SLAC-PUB-1966 June 1977 (T/E)

RECENT ADVANCES IN BOUND STATE QUANTUM ELECTRODYNAMICS*

Stanley J. Brodsky[†] and G. Peter Lepage

Stanford Linear Accelerator Center Stanford University, Stanford, California 94305

ABSTRACT

We review recent developments in four areas of computational quantum electrodynamics: (1) a new relativistic two-body formalism equal in rigor to the Bethe-Salpeter formalism but with strong calculational advantages is discussed; (2) recent work on the computation of the decay rate of bound systems (positronium in particular) is presented; (3) limits on possible composite structure of leptons are discussed; (4) a new multidimensional integration program ('VEGAS') suitable for higher order calculations is presented.

(†Invited talk presented to the Fourth International Colloquium on Advanced Computing Methods in Theoretical Physics, Saint Maximin, France, March 21-23, 1977.)

*Work supported by the Energy Research and Development Administration.

I. INTRODUCTION

One of the most critical testing grounds of quantum electrodynamics involves the bound state spectrum of the pure QED systems, positronium (e^+e^-) and muonium (μ^+e^-) . Although the ground state splittings have now been measured to a part per million or better, calculations—which require the covariant Bethe-Salpeter equation—have been left far behind. In part, this has been due to the lack of a tractable, systematic computational procedure using the Bethe-Salpeter equation. A crucial difficulty has been the absence of known analytic bound state solutions to the equation—even for an approximate interaction kernel.

In this talk, we will report on a new approach by Lepage¹ to the two-body relativistic bound state system which is equal in rigor to the Bethe-Salpeter formalism, but which has important calculational advantages. Outstanding among these is the existence of a Coulomb-like kernel for which the exact analytic solutions of the bound state equation are known. A systematic perturbation theory has also been derived, and this has led to new results for the $\alpha^6 \log \alpha^{-1}$ relativistic recoil contributions to the ground state splitting of muonium and positronium.

Because of these new developments, it now appears that bound state computations can be carried out systematically through the ppm level. Thus the quantum electrodynamics of off-shell electrons and muon as well as the field theoretic formulation of the relativistic two-body problem can be checked to this new level of accuracy. Other applications, to the Lamb shift of muonium, the spectrum of pi-muonium $(\pi^+\mu^-)$, as well as other areas of particle physics (e.g., charmonium spectrum) also suggest themselves.

- 2 -

In this talk we shall also briefly review recent developments in the calculation of the decay rate of orthopositronium.² We also discuss the implications of the successes of QED for limits on possible lepton substructure.³ Finally a new numerical integration technique which has advantages for the very high dimension integrals encountered in QED is discussed.⁴

II. RELATIVISTIC BOUND STATES—A NEW FORMALISM¹

A general result from relativistic field theory is that the bound state of two spin 1/2 particles is exactly described by the full Bethe-Salpeter equation (Fig. 1)

$$(k-m_1)(P-k-m_2)\Psi = K\Psi$$

where K is obtained from the sum of all two particle irreducible kernels[†] (shown in Fig. 1b for QED). In the rest system $\vec{P}=0$, and $P^0 \equiv E_n$. The challenge for computation is to determine the eigenvalues E_n (i.e. the bound state energies) to ppm accuracy. In practice one would want a systematic method for determining E_n to the desired accuracy. Ideally the equation would be written in such a way as to allow algebraic computer analysis.

The problems in dealing with the Bethe-Salpeter equation though are myriad. For example, an exact solution for any kernel applicable to QED has not been available, thus making perturbation theory fraught with peril. Even so, it is known that the single one-photon exchange kernel (in any gauge) is a remarkably poor approximation to the relativistic problem. In fact, one can readily show that all crossed ladder kernels (to all orders in perturbation theory) are needed to obtain the required Dirac equation in the m_1 or $m_2 \rightarrow \infty$ limit.⁵ A further

- 3 -

[†]One includes in K those diagrams not obtainable by iteration of lower order graphs. In general K also includes self energy corrections to the fermion propagators and renormalization counter terms.

complication is that the Bethe-Salpeter equation depends on two off-shell variables $p_1^2 = k^2$, $p_2^2 = (P-k)^2$ and is difficult to interpret. In a sense the Bethe-Salpeter equation contains too much information-more than what is required to obtain the bound state spectrum.

An important advance, pioneered by F. Gross,⁶ is to realize that the bound state spectrum (i.e., the singularities in $\sqrt{s} = \sqrt{P^2}$ of the two-body Green's function) is independent of the value of the off-shell legs. Thus Gross writes an equivalent equation, equal in rigor to the Bethe-Salpeter equation, with one leg on-shell (Fig. 2). The kernel \bar{K} is irreducible in the sense that it contains no two-particle cuts with line 1 on-shell, and it is obtained from the Bethe-Salpeter kernel as shown in Fig. 2b. In fact \bar{K} is the full two particle T-matrix with pole contributions, $\delta^+(k^2-m_1^2)$, removed from each loop integration.

