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Large-Scale Calculations for Hadron Spectroscopy

Claudio Rebbi[1]

Some recent Monte Carlo calculations for quantum chromodynamics, performed on Euclidean lattices of rather large extent, are reviewed. The purpose of the calculations is to provide accurate determinations of quantities, such as interquark potentials or mass eigenvalues, which are relevant for hadronic spectroscopy. Results obtained in quenched QCD on $16^3 \times 32$ lattices are illustrated, and a discussion of computational resources and techniques required for the calculations is presented.

KEY WORDS: Quantum field theories (QFT); numerical simulations of QFT; lattice quantum chromodynamics (QCD).

It was a great pleasure for me to give a talk at the meeting, at which the papers in this issue were presented, dedicated to Professor Metropolis, to whom all of us working on computer simulations owe so much.

I first heard about the Metropolis method many years ago at a conference held at the International Centre for Theoretical Physics in Trieste. I was not doing research in the field of computer simulations at the time, and I do not even remember the year or what exactly the conference was about. I just attended a few talks out of general interest, and I heard about this method for approximating the weighted integral over configuration space by letting particles perform random moves and then accepting or rejecting the moves with a probability related to the variation of the weight factor. It appeared to me a very clever algorithm, and it stayed in the background of my mind. So when several years later at BNL I heard from Robert Swendsen about his studies of critical behavior of spin systems, the Metropolis method he was using for the computer simulations sounded

[1] Physics Department, Brookhaven National Laboratory, Upton, N.Y., 11973 U.S.A.

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familiar and natural. It was then that Mike Creutz, Laurence Jacobs, and I began to do computer studies of the simplest lattice gauge models.

A long time has passed since that conference at the ICTP, and the power of computational devices has increased enormously, to the point that computer simulations can be used to obtain rather accurate results for many problems in quantum fields theories. The numerical study of quantum field theories represents one of the most demanding applications of computers. This follows from the four-dimensional nature of the problem and the very large number of degrees of freedom that realistic simulations have to contend with.

The most important applications of Monte Carlo simulations to quantum field theories relate to the theory of strong interactions known as quantum chromodynamics (QCD) in which, when the theory is formulated on a Euclidan lattice, the dynamical variables are gluon fields U_x^μ, i.e., finite elements of the $SU(3)$ group of color transformations, defined over the oriented links of the lattice, and quark fields $\Psi_x \bar{\Psi}_x$, transforming according to the fundamental representation of the color group, defined over the sites of the lattice.[1] The goal is to evaluate integrals

$$\begin{aligned} \langle O \rangle &= Z^{-1} \int \prod_{x,\mu} dU_x^\mu \prod_x d\bar{\Psi}_x d\Psi_x \, O(U, \Psi, \bar{\Psi}) \, e^{-S_G - S_M} \\ Z &= \int \prod_{x,\mu} dU_x^\mu \prod_x d\bar{\Psi}_x \, d\Psi_x \, e^{-S_G - S_M} \end{aligned} \tag{1}$$

which give the observables of the theory. The action S in (1) is the sum of two terms, the gauge field action S_G and the quark field action S_M. There is a large degree of freedom in formulating a lattice action, although all choices should produce the same continuum limit. A typical form for the gauge field action is

$$S_G = \frac{6}{g^2} \sum_{\substack{x \\ \mu < \nu}} \left(1 - \frac{1}{3} Re \, \mathrm{tr} \, U_x^{\mu\nu} \right) \tag{2}$$

where $U_x^{\mu\nu} = U_x^{\nu\dagger} U_{x+\hat{\nu}a}^{\mu\dagger} U_{x+\hat{\mu}a}^{\nu} U_x^\mu$, a is the lattice spacing, and g is the unrenormalized coupling constant. (In numerical calculations one frequently parametrizes results in terms of a coupling parameter $\beta = 6/g^2$ rather than g). The action of the quark field is a bilinear function of the quark variables

$$\sum_{xy} \bar{\Psi}_x \, D(U)_{xy} \, \Psi_y + m \sum_x \bar{\Psi}_x \Psi_x \tag{3}$$

connecting quark fields at neighboring sites through the kinetic term $D(U)_{xy}$. The kinetic term contains factors of U_x^μ required to make the couplings between neighboring quark fields gauge-invariant. These factors

couple the Ψ fields to the U field, just as in the continuum theory the kinetic term $\bar{\Psi}\gamma^{\mu}(\partial_{\mu} - igA_{\mu})\Psi$ couples matter fields to gauge fields through the covariant derivatives.

