Relativistic effects in heavy-quarkonium spectroscopy

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(Received 3 September 1982; revised manuscript received 5 July 1983)

It is shown that the discrepancy between the measured rate for $\psi' \to \chi_0 \gamma$ and that predicted by nonrelativistic models can be accounted for by $(v/c)^2$ relativistic corrections. A Breit-Fermi Hamiltonian is used to predict the energy level structure and $E1$ transition rates in the charmonium and Υ systems. It is obtained from an instantaneous approximation to a Bethe-Salpeter equation whose kernel is composed of Coulomb-gauge gluon exchange and a scalar confining piece. The model accounts for the observed fine and hyperfine structure of the charmonium levels and for the $E1$ transition rates. It is used to predict the level structure and $E1$ rates in the Υ system. It is shown that an extension of Siegert's theorem is valid in the relativistic regime. This result is useful in analyzing $E1$ transition-matrix elements.

I. INTRODUCTION

Nonrelativistic theories of quarkonium have been notably successful in accounting for the energy-level spectrum of heavy mesonic states.[1] However, such theories do not account for the fine structure and hyperfine structure of the energy levels, and in addition they cannot account for the measured rates for $\psi' \to \chi_J \gamma$ decays.[2] As in positronium, relativistic corrections will give the spin-spin, spin-orbit, and tensor forces that cause the hyperfine- and fine-structure splitting of the levels. In this paper we report a study of a Breit-Fermi Hamiltonian that contains $(v/c)^2$ corrections to the nonrelativistic theory. The Hamiltonian reduces to the one-gluon-exchange-plus-linear-confinement model of Eichten *et al.*[3] in nonrelativistic approximation. It can be derived from a Bethe-Salpeter equation with a kernel evaluated in instantaneous approximation.[4] The kernel includes transverse- as well as timelike-gluon exchange taken in Coulomb gauge. The transverse-gluon exchange gives rise to spin-spin and tensor forces, and the spin-orbit interaction has contributions from both the gluon exchange and the linearly confining potential. We solve the Breit-Fermi Hamiltonian and find that we can fit the observed charmonium and Υ spectra using the parameters of Eichten *et al.* with minor modifications. The interaction is taken to be flavor independent, aside from the slow decrease in the running coupling constant. We calculate $E1$ radiative transition rates and find that relativistic effects reduce appreciably the $\psi' \to \chi_0 \gamma$ rate and also to a lesser degree the $\psi' \to \chi_1 \gamma$ rate. When these corrections are combined with the coupled-channel effects estimated by Eichten *et al.*,[3] predicted and measured rates agree within errors. Relativistic effects will also be appreciable in certain $b\bar{b}$ radiative transitions. We have used our model to calculate $E1$ transition rates for the states expected to be present below the open-b-flavor threshold. Comparison of our predicted $b\bar{b}$ level structure and $E1$ transition rates with measured values will check the validity of our model.

In a previous paper, we reported that there are numerous $(v/c)^2$ corrections to the nonrelativistic (convection-current) operator that describes radiative transitions.[5] To get all $(v/c)^2$ effects one must evaluate matrix elements using eigenfunctions of a Breit-Fermi Hamiltonian. It turns out that there are cancellations in the long-wavelength limit and $E1$ transition amplitudes correct to order $(v/c)^2$ are given by matrix elements of r (aside from small retardation and recoil corrections). In nuclear physics, this result is known as Siegert's theorem.[6]

Using this result, it is easy to see why small relativistic corrections appreciably alter some $E1$ transition amplitudes. Consider for example $\psi' \to \chi_J \gamma$. The ψ' is a $2\,^3S_1$ state whose wave function has one node, while the χ_J are $1\,^3P_J$ states.[7] There is a strong cancellation in the matrix element of r due to this node and the result is sensitive to small changes in the wave function. This is to be contrasted with $\chi_J \to (J/\psi)\gamma$ transitions where there is no such cancellation. Relativistic corrections are not appreciable in the $\chi_J \to (J/\psi)\gamma$ rates.

Similar effects occur in $b\bar{b}$ transitions. The $1P \to 1S$ transition rates are insensitive to relativistic corrections while there are appreciable effects, though not as large as in charmonium, in $2S \to 1P$ rates. In $b\bar{b}$ we expect to see other transitions where relativistic effects may be large; for example, $(n+1)\,^3P_0 \to n\,^3S_1$ transitions. The matrix elements for such transitions are small, but the photon frequencies are large and compensate. Generally, for example, $2P \to 1S$ rates are expected to be comparable to $2P \to 2S$ rates. However, in some cases, there is a strong suppression due to relativistic effects. We find, for example, that the $2\,^3P_0 \to 1\,^3S_1$ rate is reduced by a factor of 5. Generally our results for such transitions are model dependent and are at best rough estimates.

In charmonium $\langle v/c \rangle^2$ is much bigger than in positronium (~ 0.2). Consequently, spin-spin, spin-orbit, and tensor forces are relatively large. In positronium these forces are usually treated as first-order perturbations. Indeed, since $(v/c)^4$ and higher-order corrections are neglected in the Breit-Fermi Hamiltonian, it would be inconsistent to do otherwise. In fact, they cannot be treated otherwise because the spin-spin interaction is a contact δ function and the spin-orbit and tensor-force potentials

diverge like r^{-3} at small distances. When such interaction energies are attractive, as they are in the $^1S_0$ and $^3P_0$ states, the eigenvalues of the Hamiltonian have no lower bound.[8] This is a spurious divergence which, presumably, is cured by taking $(v/c)^4$ and higher-order corrections into account (radiative corrections also must be included). Though these potentials become very large at small distances, their effects are small because they become large only at distances smaller than the Compton wavelength of the electron. Since the Compton wavelength of the electron is very small compared to the radius of the bound state, when these potentials become large the radial wave functions of the bound states tend to zero sufficiently rapidly for the matrix elements to remain small. This is the reason why perturbation theory adequately accounts for their effects. In charmonium as in positronium one has $R \simeq (\alpha m)^{-1}$, where R is the radius of the bound state; however, for charmonium $\alpha = \alpha_s \simeq \frac{1}{5}$, whereas for positronium $\alpha \simeq \frac{1}{137}$. Nevertheless, we find that in charmonium also $(v/c)^2$ effects are perturbative or nearly so. When this is the case, the detailed behavior of these effects at small distances is not important.

In order to use our extension of Siegert's theorem, we need the eigenvalues and eigenfunctions of the Breit-Fermi Hamiltonian with relativistic corrections to order $(v/c)^2$. To obtain such wave functions it is necessary to soften the singular nature of the potentials at small distances. Since those singularities are spurious and, presumably, cured by the $(v/c)^4$ and higher-order corrections, we attempt to include such effects in our calculation simply by smearing out the color charge. Instead of taking the Coulomb potential of a point charge, we take the gluon-exchange potential to be that due to a Gaussian-distributed color charge whose mean-square radius is given by the Compton wavelength of the quark. Precisely, the radius is given by a parameter f, where $\langle r^2 \rangle = 1.5(fm)^{-2}$. With our assumption that perturbation theory is valid, our results should not depend upon f provided f is not too small nor too large. If f is too large, we will get the "fall" to the center in $^3P_0$ and $^1S_0$ states when we solve the Hamiltonian for its eigenvalues and eigenfunctions. If f is too small, the color charge will be smeared over distances comparable with the quarkonium radius which would be unacceptable. These considerations restrict f to the range $1 < f < 2$. For convenience we took $f = \sqrt{2}$. This value gives a nonrelativistic potential that is essentially the same as that of Eichten *et al.*[3] for $r \gtrsim 0.1$ fm (see Fig. 1), and therefore also agrees with the "universal" potential-energy curve for $0.1 \lesssim r \lesssim 1$ fm found in other models that also fit the charmonium and Υ spectra.[1] We studied how our results vary with f and found that the $E1$ transition rates are insensitive to changes in f as are most of the charmonium and Υ energy levels. However, we found that the hyperfine splitting was sensitive to f; and also, but to a lesser degree, the position of the $1\,^3P_0$ state of charmonium. Perhaps it was fortuitous, but we found that the value $f = \sqrt{2}$ gave good agreement with the observed J/ψ-η_c mass splitting.

Since our value of $f = \sqrt{2}$ gives reasonable values for the hyperfine splitting in charmonium, we used it to calculate the Υ level structure and $E1$ transition rates. In this case, of course, the color charge is smeared out over distances of the order of the Compton wavelength of the b quark. For the $b\bar{b}$ system we used the same slope for the linear-confining part of the interaction and slightly weaker color charge consistent with asymptotic freedom. Our results are displayed in Fig. 3.

The linearly confining part of the interaction contributes to the spin-orbit force. (Tensor and spin-spin interactions come only from transverse gluon exchange.) The spin-orbit interaction that arises from the linear confinement varies like r^{-1}; its sign depends on the Lorentz-transformation properties of the confining potential. We assumed that it transformed as a scalar and/or vector exchange. In order to fit the observed fine structure of the charmonium ^3P_J levels, we found that the linear confinement should be taken to transform like a scalar exchange. It is perhaps of some interest to note here that there is a constant associated with the linear confinement which is needed to get the right masses and also to have the nonrelativistic potential energy fall on the universal curve which Berkelman[1] found. It turns out that this constant gives rise to some spin-independent $(v/c)^2$ corrections to the energy levels and wave functions (see Appendix B). We found it necessary to assume this constant was associated with the linearly confining piece as part of our scalar-exchange contribution. We studied the possibility that it was part of the vector-exchange contribution and found that assumption gave very large corrections that were inconsistent with a perturbative treatment and seriously distorted the energy-level spectrum.

The contents of this paper are organized as follows. In Sec. II we outline the derivation of the Breit-Fermi Hamiltonian. In Sec. III we derive the $(v/c)^2$ corrections to the nonrelativistic expression for the interaction of a quark-antiquark bound state with the radiation field and show that Siegert's theorem applies to this case. Here we also include the possible effects of an anomalous quark magnetic moment. In Sec. IV, we discuss the specific parameter values we use in our model and the results we obtain for the energy-level structure of the Υ and charmonium systems. Sections V and VI contain discussions of spin-dependent and spin-independent forces, respectively, in our model. In Sec. VII we report our results for the $E1$ transition rates and discuss them. In Sec. VIII we summarize our conclusions. Appendix A contains a discussion of finite-size corrections to $E1$ transition amplitudes, and Appendix B outlines our method of calculating Breit-Fermi wave functions.

