Lattice calculation of muon-pair production with capture in relativistic heavy-ion collisions

M. R. Strayer and C. Bottcher
Physics Division, Oak Ridge National Laboratory
Oak Ridge, Tennessee 37831

V. E. Oberacker and A. S. Umar
Department of Physics and Astronomy, Vanderbilt University
Nashville, Tennessee 37235

(Received 7 August 1989)

We present a schematic study of muon-pair production with capture of the negative muon into the $1s_{1/2}$ ground state in relativistic heavy-ion collisions. The muon pairs are generated by a time-dependent, screened electromagnetic field. Our numerical calculations are carried out on a three-dimensional lattice with 20–30 mesh points in each direction, utilizing the B-spline collocation method. Numerical convergence has been demonstrated using a Lorentz-boosted screened Coulomb potential. For the system ^{197}Au+^{197}Au at collider energies of 0.2, 1.0 and 2.0 GeV/nucleon, we obtain probabilities for dimuon production with capture between 1.0×10^{-3} and 7.0×10^{-2} at grazing impact parameters. This may indicate that the electromagnetic lepton-pair production is strongly nonperturbative.

I. INTRODUCTION

In ultrarelativistic heavy-ion collisions, electron- and muon-pair production have been widely discussed as a possible tool to help probe the formation and the decay of the quark-gluon plasma phase of matter.[1,2] In the conditions of such collisions, lepton-hadron final-state interactions are usually small, and hence the leptons carry direct information on the space-time region of creation. The processes are also of fundamental interest in their own right.

We have pointed out that the dominant background to the hadronic (Drell-Yan) production of lepton pairs will come from electromagnetic (em) sources and might possibly mask the signals from the plasma phase.[3,4] The heavy ions in relativistic motion generate strong time-dependent em fields with large Fourier components, which give rise to sizable pair production. We want to examine the latter process in detail. Several experimental groups at Brookhaven and at European Organization for Nuclear Research (CERN) are concerned with designing and building dilepton spectrometers with which to probe the complex hadronic phases of relativistic heavy-ion collisions. Detailed predictions of the electromagnetic signals are important for these design studies.

The electromagnetic production of lepton pairs with heavy ions is fundamentally different from the production mechanism with protons or electrons because the coupling constant is strongly enhanced. For very heavy systems (Au+Au,U+U) the effective coupling constant $Z\alpha \approx 0.5$; therefore, heavy-ion colliders provide a unique opportunity to study nonperturbative QED in an entirely new energy regime. Currently, such heavy-ion experiments are carried out at energies of about 10 MeV/nucleon.[5,6] At these low energies, one studies mainly the longitudinal part of the interaction, whereas at relativistic energies the electromagnetic fields become increasingly transverse.

As Gould[7] has pointed out, electromagnetically produced lepton pairs may also impose severe constraints on the design of colliding beam accelerators such as the proposed relativistic heavy-ion collider (RHIC) and the superconducting supercollider (SSC). Pair production with the capture of an electron is a leading mechanism for destroying the intersecting collider beams, because it changes the ionic charge state. Furthermore, if the cross section for em pair production turns out to be large, it will also have implications on the design of dilepton spectrometers which will search for decay products from the quark-gluon plasma phase transition.

In the collision of two relativistic nuclei, the near-zone electromagnetic fields become very large. Estimates indicate that both muon- and tauon-pair production take place with moderate probability.[7] These estimates are based on perturbative treatments in which vacuum excitations decay into pairs via timelike virtual photons. In the case of real photons coupled to slowly varying fields, the dimensionless parameter which sets the scale for pair production is,[8]

$$\kappa = \frac{\omega e E}{m_\ell^3}\,, \tag{1}$$

where ω is the frequency of the photon field, m_ℓ is the lepton mass, and E is the electric field. If the transverse fields near heavy ions are sufficiently large and rapidly varying, we expect to observe lepton-pair production corresponding to large values of κ from these fields.

