Monte Carlo Calculation of the Spin-Dependent Potentials for Heavy-Quark Spectroscopy

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(Received 2 April 1986)

We calculate by lattice numerical methods the spin-dependent potentials relevant for heavy-quark spectroscopy. We find a long-ranged nonperturbative component in one of the spin-orbit potentials, whereas all other potentials exhibit a short-ranged perturbative behavior.

PACS numbers: 12.38.Gc, 12.40.Qq

The complex dynamics which governs the binding of quarks and antiquarks into hadrons simplifies under the assumption that the quarks are very massive. It then becomes possible to perform an expansion in inverse powers of the quark mass and, to the leading orders, the dynamics is determined by the two-body Hamiltonian[1,2]

$$H=\frac{\mathbf{p}^2}{m}+V(r)+\frac{\mathbf{S}_+\cdot\mathbf{L}_++\mathbf{S}_-\cdot\mathbf{L}_-}{2m^2}\frac{1}{r}\left(\frac{dV}{dr}+2\frac{dV_1}{dr}\right)+\frac{\mathbf{S}_+\cdot\mathbf{L}_-+\mathbf{S}_-\cdot\mathbf{L}_+}{m^2}\frac{1}{r}\frac{dV_2}{dr}$$
$$+\frac{1}{m^2}[(\mathbf{S}_+\cdot\hat{\mathbf{r}})(\mathbf{S}_-\cdot\hat{\mathbf{r}})-\tfrac{1}{3}\mathbf{S}_+\cdot\mathbf{S}_-]V_3(r)+\frac{1}{3m^2}\mathbf{S}_+\cdot\mathbf{S}_-V_4(r). \quad (1)$$

The static potential V in Eq. (1) is related to the expectation value of Wilson-loop factors, whereas the spin-dependent potentials V_i, $i=1$–4, are given by

$$\epsilon_{ijk}\hat{r}_k\frac{d\tilde{V}_1(r,T)}{dr}=\int_0^T dt\int_0^T dt'(t'-t)\langle g^2B_i(0,t)E_j(0,t')\rangle_W, \quad (2)$$

$$\epsilon_{ijk}\hat{r}_k\frac{d\tilde{V}_2(r,T)}{dr}=\int_0^T dt\int_0^T dt'(t'-t)\langle g^2B_i(0,t)E_j(\mathbf{r},t')\rangle_W, \quad (3)$$

$$(\hat{r}_i\hat{r}_j-\tfrac{1}{3}\delta_{ij})\tilde{V}_3(r,T)+\tfrac{1}{3}\delta_{ij}\tilde{V}_4(r,T)=\int_0^T dt\int_0^T dt'\langle g^2B_i(0,t)B_j(\mathbf{r},t')\rangle_W, \quad (4)$$

$$V_i(r)=\lim_{T\to\infty}\frac{1}{T}\frac{\tilde{V}_i(r,T)}{\langle 1\rangle_W}. \quad (5)$$

The symbol $\langle B_iE_j$ (or $B_j)\rangle_W$ in (2)–(5) stands for the expectation value of the path-ordered product of color fields and transport factors along the sides of rectangular loops of extent r in space and T in time. $\langle 1\rangle_W$ is the Wilson-loop factor itself. The quantum averages in (2)–(5) can be calculated numerically within the lattice formulation of QCD. Thus the static potential has been evaluated with a high degree of accuracy[3–7] and successfully used for a calculation of the spin-independent properties of the J/ψ and Υ families.[8] Here we report about the numerical determination of the spin-dependent potentials. Calculations along similar lines, albeit with less statistics or for different gauge groups, have been recently presented.[9–11]

We considered a $16^3\times 32$ hypercubical lattice with periodic boundary conditions. We calculated the quantum averages by the Monte Carlo method, using Wilson's form of the lattice action, with coupling parameter $\beta=6/g^2=6.2$, and the quenched approximation, whereby vacuum polarization effects due to light quarks are neglected. We denote by a the lattice spacing, and by U_x^μ the gauge dynamical variables defined over the links from x to $x+\hat{\mu}a$. It will be convenient to denote by $U_{x,ss'}^{\mu\nu}$ the product of the link variables U along a counterclockwise path originating at x and threading the sides of a plaquette in the (s,s') quadrant of the μ-ν plane. Thus, e.g.,

$$U_{x,-+}^{\mu\nu}=U_{x-\hat{\mu}a}^{\mu}U_{x-\hat{\nu}a}^{\nu\dagger}U_{x-\hat{\mu}a+\hat{\nu}a}^{\mu\dagger}U_x^{\nu}. \quad (6)$$