II. THE HAMILTONIAN

To include relativistic corrections in a description of quarkonium, we used a Breit-Fermi Hamiltonian which has $(v/c)^2$ corrections to a nonrelativistic Hamiltonian. The nonrelativistic Hamiltonian is one in which there is one-gluon exchange and linear confinement. Our Breit-Fermi Hamiltonian was obtained by a reduction to Pauli spinor form of Sucher's[4] instantaneous approximation to a Bethe-Salpeter equation. The kernel contains one-gluon exchange in Coulomb gauge and a linearly rising confining piece that transforms like scalar exchange. We allowed the linearly rising confining piece to have a part

that transformed like vector exchange and a part that transformed like scalar exchange, and we found from a fit to the fine-structure splitting of the charmonium levels that the vector-exchange part of the confining piece is small compared to the scalar part. We therefore took the confining piece to transform as scalar exchange. We obtained our Breit-Fermi Hamiltonian from the Hamiltonian,

$$H = h_1 + h_2 + V \ , \tag{2.1}$$

where the quark is particle 1 and the antiquark particle 2

$$\begin{aligned} h &= \vec{\alpha}\cdot\vec{p} + \beta m \ , \\ V &= V_V + \vec{\alpha}_1\cdot[(I - \vec{\nabla}\,\vec{\nabla}/\nabla^2)V_V]\cdot\vec{\alpha}_2 + \beta_1\beta_2 V_S \ . \end{aligned} \tag{2.2}$$

We took the potentials V_V and V_S to be spherically symmetric functions of $\vec{r} = \vec{r}_1 - \vec{r}_2$. The nonrelativistic approximation to (2.1) is a Schrödinger Hamiltonian with potential energy $V_{\rm NR} = V_V + V_S$. The transverse-gluon-exchange term in V is a $(v/c)^2$ correction to $V_{\rm NR}$. As written it must be taken as a first-order effect only; it is not correct for second- and higher-order transitions which involve negative-energy fermions in intermediate states.[9] Such intermediate states give rise to what are called pair terms, and these terms must be included separately.[4]

In this paper we only consider relativistic effects of order $(v/c)^2$. To this order the pair terms do not contribute to the Hamiltonian and we can replace the V in (2.1) by its positive-energy projection

$$V_{++} = \Lambda_{++} V \Lambda_{++} \ , \tag{2.3}$$

where

$$\Lambda_{++} = (\epsilon_1 + h_1)(\epsilon_2 + h_2)/2\epsilon_1 2\epsilon_2$$

and

$$\epsilon = [\vec{p}^{\,2} + m^2]^{1/2} \ .$$

With this replacement, the bound-state eigenfunctions of H satisfy

$$\psi^{++} = \Lambda_{++}\psi^{++} \tag{2.4}$$

and this condition allows us to write the Dirac-spinor wave functions as Pauli-spinor wave functions ϕ. The ϕ are related to the ψ by the unitary free-particle Foldy-Wouthuysen operator U (Ref. 10); viz.,

$$\phi = U\psi^{++} \ , \tag{2.5}$$

$$U = \exp\left\{ \sum_i \vec{\gamma}_i\cdot\hat{p}_i\theta \right\} \tag{2.6}$$

with

$$\sin 2\theta = |\vec{p}\,|/\epsilon, \quad \cos 2\theta = m/\epsilon \ .$$

It is easy to verify that

$$U\Lambda_{++}U^{-1} = (1+\beta_1)(1+\beta_2)/4 \ .$$

Consequently one sees that the ϕ are Pauli spinors since

$$\phi = \tfrac{1}{4}(1+\beta_1)(1+\beta_2)\phi \ . \tag{2.7}$$

The Breit-Fermi Hamiltonian acts on ϕ. It is related to H by

$$H_{\rm BF} = UHU^{-1} - 2m \ , \tag{2.8}$$

where one expands the right-hand side in powers of $\vec{p}/m$ and keeps only the $(\vec{p}/m)^2 = (v/c)^2$ corrections to the nonrelativistic Hamiltonian.

We use the instantaneous approximation and Coulomb-gauge gluon-exchange in the quarkonium rest frame, so it is understood that $H_{\rm BF}$ refers to this frame. Taking $\vec{p}_1 = -\vec{p}_2 = \vec{p}$ in (2.8), we obtain

$$\begin{aligned} H_{\rm BF} = {} & p^2/m - p^4/4m^3 + V_{\rm NR} + (3V_V' - V_S')\vec{S}\cdot\vec{L}/2m^2 r \\ & + (r^{-1}V_V' - V_V'')(3\vec{\sigma}_1\cdot\hat{r}\,\vec{\sigma}_2\cdot\hat{r} - \vec{\sigma}_1\cdot\vec{\sigma}_2)/12m^2 \\ & + \vec{\sigma}_1\cdot\vec{\sigma}_2\nabla^2 V_V/6m^2 + \nabla^2 V_{\rm NR}/4m^2 - \vec{p}\,V_S\cdot\vec{p}/m^2 \\ & + \vec{p}\cdot\left[I - \frac{\vec{\nabla}\,\vec{\nabla}}{\nabla^2} \right] V_V\cdot\vec{p}/m^2 \ , \end{aligned} \tag{2.9}$$

where $V_{\rm NR} = V_V + V_S$, $\vec{S} = (\vec{\sigma}_1 + \vec{\sigma}_2)/2$, and $\vec{L} = \vec{r}\times\vec{p}$. If we were to take $V_S = 0$ and $V_V = -\alpha/r$, (2.9) would give the Breit-Fermi Hamiltonian for positronium with the one-photon-annihilation term omitted.[11] In a later section we describe how we solved (2.9) for its eigenfunctions and eigenvalues.

For analyzing the interactions with the radiation field it is convenient to have $H_{\rm BF}$ expressed in terms of $\vec{p}_1$ and $\vec{p}_2$. The expression is

$$\begin{aligned} H_{\rm BF} = {} & (p_1^{\,2} + p_2^{\,2})/2m - (p_1^{\,4} + p_2^{\,4})/8m^3 + V_{\rm NR} \\ & + (V_V' - V_S')(\vec{\sigma}_1\cdot\hat{r}\times\vec{p}_1 - \vec{\sigma}_2\cdot\hat{r}\times\vec{p}_2)/4m^2 \\ & - V_V'(\vec{\sigma}_1\cdot\hat{r}\times\vec{p}_2 - \vec{\sigma}_2\cdot\hat{r}\times\vec{p}_1)/2m^2 \\ & + (r^{-1}V_V' - V_V'')(3\vec{\sigma}_1\cdot\hat{r}\,\vec{\sigma}_2\cdot\hat{r} - \vec{\sigma}_1\cdot\vec{\sigma}_2)/12m^2 \\ & + \vec{\sigma}_1\cdot\vec{\sigma}_2\nabla^2 V_V/6m^2 + \nabla^2 V_{\rm NR}/4m^2 - \vec{p}_1 V_S\cdot\vec{p}_1/2m^2 \\ & - \vec{p}_2 V_S\cdot\vec{p}_2/2m^2 - \vec{p}_1\cdot(I - \vec{\nabla}\,\vec{\nabla}/\nabla^2)V_V\cdot\vec{p}_2/m^2 \ . \end{aligned} \tag{2.10}$$

III. ELECTROMAGNETIC INTERACTION AND SIEGERT'S THEOREM

We start with minimal electromagnetic coupling and later add the effect of an anomalous magnetic moment. We assume amplitudes for one-photon emission are given by

$$\mathcal{M}_{\lambda fi} = q(\psi_f, [\vec{\alpha}_1\cdot\vec{A}_\lambda(1)^* - \vec{\alpha}_2\cdot\vec{A}_\lambda(2)^*]\psi_i) \ , \tag{3.1}$$

where ψ_i and ψ_f are eigenstates of the Dirac Hamiltonian (2.1). We reduce (3.1) to Pauli-spinor form using the Foldy-Wouthuysen reduction described in the previous section. As there, we keep only $(v/c)^2$ corrections, and obtain for (3.1)

$$\mathcal{M}_{\lambda fi} = q(\phi_f, h_\lambda \phi_i) \ , \tag{3.2}$$

where the ϕ are eigenstates of the Breit-Fermi Hamiltonian. To obtain the correct expression for h_λ care must be taken with pair effects. As stated in the previous section, the transverse-gluon term in V is not right, in general,

when one has negative-energy fermions in intermediate states. However, the work of Drake[12] shows that one can use it in this case where we calculate radiative transitions to order $(v/c)^2$ only. We assume the confining part of the potential also can be used in the same way and we derive an expression for h_λ including pair effects perturbatively as follows. We write ψ in terms of solutions ψ_{++} to the no-pair equation,

$$(h_1+h_2+V_{++})\psi_{++}=E\psi_{++} \tag{3.3}$$

as

$$\psi=\psi_{++}+(V-V_{++})\psi_{++}/2m\ . \tag{3.4}$$

Keeping terms of order $(v/c)^2$ only, we obtain $\mathcal{M}_{\lambda fi}$ as a matrix element between eigenstates of (3.3); viz.,

$$\mathcal{M}_{\lambda fi}=q(\psi_{++f},\{\vec{\alpha}_1\cdot\vec{A}_\lambda(1)^*+[\vec{\alpha}_1\cdot\vec{A}_\lambda(1)^*\Lambda_-(1)V+V\Lambda_-(1)\vec{\alpha}_1\cdot\vec{A}(1)^*]/2m-(1\to2)\}\psi_{++i})\ , \tag{3.5}$$

where $\Lambda_-=(\epsilon-h)/2\epsilon$ and $\epsilon=[\vec{p}^{\,2}+m^2]^{1/2}$ as before. Now using (2.5) one easily obtains h_λ and finds

$$\begin{aligned}h_\lambda=&[\vec{p}_1\cdot\vec{A}_\lambda(1)^*+\vec{A}_\lambda(1)^*\cdot\vec{p}_1]/2m+\vec{\sigma}_1\cdot\vec{B}_\lambda(1)^*/2m+\vec{\sigma}_1\cdot\vec{E}_\lambda(1)^*\times\vec{p}_1/4m^2\\&-\{\vec{p}_1^{\,2},[\vec{p}_1\cdot\vec{A}_\lambda(1)^*+\vec{A}_\lambda(1)^*\cdot\vec{p}_1]\}/8m^3+\vec{\sigma}_1\cdot\hat{r}\times\vec{A}_\lambda(1)^*(V_V'-V_S')/4m^2\\&+\vec{\sigma}_2\cdot\hat{r}\times\vec{A}_\lambda(1)^*V_V'/2m^2-[\vec{A}_\lambda(1)^*V_S\cdot\vec{p}_1+\vec{p}_1V_S\cdot\vec{A}_\lambda(1)^*]/2m^2-\vec{A}_\lambda(1)\cdot(I-\vec{\nabla}\,\vec{\nabla}/\nabla^2)V_V\cdot\vec{p}_2/m^2-(1\rightleftarrows2)\ .\end{aligned} \tag{3.6}$$