The excitation of pairs from such fields has been studied with a one-dimensional model.[3] The nonperturbative creation of lepton pairs from the vacuum was estimated by solving the time-dependent Dirac equation on a one-dimensional collocation lattice. The electric field was taken as uniform throughout the spatial lattice; its time dependence was described by a Gaussian. The size of the lattice and the strength and duration of the em pulse were fixed to approximately correspond to those in a grazing relativistic collision of two heavy nuclei. Preliminary estimates from these one-dimensional calculations suggested that relativistic heavy-ion colliders might serve as factories for producing heavy leptons and could even be used to search for possible new generations of leptons, with rest energies up to 200 GeV.[9,3]

In this paper, we present for the first time results of *three-dimensional* calculations of muon-pair production with capture. We solve nonperturbatively the equations for the evolution of the vacuum perturbed by strong, time-dependent electromagnetic fields. The advent of supercomputer technology has stimulated the development of new techniques for obtaining highly accurate numerical solutions to problems in quantum field theory.[10] These approaches, developed for solving gauge field theories of strongly interacting particles on lattices, are applicable to problems in nuclear and atomic physics and, generally, to the nonlinear dynamics of complex systems. For relativistic fermion fields on lattices, problems relating to the doubling of the spectrum and gauge invariance play a central role in the numerical formulation.

Over the past several years, we have pursued a distinct approach which preserves the spirit of lattice gauge theory.[9,3,11,12] We eliminate the field operators from the theory in favor of representations of quantum state vectors on a space-time lattice of collocation points. Both state vectors and fields are given by expansions in terms of basis splines. Lattice variational equations are obtained from a discrete action formulation, yielding a set of coupled matrix equations for the state vectors. This method is particularly well suited to solve systems of fermions coupled to classical fields on a lattice. The advantages of this method include the following.

(1) *Accuracy and efficiency.* Since the solutions can be represented by piecewise polynomials of any degree, unlimited accuracy is possible in principle. More to the point, sufficient accuracy for practical purposes can be achieved with a modest number of lattice points. This is the crucial advantage which enables us to study three-dimensional problems.

(2) *Stability.* The basis spline collocation method is in itself extremely resistant to instabilities. We have developed techniques of building into our algorithms physical criteria such as dispersion relations and conservation laws. In this way, many notorious pathologies can be eliminated, e.g., fermion doubling.

II. FORMALISM

The formalism of nonperturbative lepton-pair production in relativistic heavy-ion collisions can be derived from a semiclassical least action principle.[9] In the following, we present an alternative derivation which is more closely related to the approach by Reinhardt, Müller, and Greiner[13] of e^+e^- production in nonrelativistic heavy-ion reactions. The main difference between the two treatments is that we neglect here the residual interaction among the leptons at an earlier stage.[9]

Throughout this paper, we use a system of units with $\hbar = c = m_0 = 1$. This implies that energies are measured in units of the lepton rest mass, m_0c^2, and that our length and time units are the lepton Compton wavelength $\lambda_c = \hbar/m_0c$ and Compton time $\tau_c = \lambda_c/c$, respectively. For the specific case of muon-pair production we have

$$\begin{aligned} m_0c^2 &= 105.7\ \text{MeV}\ , \\ \lambda_c &= 1.87\ \text{fm}\ , \\ \tau_c &= 6.2\times 10^{-24}\ \text{s}\ . \end{aligned} \tag{2}$$

We start from the standard QED Lagrange density

$$L_{\text{QED}} = \hat{\psi}^\dagger\gamma^0(\gamma^\mu i\partial_\mu - 1)\hat{\psi} - \tfrac{1}{4}\hat{F}_{\mu\nu}\hat{F}^{\mu\nu} - \hat{\jmath}^\mu\hat{A}_\mu\ , \tag{3}$$

where

$$\hat{\jmath}^\mu = \hat{\jmath}^\mu_{\text{lepton}} + \hat{\jmath}^\mu_{\text{ext}} = -e\hat{\psi}^\dagger\gamma^0\gamma^\mu\hat{\psi} + \hat{\jmath}^\mu_{\text{ext}}\ . \tag{4}$$

In general, we denote quantum field operators by a hat over the mathematical symbol, e.g. $\hat{\psi}$ is the lepton field operator. The first two terms describe the free lepton field and the free radiation field, respectively. The coupling term between the two fields, $\hat{\jmath}^\mu\hat{A}_\mu$, arises naturally from the requirement of local $U(1)$ gauge invariance of the QED Lagrange density. The quantity $\hat{\jmath}^\mu_{\text{ext}}$ is a conserved external current, generated by the moving heavy ions.