The Gross equation has the Dirac form

$$(\mathcal{P}-\mathcal{K}-\mathbf{m}_2) \ \psi(\mathbf{\vec{k}} \mathbf{P}) = \int \frac{d^3 \ell}{2E_{\ell}(2\pi)^3} \widetilde{\mathbf{K}}(\mathbf{\vec{k}} \ \ell \mathbf{P}) \ \psi(\mathbf{\vec{\ell}} \mathbf{P})$$
(*)

where ψ is a 4 \otimes 2 component spinor (i.e., Pauli matrix representation for spin of on-shell particle 1) and \tilde{K} is defined via

$$\mathbf{\bar{u}}_{(1)}\mathbf{\bar{K}}\mathbf{u}_{(1)} = \chi^{\dagger}_{(1)}\mathbf{\tilde{K}}\chi_{(1)}$$

An awkward feature of this equations is the presence of the variable $k_0 = \sqrt{k^2 + m_1^2}$ on the left hand side. However, as pointed out in Ref. 1, this can be remedied by multiplying through by $\gamma^{0}(\not P+\not k-m_2)$, giving simply

$$\begin{bmatrix} \widetilde{E}\gamma^{0} + \overrightarrow{\gamma} \cdot \overrightarrow{k} - m_{2} \end{bmatrix} \frac{\psi(\overrightarrow{k} P)}{2E_{k}} = \frac{\gamma_{0}(\overrightarrow{P} + \cancel{k} - m_{2})}{4E_{k}P_{0}} \int \frac{d^{3}\ell}{2E_{\ell}(2\pi)^{3}} \widetilde{K}(\overrightarrow{k} P) \psi(\overrightarrow{\ell} P)$$
$$\widetilde{E} \equiv \frac{P_{0}^{2} + m_{2}^{2} - m_{1}^{2}}{2P_{0}}$$

with

Remarkably, this has the form of a standard Dirac equation (with a generalized potential), but it is the exact equation for the Bethe-Salpeter amplitude with one leg on-shell. In fact if one now chooses as the initial approximation the Coulomb-like kernel

$$\widetilde{\mathbf{K}}_{0} = \frac{2\mathbf{E}_{\mathbf{k}}^{2}\mathbf{m}_{1}}{\mathcal{P} + \mathbf{k} - \mathbf{m}_{2}} \left(\frac{-\mathbf{Z} \mathbf{e}^{2}}{|\mathbf{k} - \boldsymbol{\ell}|^{2}} \right)$$

one has the standard Dirac equation for particle (2) in a Coulomb field

$$\widetilde{\mathbf{E}} \gamma_0 + \overrightarrow{\gamma} \cdot \overrightarrow{\mathbf{k}} - \mathbf{m}_2) \psi_{\mathbf{D}}(\overrightarrow{\mathbf{k}}) = - \mathbf{Z} \mathbf{e}^2 \int \frac{\mathrm{d}^3 \boldsymbol{\ell}}{(2\pi)^3} \frac{\gamma_0 \psi_{\mathbf{D}}(\overrightarrow{\ell})}{|\overrightarrow{\mathbf{k}} - \overrightarrow{\ell}|^2}$$

where $e^2 = e^2 m_1/P_0$ and E is given above. One obtains the standard Dirac-Sommerfeld spectrum ($\tilde{E}=\tilde{E}(e^2)$) and Dirac-Coulomb wavefunctions. Thus for this simple choice of kernel one finally has an exact solution for a Bethe-Salpeter wavefunction. It is important to note that for $m_1 - \infty$,

$$e^{2} \rightarrow e^{2}$$

$$\widetilde{E} \equiv m_{2} - \epsilon \frac{m_{1}}{P_{0}} + \frac{\epsilon^{2}}{2P_{0}} \rightarrow m_{2} - \epsilon$$

$$(\epsilon = m_{1} + m_{2} - P_{0})$$

and so the simplest kernel gives the Dirac-Coulomb limit as $m_1 \rightarrow \infty$ [The corrections of order m_2/m_1 agree with the Grotch-Yennie results,⁷ obtained by approximating $k_0 \sim m_1 + \overline{k}^2/2m_1$ in an effective potential equation similar to (*).].

Since an exact solution is known to lowest order, a straightforward perturbation theory can be developed from $\tilde{K}-\tilde{K}_0$ to compute the spectrum to the desired accuracy.