In h_λ we have written

$$[\vec{p}^{\,2},i\vec{\sigma}\cdot\vec{A}\times\vec{p}]/2m=\vec{\sigma}\cdot\vec{E}\times\vec{p}+\vec{\sigma}\cdot\vec{A}\times\vec{\nabla}V_{\rm NR}\ , \tag{3.7}$$

because matrix elements of $[H_{\rm NR},i\vec{\sigma}\cdot\vec{A}\times\vec{p}]$ with $H_{\rm NR}=p_1^{\,2}/2m+p_2^{\,2}/2m+V_{\rm NR}$ between eigenstates of $H_{\rm BF}$ are equal to those of $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ to the accuracy of our calculations. The terms proportional to $\vec{A}$ in (3.6) are just the terms linear in $\vec{A}$ which are obtained from the Breit-Fermi Hamiltonian (2.10) by the gauge-covariant replacements $\vec{p}_1\to\vec{p}_1-q\vec{A}(1)$ and $\vec{p}_2\to\vec{p}_2+q\vec{A}(2)$. To obtain the $\vec{\sigma}\cdot\vec{B}$ and $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ terms one must do the Foldy-Wouthuysen reduction of (3.1).

If the quarks have anomalous magnetic moments given by κ, we can include that by adding terms

$$q\kappa\beta\sigma_{\mu\nu}F^{\mu\nu}/4m \tag{3.8}$$

to (3.1). Then the Foldy-Wouthuysen reduction gives $\vec{\sigma}\cdot\vec{B}$ and $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ contributions that can be included if one multiplies the $\vec{\sigma}\cdot\vec{B}$ term in (3.6) by $(1+\kappa)$ and the $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ term by $(1+2\kappa)$. This is as in the usual Foldy-Wouthuysen reduction[10] of the interaction of Dirac particles with an external field. Hereafter we shall include anomalous-magnetic-moment effects.

A great simplification arises if we evaluate (3.6) for electric multipole transitions in the long-wavelength limit. To see this it is convenient to write h_λ as the convection-current, $\vec{\sigma}\cdot\vec{B}$ and $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ terms, and a remainder; viz.,

$$h_\lambda=[\vec{p}_1\cdot\vec{A}_\lambda(1)^*+\vec{A}_\lambda(1)^*\cdot\vec{p}_1]/2m+(1+\kappa)\vec{\sigma}_1\cdot\vec{B}_\lambda(1)^*/2m+(1+2\kappa)\vec{\sigma}_1\cdot\vec{E}_\lambda(1)^*\times\vec{p}_1/4m^2-(1\to2)+h_\lambda'\ . \tag{3.9}$$

For electric multipole transitions where the wavelength of the emitted radiation is much larger than the size of the bound state, the convection-current term in (3.9) can be replaced by the photon energy times the electric multipole operator minus h_λ', so that all that is left is this multipole-operator term and the $\vec{\sigma}\cdot\vec{B}$ and $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ terms. In nonrelativistic approximation, the latter two terms are neglected and this result is known as Siegert's theorem.[6] To see how this result comes about, consider an electric dipole transition, where in the long-wavelength approximation, one replaces the exponential in $\vec{A}_\lambda=\hat{\epsilon}_\lambda e^{i\vec{k}\cdot\vec{r}}$ by unity. Using the commutation relation $\vec{p}=i[p^2,\vec{r}]/2$, one can rewrite the convection-current term as a commutator of $H_{\rm BF}$ with $\hat{\epsilon}_\lambda^*\cdot\vec{r}$. Using (2.10) we get, e.g.,

$$\begin{aligned}\vec{p}_1\cdot\vec{A}^*/m=&\,i[H_{\rm BF},\hat{\epsilon}^*\cdot\vec{r}_1]+i[p_1^{\,4},\hat{\epsilon}^*\cdot\vec{r}_1]/8m^3-(V_V'-V_S')i[\vec{\sigma}_1\cdot\hat{r}\times\vec{p}_1,\hat{\epsilon}\cdot\vec{r}_1]/4m^2-V_V'i[\vec{\sigma}_2\cdot\hat{r}\times\vec{p}_1,\hat{\epsilon}\cdot\vec{r}_1]/2m^2\\&+i[\vec{p}_1V_S\cdot\vec{p}_1,\hat{\epsilon}^*\cdot\vec{r}_1]/2m^2+i[\vec{p}_1\cdot\{(I-\vec{\nabla}\,\vec{\nabla}/\nabla^2)V_V\}\cdot\vec{p}_2,\hat{\epsilon}^*\cdot\vec{r}_1]/m^2\ ,\end{aligned} \tag{3.10}$$

and the extra terms aside from the first on the right-hand side are just equal and opposite in sign to the corresponding terms in the remainder term h_λ' in (3.9). That this cancellation takes place stems from the fact that those terms in h_λ' are generated from the corresponding terms in $H_{\rm BF}$ by the gauge-covariant replacement $p\to p-qA$. Thus taking $k=E_i-E_f$ we obtain

$$(\phi_f,h_\lambda\phi_i)=(\phi_f,[-ik\hat{\epsilon}_\lambda^*\cdot\vec{r}+(1+2\kappa)\hat{\epsilon}_\lambda^*\cdot\vec{S}\times\vec{r}k^2/4m+(1+2\kappa)\hat{\epsilon}_\lambda^*\cdot(\vec{\sigma}_1-\vec{\sigma}_2)\times(\vec{r}_1+\vec{r}_2)k^2/8m]\phi_i)\ . \tag{3.11}$$

Here $\vec{S}=(\vec{\sigma}_1+\vec{\sigma}_2)/2$. A term proportional to $\vec{\sigma}_1-\vec{\sigma}_2$ only contributes to triplet-singlet transitions. We do not consider such transitions here and therefore will ignore such terms.

To the accuracy of (3.11), we must include the first retardation correction in the $\vec{\sigma}\cdot\vec{B}$ term; i.e., we must take

$$\vec{B}_\lambda(\vec{r}) = -\vec{k}\cdot\vec{r}\vec{\epsilon}_\lambda\times\vec{k} \tag{3.12}$$

in that term. Adding this in we obtain

$$(\phi_f, h_\lambda\phi_i) = (\phi_f, [-ik\hat{\epsilon}^*_\lambda\cdot\vec{r} - (1+\kappa)\hat{\epsilon}^*_\lambda\cdot\vec{S}\times\vec{k}\,\vec{k}\cdot\vec{r}/2m + (1+2\kappa)\hat{\epsilon}^*_\lambda\cdot\vec{S}\times\vec{r}k^2/4m$$
$$-(1+\kappa)\hat{\epsilon}^*_\lambda\cdot\vec{D}\times\vec{k}\,\vec{k}\cdot\vec{R}/2m + (1+2\kappa)\hat{\epsilon}^*_\lambda\cdot\vec{D}\times\vec{R}k^2/4m]\phi_i) , \tag{3.13}$$

where $\vec{D}=(\vec{\sigma}_1-\vec{\sigma}_2)/2$ and $\vec{R}=\vec{r}_1+\vec{r}_2$. This expression contains both $E1$ and $M2$ transition operators for singlet-singlet and triplet-triplet transitions. The $M2$ piece in (3.13) is

$$(1+\kappa)\hat{\epsilon}^*_\lambda\cdot\vec{S}\times(\vec{r}-2\hat{k}\,\hat{k}\cdot\vec{r})k^2/4m \tag{3.14}$$

and the $(v/c)^2$ correction to the $E1$ piece is

$$\kappa\hat{\epsilon}^*_\lambda\cdot\vec{S}\times\vec{r}k^2/4m . \tag{3.15}$$

If we neglect the retardation correction in the $\vec{r}$ term, the electric dipole operator is

$$-ik\hat{\epsilon}^*_\lambda\cdot(\vec{r}+i\kappa\vec{r}\times\vec{S}k/4m) \tag{3.16}$$

to order $(v/c)^2$. We studied the retardation corrections and found them to be small (3% in charmonium). Lowest-order retardation corrections are given by (see Appendix A)

$$1\mp k/12m - k^2\langle r^3\rangle/120\langle r\rangle , \tag{3.17}$$

where the upper (lower) sign refers to $P\to S$ ($S\to P$) transitions. An additional correction to (3.16) arises owing to the effect of recoil in the final state. Kinematically this effect is included by taking for k the observed photon energy. There may be some dynamical effect of this recoil on the final bound-state wave function; this has not been included.