The lattice spacing a is related to the (unrenormalized) coupling constant g in (2) by the renormalization procedure and, in asymptotically free theories such as QCD, the continuum limit $a \to 0$ is approached for $g \to 0$. In actual QCD calculations one finds that a reasonably good approximation to the continuum limit is achieved for many observables when $a \sim 0.1$ Fm, which is not unreasonable since 1 Fm is a typical scale for strong interactions. This, however, implies that lattices extending for at least 10 sites in each direction should be used for realistic calculations. To see what this implies in terms of computational requirements, let us consider explicitly a lattice with $16^3 \times 32$ sites, such as the one used to obtain some of the results which I describe later[2-5] and which represents one of the largest sizes utilized up to now for QCD calculations. A lattice of this size involves $4 \times 2^{17} \sim 520000$ U variables. Since it is convenient to represent these in memory in explicit 3×3 matrix notation, over 9 million real variables must be stored in memory. About the simulation procedure, the typical upgrading step in the Metropolis algorithm, $U_x^{\mu} \to U_x^{\mu\prime}$, requires approximately 4000 arithmetic operations if one is content with reproducing the $\exp\{-S_G\}$ distribution, neglecting the influence on the measure of the quark fields. Since a typical calculation may involve hundreds or thousands of sweeps through the whole lattice, the simulation is practical only if the upgrade $U_x^{\mu} \to U_x^{\mu\prime}$ can be done in microseconds. This is possible with today's most powerful supercomputers, exploiting their vectorized architecture.

If one wants to take into account the dynamical effects of the quark fields, the situation becomes more complicated. The Ψ, $\bar{\Psi}$ variables are anti-commuting elements of a Grassman algebra rather than ordinary c numbers, and it is problematic to incorporate them directly in a simulation because, for space-time dimensionality larger than 2, one runs into negative probabilities. One can, however, perform the integration over $d\bar{\Psi}d\Psi$ explicitly, since the measure is Gaussian in these variables, obtaining

$$\begin{aligned} \langle O \rangle &= Z^{-1} \int \prod_{x,\mu} dU_x^{\mu} \langle O \rangle_U e^{-S_G} \det[D(U) + m] \\ Z &= \int \prod_{x,\mu} dU_x^{\mu} e^{-S_G} \det[D(U) + m] \end{aligned} \tag{4}$$

where $\langle O \rangle_U$ stands for the expectation value of $O(U, \Psi, \bar{\Psi})$ over the quark fields at given background U_x^{μ}.

The integration is now over the gauge field variables only, and it can be shown that the measure is positive-definite. However, the fermionic

determinant, which appears as a new factor in the measure and which accounts for the dynamical effects of the quarks, is a nonlocal function of the gauge variables U_x^μ. An exact calculation of the variation of the determinant at each upgrading step $U_x^\mu \to U_x^{\mu\prime}$ is way too time-consuming for any lattice but those of the smallest size.

It is an established fact that the most important properties of QCD emerge from the quantum fluctuations of the gauge field. This prompted an approximation, called the quenched[6] or valence[7] approximation, whereby the determinantal factor in the measure is neglected altogether. Neglecting the $\det[D(U)+m]$ factor in the measure corresponds to leaving out of the calculation all corrections induced by the creation and annihilation of virtual $q-\bar{q}$ pairs. One does not claim that the quenched approximation has no effect; there are certainly problems where the quantum mechanical fluctuations of the quark field play a crucial role, an example being the thermodynamical properties of the quark–gluon plasma. Also, in general, the relationship between lattice spacing and the unrenormalized coupling constant will be affected by the inclusion of virtual $q-\bar{q}$ processes. The hope is, however, that for many problems, apart from the change of scale induced by the different renormalization, the inclusion of dynamical fermions may induce only corrections negligible in first approximation.

Methods to incorporate the effects of the $\det[D(U)+m]$ factor in Monte Carlo simulations have been proposed.[8] For lattices of realistic size this can be done only approximately, and the time per step increases very substantially anyway.

