carlo simulations at successively lower and lower temperatures. The formalism on which the simulations are based requires the partition function of the model in terms of the Feynman path integral.[4,5] In general,

$$Z = \int D\phi\, e^{-S\{\phi\}}$$

where $S\{\phi\}$ is the action associated with the scalar field ϕ. In terms of (2), we find that

$$S\{\phi\} = \epsilon \sum_n \int_0^\beta d\tau \left[\frac{1}{2}\left(\frac{\partial\phi_n}{\partial\tau}\right)^2 + \frac{\gamma}{2}(\phi_n - \phi_{n+1})^2 + \frac{1}{4}(\phi_n^2 - 1)^2 \right] \tag{3}$$

where τ is the imaginary-time variable and β is the inverse of the temperature T.

An implicit parameter in (1) is the lattice constant a. If we let a vanish while keeping ωa constant, we can show that in the ground state ($\beta \to \infty$)

$$S\{\phi\} = \epsilon\gamma \int_{-\infty}^{\infty} dx \int_0^{\infty} d\tau \left[\frac{1}{2}\left(\frac{\partial\phi}{\partial\tau}\right)^2 + \frac{1}{2}\left(\frac{\partial\phi}{\partial x}\right)^2 + \frac{1}{4}(\phi^2 - 1)^2 \right] \tag{4}$$

This expression is the continuum version of the ϕ^4 field theory we are investigating. If treated classically, this field theory has the well known ground states of $\phi = \pm 1$ with energy $E_g = 0$ and has soliton solutions representing excitations from the ground state. If treated quantum mechanically, the ground state properties are renormalized. The lowest order correction (at the one-loop level) has been calculated,[2] and in this approximation

$$E_g = \frac{2\sqrt{2}}{3}\epsilon\sqrt{\gamma} + \frac{1}{\sqrt{\gamma}}\left(\frac{-3}{\pi\sqrt{2}} + \frac{1}{2\sqrt{2}}\right) \tag{5}$$

When

$$\epsilon < \frac{18 - \sqrt{3}\pi}{8\pi\gamma} = \frac{0.49969}{\gamma} \tag{6}$$

E_g becomes negative, then the broken symmetry ground state is unstable to the formation of kink/anti-kink pairs. This instability is an indication of the restoration of symmetry. We will find that the above estimate, while not very useful quantitatively, does point to the correct physical picture.

NUMERICAL METHODS

For the simulations, we discretize the integration in imaginary time into L steps of size Δ defined by $L\Delta = \beta$ and express the action $S\{\phi\}$ in terms of variable $\phi_{i,j}$,

$$S\{\phi\} = \Delta\epsilon \sum_{i,j}^{L,N} \left[\frac{\gamma}{2}\left(\frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta}\right)^2 + \frac{\gamma}{2}(\phi_{i,j} - \phi_{i,j+1})^2 + \frac{1}{4}(\phi_{i,j}^4 - 1)^2 \right] \tag{7}$$

Here, the subscripts i and j are the labels for the imaginary time and space dimensions.

Formally, this action is similar to the discrete, classical, two dimensional ϕ^4 system.[6,7] In the present case, however, to insure we are describing quantum behavior, we have to require Δ to be much smaller than the reciprocal of Ω. In contrast to the classical ϕ^4 system, this requirement poses an extreme anisotropic nature on the problem. It also makes measurements of quantum quantities, such as the energy, specific heat, *etc.*, different from those of their classical counterparts. We will now describe how we performed the simulations and how we made our measurements.

Hybrid Monte Carlo Algorithm

The conventional, path integral Monte Carlo procedure evaluates the expectation value of a physical quantity $A = A\{\phi\}$,

$$\langle A \rangle = \int D\phi\, A\{\phi\} \frac{e^{-\beta S\{\phi\}}}{Z}$$

by generating a sequence ϕ_i of independent configuration of the ϕ fields with weight $e^{-\beta S}/Z$. The procedure reduces the computation of the expectation values to the simple summation

$$\langle A \rangle = \frac{1}{M}\sum_{i=1}^{M} A\{\phi_i\}$$

where M is the number of independent configurations generated.

