# Charge-Density-Wave to Spin-Density-Wave Transition in the Extended Hubbard Model

J. E. Hirsch
*Department of Physics, University of California, San Diego, La Jolla, California 92093*
(Received 10 September 1984)

Monte Carlo simulations are used to study the charge-density-wave to spin-density-wave transition in the one-dimensional Hubbard model with on-site ($U$) and nearest-neighbor ($V$) repulsion. The transition is found to be continuous for small $U$ and first order for large $U$, with the crossover occurring around $U \sim 3$. The transition line deviates somewhat from the theoretical prediction $U = 2V$ towards the charge-density-wave phase for intermediate coupling. A qualitative explanation for the results is given by use of strong-coupling arguments.

PACS numbers: 72.15.Nj, 64.70.Kb

The properties of the one-dimensional electron gas have been extensively studied in recent years.[1,2] With use of renormalization-group (RG) techniques a phase diagram, valid in the weak-coupling regime, is obtained. Furthermore, strong-coupling expansions[3-5] provide additional information and in general the results of these agree with the weak-coupling predictions so that one can assume a smooth matching of both solutions. The relations between weak- and strong-coupling results are discussed in detail by Emery.[2]

Recently developed quantum Monte Carlo techniques[6] allow the picture to be completed by providing quantitative information about the system in intermediate-coupling regimes. These techniques are most useful to study quantitatively phenomena that occur away from the range of validity of either weak- or strong-coupling expansions, and I discuss here such a situation.

We will be concerned with the charge-density-wave (CDW) to spin-density-wave (SDW) transition in the extended half-filled Hubbard model. The Hamiltonian is

$$H = -t\sum_{i,\sigma}(c_{i\sigma}^{\dagger}c_{i+1\sigma} + \text{H.c.}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow} + V\sum_{i} n_i n_{i+1} \tag{1}$$

with $n_i = n_{i\uparrow} + n_{i\downarrow}$. Both weak-[1,2] and strong-coupling[7] theory predict the CDW-SDW transition to occur at $U = 2V$. One may speculate that a symmetry of the model forces the transition to occur at $U = 2V$ for all values of $U$. Such a situation occurs for the transition between singlet pairing (SP) and CDW phases for $U < 0$: Both weak- and strong-coupling theories predict the transition to occur at $V = 0$.[4] In addition, because the symmetry transformation

$$\begin{aligned} c'_{i\uparrow} &= \cos\theta\, c_{i\uparrow} + (-1)^i \sin\theta\, c_{i\downarrow}^{\dagger}, \\ c'_{i\downarrow} &= -\sin\theta\, c_{i\uparrow} + (-1)^i \cos\theta\, c_{i\downarrow}^{\dagger}, \end{aligned} \tag{2}$$

for $\theta = \pi/2$ interchanges SP and CDW correlation functions and leaves the Hamiltonian invariant if $V = 0$, one can conclude that the CDW-SP transition occurs at $V = 0$ for all values of $U$.

One of the purposes of this Letter is to show that such a symmetry does not exist for the CDW-SDW transition. The simulations clearly indicate small deviations from the $U = 2V$ line for intermediate values of $U$. This was also found recently by Fourcade and Spronken[8] from exact diagonalization of small chains. The other purpose is to study the character of the transition. Haldane[9] recently predicted, using weak-coupling arguments, that the transition should change from continuous to first order as $U$ is increased. The simulations show that indeed such a change in the character of the transition occurs, at a value of $U$ of approximately 3. A similar change from continuous to first-order transition was recently found in the two-dimensional classical $xy$ model[10]; one may speculate that both problems are related.

I have performed simulations on lattices of up to $N = 32$ sites, using the method of Ref. 6. The number of time slices was taken to be $L = N$, and the time slice size $\Delta\tau = 0.25$, so that $\beta = N/4$. This temperature is sufficiently low that fluctuations are expected to be quantum rather than thermal. A typical simulation involved 10 000 sweeps through the lattice, with measurements performed every five sweeps.