The largest lattices have been considered in the context of the quenched approximation. One of the most fundamental problems of QCD is the calculation of the spectrum of masses from the first principles of the theory, and in the rest of my talk I shall concentrate on this problem since it exemplifies what can be achieved by numerical methods.

One may pursue two different approaches, one likely to be more accurate but applicable only to the spectroscopy of heavy quark systems, the other of more general validity. One may use a lattice numerical calculation to evaluate the static potential, and possibly also its higher-order corrections, to be used in a Schrödinger equation for the calculation of the bound states of heavy quarks. The static potential is derived from the numerical evaluation of the so-called Wilson loop factors, i.e., the expectation values of the transport factors obtained by multiplying the U variables along the sides of a rectangle of sides ma and na

$$W_{mn} = \langle \tfrac{1}{3} \operatorname{Re} \operatorname{tr}(U_x^{\nu+} \cdots U_{x+n\hat{\nu}a}^{\mu+} \cdots U_{x+m\hat{\mu}a+(n-1)\hat{\nu}a}^{\nu} \cdots U_{x+(m-1)\hat{\mu}a}^{\mu} \cdots U_x^{\mu}) \rangle \tag{5}$$

It can be shown that W_{mn}, which describes the variation of the vacuum–vacuum transition amplitude induced by a static $q-\bar{q}$ pair at separation ma (identifying the ma side with a space-like displacement and the na side with a time-like one), behaves for large n as

$$W_{mn} \sim e^{-na\,V(ma)} \tag{6}$$

V being the static $q-q$ potential. This allows one to extract V from a sufficiently accurate determination of W_{mn}.

The calculations of largest scale for the evaluation of the static potential have been presented in Refs. 2, 3, 9, and 10). Figure 1 illustrates the results (the attractive force, rather than the potential, is displayed in the figure). The numerically determined potential has been used in Ref. 11 to

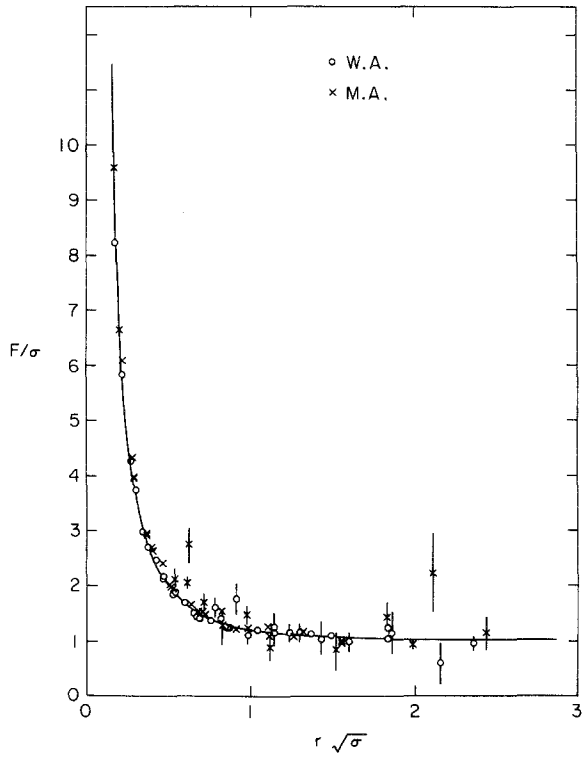

Fig. 1. A determination of the force between static $q, \bar{q}$ by Monte Carlo methods. The two symbols correspond to numerical results obtained with two different lattice actions, which should give the same value for the force in the continuum limit. The solid line represents a fit to the numerical data incorporating the expected behavior at short distances, which can be calculated from perturbative QCD. Units are in suitable powers of the string tension $\sigma \approx (420\ \mathrm{MeV})^2$.

calculate properties of the J/Ψ and Υ families. The results obtained in Ref. 11 are reproduced in the table. The agreement between calculated values and experimental data is impressive. It is worth emphasizing that the entire calculation is from first principles, the heavy quark mass and an overall scale being the only parameters in the calculation. By considering the expectation value of more elaborate transport factors, namely for rectangular loops with space-like or time-like plaquette insertions, one can also calculate the spin-dependent potentials responsible for the fine and hyperfine splitings. Some preliminary results have been reported, and large-scale calculations are in progress.[12]