With the commonly-used Metropolis algorithm, the configurations are generated by making local, trial changes of ϕ-fields, thereby changing the action from $S\{\phi\}$ to $S\{\phi'\}$, and then deciding to accept or reject the proposed configuration with the probability of $\min(1, e^{\delta S})$ where $\delta S = S\{\phi'\} - S\{\phi\}$. This movement of the $\phi_{i,j}$ is diffusive, and strong correlations can exist between consecutive configurations. Related simulation methods based on Lanegvin or molecular dynamics motions are also used, but often they share similar difficulties in efficiently generating independent configurations. Hybrid methods, which combine two or more different simulation methods, can greatly reduce this problem. In our simulations, we used the Hybrid Method proposed by Duane *et al.*[6]

In the Hybrid Method, a fictitious time t is added to the problem to allow the $\phi_{i,j}$ to evolve globally. Instead of the particles drifting in the phase space by diffusion, fictitious momenta (usually called pseudo-momenta) are introduced to guide their motion. The equations of motion are given by the Hamilton-Jacobi equations derived from the pseudo-Hamiltonian H_p. In our case, we assign each $\phi_{i,j}$ a pseudo-mass μ, such that the pseudo-Hamiltonian of the new system can be written as

$$H_p\{\phi, p\} = \sum_{i,j} \frac{p_{i,j}^2}{2\mu} + S\{\phi\}$$

The partition function of this system is

$$Z_p = \int \prod_{i,j} d\phi_{i,j}\, dp_{i,j}\, e^{-H_p\{\phi,p\}}$$

and since integrand for the $p_{i,j}$ integration is Gaussian, the integration can be carried out easily to give to $Z_p = (2\pi\mu)^{NL/2} Z$. Thus, the pseudo-partition function Z_p differs from the true partition function Z only by a multiplicative constant so the physical observables will have the same expectation values as in the original system.

In our simulations, we first generate a Gaussian distribution for momentum $p_{i,j}$, and then let we let $\phi_{i,j}$ and $p_{i,j}$ evolve in a fictitious time t under the following equations of motion

$$\begin{aligned}
\frac{d\phi_{i,j}}{dt} &= \frac{p_{i,j}}{\mu} \\
\frac{dp_{i,j}}{dt} &= \epsilon\Delta\Big[\frac{\gamma}{\Delta^2}(2\phi_{i,j} - \phi_{i+1,j} - \phi_{i-1,j}) \\
&\qquad \gamma(2\phi_{i,j} - \phi_{i,j+1} - \phi_{i,j-1}) - \phi_{i,j} - \phi_{i,j}^3\Big]
\end{aligned}$$

This propagation should be energy conserving, but after the system has evolved for a while in t with time step δt, the energy will begin to deviate from its starting value because of the numerical errors in the integration procedure. We stop the evolution and then calculate the difference between the current and initial energies, $\delta H_p\{\phi\} = H_p\{\phi'\} - H_p\{\phi\}$, and accept the new configuration of the ϕ fields according to Metropolis Algorithm, i.e., accept with a probability of $\min(1, e^{-\delta H_p})$. This step removes the cumulative errors that arise from the numerical integration because of the finite size of the integration step. We carry out this procedure repeatedly until the statistical errors of the measured quantities are as small as required.

Because of the integration error is removed by the Metropolis step, the simple leap frog algorithm[8,9] is more than adequate for evolving the configurations of the

$\phi_{i,j}$. This algorithm evolves the system with accuracy second order in δt, with the same computational efficiency as first order integrations. Since we can allow the $\phi_{i,j}$ to drift far away from from their starting configuration, this method also has the advantage of reducing correlations among consecutive measurements. Because of parallel nature of the equations of motion, the hybrid method is very efficient on parallel (and vector) computers. This efficiency allows us to study long chains at low temperatures.

Measurements

To study whether the symmetry of the ground state is broken, we adopt the following strategy: for successively lower values of the temperature T, we study the behavior of the order parameter, the energy, and their mean-squared fluctuations as a function of ϵ and γ. In terms of the discretized action (7), we define a "quasi" inverse temperature $\beta_q \equiv \epsilon$ and a "quasi" (classical) two-dimensional Hamiltonian

$$H_q \equiv \sum_{i,j} \left[\frac{\gamma}{2\Delta}(\phi_{i+1,j} - \phi_{i,j})^2 + \frac{\Delta\gamma}{2}(\phi_{i,j+1} - \phi_{i,j})^2 + \frac{\Delta}{4}(\phi_{i,j}^2 - 1)^2 \right] \tag{8}$$

such that $\beta_q H_q\{\phi\} = S\{\phi\}$. At each value of the physical temperature, we fix γ and then use standard methods to study the energy, specific heat, and their mean-squared fluctuations to determine whether the system defined by H_q undergoes a transition from the broken to the restored symmetry state at some critical value of β_q, $\beta_{qc} \equiv \epsilon_c$.