III. APPLICATION: GROUND STATE SPLITTING

MUONIUM AND POSITRONIUM

The ground state splitting due to the spin-spin interactions of a hydrogenic atom is given in lowest order by the Fermi formula $(\gamma = Z\alpha m_1 m_2 / (m_1 + m_2))$:

$$E_{F} = \frac{2}{3} \frac{Z\alpha\gamma^{3}}{m_{1}m_{2}} \langle \vec{\sigma}_{1} \cdot \vec{\sigma}_{2} \rangle \Big|_{j=0}^{j=1} (1+a_{1})(1+a_{2})$$
$$= \frac{8}{3} \frac{Z\alpha\gamma^{3}}{m_{1}m_{2}} (1+a_{1})(1+a_{2})$$

where a_1 and a_2 are the anomalous magnetic moments of the two spin 1/2 constituents. Through the years Dirac binding corrections of order $(Z\alpha)^2 E_F$, radiative corrections of orders $\alpha(Z\alpha)E_F$, $(\alpha(Z\alpha)^2 \log^2 Z\alpha, \alpha(Z\alpha)^2 \log Z\alpha, \alpha(Z\alpha)^2)E_F$, and recoil corrections of order $(Z\alpha)m_2/m_1E_F$ have been systematically evaluated,⁸ but the terms of order $(Z\alpha)^2m_2/m_1E_F$ from the Bethe-Salpeter formalism (relativistic recoil) have been extraordinarily difficult to obtain. At present, theorists have set a temporary goal of calculating the terms of order $(Z\alpha)^2 \log (Z\alpha)m_2/m_1E_F$, although it should be emphasized that all terms of order $(Z\alpha)^2 E_F$ will be required to make comparisons with experiment within the experimental precision. Further it should be noted that terms of order $(Z\alpha)^2 m_2/m_1 \log (m_2/m_1)E_F$ are present and will be important for the muonium comparison. Progress has recently been made in calculating individual $\alpha^3 E_F$ contributions; an example is a new result by Cung, Fulton <u>et al.</u> for the three photon annihilation kernel in positronium.⁹

A summary of Lepage's results¹ for the $\alpha^2 \log \alpha E_F$ contribution to the ground state splitting of positronium and muonium is shown in Fig. 3 (annihilation contributions obtained by Barbieri and Remiddi,¹⁰ and by Owen¹¹ are not shown here but give a coefficient - 5/2). The contribution of (a) (from the difference between the Coulomb interaction and K_0) agrees with a recent calculation by Cung et al.¹²—the spin interaction comes from the small components of the wave function. The two transverse photon contribution (e) agrees with the result of Fulton, Owen and Repko.¹³ The contributions of (f) and (g) agree with the results of Barbieri and Remiddi,¹⁰ and Fulton, Owen and Repko¹³ respectively. The contributions of graphs (b), (c) and (d) are new results obtained by the formalism described above. Previous calculational methods, lacking a 0th order solution of the Bethe-Salpeter equation, cannot readily determine contributions such as (d) which require two iteraction of the interaction kernel.

It is believed this is now the complete set of $\alpha^2 \log \alpha E_F$ contributions. It is reassuring that the m_e/m_{μ} terms in the last column of Fig. 3 cancel, reflecting the fact that it is immaterial which particle is put on the mass-shell in this new formalism.

A summary of the current experimental and theoretical results for the spectra of muonium and positronium is given in Table I. The agreement is remarkable—the experiment-theory differences are within the nominal order expected for the uncalculated terms ($\alpha^2 E_F$ for positronium, $\alpha^2 m_e/m_\mu \log(m_e/m_\mu) E_F$ for muonium).

As an example of the types of terms encountered in the calculation, the one transverse exchange kernel leads to a structure for \vec{k}^2 and $\vec{l}^2 \ll m^2$

$$\sim \int^{\sim \mathbf{m}} \frac{\mathrm{d}^{3}\mathbf{k}}{(\mathbf{k}^{2}+\gamma^{2})^{2}} \int^{\sim \mathbf{m}} \frac{\mathrm{d}^{3}\boldsymbol{\ell}}{(\boldsymbol{\ell}^{2}+\gamma^{2})^{2}} \frac{\overrightarrow{\mathbf{k}^{2}}(\overrightarrow{\mathbf{k}\cdot\boldsymbol{\ell}}-\overrightarrow{\boldsymbol{\ell}}^{2}) - \frac{\mathbf{m}_{\mathrm{e}}}{\mathbf{m}_{\mu}} \overrightarrow{\mathbf{k}^{2}} \overrightarrow{\boldsymbol{\ell}}^{2}}{|\overrightarrow{\mathbf{k}-\boldsymbol{\ell}}|^{2}}$$

giving a $\log \gamma/m$ contribution. In the loop diagrams of Fig. 3 one does the k₀ integration as a contour integral, picking up all poles except the reducible contributions.

-7-

It is expected that all terms of order $\alpha^2 m_e/m_\mu \log (m_e/m_\mu) E_F$ can be readily identified and computed. The goal of computing all terms of order $\alpha^2 E_F$ looks more arduous, but much of the calculation should be amenable to algebraic computer analysis since

- (a) the perturbation theory has been systematized;
- (b) the spin projection analysis and numerator algebra can be performed automatically.