In terms of these variables we define lattice field

strengths:

$$F^{\mu\nu}_{x,ss'} = \mathrm{Im}\, U^{\mu\nu}_{x,ss'} \equiv -\tfrac{1}{2} i (U^{\mu\nu}_{x,ss'} - U^{\mu\nu\dagger}_{x,ss'}), \quad (7)$$

$$F^{\mu\nu}_{x,s} = \tfrac{1}{2} \sum_{s'} F^{\mu\nu}_{x,ss'}, \quad (8)$$

$$F^{\mu\nu}_{x} = \tfrac{1}{2} \sum_{s} F^{\mu\nu}_{x,s}. \quad (9)$$

We made the identifications $ga^2 B_i(x) \rightarrow F^{jk}_x$, ijk in cyclical order,

$$ga^2 E_i(x) \rightarrow F^{4i}_x,$$

for the correlations between fields B and E and for the correlation between the components of B in the direction of separation $\hat{\mathbf{r}}$ (i.e., the fields defined over spatial plaquettes orthogonal to $\hat{\mathbf{r}}$); but we used

$$\tfrac{1}{2} \sum_s \langle F^{ij}_{x,s} F^{ij}_{x',s} \rangle$$

to reproduce the correlation between components B^k orthogonal to the direction of separation (assumed to be along the i axis). These definitions were found in Ref. 9 to produce results in good agreement with perturbation theory also at small distances with the Abelian gauge group $U(1)$. In our Monte Carlo calculation we performed 2000 iterations (with the Metropolis algorithm and 10 hits per link) to equilibrate the system and proceeded then to 200 measurements, separated from each other by 20 Monte Carlo iterations, of the correlation functions for all rectangular loops with one spatial side of length varying from 0 to 7 links and one temporal side of length ranging from 4 to 12 links. The computation is not straightforward, because of the large number of operations needed to calculate all individual loop factors with insertions and the very large number of variables involved. The details of the program that we developed for the calculation will be presented in a separate publication.[12] We wish, however, to mention here the following points which may be of general interest.

As a first step for the measurement of the observables, the configuration of the gauge variables is transformed to the temporal gauge $U^4_x = 1$, extending the lattice by the amount necessary to contain all measurable loops (periodic boundary conditions in time cannot be maintained in the temporal gauge). The advantage of the temporal gauge is that the transport factors along the sides of the loops with the field insertions become equal to the identity, so that no matrix multiplications are needed to reconstruct the factors corresponding to the temporal sides once the lattice field strengths are calculated; moreover, the summations of the field strengths corresponding to the integrals over t and t' can be performed before the loops are closed, with enormous saving in computer time. The transport factors corresponding to the spatial bases of the loops are calculated by the "multihit" method to reduce variance as proposed by Parisi, Petronzio, and Rapuano[13]; i.e., the U^{μ}_x variables in the basis factor are first averaged in the fields of the neighboring U's and then multiplied. In the process, the field strengths are calculated as well and transport factors and field strength are temporarily stored in large memory. Finally, in a double loop over time coordinate and time extent of the loop, the field strengths are summed and combined with the transport factors for the bases in such a way as to reproduce the required integrals.

Our results are displayed in Figs. 1–4, where the functions $-dV_1/dr$, dV_2/dr, V_3, and $-V_4$ are expressed in lattice units. The potentials have been determined by performing linear fits to the dependence of the integrals on the time extent of the loops. We included all data from $T=4a$ to $T=12a$ in the fits. Fits based on the interval $5a$–$12a$, as well as a determination from the finite differences at subsequent values of t, give consistent results, although generally with larger errors. We estimated the statistical errors by repeating all calculations over subsamples of measurements, obtained by leaving out of the total sample sets of approximately 20 consecutive measurements, following a procedure very similar to the one outlined by Gottlieb *et al.*[14] We also evaluated the errors from the quadratic fluctuations, finding generally consistent results. At the lowest separations one expects distortions due to lattice artifacts. To estimate the possible size of such errors, we computed correction factors based on the following idea. The field strengths are given by averages which involve several plaquettes; as a consequence, the central points of the plaquettes are not all at separation r, but rather they are at separations r' which may substantially differ