Within this strategy, finding the condition for the broken symmetry at a fixed physical temperature for our one-dimensional quantum model is equivalent to finding the critical inverse quasi-temperature ϵ_c for the two-dimensional Hamiltonian H_q. In the absence of infinite-ranged interactions, however, a true phase transition in one-dimension can only occur for an infinite-sized system at zero temperature (i.e. for N and $L \to \infty$). Within our strategy, we search for a phase transition in a two-dimensional system whose inverse temperature is ϵ. Again, a true transition will only occur in an infinite system (i.e., for $N \to \infty$), but it can occur at a finite value of inverse quasi-temperature ϵ. We seek to determine if such a transition is indicated and if these indications remain as we increase L and N. What will distinguish our quantum simulations from those for the classical system H_q is the need to require that the physical quantities we compute to be independent of Δ to within the accuracy of our calculation.

In our simulations, we chose $L = N$ or $L = 2N$. These choices were a compromised concession to the intuitive and empirical fact that high aspect ratio rectangular space time lattices inhibit efficient propagation of the $\phi_{i,j}$ configurations. As we lower the temperature, we also reduce finite-size effects by making L increasingly larger.

Order Parameter and Susceptibility. A criterion for the symmetry state of the system is the expectation value of $\Phi = \sum_{i,j}^{L,N} \phi_{i,j}$. Since only finite sized systems can be simulated, this definition of an order parameter will change its sign as the simulation progresses and in general averages to zero independent of whether the ground state exhibits broken symmetry or not. Thus, as an indicator of the symmetry state of the system, we take for the order parameter

$$\Lambda(\epsilon) = \frac{1}{LN} \langle |\Phi| \rangle \tag{9}$$

As the size of the system N becomes very large and the true temperature $T = 1/NL$ approaches zero, the value of the order parameter will change from a finite positive value to zero if quantum fluctuations are restoring the symmetry.

Although the order parameter $\Lambda(\epsilon)$ gives direct evidence of the quantum symmetry, simply measuring it is not always a very accurate way of finding the critical

value ϵ_c. For determining a critical value, the susceptibility is more useful since it will diverge near ϵ_c. This susceptibility is defined as

$$\chi(\epsilon) = NL\beta(\langle\Phi^2\rangle - \langle|\Phi|\rangle^2) \tag{10}$$

Energy and Specific Heat. The expectation value $\langle S\{\phi\}\rangle$ is not a meaningful estimator for the energy $E(\beta)$ of the quantum system, since it diverges as $\Delta \to 0$. The difficulty lies in using

$$K_q(\epsilon) \equiv \frac{\gamma}{2\Delta}\sum_{i,j}(\phi_{i+1,j} - \phi_{i,j})^2$$

as an estimator for the kinetic energy.[4,5] To estimate the kinetic energy $K(\beta)$ of the quantum system correctly, we used the following estimator based on the Virial Principle[5]

$$K(\beta) = \frac{1}{2}\langle\phi V'\{\phi\}\rangle$$

where in the present case

$$V\{\phi\} = \Delta\sum_{i,j}\left[\frac{\gamma}{2}(\phi_{i,j+1} - \phi_{i,j})^2 + \frac{1}{4}(\phi_{i,j}^2 - 1)^2\right] \tag{11}$$

Hence, $E(\beta) \equiv K(\beta) + V(\beta)$ where $V(\beta)$ is given by (11). The specific heat $C(\beta)$ for the quantum system is simply

$$C(\beta) = \beta^2(\langle E(\beta)^2\rangle - \langle E(\beta)\rangle^2) \tag{12}$$

To find ϵ_c, on the other hand, we take $E_q(\epsilon) = \langle H_q\rangle$ and

$$C_q(\epsilon) = \epsilon^2(\langle E_q(\epsilon)^2\rangle - \langle E_q(\epsilon)\rangle^2) \tag{13}$$

It is important to note that a divergence of $C_q(\epsilon)$ does *not* necessarily imply divergent behavior in actual energy $E(\beta)$ or the specific heat $C(\beta)$. The actual and quasi energies are computed differently. This difference again underscores the intrinsic difference between a two-dimensional classical system and a $1+1$ dimensional quantum system, despite of their formal similarity.