Ignoring recoil entirely, we can give a simple derivation of our extension of Siegert's theorem which directly shows its relation to gauge invariance. This derivation holds for all electric multipoles. Therefore consider a 2^L electric multipole transition. In the long-wavelength approximation, the leading term in the vector potential may be written as[13]

$$\vec{A}_\lambda(\vec{r}) = \vec{\nabla} f_{L\lambda}(\vec{r}) , \tag{3.18}$$

where

$$f_{L\lambda}(\vec{r}) = k^{-1}N_L(kr)^L D^{(L)}_{\lambda 0}(\hat{r}) . \tag{3.19}$$

Using (3.18) and the relation $\vec{\alpha}_1\cdot\vec{A}_\lambda = i[H, f_{L\lambda}(1)]$ with H given by (2.1), one obtains for (3.1)

$$\mathcal{M}_{\lambda fi} = iq(\psi_f, [H, \{f_{L\lambda}(1)^* - f_{L\lambda}(2)^*\}]\psi_i)$$
$$= -ikq(\psi_f, \{f_{L\lambda}(1)^* - f_{L\lambda}(2)^*\}\psi_i) , \tag{3.20}$$

where $k = E_i - E_f$. To compare this with (3.13) we must write $\psi = \psi_{++} = U^{-1}\phi$ and consider $Uf_{L\lambda}U^{-1}$ keeping $(v/c)^2$ terms. The pair terms in (3.4) do not contribute to h_λ to this order. Since $\nabla^2 f_{L\lambda}=0$, one has

$$U^{-1}f_{L\lambda}U \simeq f_{L\lambda} + \vec{\sigma}\cdot(\vec{\nabla} f_{L\lambda})\times\vec{p}/4m^2 . \tag{3.21}$$

Writing

$$\vec{E}_{L\lambda} = ik\vec{\nabla} f_{L\lambda} , \tag{3.22}$$

we get

$$\mathcal{M}_{\lambda fi} = q(\phi_f, [-ikf_{L\lambda}(1)^* + \vec{\sigma}_1\cdot\vec{E}_{L\lambda}(1)^*\times\vec{p}_1/4m^2$$
$$-(1\to 2)]\phi_i) . \tag{3.23}$$

Here we have neglected the magnetic $\vec{\sigma}\cdot\vec{B}/2m$ interaction by assuming (3.18). It must be included because the first-order retardation correction to (3.18) gives a nonvanishing contribution from the $\vec{\sigma}\cdot\vec{B}$ term of the same order as the $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ term in (3.23). This can be included. One takes for $\vec{B}$ (Ref. 13)

$$\vec{B}_{L\lambda} = -k^2\vec{r}\times\vec{\nabla} f_{L\lambda}/(L+1) \tag{3.24}$$

and includes it in $\mathcal{M}_{\lambda fi}$ by taking

$$\mathcal{M}_{\lambda fi} = q(\phi_f, [-ikf_{L\lambda}(1)^* + \vec{\sigma}_1\cdot\vec{E}_{L\lambda}(1)^*\times\vec{p}_1/4m^2$$
$$+\vec{\sigma}_1\cdot\vec{B}_{L\lambda}(1)^*/2m - (1\to 2)]\phi_i) . \tag{3.25}$$

For $L=1$, this result simply gives

$$\mathcal{M}_{\lambda fi} = q(\phi_f, -ik\hat{\epsilon}^*_\lambda\cdot\vec{r}\phi_i) , \tag{3.26}$$

which agrees with (3.16) for $\kappa=0$. In these electric dipole transitions, the $\vec{\sigma}\cdot\vec{B}$ and $\vec{\sigma}\cdot\vec{E}\times\vec{p}$ contributions are equal and opposite and cancel.[14] All the $(v/c)^2$ corrections to the radiative transition amplitudes are contained in the Breit-Fermi energy eigenvalues and eigenfunctions. For electric multipole transitions, it is not necessary to compute all the correction terms in (3.6). If one were to use (3.6), one must compute its matrix elements between Breit-Fermi wave functions for consistency. Our extension of Siegert's theorem shows that the many $(v/c)^2$ correction terms in (3.6) simply correct the convection-current term, in the long-wavelength limit, so that its contribution is simply given by the electric multipole operator as in (3.23).

So, we see that the problem of computing the $(v/c)^2$ corrections to electric multipole amplitudes in the long-wavelength limit is reduced to the problem of computing eigenfunctions and eigenvalues of the Breit-Fermi Hamiltonian. For $E1$ transitions, one need only calculate the matrix elements of r between these wave functions. From (3.16) by direct calculation it is easy to show that the anomalous magnetic-moment contribution to ${}^3P_J\to{}^3S_1+\gamma$ transitions can be taken into account simply by multiplying the radial matrix element of r by the factor[14]

$$1+\kappa k[J(J+1)-4]/8m . \tag{3.27}$$

For ${}^3S_1\to{}^3P_J+\gamma$ transitions, (3.27) applies with the

correction term $\propto\kappa$ of opposite sign. Clearly there is no such correction for the singlet-singlet case.

For $E1$ transitions, the effective interaction Hamiltonian h_λ depends only on the relative coordinate $\vec{r}$. The center-of-mass coordinate simply cancels out in the derivation of (3.16). In general, it is not so simple to separate out the center-of-mass motion. Krajcik and Foldy[15] have given an extensive discussion of the problem of defining relativistic center-of-mass variables. They find $1/c^2$ corrections to the Hamiltonian for the interaction of a composite system with an external electromagnetic field when one carefully separates out the center-of-mass motion. Those corrections do not contribute to $E1$ transitions in quarkonium. We can obtain the $(v/c)^2$ corrections by using eigenvalues of $H_{\rm BF}$ to compute k and calculating matrix elements of r with Breit-Fermi wave functions.

IV. EIGENVALUES AND EIGENFUNCTIONS OF $H_{\rm BF}$

As shown in the previous section, we can obtain the $(v/c)^2$ corrections to the $E1$ amplitudes simply by calculating matrix elements of r with wave functions correct to this order. We can either treat the $(v/c)^2$ terms perturbatively or find the eigenfunctions of $H_{\rm BF}$. To the degree that $(v/c)^4$ and higher-order corrections are small, both methods should yield the same results. Treating the $(v/c)^2$ correction terms in $H_{\rm BF}$ perturbatively, one easily obtains the corresponding energy-level shifts. However, it is not so simple to obtain the wave functions correct to this order. This is because the perturbation-theory correction to the wave function is given by an infinite sum over states of the nonrelativistic Hamiltonian, and this sum diverges for potentials that become infinite like r^{-1} at the origin. This is well known for the case of positronium, where the hyperfine interaction, for example, is a δ function at the origin and the spin-orbit and tensor forces diverge like r^{-3}. Indeed, the Breit-Fermi Hamiltonian with these potentials is not soluble because the energy levels for the $^1S_0$ and $^3P_0$ states are unbounded from below; in these states the hyperfine- and fine-structure interactions are attractive and produce the so-called fall to the center phenomenon where the wave function all piles up at the origin.[8] Correspondingly, one finds that the perturbation-theory sum for the first-order change in the wave functions diverges for large momenta when one includes the continuum. Matrix elements of r are insensitive to the detailed behavior of the wave function near the origin. Consequently, one can ignore this divergence by truncating the perturbation-theory sum or one can remove the singularities by replacing the Coulomb potential of a point charge by the Coulomb potential of a smeared charge. Both methods yield essentially the same results for the energy-level shifts and for the $E1$ matrix elements in the low-lying states.

In our work we assumed that the nonrelativistic potential was a Coulomb potential for the color charge and linear confinement. Arafune and Fukugita[16] used the same model. They calculated the spin-dependent $(v/c)^2$ corrections to the wave functions by perturbation theory taking only the bound states into account. We, on the other hand, smoothed the singular behavior by assuming that the color charge was Gaussian distributed instead of a point charge and solved $H_{\rm BF}$ for its eigenvalues and eigenfunctions. We took into account both the spin-dependent and spin-independent $(v/c)^2$ effects. Arafune and Fukugita did not calculate spin-independent $(v/c)^2$ effects. These are difficult to take into account. Our method of doing so is given in Appendix B. We found that the spin-independent $(v/c)^2$ effects are comparable to the spin-dependent ones.

The Breit-Fermi Hamiltonian we used is given in Sec. II. We assumed (2.2) with the V_V terms the instantaneous potential for one-gluon exchange in Coulomb gauge and V_S a linearly confining potential. In nonrelativistic approximation our model is essentially the one-gluon-exchange-plus-linear-confinement model of Eichten *et al.*[3] We used their value for the slope of the linear confining potential. It was necessary to take the linear confining potential to be the scalar-exchange part of V in order to fit the $1\,^3P_J$ levels in charmonium (see Sec. V).

We also assumed the Cornell values for the constituent quark masses. They chose the charmed quark mass guided partly by their desire to keep it close to the mass of the lightest charmed meson and by their desire to keep relativistic effects relatively small. Their choice of m_b gave with the same potential (with slight adjustment for a running coupling constant in the Coulomb piece) a fit to the low-lying $b\bar{b}$ S-state mass differences. Martin arrived at similar quark masses by fitting his flavor-independent potential to the $s\bar{s}$, $c\bar{c}$, and $b\bar{b}$ mass spectra.[17]

In potential models which include relativistic effects, the choice of quark mass is more constrained than in the nonrelativistic case. We found that a charmed quark mass smaller than that used by the Cornell group tends to give too large a fine-structure splitting in the $1\,^3P_J$ levels.

The quark masses we use require a negative constant in the nonrelativistic potential. This constant, which we call C, is chosen so that the $1\,^3S_1$ $c\bar{c}$ mass agrees with the measured J/ψ mass. The constant C not only corrects the nonrelativistic bound-state masses, it also contributes to certain $(v/c)^2$ spin-independent corrections. Owing to these corrections, we found that the $c\bar{c}$ energy levels could only be fit if C was included as part of the scalar potential (see Sec. VI).[18] Therefore, we assumed $V_S=r/a^2+C$.