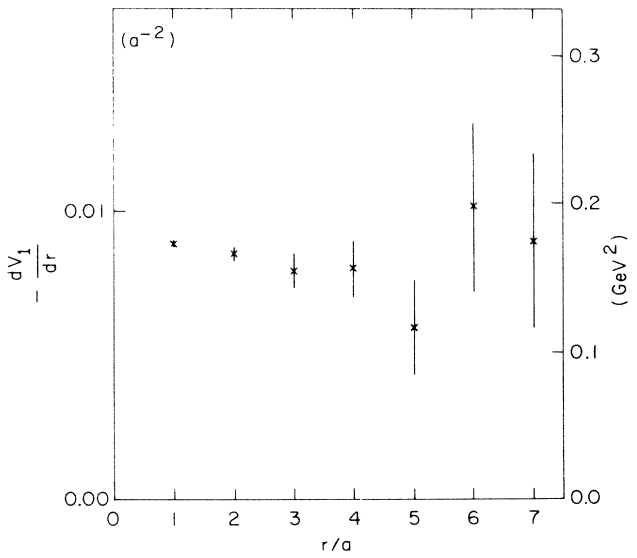

FIG. 1. Monte Carlo results for the spin-dependent potential V_1.

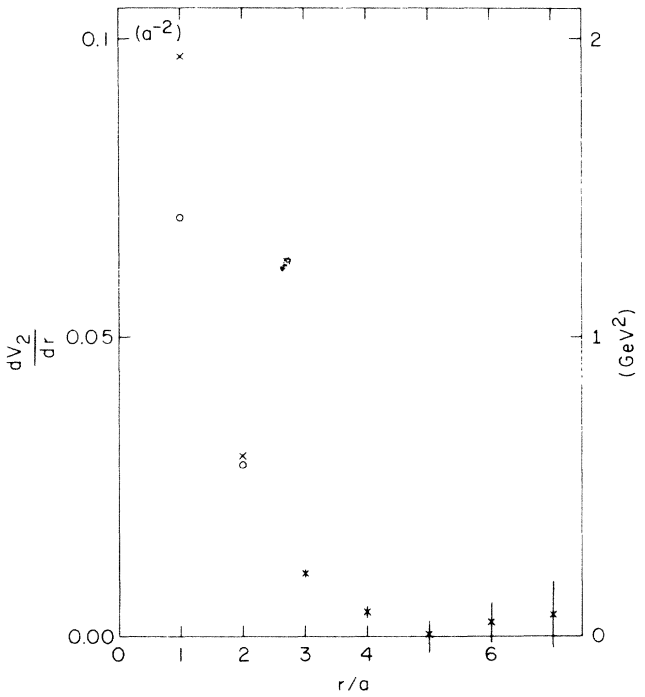

FIG. 2. Monte Carlo results for the spin-dependent potential V_2, before (crosses) and after (circles) the correction for lattice artifacts discussed in the text.

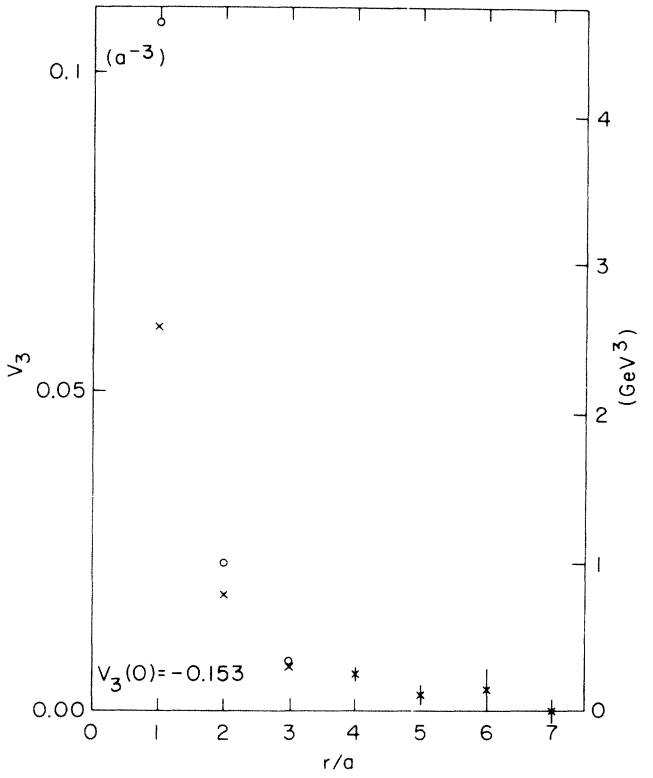

FIG. 3. Same as in Fig. 2, but for the spin-dependent potential V_3.

from r at close lattice distance. The correction is made by rescaling the contributions of the plaquettes by the factors [either $(r/r')^2$ or $(r/r')^3$] which would follow from first-order perturbation theory. One sees from the figures that the correction is indeed substantial for $r=a$ (and tends to make the points conform better with the perturbative behavior expected at short distances), but becomes almost negligible already at $r=2a$, giving one some confidence that for all but the smallest separations lattice artifacts may be under control.