RESULTS

We simulated a variety of system sizes, ranging from $N = 7$ ($\beta = 4.95$) to $N = 128$ ($\beta = 45.25$). The $N = 128$ calculations were done on a Thinking Machines CM 2 computer. The remainder were done on a Sun Sparcstation 1, a Convex 230, and a Cray X MP. The Cray computer ran our programs about up to 20 times faster than the Sun computer and about twice as fast as the Convex computer. The Cray computer was, however, at least 10 times slower, and sometimes 20 times slower, than the Thinking Machines computer. The speed of the latter provided us the opportunity to simulate efficiently a rather large system at a very low temperature. The simulations on the CM 2 took about 65 minutes of computation time for 40,000 measurements and about 120 minutes for 80,000.

We found that Δ satisfying $\Delta\Omega \approx \frac{1}{4}$ was sufficient to reduce the Δ dependence of our results to within our statistical error. This choice is a comprise between the need to have Δ small to be in the quantum regime, at the cost of increased computation

time, and to have Δ sufficiently large to control computation time, at the risk of being in the classical regime.

For the pseudo-time-step δt, we typically chose $\delta t\Omega \approx 3.5$. With this choice our Monte Carlo acceptance rate was 90% to 95%. This rate seemed reasonable. In the Hybrid Method, one of the things that we are trying to achieved is a global updating of the configurational variables $\phi_{i,j}$. We accomplish this by integrating the equations of motion and using the Monte Carlo step to eliminate the need to monitor and adjust the integration step size δt. The idea is to choose this step-size to keep things close and to use the Metropolis algorithm to cull out cases that deviate a bit too far from the initial energy. The average, absolute value of the relative deviation from energy conservation was approximately 1.5×10^{-4}.

To promote decorrelated measured values, we usually made measurements after every second Monte Carlo step. For the smaller chain lengths, we made 20 000 measurements, while for the larger ones, 100,000 measurements. The measurements were grouped into bins, and the average of each bin was computed. The desired expectation values were the average of the bin averages. Our error estimates were based on the sample estimate of the variance of the bin averages.[10]

To estimate ϵ_c, we used the Cumulant Intersection Method.[6,10,11] Here, one computes

$$U_N = 1 - \frac{\langle \phi^4 \rangle_N}{3\langle \phi^2 \rangle_N} \tag{14}$$

for each chain length (and hence T) as a function of the inverse quasi-temperature ϵ. This quantity measures the size of the system relative to the coherence length ξ. To find ϵ_c, one plots the ratio $R(\epsilon) = U_{N'}/U_N$ for various pairs of lattice sizes as a function of ϵ. At the critical point, $R(\epsilon_c) = 1$. Accordingly, ϵ_c is found by searching for the point of common intersection of the curves . Since the point of intersection is independent of system size, this method returns an estimate for ϵ_c extrapolated to the thermodynamic limit and to zero temperature.

In practice, the curves never intersect precisely at a point and care must be taken in interpolation between measure values of $R(\epsilon)$. To reduce the computation time near the critical point, we used the Histogram Method of Ferrenberg and Swendsen.[12] In this method, at a given inverse quasi-temperature ϵ' (and actual inverse temperature β), one collects a histogram of the measured values of the energy to construct an estimate of the density of states $\rho(E)$ and the dependence of ϕ on E. With these, one then estimates the moments of $\phi(E)$ as a function of ϵ by using

$$\langle \phi^n \rangle_{N,\epsilon'} = \frac{\int \rho(E)\phi(E)^n e^{(\epsilon - \epsilon')E} dE}{\int \rho(E) e^{(\epsilon - \epsilon')E} dE}$$

and then obtains (14) and hence $R(\epsilon)$ for the different pairs of N and N'. This estimate for (14) is accurate in a narrow region around ϵ', but this region is wide enough so that the overlap of ϵ dependence from adjacent values of ϵ' will allow a smooth accurate curve for $R(\epsilon)$ to be produced with fewer simulations than needed to compute the same curve with another sequence of necessarily more closely spaced ϵ' values.