In order to be able to solve for the eigenfunctions of $H_{\rm BF}$, we smeared the color charge over the Compton wavelength of the quark. We took V_V to be the potential of a Gaussian distributed color charge; viz.,

$$V_V=-\kappa\,\mathrm{erf}(\sqrt{2}mr)/r\ , \tag{4.1}$$

where m is the mass of the constituent quark and erf is the usual error function; viz.,

$$\mathrm{erf}(x)=(4/\pi)^{1/2}\int_0^x e^{-y^2}dy \tag{4.2a}$$

$$\underset{x\to 0}{\longrightarrow}(4/\pi)^{1/2}x \tag{4.2b}$$

$$\underset{x\to\infty}{\to} 1 \,. \tag{4.2c}$$

The $\sqrt{2}$ in the argument of erf is somewhat arbitrary. If we call this factor f, a range of acceptable values for f can be determined in the following way. A lower limit to f is set by the requirement that V_V does not differ too much from the Cornell potential over the range of r where the quarkonium wave functions are appreciable. An upper limit on f is set by the requirement that the fine-structure splitting of the ^3P_J eigenvalues of $H_{\rm BF}$ is not very different from that given by first-order perturbation theory with a point color charge. Those considerations require that $1<f<2$. With $f=\sqrt{2}$ our $V_{\rm NR}$ is very similar to the Cornell potential for $r>0.1$ fm; both are shown in Fig. 1. To compensate for the decreased attraction near $r=0$, we used a slightly larger value of κ than the Cornell group used.

Our value of κ was chosen to fit the experimental value of ($M_{1P}=M_{\chi_{\rm c.g.}}$)

$$R=(M_{2S}-M_{1P})/(M_{1P}-M_{1S}) \,, \tag{4.3}$$

as in the Cornell model. Our parameter values are displayed in Table I with the Cornell values in parentheses where they are different. For the $b\bar{b}$ potential our κ value was similarly chosen. It was chosen so that our $H_{\rm NR}$ gave the same mass difference ratio,

$$r=(M_{3S}-M_{2S})/(M_{2S}-M_{1S}) \,, \tag{4.4}$$

as the Cornell model. The Cornell group used the observed Υ'', Υ', and Υ masses to determine r. As asymptotic freedom requires, κ is smaller for $b\bar{b}$ than for $c\bar{c}$. The constant C was chosen to fit the $1\,^3S_1$ eigenvalue of $H_{\rm BF}$ to the J/ψ mass; the same value also fits the Υ mass. Berkelman[1] has shown that fits to quarkonium spectrum determine a potential-energy function which is (almost) flavor independent and universal in the range $0.1\le r\le 1$ fm in the sense that many different analytical forms give approximately the same potential energy in this range when the parameters are adjusted to fit the spectra. Our $V_{\rm NR}$ for $0.1\le r\le 1$ fm agrees with this universal curve.

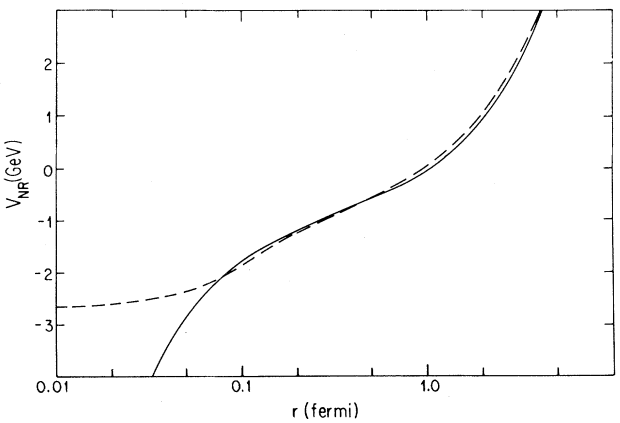

FIG. 1. $V_{\rm NR}$ vs r. The solid curve is the Coulomb-plus-linear-potential model of Ref. 3. The dashed curve is the nonrelativistic approximation to the interaction energy used in this paper.

TABLE I. Parameter values for V. We use $V_V=-\kappa\,\mathrm{erf}(\sqrt{2}mr)/r$ and $V_S=r/a^2+C$ with $a=0.46$ f and $C=-0.80$ GeV (-0.85 GeV). Parameters of Eichten *et al.* (Ref. 3) are in parentheses where they are different from those we use.

$q\bar{q}$	m (GeV)	κ
$c\bar{c}$	1.84	0.65 (0.52)
$b\bar{b}$	5.17	0.53 (0.48)

Our calculated masses are shown in Tables II and III. The agreement between the calculated and measured masses of the Υ states in Table III is evidence for the flavor independence of the nonrelativistic potential. The level structure we obtain, aside from the fine and hyperfine structure, is very similar to that obtained by the Cornell group. The spin-dependent and spin-independent $(v/c)^2$ effects on the energy levels are discussed in the next two sections. We conclude this section by discussing the sensitivity of our results to the smearing parameter f. We calculated $c\bar{c}$ masses with various values of f and found that the hyperfine mass splittings exhibit the largest f dependence. This is because the hyperfine interaction is concentrated near the origin where the details of the smearing of the color charge are important. Since the effect of this smearing does not extend much beyond a quark Compton wavelength, matrix elements which depend on large values of r such as $E1$ matrix elements are insensitive to the color-charge smearing. A moderate amount of sensitivity ($\sim$20%) to the value of f was found in the position of the $1\,^3P_0$ state. This occurs because both the spin-orbit and tensor forces are attractive in this state and also are concentrated near the origin. The fine-structure effects in the other ^3P_J states for $J=1$ and 2 are less sensitive to f because the interactions here are less attractive (see Table IV).

TABLE II. Charmonium masses in MeV relative to the $1\,^3S_1$ mass. Parameters m and a^2 are those of Ref. 3; κ has been adjusted to give the same mass ratio $(M_{2S}-M_{1P})/(M_{1P}-M_{1S})$ as Ref. 3.

	Nonrelativistic results	With $(v/c)^2$ corrections	Measured charmonium values[a]
$1\,^3D_1$	757	670	670.7±3.8
$2\,^3S_1$	625	560	589.2±0.9
$2\,^1S_0$		490	497 ±5
$1\,^3P_2$	455	428	458.9±0.5
$1\,^3P_1$		391	413.4±0.4
$1\,^3P_0$		285	317.9±0.6
$1\,^1P_1$		405	?
$1\,^1S_0$	0	−113	−111 ±5

[a]Hyperfine splittings are taken from Ref. 2 and P-state masses from Ref. 19.

TABLE III. $b\bar{b}$ bound-state masses in MeV relative to $1\,^3S_1$ mass.

	Nonrelativistic results	With $(v/c)^2$ corrections	Measured $b\bar{b}$ values (Ref. 1)
$3\,^3D_1$	1278	1231	
$4\,^3S_0$	1204	1160	1114±5
$4\,^1S_0$		1133	
$3\,^3P_2$		1091	
$3\,^3P_1$	1120	1074	
$3\,^3P_0$		1037	
$3\,^1P_1$		1081	
$2\,^3D_1$	1026	991	
$3\,^3S_1$	928	895	889±4
$3\,^1S_0$		864	
$2\,^3P_2$		820	
$2\,^3P_1$	838	801	
$2\,^3P_0$		761	
$2\,^1P_1$		809	
$1\,^3D_1$	734	710	
$2\,^3S_1$	585	560	560±3
$2\,^1S_0$		520	
$1\,^3P_2$		478	
$1\,^3P_1$	483	456	
$1\,^3P_0$		407	
$1\,^1P_1$		465	
$1\,^1S_0$	0	−101	

V. SPIN-DEPENDENT FORCES

The spin-orbit and tensor-force effects on the ^3P_J wave functions have important consequences for some $E1$ decay amplitudes as is shown in detail in Sec. VII. The tensor-force term in the Breit-Fermi Hamiltonian is

$$(r^{-1}V_V'-V_V'')(3\vec{\sigma}_1\cdot\hat{r}\,\vec{\sigma}_2\cdot\hat{r}-\vec{\sigma}_1\cdot\vec{\sigma}_2)/12m^2\,, \tag{5.1}$$

and the spin-orbit interaction term is

$$(3V_V'-V_S')\vec{L}\cdot\vec{S}/2m^2r\,. \tag{5.2}$$

The tensor force comes entirely from the transverse-gluon-exchange interaction term (proportional to $\alpha_{1i}\alpha_{2j}$) in V. Besides contributing to fine-structure effects, the tensor force causes mixing between triplet S and D states. In our model this mixing is small (slightly less than 1%).[18] This mixing is smaller by a factor of about 3 than that found by the Cornell group when they included coupling to open charm channels.[3]

The spin-orbit interaction term has contributions from both the gluon-exchange term (V_V) and the scalar confining potential (V_S). One unit of the V_V term in (5.2) comes from the Coulomb term in V and two from the transverse-gluon-exchange term. In our one-gluon-exchange-plus-linear-confining potential, the vector and scalar contributions to the spin-orbit interaction energy tend to cancel for low-lying P states. To see this consider the point-charge case with $V_V=-\kappa/r$ and $V_S=r/a^2+C$. Then the coefficient of $\vec{L}\cdot\vec{S}$ is

$$[3\kappa-(r/a)^2]/2m^2r^3\,, \tag{5.3}$$

and with parameter values $\kappa=0.65$ and $a=0.46$ fm the two contributions tend to cancel over the range of r where the $1P$ wave function is appreciable (see Fig. 2). If the confining potential were in V_V, it would contribute an $(r/a)^2$ term of opposite sign and produce fine-structure splitting of charmonium levels considerably larger than that which is observed.

The fine structure of the $1\,^3P_2$ and $1\,^3P_1$ levels is insensitive to the smearing of color charge. The position of the $1\,^3P_0$ state, on the other hand, is somewhat sensitive to the choice of the smearing parameter f; the mass difference $M_{\psi}-M_{\chi_0}$ varied by about 20% when we varied f over its allowed range. This mass difference calculated in our model with $f=\sqrt{2}$ is about 20% larger than that given by first-order perturbation theory using the Cornell value for κ. The position of the $^3P_0$ state is most sensitive to details of the interaction at short distances because both the spin-orbit and tensor forces are attractive in this state and are relatively large. In the $b\bar{b}$ system we found the fine-structure splittings of the $1\,^3P_J$ states to be about half as large as in charmonium (see Table III). Also we found that the fine structure of the ^3P_J states decreases in magnitude as the level of excitation increases.