Hopefully the bound state calculations can be systematized to the same extent as (g-2) calculations. It should be noted that some of the $\alpha^2 E_F$ contributions will probably require a Bethe-type sum-over-states calculation.

The new formalism will also clearly be useful for analyzing other bound state problems, as we have discussed in the Introduction. Further work on the analysis of high order corrections within this bound state formalism is in progress. Some clues may also be provided to the formal question of what happens to bound state solutions in QED when α becomes large.

IV. ORTHOPOSITRONIUM $DECAY^2$

The rate for positronium in the 1s, J=1 state to decay into 3 photons is particularly important since it is the only annihilation decay rate of a pure QED system measured to better than 1% precision. In fact experiment has now reached the .1% level and it now appears that there is a serious discrepancy between theory and experiment.

To lowest order, neglecting radiative and relativistic corrections, the positronium decay rate (Fig. 4) is

 $\Gamma_0 = \alpha^6 \,\mathrm{m_e} \frac{2(\pi^2 - 9)}{9\pi}$ = 7.2112×10⁶ sec⁻¹. The complete decay amplitude can be written in exact form as:

$$\mathbf{T} = \int \frac{d^4 \mathbf{k}}{(2\pi)^4} \psi_{\rm BS}(\mathbf{k} \mathbf{P}) \mathcal{M}_{\rm e^+e^- \rightarrow 3\gamma}^{\rm irred}$$

where ψ_{BS} is the full Bethe-Salpeter amplitude and \mathscr{M}^{irred} is the entire set of Feynman graphs for $e^+e^- \rightarrow 3\gamma$, excepting two particle reducible graphs obtained by iteration of the Bethe-Salpeter kernel. Thus, if ψ_{BS} is approximated by solving the Bethe-Salpeter equation with only the Coulomb exchange graph (Coulomb ladder approximation), then \mathscr{M}^{irred} does not include the exchange of Coulomb photons between the e^+, e^- . Working to relative order α , all contributing graphs for \mathscr{M}^{irred} are shown in Fig. 4a to 4g. All contributions are assumed renormalized where required. Notice that even for on-mass lines, \mathscr{M}^{irred} is not infrared divergent; all log λ contributions must cancel by Kinoshita's theorem,¹⁸ or by charge conjugation arguments.

In a new analysis by Caswell, Lepage, and Sapirstein (CLS),² it is noticed that it is actually very useful to include in $\mathcal{M}^{\text{irred}}$ the contribution due to the exchange of a Coulomb photon. When this extra graph is convoluted with ψ_{BS} in the nonrelativistic (Schrædinger) approximation, one simply obtains back the lowest order contribution, Γ_0 . However, as shown by Fulton and Martin^{19,13} the first iteration of the Coulomb kernel with the Schrædinger vertex function and external free Dirac propagators yields the relativistic two-body wavefunction corrections with sufficient accuracy for the order $\alpha \Gamma_0$ calculations. The calculation to this order then simply reduces to

$$T = \psi_{NR}(\vec{x}=0) \operatorname{Re}\left[\mathcal{M}_{b-f}\right]_{\text{on-shell}}(\vec{p}=0)$$
$$+ \int \frac{d^3\vec{p}}{(2\pi)^3} \psi_{NR}(\vec{p}) \operatorname{Re}\left[\mathcal{M}_{g}(\vec{p})\right]$$

- 9 -

where the \mathcal{M} 's are computed with on-shell spinors for the e^+ and e^- . The result is obviously gauge invariant, and the Feynman gauge can be used for convenience.

The CLS results for the self-energy, and vertex corrections (\mathcal{M}_{b-e}) agree with earlier results by Holt and Stroscio (HS);²⁰ however for the annihilation kernel

$$\Gamma_{f} = \frac{\alpha}{\pi} \Gamma_{0} \begin{cases} -.5 \pm .2 & \text{HS} \\ -.741 \pm .017 & \text{Pascual and de Rafael}^{21} \\ -.809 \pm .004 & \text{CLS} \end{cases}$$

and for one photon exchange

$$\Gamma_{\mathbf{g}} = \Gamma_0 + \frac{\alpha}{\pi} \Gamma_0 \left(2 \log \frac{\lambda}{m_e} - 2 \right)$$
$$+ \frac{\alpha}{\pi} \Gamma_0 \begin{cases} 5.8 \pm .4 & \text{HS} \\ -5.90 \pm .07 & \text{CLS} \end{cases}$$

The Γ_0 term in Γ_g , is computed from an explicit 1/v term in \mathcal{M}_g . The next term is associated with the infrared structure of the kernel and can be done analytically. The remaining term disagrees in sign with the Holt and Stroscio result, and leads to a significant change in the theoretical results.