Our principal result is shown in Fig. 1 where we plot the phase diagram as a function of the model parameters ϵ and $1/s$. The straight line with a slope of approximately 2 is the phase boundary estimated from the continuum theory results of (5) and (6). It predicts the existence of a restored symmetry phase above this line. The markers in this figure are the results from the quantum Monte Carlo simulation. Above the curve represented by these points lies the restored symmetry phase. We

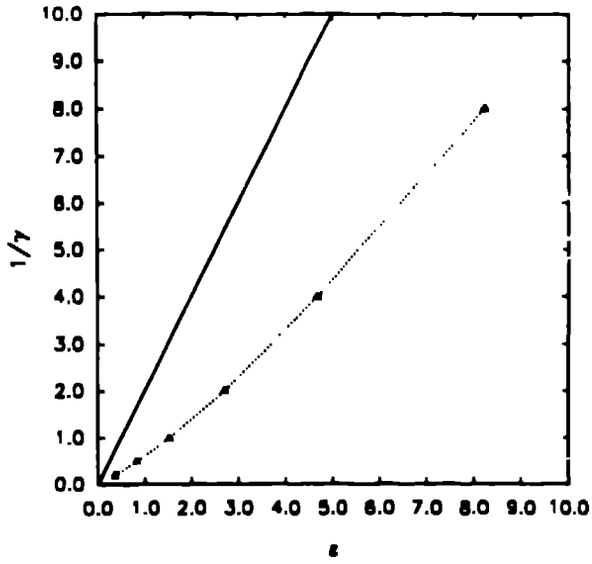

Fig. 1. The phase diagram. The straight line is the phase boundary predicted from the perturbation analysis of the continuum limit; the makers are the results obtained from the simulations. The restored symmetry phase lies above the curve represented by these markers.

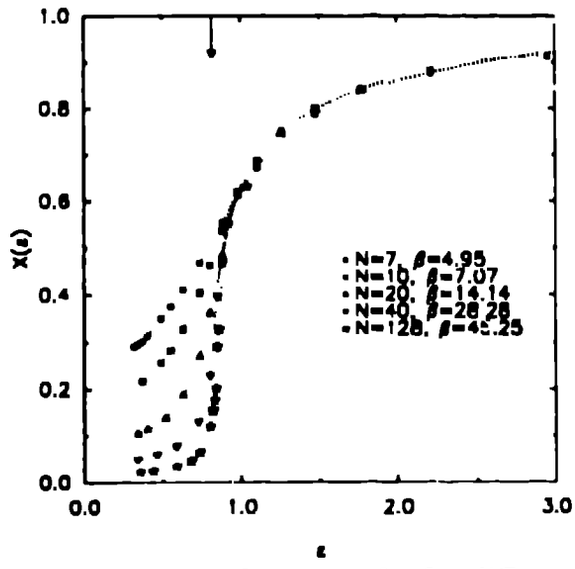

Fig. 2. The order parameter as a function of ϵ for different system sizes. Its value for a classical system is unity. The down-ward arrow marks $\epsilon_c \approx 0.82$. Here, $\gamma = 2$.

see that the continuum theory qualitatively predicts the correct physics, but quantitatively the the transition actually occurs more easily.

The behavior of the order parameter from different chain lengths as a function of ϵ is shown in Fig. 2. Out normalizations are such that the classical value of $X(\epsilon)$ is unity, independent of size and ϵ. From this figure, we see that quantum effects always reduce the order parameter relative to the classical value and that above an $\epsilon_c \approx 0.82$ the symmetry is broken. Clearly, as N (and hence β becomes large) the quantum order parameter curves are tending toward a definite value of ϵ_c.