Table I. Results (from Ref. 11) for the Spectroscopy of the J/4 and γ families[a]

State	Mass (GeV) (experiment)	$\Gamma(e^+e^-)/\Gamma(1S\to e^+e^-)$ (experiment)	$\langle v^2/c^2\rangle$	$\langle r^2\rangle^{1/2}$ (fm)
	$\Gamma(1S\to e^+e^-)=6.17$ keV (experiment: 4.6 ± 1.4 keV)			
$1S$	3.10 (3.10)	1.00	0.20	0.40
$1P$	3.51 (3.50)		0.22	0.62
$2S$	3.69 (3.69)	0.48 (0.41 ± 0.15)	0.26	0.79
$1D$	3.80 (3.77)		0.25	0.81
$2P$	3.96		0.29	0.97
$3S$	4.11 (4.03 ± 0.05)	0.34 (0.2)	0.32	1.12
$2D$	4.19 (4.16 ± 0.02)		0.32	1.13
$3P$	4.34		0.35	1.27
$4S$	4.48 (4.42 ± 0.01)	0.26	0.38	1.40
$3D$	4.53		0.38	1.41
$5S$	4.80	0.22	0.43	1.65
	$\Gamma(1S\to e^+e^-)=1.17$ keV (experiment: 1.22 ± 0.03 keV)			
$1S$	9.46 (9.46)	1.00	0.070	0.23
$1P$	9.87 (9.90)		0.064	0.39
$2S$	9.99 (10.02)	0.47 (0.42 ± 0.02)	0.072	0.50
$1D$	10.11		0.068	0.53
$2P$	10.22 (10.26)		0.076	0.64
$3S$	10.33 (10.36)	0.35 (0.31 ± 0.02)	0.083	0.73
$2D$	10.41		0.081	0.75
$3P$	10.51		0.088	0.85
$4S$	10.60 (10.58)	0.29 (0.24 ± 0.03)	0.095	0.94
$4P$	10.75		0.099	1.04
$5S$	10.84 (10.87)	0.26	0.107	1.11

[a] $m_c=1.70$ GeV and $m_b=5.07$ GeV.

In a more direct approach to mass calculations one starts by evaluating Green's functions such as (for mesons)

$$G_t = \sum_{\vec{x}} \langle (\bar{\Psi}\Psi)_{\vec{x},t} (\bar{\Psi}\Psi)_0 \rangle \tag{7}$$

(spin indices are left implicit in this and subsequent equations.)

Expanding into a complete set of intermediate states and recalling that the propagation is in Euclidean space-time, we may express G_t in the form

$$G_t = \sum_{\substack{n \\ \vec{p}_n = 0}} |\langle n | \bar{\Psi}\Psi | O \rangle|^2 e^{-m_n t} \tag{8}$$

where we have also made use of the fact that the sum over final space positions in (7) projects over states of 0 spatial momentum, so that $E(\vec{p}=0) = m$.

If one can calculate G with sufficient accuracy and for sufficiently long propagations in time so that the leading exponential behavior(s) can be isolated, then the mass(es) of the lowest state(s) in the channel with the quantum numbers of $(\bar{\Psi}\Psi)$ can be determined.

G itself can be computed as average over configurations in the Monte Carlo sequence of suitable products of quark propagators

$$G_t \approx \sum_{\vec{x}} \frac{1}{n} \sum_{i=i_0+1}^{i_0+n} \langle \Psi_{\vec{x},t} \bar{\Psi}_0 \rangle_{\{U\}_i} \langle \Psi_0 \bar{\Psi}_{\vec{x},t} \rangle_{\{U\}_i} \tag{9}$$

The most demanding part of the calculation becomes then the computation of the quark propagators themselves, which must be performed repeatedly and which requires solving the very large of simultaneous linear equations

$$[D(U) + m]_{xy} \langle \Psi_y \bar{\Psi}_0 \rangle = \delta_{x0} \tag{10}$$

The task is made less severe by the fact that the matrix of the system is very sparse, so that iterative procedures such as the algorithm of conjugate gradients can be used very efficiently, and by the fact that the individual quark propagators themselves exhibit an exponential rate of decay (albeit modulated by irregular fluctuations) so that, at least for not too small quark masses and not too long propagations in time, a limited statistics may be sufficient to obtain reasonably accurate hadronic propagators.