The hyperfine interaction in $H_{\rm BF}$ is

$$V_{\rm hf}=\vec{\sigma}_1\cdot\sigma_2\nabla^2V_V/6m^2\,. \tag{5.4}$$

This interaction is entirely due to the transverse-gluon-exchange term in (2.2). With our choice of V_V, (5.4) has the form of a Gaussian:

$$V_{\rm hf}=\vec{\sigma}_1\cdot\vec{\sigma}_2(2/3\sqrt{\pi})\kappa f^3m\exp(-f^2m^2r^2)/3\,. \tag{5.5}$$

As $f\to\infty$, (5.5) goes uniformly over to the familiar δ-function contact interaction. For triplet states, the hyperfine interaction is repulsive. For single states it is attractive and is three times as large in magnitude as in the triplet case. In the limit $f\to\infty$, the singlet energy levels have no lower bound and the hyperfine interaction (5.4) only makes sense if it is used in first-order perturbation theory.

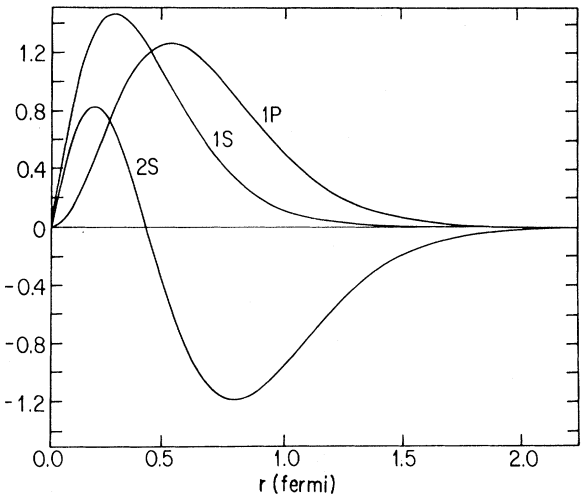

FIG. 2. Radial wave functions plotted as functions of r. These are eigenstates of the nonrelativistic approximation to our Hamiltonian.

From this point of view it is not surprising that our result for the mass difference is sensitive to our choice of parameter f. We regard it as fortuitous that our calculated value of 113 MeV is so close to the experimental value of 111 ± 5 MeV. We choose $f=\sqrt{2}$ somewhat arbitrarily, guided only by the requirement that our nonrelativistic potential agree with the "universal curve" of Berkelman[1] in the range $0.1<r<1$ fm. Owing to the fact that this value gave such a good mass splitting, we kept it as a constant and used $f=\sqrt{2}$ and $b\bar{b}$ system. Our predictions for the hyperfine splitting of the levels in the $b\bar{b}$ system are sensitive to this choice of f and we therefore regard them only as rough estimates. The magnitude of the hyperfine splitting in the $b\bar{b}$ system is not much smaller than that in the $c\bar{c}$ case. On reflection this is not surprising though the hyperfine interaction is proportional to m^{-2} because this interaction is concentrated near the origin and the $b\bar{b}$ wave function is relatively larger near the origin.

We used our model to calculate values of $c\bar{c}$ and $b\bar{b}$ wave functions at the origin. These are changed substantially from nonrelativistic values by the hyperfine interaction—particularly for singlet states. Our results are very sensitive to our smearing parameter f.

Finally, we mention that we calculated $E1$ transition rates between $^1P_1$ and $^1S_0$ states. The hyperfine interaction has an effect here through its effect on the wave functions, but the results are insensitive to the value of f because the matrix elements are matrix elements of r and are therefore insensitive to details near the origin.

VI. SPIN-INDEPENDENT TERMS

The spin-independent $(v/c)^2$ terms in $H_{\rm BF}$ cause effects on eigenvalues and eigenfunctions as large as those due to spin-dependent terms. Collectively, these spin-independent terms act effectively like an attractive potential. They tend to reduce all $c\bar{c}$ and $b\bar{b}$ bound-state energies relative to nonrelativistic values. They also reduce the $E1$ radiative transition amplitudes.

Values of wave functions at the origin are changed as much by the spin-dependent $(v/c)^2$ terms as by the hyperfine interaction. However, as is the case with the hyperfine interaction, spin-independent corrections to wave functions at the origin depend upon the potential at small distances and are therefore cutoff dependent. Appendix B contains a description of the method we used to calculate the effects of the spin-independent terms.

In our study of spin-independent effects, we had to decide how to treat the additive potential constant C. We found widely differing results depending on whether we took C to contribute to V_V or V_S.[18] In order to get agreement with the measured $c\bar{c}$ and $b\bar{b}$ mass values, we were forced to take C to be part of the scalar potential. We found that if we put C in V_V or even if we just ignored the contribution of C altogether, we then got very large spin-independent corrections which seriously distorted the energy-level spectrum.

VII. RADIATIVE TRANSITION RATES

The tensor forces in our Breit-Fermi Hamiltonian are weak and produce negligible S-D mixing. Therefore the $E1$ rates can be calculated neglecting mixing. Then with relativistic effects included the rates are given by matrix elements of r; viz.,

$$\Gamma(^3S_1\rightarrow{}^3P_J)=4(2J+1)\alpha_q k^3\langle r\rangle^2/27\ , \tag{7.1}$$

$$\Gamma(^3P_J\rightarrow{}^3S_1)=4\alpha_q k^3\langle r\rangle^2/9\ , \tag{7.2}$$

$$\Gamma(^1S_0\rightarrow{}^1P_1)=4\alpha_q k^3\langle r\rangle^2/3\ , \tag{7.3}$$

$$\Gamma(^1P_1\rightarrow{}^1S_0)=4\alpha_q k^3\langle r\rangle^2/9 \tag{7.4}$$

with $\alpha_q=q^2/4\pi$ where q is the quark charge.

We calculate radiative widths using these formulas with experimental values for the photon frequencies where they are known. We calculate matrix elements of r using eigenfunctions of $H_{\rm BF}$ and compare them with the nonrelativistic results using eigenfunctions of $H_{\rm NR}$ with $V_{\rm NR}=V_V+V_S$. Our results for charmonium are shown in Table IV where we also display experimental magnitudes.

Notice that the $2\,^3S_1\rightarrow1\,^3P_0$ matrix element is decreased in magnitude from 0.47 to 0.30 by relativistic ef-

TABLE IV. Matrix elements of r calculated with nonrelativistic and Breit-Fermi wave functions for charmonium states.

	J	Nonrelativistic result (fm)	With $(v/c)^2$-corrected wave functions (fm)	Experimental magnitudes[a] (fm)
$\langle 1\,^3P_J \mid r \mid 2\,^3S_1\rangle$	0	−0.47	−0.30	0.31±0.04
	1		−0.42	0.33±0.04
	2		−0.47	0.37±0.06
$\langle 1\,^1P_1 \mid r \mid 2\,^1S_0\rangle$			−0.48	?
$\langle 1\,^3S_1 \mid r \mid 1\,^3P_J\rangle$	0	0.36	0.37	0.31±0.06
	1		0.37	<3
	2		0.36	0.35±0.1
$\langle 1\,^1S_0 \mid r \mid 1\,^1P_1\rangle$			0.31	?

[a]Experimental magnitudes are magnitudes of the matrix elements of r calculated assuming that the observed rates are given by (7.1) and (7.2).

fects. The relativistic effects are of three types: (i) spin-orbit and tensor-force effects which vanish in S states, (ii) the hyperfine interaction $\vec{\sigma}_1\cdot\vec{\sigma}_2\nabla^2 V_V/6m^2$ which acts mainly in S states, and (iii) spin-independent effects. Effects (i) and (iii) are attractive in the $^3P_0$ state while (ii) is repulsive in the $^2S_1$ state, and they all act to decrease the magnitude of the matrix element. To understand why the effect is so large, consider Fig. 2, where the nonrelativistic $2S$ and $1P$ radial wave functions are displayed. The node of the $2S$ wave function is near the maximum of the $1P$ wave function; consequently there is a large cancellation in the $2S\rightarrow 1P$ matrix element of r. Because of this, small $(v/c)^2$ corrections have a surprisingly large effect. The spin-orbit and tensor-force corrections are largest in the $^3P_0$ state. In the $^3P_1$ state similar effects occur but are smaller because the tensor force tends to cancel out the effect of the spin-orbit force; see Table V. In the $J=2$ state, the combined effect of the spin-orbit and tensor force is repulsive and tends to cancel the attractive spin-independent effects.

Relativistic corrections to the $1\,^3P_J\rightarrow 1\,^3S_1$ transition matrix elements are small because there is no node in either wave function and no cancellation like that in the $2S\rightarrow 1P$ case. Triplet $1P\rightarrow 1S$ matrix elements are relatively insensitive to $(v/c)^2$ corrections.

In the singlet transitions relativistic corrections are negligible in the $2\,^1S_0\rightarrow 1\,^1P_1$ case, but produce a 20% reduction in the matrix element of r for the $1\,^1P_1\rightarrow 1\,^1S_0$ case. The main effect here is the hyperfine interaction which is attractive in the $^1S_0$ state and three times as large as in the $^3S_1$ state (where it is repulsive). This attraction reduces the overlap of the wave functions and moves this overlap to smaller values of r, thus appreciably reducing the matrix element. In the $2\,^1S_0\rightarrow 1\,^1P_1$ case, the overlap is improved but moved to smaller r values; these effects tend to cancel, and the overall change in the matrix element is therefore small.

TABLE V. Diagonal ^3P_J matrix elements of the spin-orbit and tensor operators. $\langle S_T\rangle=\langle 3\vec{\sigma}_1\cdot\hat{r}\,\vec{\sigma}_2\cdot\hat{r}-\vec{\sigma}_1\cdot\vec{\sigma}_2\rangle$.