The susceptibility (10) for different chain lengths as a function of ϵ is shown in Fig. 3. As N increases, the peak in $\chi(\epsilon)$ is clearly diverging around the same value

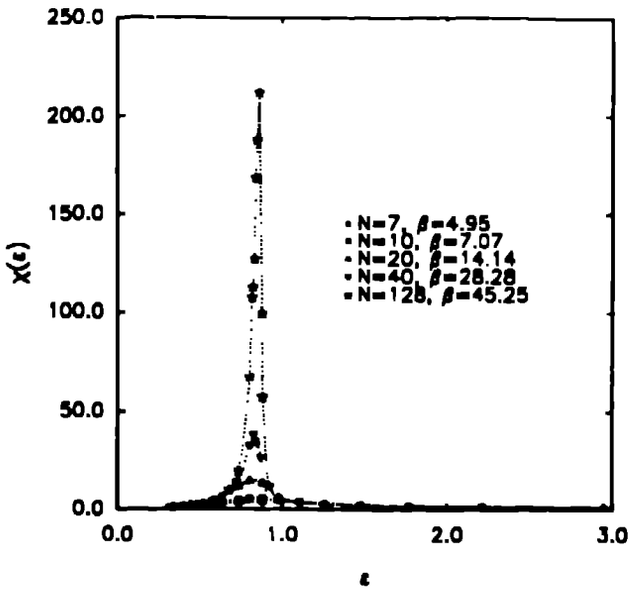

Fig. 3. The susceptibility $\chi(\epsilon)$ as a function of ϵ for different sizes. $\gamma = 2$. The peak in $\chi(\epsilon)$ occurs at approximately the same value of ϵ at which the order parameter, shown in Fig. 2, is vanishing.

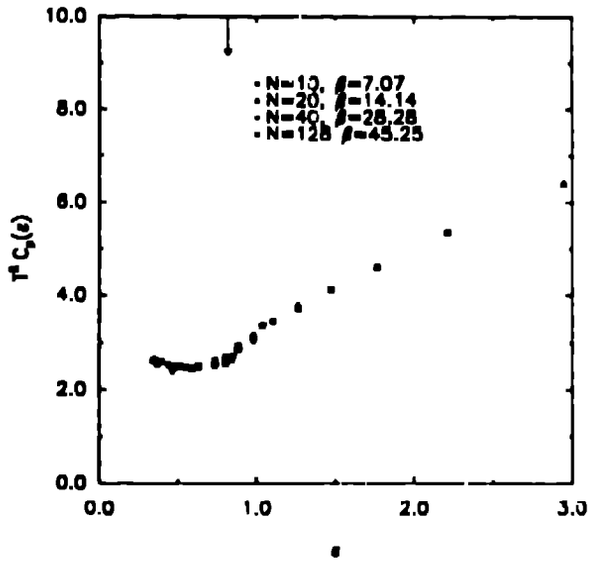

Fig. 4. The specific heat $C_p(\epsilon)$ times the temperature T squared as a function of ϵ for different system sizes. The approximate universality of the curve for different system sizes suggests that specific heat critical exponent α is around 2. The down-ward arrow marks $\epsilon_c \approx 0.82$. $\gamma = 2$.

of ϵ (≈ 0.82) at which the order parameter was disappearing in Fig. 2. On the other hand, in Fig. 1, we plotted T^2 times the specific heat $C_q(\epsilon)$ (13) as a function ϵ, and we see an absence of a peak and any size dependence in the results. These observations suggest that the specific heat critical exponent α is approximately 2. This is an unusual finding. For narrow deep wells, as found in simulations of the isotropic, two-dimensional, classical version of a discrete ϕ^4 theory, this exponent is Ising-like, i.e., approximately zero, plus log corrections, while in the other extreme of shallow broad wells, the exponent seems to be mean-field-like with a value of 1.[6,7] In one-dimension, the specific heat of the Ising model vanishes exponentially as $T \to 0$

and $\alpha = \frac{3}{2}$ for mean-field theory.[13]

CONCLUDING REMARKS

We have presented numerical evidence that quantum fluctuations can produce a symmetric ground-state in the double-well chain, restoring the symmetry that is broken classically. We presented the phase diagram for this model that shows the symmetry restoration occurs more easily than predicted by a perturbation theory calculation of the continuum limit of the model. In another paper will report the full details of our analysis and results.[14]

The suggestion from our numerical results on the specific heat that the phase transition from the restored symmetry state to the broken one does not lie in the Ising or Gaussian universality classes as suggested for the classical model perhaps should not be surprising.[15] We are currently trying to determine the universality class for the model by a combination of standard finite-size scaling methods[10] and more novel conformal-charge methods.[16,17]

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