This approach has been pursued by many investigators, from the earliest investigations in Refs. 13, 14, 15 to the most recent large-scale calculations.[16,5] I would like to illustrate the method by presenting results obtained in collaboration with D. Barkai and K. Moriarty[5] working on a $16^3 \times 32$ lattice at a value of the coupling parameter $\beta = 6/g^2$, in the

quenched approximation. This is the value of β where one observes the onset of the continuum limit.

Before presenting the actual results, I must mention that the so-called Kogut-Susskind or staggered formulation of lattice fermions has been used. In this lattice transcription of the Dirac equation different spin and flavor components of four degenerate species of quarks (16 components altogether) are assigned to the sites of a 2^4 cell of the lattice. This formulation offers the advantage that a continuous chiral symmetry is present for zero quark mass even at finite lattice spacing; moreover the thinning of degrees of freedom reduces substantially the dimensionality of the matrix of the linear system that must be solved for obtaining the quark propagators. A peculiarity of staggered fermions is that factors such as $(-1)^{x_1/a}$ which change the sign from point to point of the 2^4 cell play the role of spin and flavor matrices. Moreover, the Green's functions must be expanded in terms of two contributions

$$\sum_n A_n e^{-m_n t} + (-1)^{t/a} \sum_n A'_n e^{-m'_n t} \tag{11}$$

where the two terms correspond to intermediate states of opposite parity. (On a finite lattice with periodic boundary conditions, reflected exponentials appear also in the expression for m, so that the expansion is in terms of hyperbolic cosines rather than exponentials).

We used in our calculation values for the bare (Lagrangean) quark mass $m_q a = 0.5, 0.16, 0.09, 0.04, 0.01$ and spin-flavor factors which allowed us to determine the masses of states with the following quantum numbers

mesons: $0^{-+}(\pi)$, $1^{--}(\rho)$, $1^{++}(A_1)$, $0^{++}(S)$

baryons: $\frac{1}{2}^+$ (nucleon), $\frac{1}{2}^-$ (Λ^*, but with $m_s = m_u = m_d = m_q$)

The results are illustrated in Figs. 2 and 3. Figure 2 shows that, especially for small quark masses, the mass of the state with the quantum numbers of the π is proportional to $m_q^{1/2}$, giving strong indication that chiral symmetry is dynamically broken with a massless Goldstone boson for zero quark mass even with finite lattice spacing. The behavior of all other masses as functions of m indicates instead that they tend to finite values for $m_q \to 0$. It is also interesting to notice that whereas for large quark mass the mesons and baryons have masses in a ratio of 2/3, corresponding to additivity in the heavy quark mass (renormalized, however, from its Lagrangean value), for lower quark masses baryons and meson resonances have comparable masses, in agreement with experimental data.

One can use the values of the π and ρ masses to determine the overall

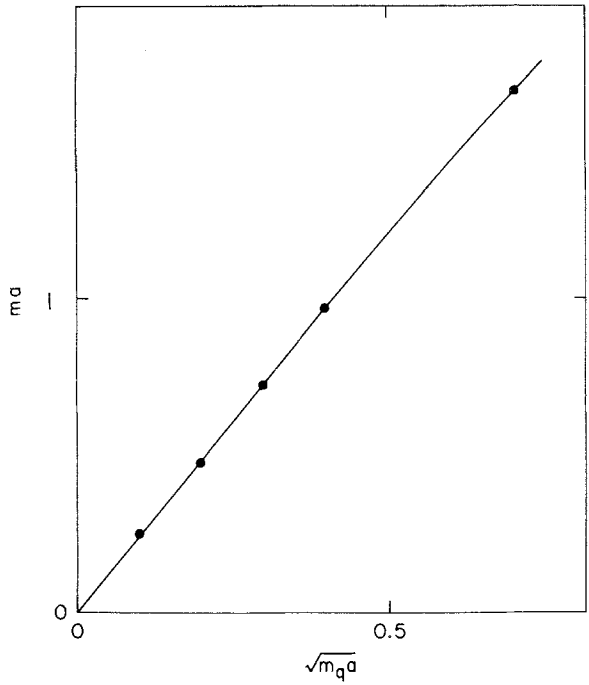

Fig. 2. Mass of the lowest pseudo-scalar meson versus square root of the quark mass, as calculated in Ref. 5.