By varying the action integral

$$S_{\text{QED}} = \int d^4x\ L_{\text{QED}} \tag{5}$$

with respect to the field operators $\hat{\psi}$ and $\hat{A}$ we obtain the Euler-Lagrange equations of motion for the quantum fields

$$[\gamma^\mu(i\partial_\mu + e\hat{A}_\mu) - 1]\hat{\psi}(x) = 0 \tag{6}$$

and

$$\partial_\mu\hat{F}^{\mu\nu}(x) = \hat{\jmath}^\nu(x)\ . \tag{7}$$

Because the external heavy-ion current is much larger than the leptonic current, one may neglect the latter in first approximation. Furthermore, we shall assume that the external gauge field may be treated classically

$$\partial_\mu F^{\mu\nu}_{\rm ext}(x) = j^\nu_{\rm ext}(x) \ . \tag{8}$$

Thus, the two field equations decouple and we are left with the Dirac equation (6) for the lepton field $\hat{\psi}$ which may be recast in Schrödinger form

$$H_D \hat{\psi}(\mathbf{r},t) = i\frac{\partial}{\partial t}\hat{\psi}(\mathbf{r},t) \tag{9}$$

with

$$H_D = \boldsymbol{\alpha}\cdot(-i\boldsymbol{\nabla} + e\mathbf{A}_{\rm ext}) + \beta - eA^0_{\rm ext} \ . \tag{10}$$

We study the electromagnetic production of lepton pairs in a reference frame in which one of the nuclei, henceforth referred to as the target, is at rest. For simplicity, recoil effects are neglected. The target nucleus and the muon interact via the static Coulomb field A^0_T. The only time-dependent interaction $A^\mu_P(t)$ arises from the classical motion of the projectile. It is natural to decompose the Hamiltonian H_D into a static Hamiltonian H_0 and the time-dependent em coupling between the muon field and the projectile nucleus

$$H_D(t) = H_0 + H_P(t) \ , \tag{11}$$

where the static *Furry Hamiltonian* is given by

$$H_0 = -i\boldsymbol{\alpha}\cdot\boldsymbol{\nabla} + \beta - eA^0_T \tag{12}$$

and the interaction term

$$H_P(t) = e\boldsymbol{\alpha}\cdot\mathbf{A}_P(t) - eA^0_P(t) \ . \tag{13}$$

The static part of this Hamiltonian, originally introduced by Furry[14] for atomic physics problems, describes the lepton field in the presence of the strong external Coulomb field of the target nucleus. In this way, binding energy effects to all orders in the coupling constant $(Z\alpha)$ are taken into account. By contrast, the perturbative treatment of QED developed by Feynman and Dyson uses the free Dirac Hamiltonian for H_0, and is thus limited to weak fields.

Following the usual practice, we expand the field operator $\hat{\psi}(\mathbf{r},t)$, defined in Eq. (9), into a complete orthonormal set of single-particle basis states. We consider two convenient choices for this basis.

(1) The *Furry basis* $\{\chi_k(\mathbf{r})\}$, i.e., the *stationary* eigenstates corresponding to the static Hamiltonian H_0 defined in Eq. (12)

$$H_0\chi_k(\mathbf{r}) = E_k\chi_k(\mathbf{r}) \ . \tag{14}$$

(2) The time-dependent basis $\{\phi_j(\mathbf{r},t)\}$ corresponding to the full Dirac Hamiltonian $H_D(t)$ given in Eq. (11)

$$H_D(t)\phi_j(\mathbf{r},t) = i\frac{\partial}{\partial t}\phi_j(\mathbf{r},t) \ . \tag{15}$$

Let us first expand the fermion field operator in terms of the Furry basis, with operator-valued expansion coefficients $\hat{a}_k(t)$

$$\hat{\psi}(\mathbf{r},t) = \sum_k \hat{a}_k(t)\chi_k(\mathbf{r})\exp(-iE_kt) \ . \tag{16}$$