The comparison of theory and experiment is as follows:

$$\Gamma_{J=1}(e^+e^- \rightarrow 3\gamma)$$

 $\Gamma_{expt} = \begin{cases} 7.09 \pm .02 \times 10^{6} \text{ sec}^{-1} & \text{Gidley } \underline{et al.}^{22} \text{ (Vacuum 1976)} \\ 7.104 \pm .006 \times 10^{6} \text{ sec}^{-1} & \text{Gidley } \underline{et al.}^{23} \text{ (Powder 1976)} \\ 7.262 \pm .015 \times 10^{6} \text{ sec}^{-1} & \text{Coleman } \underline{et al.}^{24} \text{ (Gas 1973)} \\ 7.269 \pm .015 \times 10^{6} \text{ sec}^{-1} & \text{Hughes } \underline{et al.}^{25} \text{ (Gas 1973)} \end{cases}$

that is if
$$\Gamma_{expt} = \Gamma_0 \left(1 + \frac{\alpha}{\pi} a_{expt} \right)$$
,

$$\mathbf{a}_{expt} = \begin{cases} -7 \pm 1 & \text{Gidley et al. (Vacuum)} \\ -6.4 \pm 0.4 & \text{Gidley et al. (Powder)} \\ 3.5 \pm 0.9 & \text{Coleman et al., Hughes et al. (Gas)} \end{cases}$$

compared to

$$\mathbf{a}_{\text{theory}} = \begin{cases} -10.35 \pm 0.07 & \text{Caswell, Lepage, Sapirstein (1976)} \\ 1.86 \pm 0.45 & \text{Stroscio, Holt (1974)} \end{cases}$$

Comparing the new CLS result, $\Gamma_{\text{theory}} = 7.0379(12) \times 10^6/\text{sec}$, and the most precise measurements (extrapolated to a zero powder density environment), there appears to be a serious discrepancy of almost 10 standard deviations! It is of course extremely important that this discrepancy be understood. We note that the nominal size of the next contribution from QED (order $\alpha^2 \log \alpha^{-1} \Gamma_0$) is $\sim .002 \times 10^6/\text{sec}$.

The current status of the parapositronium decay

$$\Gamma_{J=0}(e^{-}e^{-} \rightarrow 2\gamma)$$

 $\Gamma_{expt} = 7.99(11) \text{ n sec}^{-1}$ Theriot <u>et al.</u>²⁶ $\Gamma_{th} = 7.98 \text{ n sec}^{-1}$ Harris (1957)²⁷

v. Qed limits on lepton structure³

It is truly extraordinary that the experimental determination of the g factor:

$$g_e = 2(1.001159652410(200))$$
 (Ref. 28)
 $g_{\mu} = 2(1.001165922(9))$ (Ref. 29)

is predicted by QED correctly through eleven significant figures for the electron and nine for the muon.³⁰Note that there is no a priori reason for a spin 1/2particle to have g near 2 (as witnessed by the nucleon). The Dirac value holds only if the fermion is elementary. Thus, suppose the electron was actually a composite structure—a bound state of say two or three more 'fundamental' subunits. Then the coupling to an internal charged current leads to the general contribution to (g-2)/2 of

$$\mathbf{a_e} \sim \mathscr{O}\left(\frac{\mathbf{m_e}}{\mathbf{m^*}}\right)$$

where m* is a characteristic internal mass, the mass of the first excited state, or continuum threshold. Alternately, we can use the Drell-Hearn-Gerasimov³¹ sum rule:

$$\mathbf{a}_{\mathbf{e}}^{2} = \frac{\mathbf{m}_{\mathbf{e}}^{2}}{8\pi\alpha} \int_{\mathbf{s}_{\text{th}}}^{\infty} \left[\sigma_{\gamma \mathbf{e}}^{\mathbf{P}} - \sigma_{\gamma \mathbf{e}}^{\mathbf{A}} \right] \frac{\mathrm{ds}}{\mathrm{s}}$$

where $\sigma_{\gamma e}^{\mathbf{P} \mathbf{A}}$ is the photoabsorption cross section with parallel (antiparallel) photon and target spins. In general $\langle \sigma \rangle \sim \mathcal{O}\left[\alpha/\mathrm{m}^{*2}\right]$ for the contribution of the excited states of the bound system. This contribution (together with the modification of the near-threshold region of $\sigma_{\gamma\mu}$) again gives $a_e \sim \mathcal{O}(m_e/\mathrm{m}^*)$. Taking this effect to be less than the uncertainties in g gives a bound

> $m^* \gtrsim 5 \times 10^4 \text{ GeV}$ for the electron $m^* \gtrsim 3 \times 10^6 \text{ GeV}$ for the muon.