scale of the calculation (i.e., the value of the lattice spacing a) and the quark mass. This gives

$$a^{-1} = 1659 \pm 134 \text{ MeV}$$
$$M_{u,d} \approx 2.0 \text{ MeV} \tag{12}$$

One then derives values for the other masses

$$m_{A_1} = 1497 \pm 162 \text{ (exp 1275) MeV}$$
$$m_S = 1063 \pm 79 \text{ (exp 975) MeV}$$
$$m_N = 1073 \pm 91 \text{ (exp 939) MeV}$$
$$m_{N^*} = 1300 \pm 130 \text{ (exp 1405} - \approx 177 \text{ to account for } m_s = m_u = m_d) \text{ MeV}$$

and we see that the agreement between the calculated values and the experimental data is reasonably good.

The numerical calculations such as the one described above are affected by various errors, and it is important to be able to estimate their magnitude. Sources of error are the statistical errors, inherent in the

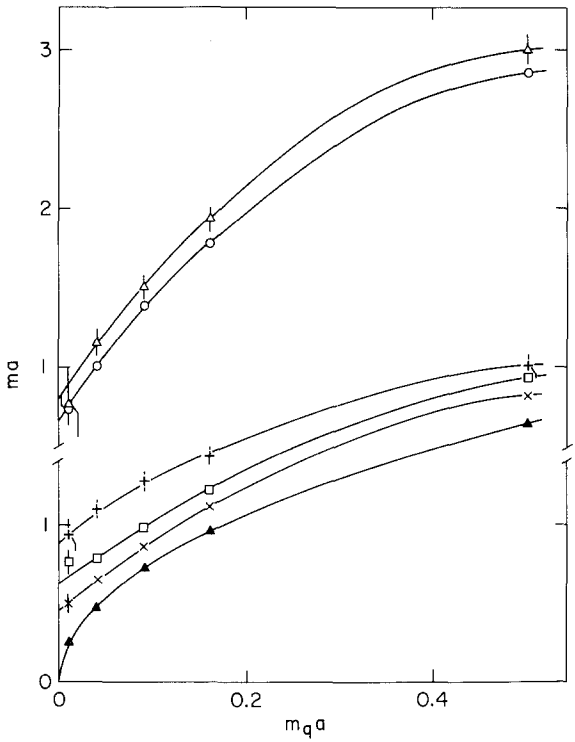

Fig. 3. Masses of several hadrons: $A^*(\frac{1}{2}^-)(\Delta)$, p, n (○), $A_1(1^{++})$ (+), $S(0^{++})$ (□), $\rho(1^{--})(x)$, π(▲), as functions of the quark mass (from Ref. 5)

simulation procedure. These are the most straightforward to estimate by standard methods of error analysis. There are then the errors induced by the finiteness of the lattice spacing and lattice volume (the ultraviolet and infrared cutoffs). Their magnitude can in principle be estimated by repeating the calculations on lattices of different sizes and with different lattice spacings (varied by varying the unrenormalized coupling constant), although it is not always practical to do so. Finally, the most insidious source of error may come from the use of the quenched approximation, i.e., the neglect of virtual $q-\bar{q}$ pairs. This can be checked only by performing calculations which incorporate the effects of dynamical fermions. Such calculations have been performed on lattices of smaller extent, especially in order to investigate chiral and finite temperature properties.[17] Recently a calculation of the spectrum with dynamical fermions has also been made.[18] While one could obtain interesting information about the scale and general features of the spectrum, the errors are still too large to make a meaningful estimate of the errors induced by the quenched approximation.

These are years when the power and availability of computational resources are progressing at an outstanding pace. This augurs very well for the future. The numerical methods introduced by Prof. Metropolis have already produced many valuable results for field theories, and we look forward to many more important and impressive applications of such powerful computational tools.