One observes a clear nonperturbative long-ranged component in the spin-orbit potential V_1, whereas all the other spin-dependent potentials appear to be short ranged and similar to what one would expect from perturbation theory. Such behavior appears compatible with the experimental data, according to the most recent phenomenological analyses.[15] Of course, the real test would come from a direct computation of the spectroscopic observables from the calculated potentials. For this, one must be able to rescale the spin-dependent potentials, according to a suitable renormalization factor. As a heuristic argument for the determination of such factor, we offer the following consideration. The spin-dependent potentials always appear in the Hamiltonian divided by m^2, m being the quark mass. Since the energy levels must be a renormalization-group invariant, it appears plausible that the lattice values for the potentials be divided by

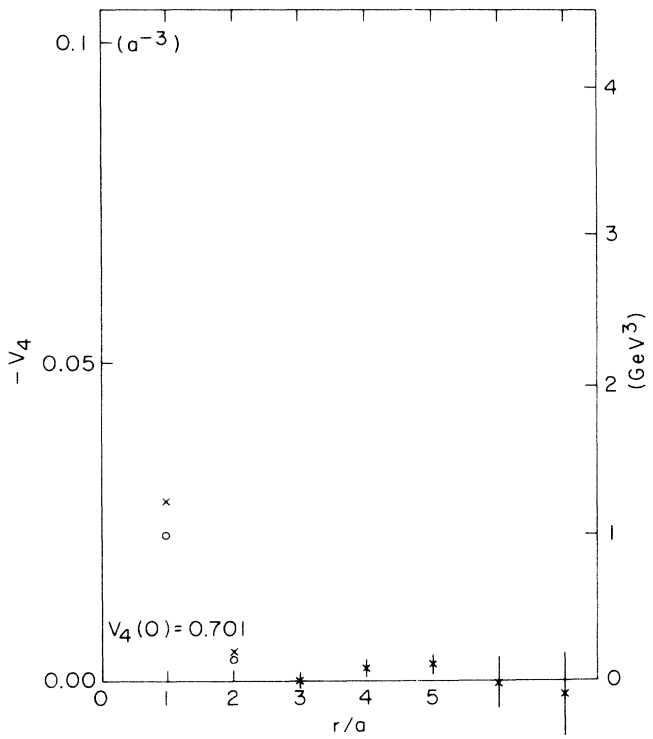

FIG. 4. Same as in Fig. 2, but for the spin-dependent potential V_4.

the bare, Lagrangean mass squared. Equivalently, they should be rescaled by a factor $f=(m_R/m)^2$, m_R being the renormalized quark mass effectively used in the solution of the Schrödinger equation. A recent calculation of hadronic masses in the quenched approximation,[16] on a lattice equal in size to the present one and at $\beta=6$, suggests $m_R/m\approx 2$, for quarks giving origin to mesons comparable in mass to the lowest excitations of the J/ψ family. This gives $f\approx 4$. Accepting this renormalization and adopting the value $a=2.21$ GeV, inferred from Ref. 4, one obtains for the spin-dependent potentials in physical units the values on the scales at the right-hand sides of the figures. On the basis of Lorentz invariance, Gromes[17] has derived a relationship among the potentials, namely, $V+V_1-V_2=0$. It is noteworthy that the Gromes relation appears to be reasonably well satisfied by the potentials after renormalization.

It would be of obvious interest to verify the scaling properties of the spin-dependent potentials and to apply them to a calculation of the levels of the heavy-quark families. Work along these lines is in progress.

This calculation has been performed on the Cyber 205 computer at Rockville, Maryland, using a substantial amount of computer time granted by Control Data Corporation. We wish to thank Robert Price for his interest, encouragement, and support, and Lloyd M. Thorndyke and L. Kent Steiner of ETA Systems, Inc., for support and access to the Cyber 205 computer at Fort Collins, Colorado, where the preliminary code was developed. We also acknowledge support from CDC PACER Fellowship (Grant No. 85PCR06), the National Science and Engineering Research Council of Canada (Grant No. NSERC A8 420), and the U.S. Department of Energy under Contract No. DE-AC02-76CH00016.

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