Thus the precision measurement of g-2 leads to an important limit on possible lepton substructure.³

VI. A NEW ALGORITHM FOR MULTIDIMENSIONAL INTEGRATION⁴

One of the most important computational problems facing physicists today is the evaluation of multidimensional integrals with complicated and sometimes poorly behaved integrands. One approach, introduced by Sheppey and developed by Dufner and Lautrup,³² employs iterative and adaptive Monte Carlo integration. This algorithm (known variously as SHEP, RIWIAD, SPCINT,...) has enjoyed widespread usage in theoretical physics. The simplest Monte Carlo estimate of an integral is 33

$$\mathbf{I} = \int_0^1 d^n x \ \mathbf{f}(\vec{x}) \simeq \frac{1}{M} \sum_{i=1}^M \mathbf{f}(\vec{x}_i)$$

where the random points $\{\vec{x}_i\}$ are uniformly distributed throughout the integration volume. The variance of this estimate is approximated by

$$\sigma^{2} = \frac{1}{M} \left[\int_{0}^{1} d^{n}x f^{2}(\vec{x}) - I^{2} \right] \simeq \frac{1}{M-1} \left[\frac{1}{M} \sum_{i} f^{2}(\vec{x}_{i}) - I^{2} \right]$$

To reduce σ^2 for M fixed, Sheppey's algorithm uses stratified sampling: the integration volume is divided into Nⁿ hypercubes using a rectangular grid, and a two-point Monte Carlo integration is performed in each hypercube. The variance is minimized by adjusting increment sizes along each axis (over several iterations) such that the contributions to σ^2 from each interval are equal (= σ^2/N). Thus SHEP concentrates hypercubes where $f(\vec{x})$ is large and changes rapidly.

In high dimensions the number of increments per axis (N) SHEP uses is severely limited by the number of integrand evaluations (M):

$$M = 2N^n$$

Thus SHEP is no longer able to adapt in high dimensions. This handicap can be avoided through use of importance sampling rather than stratified sampling. To illustrate, consider the one dimensional case. The variance σ^2 can be reduced by making a variable transformation x=g(y):

$$\mathbf{I} = \int_0^1 \, dx \; f(x) = \int_0^1 \, dy \; g'(y) \; f(g(y)) \simeq \frac{1}{M} \; \sum_{i=1}^M g'(y_i) \; f(g(y_i))$$

where the points $\{y_i\}$ are uniformly distributed.

It is well known that σ^2 is minimized when

$$\frac{1}{g'(y)} = \frac{|f(x)|}{\int_0^1 dx |f(x)|} \qquad x = g(y) \qquad (**)$$

In a new algorithm called VEGAS, 4 g'(y) is chosen to be a step function with N steps:

$$g'(y) = N \Delta x_{i} \qquad \frac{i-1}{N} \leq y < \frac{i}{N}$$

i.e., $x_{i} - \Delta x_{i} \leq x < x_{i}$
$$\implies x = g(y) = \Delta x_{i} (Ny - (i-1)) + \sum_{j=1}^{i-1} \Delta x_{j}$$

Over several iterations the increments Δx_i are adjusted such that relation (**) is approximately satisfied, and σ^2 minimized. In higher dimensions the separable variable change $x_i = g_i(y_i)$ i=1,...,n is used where now the optimal $g'_i(y_i)$ is defined by projecting the integral on the ith axis.

VEGAS must concentrate integrand evaluations where the integrand is largest, whether or not it is flat there. Thus given the same number of increments per axis, SHEP should be superior. However the number of increments per axis is independent of the number of integrand evaluations in VEGAS, and so VEGAS is always adaptive, in any dimension. Thus VEGAS becomes considerably more efficient then SHEP in high dimensions $(n \ge 4)$.

In Table II VEGAS is compared with SHEP for a test integral having two spherically symmetric Gaussians equally spaced along the diagonal of the integration volume:

$$\mathbf{I_n} = \frac{1}{2} \left(\frac{1}{a\pi^{1/2}}\right)^n \int_0^1 d^n x \left[\exp\left(-\sum_{i=1}^n \frac{\left(x_i - \frac{1}{3}\right)^2}{a^2}\right) + \exp\left(-\sum_{i=1}^n \frac{\left(x_i - \frac{2}{3}\right)^2}{a^2}\right) \right]$$

The integration was done for n=2, 4, 7, 9 with a=0.1. The 'optimal standard deviation' quoted in this table is the standard deviation computed on any iteration after the optimal grid has been achieved. Results averaged over 15 iterations are also presented. As expected, SHEP is more efficient for n<4 while VEGAS is superior for n>4.

VEGAS can be (and has been) further improved through use of other well known methods of variance reduction (stratified sampling, antithetic variates, quasi-random numbers,...) applied to the smoothed integrand f(g(y))g'(y). For example, rather than choosing M random points uniformly distributed on $0 \le y \le 1$, the sampling can be stratified by selecting two points in each of M/2 equal subintervals of [0, 1]— such an algorithm would be very similar in performance to SHEP in low dimensions while remaining adaptive in arbitrarily high dimensions. Note that the optimal definition of g'(y) may differ from that given above when additional variance reduction is employed.