To obtain a rough idea of the behavior of the system, consider cycles in which the value of $V$ is first increased and then decreased in small steps for fixed $U$. Figure 1 shows results for the CDW order

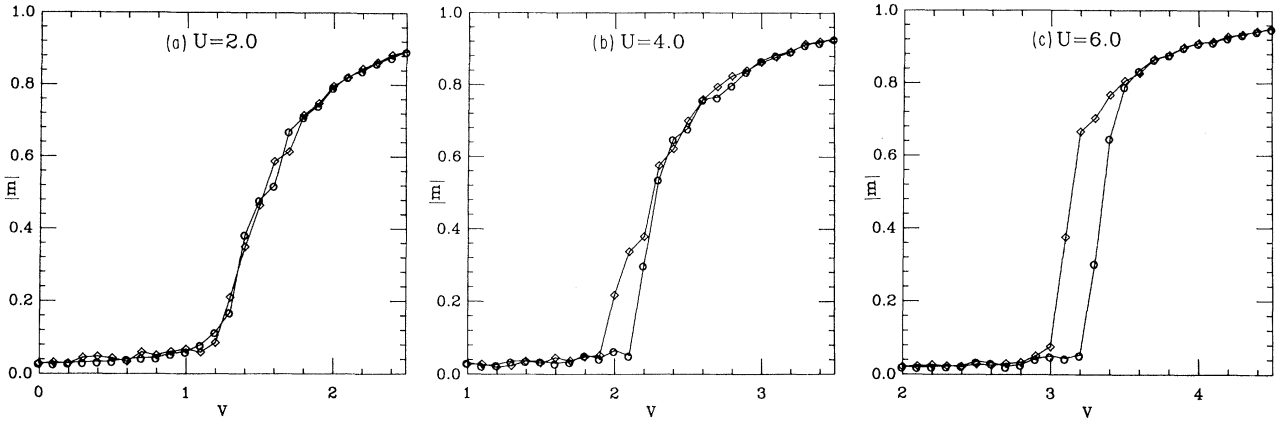


FIG. 1. Absolute value of CDW order parameter vs $V$ for $U=2$, 4, 6 on a $32\times32$ lattice. At each point 100 sweeps through the lattice were performed, and $V$ was changed in steps of 0.1. The circles (diamonds) were obtained with increasing (decreasing) $V$.

parameter

$$m=\frac{1}{N}\sum_i(-1)^i\langle n_i\rangle \tag{3}$$

for $U=2$, 4 and 6. Note that the transition does occur roughly at $V\sim U/2$. As $U$ is increased, the transition becomes sharper and wider hysteresis cycles are obtained indicating that it is turning first order. However, the presence or absence of hysteresis does not provide a precise quantitative criterion about the character of the transition since it is also dependent on the speed with which one sweeps through the transition.

To accurately determine the transition point, we study the behavior of correlation functions for different size lattices, in particular the CDW structure factor

$$S(q)=\frac{1}{N}\sum_{i,j}\exp[iq(R_i-R_j)]\langle n_i n_j\rangle \tag{4a}$$

and the zero-frequency SDW susceptibility

$$\chi(q)=\frac{1}{N}\int_0^\beta d\tau\sum_{i,j}\langle[n_{i\uparrow}(\tau)-n_{i\downarrow}(\tau)][n_{j\uparrow}(0)-n_{j\downarrow}(0)]\rangle. \tag{4b}$$

If we scale the spatial size $N$ and the inverse temperature $\beta$ by the same factor, $S(q=\pi)$ will diverge linearly with $N$ if we are in the CDW phase and $\chi(q=\pi)$ will diverge linearly in the SDW phase. As an example, Fig. 2 shows results for $U=2$. For $V=1.1$, the system is still clearly in the SDW phase, since $\chi(q)$ diverges and $S(q)$ is flat. I estimate the transition point at $V=1.15$ here. Similar calculations yielded for the transition point $V=1.675$ and 2.163 for $U=3$ and 4, respectively.

To study the character of the transition we look at histograms of the CDW order parameter. Figure 3 shows histograms for the case $U=6$, where the transition is clearly first order: the CDW and SDW phases coexist, and the relative strength of the peaks at $m=0$ and $m\sim0.5$ shifts as $V$ is changed from 3.15 to 3.1625. For $U=3$, we see still some evidence of a weakly first-order transition at $V=1.675$, as a broad peak around $m=0.25$ and some indication of another peak around 0, as shown in Fig. 4. For other values of $V$, no coexistence was found. For $U$ less than 3, I do not find coexistence

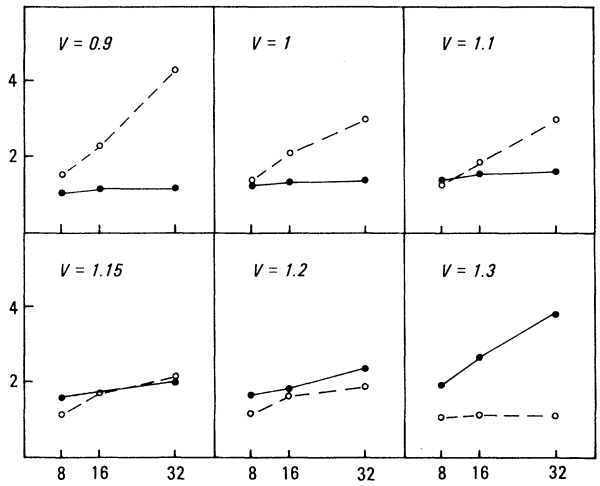


FIG. 2. CDW structure factor (solid line) and SDW susceptibility (dashed line) vs lattice size for $U=2$ and several values of $V$.