J	$\langle\vec{L}\cdot\vec{S}\rangle$	$\langle S_T\rangle$
0	-2	-4
1	-1	2
2	1	$-\frac{2}{5}$

Although $(v/c)^2$ corrections bring the $2\,^3S_1\rightarrow 1\,^3P_0$ matrix element into rather good agreement with experiment, they do not give comparably good corrected values for the $2\,^3S_1\rightarrow 1\,^3P_J$ matrix elements for $J=1$ and 2. The charmonium radiative widths calculated using (7.1)—(7.4) are given in Table VI along with measured values. The further reductions which appear to be needed for the $J=1$ and $J=2$ cases are perhaps due to coupled channel effects. Eichten *et al.*[3] have analyzed the effect of (closed) $c\bar{q}$-$q\bar{c}$ decay channels (q is a u, d, or s quark) on the $c\bar{c}$ system. They find that coupling to these channels tends to reduce $E1$ radiative decay rates; their calculations yielded the percentage reductions shown in Table VI. As shown in Table VI, if such reductions are included along with $(v/c)^2$ corrections, the calculated rates come into rough agreement with the measured rates. We have neglected S-D (and P-F) mixing. The tensor force in $H_{\rm BF}$ causes a small amount of such mixing. Coupled-channel effects produce much more mixing.

The calculated rates given in Table VI do not include retardation and recoil effects. Corrections due to retardation effects are discussed in Appendix A. Those corrections are small. We use the measured photon frequencies in evaluating (7.1)—(7.4) and in this way, presumably,

TABLE VI. $E1$ transition rates in charmonium. The first two columns are calculated in long-wavelength approximation using the matrix elements in Table V and (7.1)—(7.4). Measured values of photon momentum were used where possible; for transitions to and from the singlet P state the predicted $1\,^1P_1$ mass of 3512 MeV was used.

	J	Nonrelativistic rates (keV)	With $(v/c)^2$-corrected matrix elements[a] (keV)	Coupled-channel reduction[b]	Anomalous-magnetic-moment corrections[c]	Experimental values[d] (keV)
$\psi'\rightarrow\gamma+\chi_J$	0	45	19 (16)	86%	$1+0.14\kappa$	21±6
	1	40	31 (23)	76%	$1+0.05\kappa$	19±5
	2	27	27 (22)	82%	$1-0.04\kappa$	17±5
$\chi_J\rightarrow\gamma+\psi$	0	121	128 (117)	92%	$1-0.16\kappa$	97±38
	1	250	270 (240)	89%	$1-0.11\kappa$	<700
	2	362	347 (305)	88%	$1+0.12\kappa$	330±170
$\eta_c'\rightarrow\gamma+{}^1P_1$		15	16		none	?
${}^1P_1\rightarrow\gamma+\eta_c$		660	483		none	?

[a]The numbers in parentheses in this column are the calculated rates reduced by the percentage reductions given in the next column.
[b]Estimates given by Eichten *et al.* (Ref. 3).
[c]First-order effect only. Studies of $M2$-$E1$ interference term in angular distribution give $-0.70<\kappa<0.65$ (Ref. 19).
[d]Taken from Ref. 2. To obtain the $\psi'\rightarrow\gamma\chi_J$ rates we used $\Gamma_{\psi}=215\pm40$ keV.

most of the recoil corrections are taken into account (cf. Sec. III).

In the fourth column we give a correction factor that takes into account an anomalous magnetic moment for the quark. It is given by (3.27). The value of κ can be obtained, for example, by observation of the $M2$-$E1$ interference term in the angular distribution of the photon in one of the $^3S_1$-^3P_J transitions for $J=1$ or 2. The $M2$ amplitude is given by (3.14). So far statistics are not yet good enough to allow for a determination of κ, and the experimental results are that $-0.70 \leq \kappa \leq 0.65$.[19] Another way one might estimate κ is by using the simple nonrelativistic formula for the $M1$ transition $J/\psi \to \eta_c \gamma$. This gives for the rate

$$\Gamma(J/\psi \to \eta_c \gamma) = \tfrac{16}{3} k^3 \alpha (e_c/2m_e)^2 (1+\kappa)^2 . \quad (7.5)$$

The measured value[2] of the branching fraction $(1.2^{+0.5}_{-0.4})\%$ and the total J/ψ width of 63 keV gives for the charmed-quark mass

$$m_c = (2.8^{+0.7}_{-0.5})(1+\kappa) \text{ GeV} . \quad (7.6)$$

From this one might conclude that if the charmed-quark mass is, for example, 1.8 GeV, κ is negative and in the range -0.2 to -0.5.

Our results for the $E1$ matrix elements in the Υ system are given in Table VII. These results neglect coupled-channel effects, S-D mixing, and retardation corrections. The retardation corrections are generally smaller in the Υ than in the charmonium system and can certainly be neglected here; see Appendix A. Since $4\,^3S_1$ Υ state is above the open-b-flavor threshold, it seems likely that coupled-channel effects on the $E1$ decay rates from this state and nearby states will be significant.

Since there are many transitions in the upsilon system below the open beauty threshold, it is convenient to divide the $E1$ transitions for the triplet and singlet states into three categories: $nP \to nS$, $(n+1)P \to nS$, and $(n+1)S \to nP$. First, let us consider $n\,^3P_J \to n\,^3S_1$ rates. Those for $n=1$ are the largest; these rates are insensitive to relativistic corrections. For $n>1$, nodes in the radial wave functions cause cancellations which result in some sensitivity to $(v/c)^2$ effects. The largest effects are in transitions from $J=0$ states where the matrix elements are increased by about 15% owing to the relatively large and attractive spin-orbit and tensor forces in the $^3P_0$ state. For $J=1$ and 2, the spin-orbit and tensor forces are less attractive and/or repulsive and effects tend to cancel. In the $n\,^1P_1 \to n\,^1S_0$ transitions, the attractive hyperfine interaction decreases $\langle r \rangle$ by about 16%. For $(n+1)P \to nS$ transitions, radial wave-function nodes cause large cancellations in $\langle r \rangle$. These matrix elements are small and sensitive to $(v/c)^2$ corrections. Though the matrix elements are small, the photon frequencies are large and consequently the rates may be appreciable. We find, however, that the $(n+1)\,^3P_0 \to n\,^3S_1$ rates are suppressed by more than a factor of five compared to their nonrelativistic values. Finally, there are the $(n+1)S \to nP$ rates. These rates are small because the photon frequencies are low. The pattern of the J dependence of the relativistic effects in the $(n+1)\,^3S_1 \to n\,^3P_J$ rates is similar to that we found in charmonium; i.e., the $(v/c)^2$ effects are largest in the transitions to the $J=0$ states and not big in the $J=1$ and 2 cases. In Υ, these relativistic effects are smaller than in charmonium—about half as big. We have not included here results for decays in which the number of radial nodes in the initial and final wave functions differ by two or more. The decay rates for those transitions are very small owing to the large cancellations in the matrix elements. Predictions for these cases would be very model dependent.

For the singlet states, the main relativistic effect is that of the attractive hyperfine interaction. As in the $c\bar{c}$ case,

TABLE VII. Matrix elements for $E1$ transitions between $b\bar{b}$ states.

	Nonrelativistic $\langle r \rangle$ (fm)	J	$\langle r \rangle$ with $(v/c)^2$-corrected wave functions (fm)
$4\,^3S_1 \to 3\,^3P_J$	−0.68	0	−0.55
		1	−0.64
		2	−0.69
$4\,^1S_1 \to 3\,^1P_1$			−0.70
$3\,^3P_J \to 3\,^3S_1$	0.47	0	0.55
		1	0.48
		2	0.44
$3\,^1P_1 \to 3\,^1S_0$			0.39
$3\,^3P_J \to 2\,^3S_1$	0.064	0	0.026
		1	0.055
		2	0.067
$3\,^1P_1 \to 2\,^1S_0$			0.069
$3\,^3S_1 \to 2\,^3P_J$	−0.52	0	−0.42
		1	−0.49
		2	−0.53
$3\,^1S_0 \to 2\,^1P_1$			−0.54
$2\,^3P_J \to 2\,^3S_1$	0.34	0	0.39
		1	0.35
		2	0.32
$2\,^1P_1 \to 2\,^1S_0$			0.28
$2\,^3P_J \to 1\,^3S_1$	0.051	0	0.022
		1	0.043
		2	0.053
$2\,^1P_1 \to 1\,^1S_0$			0.054
$2\,^3S_1 \to 1\,^3P_J$	−0.33	0	−0.27
		1	−0.31
		2	−0.33
$2\,^1S_0 \to 1\,^1P_1$			−0.34
$1\,^3P_J \to 1\,^3S_1$	0.19	0	0.20
		1	0.20
		2	0.20
$1\,^1P_1 \to 1\,^1S_0$			0.16

the effect is largest in $n\,{}^1P_1 \to n\,{}^1S_0$ transitions where the attraction (mainly in the S state) causes the overlap of the wave functions to be worse and to be at smaller values of r. Consequently the amplitudes for these transitions are reduced.

To show the relative $E1$ rates for the various transitions discussed above, we present in Fig. 3 the rates calculated using the matrix elements of Table VII and our predicted photon frequencies. Since the photon frequencies are measured when the rates are measured, our predictions should be checked using our predicted matrix elements (Table VII) with experimental values for the photon frequencies to obtain rates.

VIII. CONCLUSIONS

We have calculated $c\bar{c}$ and $b\bar{b}$ spectra and $E1$ transition rates using a Breit-Fermi Hamiltonian that contains first-order $(v/c)^2$ corrections to a nonrelativistic model with one-gluon exchange and linear confinement including transverse-gluon exchange. We find that the $(v/c)^2$ corrections give fine and hyperfine structure to the energy of charmonium levels which is in accord with measured values. We find that the spin-independent $(v/c)^2$ corrections are comparable with the spin-dependent corrections.

In order to use our extension of Siegert's theorem to calculate radiative transition amplitudes, we needed wave functions correct to order $(v/c)^2$. We found these by solving a Breit-Fermi Hamiltonian with the color charge smeared out over a distance of the order of the quark Compton wave length. Our results for the $E1$ transition rates and level structure, aside from the hyperfine splitting, are not sensitive to this smearing. Arafune and Fukugita[16] have studied some of the same effects in charmonium and treated them by perturbation theory. When we calculate the same things, our results agree. They did not take into account spin-independent corrections. Hardekopf and Sucher[20] studied $(v/c)^2$ corrections to dipole transition amplitudes for quarkonium and showed that wave-function corrections are comparable to the $(v/c)^2$ corrections to the dipole operator. We agree with this result. In fact, our use of Siegert's theorem implements this.