Much work remains to be done on the development of general purpose multidimensional integration routines.³⁴ J. Friedman at SLAC is developing a new Monte Carlo routine which employs n-dimensional minimization techniques to locate important peaks in the integrand and concentrate function evaluations there (using stratified sampling).³⁵ This procedure has the advantage that it is less likely to miss peaks, even if they are very narrow and high. Furthermore hypercube subdivision and error estimates do not rely upon Monte Carlo estimates of the variance of the integrand (which can be misleading for peaky integrands and small sample sizes).

Acknowledgments

We thank W. Caswell and J. Sapirstein who collaborated on much of this work. We also thank V. Hughes for many informative discussions.

REFERENCES

- 1. G. P. Lepage, Stanford Linear Accelerator Center preprint SLAC-PUB-1900-Revised (May 1977).
- W. E. Caswell, G. P. Lepage, and J. Sapirstein, Phys. Rev. Lett. <u>38</u>, 488 (1977).
- 3. S. J. Brodsky and J. Sapirstein in preparation.
- G. P. Lepage, Stanford Linear Accelerator Center preprint SLAC-PUB-1839-Revised (November 1976).
- 5. D. R. Yennie (unpublished); S. J. Brodsky, 'Lectures on Atomic Physics and Astrophysics' Brandeis Summer Institute, 1963, Vol. 1.
- 6. F. Gross, Phys. Rev. <u>186</u>, 1448 (1969).
- 7. H. Grotch and D. R. Yennie, Rev. Mod. Phys. 41, 350 (1969).
- S. Brodsky and S. D. Drell, Ann. Rev. Nucl. Sci. <u>20</u>, 147 (1970); B. E.
 Lautrup, A. Peterman and E. de Rafael, Phys. Rep. <u>3</u>, 193 (1972).
- 9. V. K. Cung, A. Devoto, T. Fulton, and W. W. Repko, CERN preprint TH.2314 (April 1977).
- R. Barbieri, P. Christillin, and E. Remiddi, Phys. Lett. <u>B43</u>, 411 (1973);
 R. Barbieri and E. Remiddi, Phys. Lett. 65B, 258 (1976).
- 11. D. A. Owen, Phys. Rev. Lett. 30, 887 (1973).
- 12. V. K. Cung, T. Fulton, W. W. Repko, and D. Schnitzler, Ann. Phys.
 (N.Y.) <u>96</u>, 261 (1976); V. K. Cung, T. Fulton, W. W. Repko, A. Schaum, and D. Devoto, Ann. Phys. (N.Y.) <u>98</u>, 516 (1976).
- 13. T. Fulton, D. A. Owen, and W. W. Repko, Phys. Rev. A 4, 1802 (1971).
- 14. D. E. Casperson, T. W. Crane, A. B. Denison, P. O. Egan, V.-W. Hughes,
 F. G. Mariam, H. Orth, H. W. Reist, P. A. Souder, R. D. Stambaugh,
 P. A. Thompson, and G. zu Putlitz, Phys. Rev. Lett. 38, 956 (1977).

- H.G.E. Kobrak, R. A. Swanson, D. Favart, W. Kells, A. Magnon,
 P. M. McIntyre, J. Roehrig, D. Y. Stowell, V. L. Telegdi, M. Eckhouse,
 Phys. Lett. 43B, 526 (1973).
- P. O. Egan, W. E. Frieze, V. W. Hughes, and M. H. Yam, Phys. Lett.
 <u>54A</u>, 412 (1975).
- 17. A. P. Mills, Jr. and G. H. Berman, Phys. Rev. Lett. <u>34</u>, 246 (1975).
- 18. T. Kinoshita, J. Math. Phys. 3, 650 (1962).
- 19. T. Fulton and P. C. Martin, Phys. Rev. <u>93</u>, 903 (1954); <u>95</u>, 811 (1954).
- 20. M. A. Stroscio and J. M. Holt, Phys. Rev. A <u>10</u>, 749 (1974);
 M. A. Stroscio, Phys. Report 22C, 217 (1974).
- 21. P. Pascual and E. de Rafael, Lett. Nuovo Cimento 4, 1144 (1970).
- D. W. Gidley, P. W. Zitzewitz, K. A. Marko, and A. Rich, Phys. Rev. Lett. 37, 729 (1976).
- D. W. Gidley, K. A. Marko, and A. Rich, Phys. Rev. Lett. <u>36</u>, 395 (1976).
- 24. P. G. Coleman and T. C. Griffith, J. Phys. B 6, 2155 (1973).
- V. W. Hughes, Physik 1973, Plenarvortrag Physikertaguag 37th (Physik Verlag, Weinham, Germany, 1973), pp 123-155.
- 26. E. D. Theriot, Jr. et al., Phys. Rev. A 2, 707 (1970).
- I. Harris <u>et al.</u>, Phys. Rev. 105, 1656 (1957); P.A.M. Dirac, Proc.
 Cambridge Phil. Soc. <u>26</u>, 361 (1930).
- R. S. Van Dyck, P. B. Schwinberg and H. G. Dehmelt, University of Washington preprint (1977).
- 29. J. Bailey, K. Borer, F. Combley, H. Drumm, F. J. M. Farley,
 J. H. Field, W. Flegel, P. M. Hattersley, F. Krienen, F. Lange,
 E. Picasso, and W. von Ruden, CERN preprint (1977).