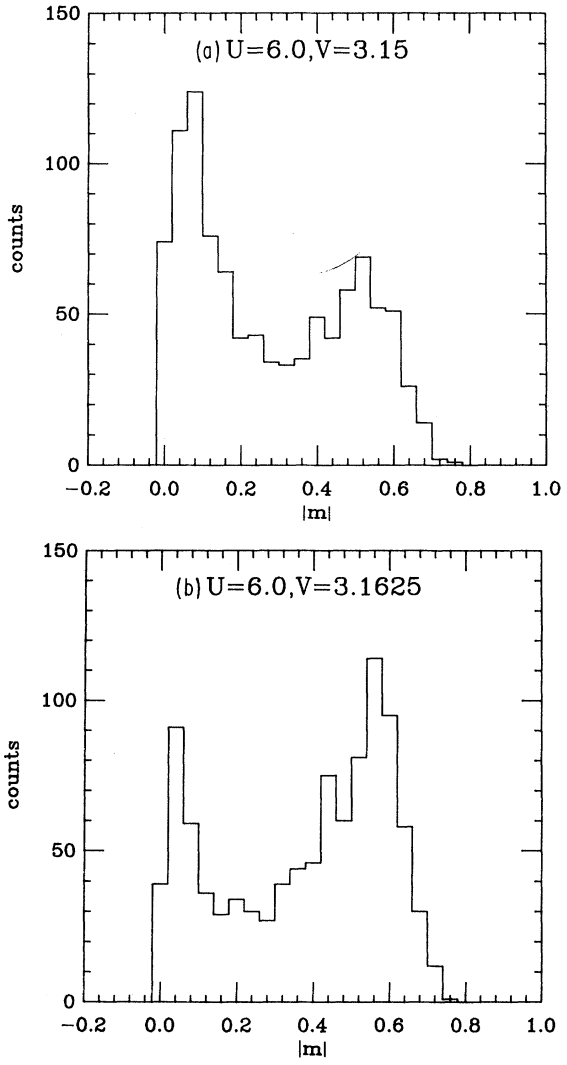


FIG. 3. Histograms of the absolute value of the CDW order parameter, Eq. (3), for $U=6$, and two values of $V$ on a $32\times32$ lattice. The double-peak structure indicates that the transition is first order.

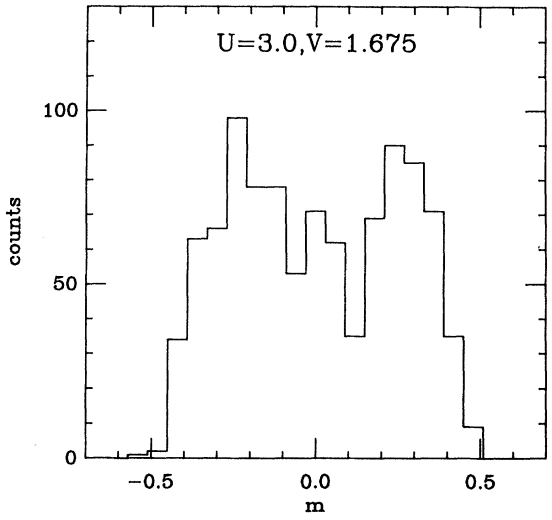


FIG. 4. Histogram of the CDW order parameter for $U=3$, $V=1.675$. The three-peak structure indicates that the transition is still weakly first order here.

of both phases. I conclude that the transition becomes first order around $U=3$, or slightly below, and becomes rapidly strongly first order as $U$ is increased.

Figure 5 summarizes the results for the CDW-SDW transition. The SDW region is slightly larger than predicted by the $U=2V$ line, and the transition changes from continuous to first order around $U=3$.