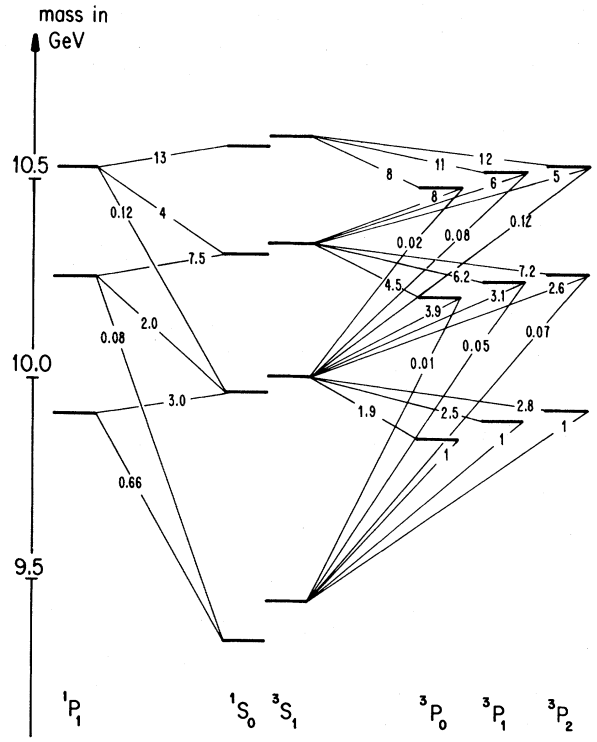

FIG. 3. Predicted $b\bar{b}$ mass spectrum below the open-b-flavor threshold with $E1$ transitions marked. The numbers on the transition lines are values of $\langle r \rangle^2$ in GeV^{-2}. These are related to the $E1$ transition rates by (7.1)—(7.4).

Note added in proof: H. J. Schnitzer [Nucl. Phys. B207, 131 (1982)] has given an analysis of ordinary-meson spectroscopy showing that the spin dependence of the forces can be interpreted as due to a short-ranged vector exchange and a confining potential that transforms as a Lorentz scalar. The compatibility of this assumption with the fine structure of charmonium P states was first demonstrated by A. B. Henriques, B. H. Kellett, and R. G. Moorhouse [Phys. Lett. 64B, 85 (1976)].

ACKNOWLEDGMENTS

We would like to acknowledge helpful conversations with Joe Sucher. This work was supported in part by the U.S. Department of Energy under Contract Number DE-AT03-81ER40024, Task B; PA DE-AM03-76DF00034.

APPENDIX A

The leading contribution to $E1$ transition amplitudes in quarkonium comes from the convection-current $(\vec{A}\cdot\vec{p}+\vec{p}\cdot\vec{A})/2m$ term where the exponential in $\vec{A}=\hat{\epsilon}e^{i\vec{k}\cdot\vec{r}}$ is replaced by unity. Such an approximation is valid when the size of the bound state is small compared to the wave length of the emitted photon. Corrections to this approximation are called finite size or retardation effects. In this appendix, we discuss such corrections for transitions in which the initial state is a P state and the final state an S state and vice versa. The radial matrix element of the convection current for such transitions is given by

$$M=(2/m)\int_0^\infty dr\, r^2 R_P(r)[j_0(kr/2)+j_2(kr/2)] \times dR_S(r)/dr\ , \tag{A1}$$

where R_P and R_S are the radial P and S wave functions, respectively, and $j_L(kr/2)$ are spherical Bessel functions

of order L. If we neglect $(v/c)^2$ corrections, we can assume that R_P and R_S satisfy nonrelativistic radial Schrödinger equations and show that[18]

$$2\int_0^\infty dr\, r^2 R_P R_S' f = \int_0^\infty dr\, r^2 R_P[(E_S-E_P)mF+2Fr^{-2} -2fr^{-1}-f']R_S\ , \quad \text{(A2)}$$

where E_S-E_P is the energy difference of the S and P states, $f(r)$ is any function of r, and $F=\int_0^r dr\, f$. Taking for f the sum j_0+j_2 in (A1) and expanding the Bessel functions as a power series in kr, one gets

$$f=1-(kr)^2/40+\cdots\ , \qquad F=r-k^2r^3/120+\cdots\ , \quad \text{(A3)}$$

and with $k=|E_S-E_P|$ (recoil neglected) one obtains, using (A2),

$$M=\pm k\langle r\rangle(1\pm k/12m-k^2\langle r^3\rangle/120\langle r\rangle+\cdots)\ , \quad \text{(A4)}$$

where the upper (lower) sign applies to $S\to P$ ($P\to S$) transitions. We denote by $\langle r^p\rangle$ the radial integrals $\int_0^\infty dr\, r^{2+p}R_P R_S$.

In charmonium $1\,^3P_J\to 1\,^3S_1+\gamma$ transitions, the retardation or finite-size effects are not more than 3% corrections. These corrections are smaller in the $2\,^3S_1\to 1\,^3P_J$ decays both because k is smaller and because the two correction terms in (A4) tend to cancel.

APPENDIX B

There are three types of problems that arise when one wants to find the eigenvalues and eigenfunctions of the Breit-Fermi Hamiltonian. First, the tensor force mixes S and D states, etc. Second, there are the momentum-dependent terms

$$-p^4/4m^3-\vec{p}\cdot V_S\vec{p}/m^2+\vec{p}\cdot\left[I-\frac{\vec{\nabla}\vec{\nabla}}{V^2}\right]V_V\cdot\vec{p}/m^2 \quad \text{(B1)}$$

and, third, the effective central potentials that arise in the various $^1S_0$, $^3S_1$, ^3P_J, etc. states require numerical methods for solutions of the eigenvalue problem. As regards the tensor-force mixing, we studied it perturbatively and found very small mixing angles. We neglect this mixing and assume that the eigenstates of $H_{\rm BF}$ are states of definite orbital angular momentum L. Then for each of these $^1S_0$, $^3S_1$, $^1P_1$, $^1D_2$, $^3D_2$, etc. states, if we neglect the terms (B1), $H_{\rm BF}$ has the form

$$p^2/m+V_{\rm eff}(r)\ . \quad \text{(B2)}$$

To include the terms (B1), one can write them as a term $V_{\rm SI}^{(1)}(r)$ which depends only on r and a commutator term

$$V_{\rm SI}^{(2)}=[p^2,U(r)]/m^2\ , \quad \text{(B3)}$$

neglecting higher-order $(v/c)^2$ effects.[18] In the commutator (B3), $U(r)$ is given by

$$U(r)=(7V_V-4Z-3V_S)/12\ , \quad \text{(B4)}$$

where

$$Z=r^{-3}\int_0^r s^3(dV_V/ds)ds\ . \quad \text{(B5)}$$

The $V_{\rm SI}^{(1)}$ term can be combined with the $V_{\rm eff}$ in (B2) to give an effective Hamiltonian

$$H_{\rm eff}=p^2/m+V_{\rm eff} \quad \text{(B6)}$$

in which the effective potential energy $V_{\rm eff}$ depends on S, L, and J. The eigenfunctions and eigenvalues of $H_{\rm eff}$ can be found using standard methods.[21] We solved for the eigenfunctions and eigenvalues of $H_{\rm eff}$ numerically. In order to evaluate the $V_{\rm SI}^{(1)}$ term, we had first to solve for the eigenvalues of the nonrelativistic Hamiltonian, $E_{NL}^{(0)}$. In terms of these and the nonrelativistic potential energy $V_{\rm NR}=V_V+V_S$, one has

$$V_{\rm SI}^{(1)}=\nabla^2\frac{U(r)}{m^2}-[(E_{NL}^{(0)}-V_{\rm NR})^2+4(E_{NL}^{(0)}-V_{\rm NR}) \times(3V_S+2Z-2V_V)/3]/4m +ZL(L+1)/m^2r^2\ . \quad \text{(B7)}$$

The remaining $V_{\rm SI}^{(2)}$ commutator term was then included perturbatively. As a first-order perturbation, this term does not change the energies since one can substitute $H_{\rm NR}$ for p^2/m in (B3). To find the effect of $V_{\rm SI}^{(2)}$ on the wave functions, one can use first-order perturbation theory

$$\psi_{NL}=\psi_{NL}^{(\rm eff)}+\sum_{M\neq N}\psi_{ML}^{(0)}(\psi_{ML}^{(0)},V_{\rm SI}^{(2)}\psi_{NL}^{(0)})/(E_{NL}^{(0)}-E_{ML}^{(0)})\ , \quad \text{(B8)}$$

where $\psi_{NL}^{(0)}$ are eigenfunctions of $H_{\rm NR}$ and $\psi_{NL}^{(\rm eff)}$ of $H_{\rm eff}$. Substituting $H_{\rm NR}$ for p^2/m in (B3), one finds for (B8)

$$\psi_{NL}=\psi_{NL}^{(\rm eff)}-\sum_{M\neq N}\psi_{ML}^{(0)}(\psi_{ML}^{(0)},U\psi_{NL}^{(0)})/m\ , \quad \text{(B9)}$$

and completing the sum over states one gets

$$\psi_{NL}(r)=\psi_{NL}^{(\rm eff)}(r)-[U(r)/m+(\psi_{NL}^{(0)},U\psi_{NL}^{(0)})/m]\psi_{NL}^{(0)}\ . \quad \text{(B10)}$$

These are the wave functions we used in our calculations of the $E1$ matrix elements. Use of eigenfunctions $\psi_{NL}^{(\rm eff)}$ of $H_{\rm eff}$ in (B10) is only a convenient way of including first-order $(v/c)^2$ corrections to the wave functions. To the accuracy of our calculations of $\langle r\rangle$, higher-order effects are negligible. We checked this numerically.

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