- 30. See R. Roskies' talk presented at this Conference.
- 31. S. Drell and A. C. Hearn, Phys. Rev. Lett. <u>16</u>, 908 (1966);
 S. B. Gerasimov, Sov. J. Nucl. Phys. <u>2</u>, 430 (1966);

S. J. Brodsky and J. Primack, Ann. Phys. (N.Y.) 52, 315 (1969).

- 32. A. Dufner, Proceedings of the Colloquium on Computational Physics, Marseille, 1970, p I-46; B. Lautrup, Proceedings of the Colloquium on Computational Physics, Marseille, 1971, p I-57.
- J. M. Hammersley and D. C. Handscomb, <u>Monte Carlo Methods</u> (Methuen, London, 1964), Chapters 3 and 5.
- 34. Another method very similar to that described here was discussed in a talk by T. Sasaki presented to this Conference.
- 35. J. Friedman, private communication.

TABLE I

- 19 -

Comparison of theory and experiment for muonium hfs. Uncertainties shown in theory due to uncertainties in $\mu_{\mu}/\mu_{\rm P}$ (Ref. 14). Terms of $\mathscr{O}\left(\alpha^2 \frac{\mathrm{m}_{\rm e}}{\mathrm{m}_{\mu}} \log \frac{\mathrm{m}_{\mu}}{\mathrm{m}_{\rm e}} \mathrm{E}_{\mathrm{F}}\right) \sim 0.01$ MHz have yet to be computed and are not included.

Theory	
$\mathbf{E}_{\mathrm{F}} + \mathcal{O}\left(\alpha \frac{\mathrm{m}_{\mathrm{e}}}{\mathrm{m}_{\mu}} \mathbf{E}_{\mathrm{F}}, \alpha^{2} \mathbf{E}_{\mathrm{F}}, \alpha^{3} \mathbf{E}_{\mathrm{F}}\right)$	4463.293 (6) MHz
$2 \alpha^2 \frac{m_e}{m_\mu} E_F \log \alpha^{-1}$.011
Total Theory	4463.304 (6) MHz
Experiment	
Ref. 14	4463.30235 (52) MHz
Ref. 15	4463.30400 (180) MHz

Comparison of theory and experiment for positronium hfs. Terms of $\mathscr{O}\left(\alpha^2 m_e^{/2}\right) \sim 0.01 \; \text{GHz}$ are not yet computed.

$\frac{\text{Theory}}{\mathscr{O}\left(\alpha^4 \text{m}_{e}, \ \alpha^5 \text{m}_{e}\right)}$	203.3812 GHz
$\frac{-1}{24} \alpha^6 m_e \log \alpha^{-1}$	0038
Total Theory	203.3774 GHz
Experiment	
Ref. 16	203.3849 (12) GHz
Ref. 17	203.3870 (16) GHz

			VEGAS		-
	n=2	n=4	n=7	n=7	n=9
No. Function Evaluations/Iteration	20 000	20 000	32 000	160 000	100 000
No. Increments/Axis	50	50	50	50	50
Optimal Standard Deviation	0.007	0.02	0.05	0.02	0.06
Cumulative Result After	0.999	1.003	1.015	0.991	0.96
15 Iterations	±.002	±.006	\pm .015	±.007	±.04
			SHEP		
	. n=2	n=4	n=7	n=7	n=9
No. Function Evaluations/Iteration	20 000	20 000	32 768	170 000	3 906 250
No. Increments/Axis	100	10	4	сл	ຽງ
Optimal Standard Deviation	0.0008	0.03	1.0 ^{a)}	0.25	(d **
Cumulative Result After	1.0001	1.004	*	0.90	* *
15 Iterations	±.0002	±.008	*	±.04	*
a 1					

TABLE II Integration of a double Gaussian in n dimensions. The exact result is 1.

^{a)}Algorithm would not converge.

^{b)}Too large to be tried.

- 20 -

FIGURE CAPTIONS

- (a) The Bethe-Salpeter equation for the bound state wave function.
 (b) The kernel for the Bethe-Salpeter equation in QED.
- 2. (a) The bound state equation for the wave function with one particle on mass shell. (b) The effective kernek K in terms of the usual Bethe-Salpeter kernel.
- 3. Diagrams contributing to $\mathcal{O}(\alpha^2 \text{ m}_e/\text{m}_\mu \log \alpha^{-1} \text{E}_F)$ hfs in muonium. The contribution to positronium hfs is found by setting $\text{m}_\mu = \text{m}_e$.
- 4. The orthopositronium decay kernels contributing to $\mathcal{O}(\alpha\Gamma^0)$. Graphs (a) and (g) may be replaced by (g').





Fig. 2