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REFERENCES

1. K. G. Wilson, *Phys. Rev. D* **10**:2445 (1974); K. G. Wilson, *Phys. Rep.* **23**:331 (1975); M. Creutz, L. Jacobs, and C. Rebbi, *Phys. Rep.* **95**:201 (1983); C. Rebbi, ed. *Lattice Gauge Theories and Monte Carlo Simulations*, (World Scientific, Singapore, 1983).
2. D. Barkai, K. J. M. Moriarty, and C. Rebbi, *Phys. Rev. D* **30**:1293 (1984).
3. D. Barkai, K. J. M. Moriarty, and C. Rebbi, *Phys. Rev. D* **30**:2201 (1984).
4. D. Barkai, K. J. M. Moriarty, and C. Rebbi, *Comput. Phys. Common.* **32**:1 (1985).
5. D. Barkai, K. J. M. Moriarty, and C. Rebbi, *Phys. Lett. B* **156**:385 (1985).
6. E. Marinari, G. Parisi, and C. Rebbi, *Nucl. Phys. B* **190**:266 (1981).
7. D. Weingarten, *Phys. Lett. B* **109**:57 (1982).
8. F. Fucito, E. Marinari, G. Parisi, and C. Rebbi, *Nucl. Phys. B* **180** [FS2]:369 (1981); D. H. Weingarten and D. N. Petcher, *Phys. Lett. B* **99**:333 (1981); H. W. Hamber, *Phys. Rev. D* **24**:951 (1981); D. J. Scalapino and R. L. Sugar, *Phys. Rev. Lett.* **46**:519 (1981); J. Polonyi and H. W. Wyld, *Phys. Rev. Lett.* **51**:2257 (1983).
9. N. A. Campbell, C. Michael, and P. Rokow, *Phys. Lett. B* **139**:288 (1984).
10. S. Otto and J. D. Stack, *Phys. Rev. Lett.* **52**:2328 (1984).
11. M. Campostrini, Phys. Lett. *B* **147**:343 (1984).
12. C. Michael and P. E. L. Rakow, Liverpool University preprint, 1985; Ph. de Forcrand and J. Stack, University of Illinois at Urbana-Champaign preprint, 1985; M. Campostrini, K. Moriarty, and C. Rebbi, in progress.
13. H. Hamber and G. Parisi, *Phys. Rev. Lett.* **47**:1792 (1981).
14. E. Marinari, G. Parisi, and C. Rebbi, *Phys. Rev. Lett.* **47**:1795 (1981).
15. A. Hasenfratz, Z. Kunszt, P. Hasenfratz, and C. B. Lang, *Phys. Lett. B* **110**:289 (1982).
16. H. Lipps, G. Martinelli, R. Petronzio, and F. Rapuano, *Phys. Lett. B* **126**:250 (1983); Ph. de Forcrand and C. Roiesnel, *Phys. Lett. B* **143**:453 (1984); K. C. Bowler, D. L. Chalmers, A. Kenway, K. D. Kenway, G. S. Pawley, and D. J. Wallace, *Nucl. Phys. B* **240** [FS12]:213 (1984); J. P. Gilchrist, G. Shierholz, H. Schneider, and M. Teper, *Nucl. Phys. B* **248**:29 (1984); A. Billoire, E. Marinari, and R. Petronzio, *Nucl. Phys. B* **251** [FS13]:141 (1985); A. König, K. H. Mütter, and K. Schilling, *Nucl. Phys. B* **259**:33 (1985); O. Martin, K. J. M. Moriarty, and S. Samuel, *Nucl. Phys. B* **261**:79 (1985).
17. F. Fucito, C. Rebbi, and S. Solomon, *Nucl. Phys. B* **248**:615 (1984); J. Polonyi, H. W. Wyld, J. B. Kogut, J. Shigemitsu, and D. K. Sinclair, *Phys. Rev. Lett. U* **53**:644 (1984); R. V. Gavai and F. Karsch, *Nucl. Phys. B* **261**:273 (1985); F. Fucito and S. Solomon, Caltech preprint CALTECH-68-1285 (July 1985).
18. F. Fucito, K. J. M. Moriarty, C. Rebbi, and S. Solomon, BNL preprint (1986).