We can understand the numerical results qualitatively starting from strong-coupling theory. For large $U$ and $V$, we can neglect the effect of $t$ and the ground state consists of either pairs occupying alternating lattice sites (CDW) with energy $E=NU/2$, or all singly occupied sites (SDW), with energy $NV$, so that the transition occurs at $U=V/2$. Consider now the system close to the transition for $V>U/2$, i.e., in the CDW state. The low-lying excitations are "droplets" of the SDW phase, with energy $\epsilon(n)=V-n(U-2V)$ for a droplet of size $n$. $V$ is the surface energy, which is the dominant term for small $n$. If we now let $V$ become smaller than the critical value $U/2$, there will be a critical droplet size $n_{\rm crit}=V/(U-2V)$ such that droplets with $n>n_{\rm crit}$ are energetically favored, and the system will tunnel to the other phase by nucleation. This clearly describes a first-order transition. For a finite value of the hopping $t$, the droplet energy is

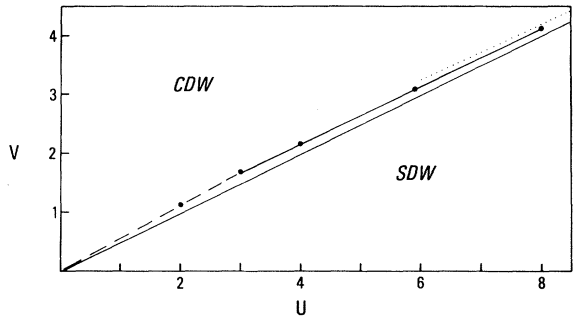


FIG. 5. Phase boundary between CDW and SDW regions. The solid line is $U=2V$, the dotted line the strong-coupling prediction. The dashed and solid lines connecting the Monte Carlo points indicate continuous and first-order transitions, respectively.

lowered by the kinetic energy term, since a droplet of size $n$ can occupy $n+1$ sites. The kinetic energy lowering is proportional to $t$ and largely independent of the size of the droplet, so that one can think of it as a surface term. It plays a role analogous to the entropy of the droplet boundary in a classical model. The energy of a droplet is then $\epsilon(n) = V - ct - n(U-2V)$ with $c$ a constant. For $V \sim t$, the two surface contributions cancel and it becomes advantageous to nucleate many droplets of arbitrary size as $V$ is reduced below $U/2$, so that the transition becomes continuous.

We can also understand the deviation of the boundary line from the $U=2V$ line in strong coupling. The energy of the CDW ground state to second order in $t$ is

$$E_{\mathrm{CDW}} = -N\left(\frac{U}{2} + \frac{2t^2}{3V-U}\right). \quad (5)$$

In the SDW phase, we obtain, to second order in $t$, an effective Hamiltonian describing a Heinsenberg antiferromagnet, with $J_{\mathrm{eff}} = t^2/(U-V)$, so that the ground-state energy, from the Bethe-*Ansatz* solution, is

$$E_{\mathrm{SDW}} = -N\left(V + \frac{4t^2 \ln 2}{U-V}\right). \quad (6)$$

For $U=2V$, $E_{\mathrm{SDW}} < E_{\mathrm{CDW}}$ so that the system is in the SDW phase. This happens because of the higher entropy of the SDW phase. For $t=0$, the CDW ground state is only doubly degenerate while the degeneracy of the SDW state is $\binom{N}{N/2}$; as $t$ is turned on, it lifts this large degeneracy and lowers the energy more than for the CDW phase. By equating the energies of both phases, a strong-coupling phase boundary is obtained, shown as the dotted line in Fig. 5. [The difference between $V$ and $U/2$ in the denominators of Eqs. (5) and (6) is neglected for consistency.] It can be seen that the numerical results do not yet make contact with the strong-coupling results in the parameter range studied.

In summary, I have for the first time studied the change in the character of a transition in a quantum system using Monte Carlo simulations: I showed that the CDW-SDW transition in the Hubbard model changes from continuous to first order as the interaction increases. I have also obtained accurate values for the transition point for intermediate coupling values, and showed that it deviates from the $V=U/2$ line. The deviation, however, was found to be remarkably small for all values of the couplings.

I am grateful to D. Haldane for a stimulating conversation on the character of the CDW-SDW transition. This work was supported by the National Science Foundation under Grant No. DMR-82-17881.

[1]J. Solyom, Adv. Phys. **21**, 201 (1979).

[2]V. J. Emery, in *Highly Conducting One-Dimensional Solids,* edited by J. Devreese, R. Evrand, and V. van Doren (Plenum, New York, 1979).

[3]P. Pincus, P. Chaikin, and C. Coll, Solid State Commun. **12**, 1265 (1973).

[4]V. J. Emery, Phys. Rev. B **14**, 2989 (1976).

[5]M. Fowler, Phys. Rev. B **17**, 2989 (1978).

[6]J. Hirsch, D. Scalapino, R. Sugar, and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).

[7]R. A. Bari, Phys. Rev. B **3**, 2662 (1971).

[8]B. Fourcade and G. Spronken, Phys. Rev. B **29**, 5096 (1984).

[9]D. Haldane, private communication.

[10]J. Van Himbergen, Phys. Rev. Lett. **53**, 5 (1984); E. Domany, M. Schick, and R. H. Swendsen, Phys. Rev. Lett. **52**, 1535 (1984).