From the anticommutation relations for the fermion field operators $\hat{\psi},\hat{\psi}^\dagger$ one readily obtains

$$\{\hat{a}_{k'},\hat{a}_k\} = \{\hat{a}^\dagger_{k'},\hat{a}^\dagger_k\} = 0, \quad \{\hat{a}_{k'},\hat{a}^\dagger_k\} = \delta_{k,k'} \ , \tag{17}$$

i.e., these operators describe the creation and annihilation of muons in the static Coulomb field of the target nucleus. After inserting the expansion of the field operator (16) into Eq. (9) and utilizing Eqs. (11)–(13) one finds the equations of motion for the annihilation operators $\hat{a}_k(t)$

$$i\frac{d}{dt}\hat{a}_k(t) = \sum_{k'} \hat{a}_{k'}(t)\langle\chi_k|H_P(t)|\chi_{k'}\rangle \times \exp[i(E_k - E_{k'})t] \ . \tag{18}$$

The last equation shows that the Fock space operators $\hat{a}_k(t)$ are time-dependent, because of the interaction Hamiltonian $H_P(t)$.

We now expand the fermion field operator in terms of the basis states $\phi_j(\mathbf{r},t)$ defined in Eq. (15). The corresponding particle destruction operators are denoted by $\hat{\alpha}_j$,

$$\hat{\psi}(\mathbf{r},t) = \sum_j \hat{\alpha}_j\phi_j(\mathbf{r},t) \ . \tag{19}$$

Inserting (19) into (9) and making use of Eq. (15) we obtain

$$i\frac{d}{dt}\hat{\alpha}_j = \sum_{j'} \hat{\alpha}_{j'}\left\langle \phi_j \middle| H_D - i\frac{\partial}{\partial t}\middle| \phi_{j'}\right\rangle = 0 \ , \tag{20}$$

i.e., the annihilation operators $\hat{\alpha}_j$ are time independent. This is not really surprising since the single-particle basis $\{\phi_j\}$ contains the full time development of the collision.

In our case, the initial state is the unperturbed QED vacuum state $|\Phi_0\rangle = |0\rangle$. All the states with energies less than $-mc^2$ are occupied in the vacuum state, while combinations of particle-antiparticle excitations correspond to other possible states.

We shall assume that the dynamics governing the time evolution is unitary. This has several important consequences. Since the initial state is a single Slater determinant, the time-evolved state will be a Slater determinant of time-dependent one-body states, which preserve completeness, orthonormality, and anticommutation relations. Thus, all of the particle-antiparticle excitations corresponding to lepton-pair production and emission are contained in a single Slater determinant. Under the external field, the single-particle states χ_k defined in Eq. (14) evolve into the perturbed states $\phi_j(t)$ according to the time-dependent Dirac equation (15).

We now perform a canonical transformation from the particle and hole operators to particles and antiparticles. From the annihilation operators $\hat{a}_k$ defined with respect to the Furry basis, Eq. (16), we define antilepton creation operators via

$$\hat{b}_k^\dagger = \hat{a}_k, \quad k < F \tag{21}$$

where $k < F$ denotes energies below the Fermi energy $-mc^2$. Similarly, we define antiparticle creation operators with respect to the full time-dependent Dirac Hamiltonian (15)

$$\hat{\beta}_k^\dagger = \hat{\alpha}_k, \quad k < F . \tag{22}$$

By equating the two representations of the field operator, Eqs. (16) and (19), one finds the following connection:

$$\hat{\beta}_k^\dagger = \sum_{n>F} \hat{a}_n \langle \phi_k | \chi_n \rangle + \sum_{n<F} \hat{b}_n^\dagger \langle \phi_k | \chi_n \rangle , \tag{23}$$

where $k < F$. We can now calculate the number of antileptons generated from the time-evolved QED vacuum state $|0(t)\rangle = U(t)|0\rangle$,

$$N_-(t) = \left\langle 0(t) \left| : \sum_{k<F} \hat{b}_k^\dagger \hat{b}_k : \right| 0(t) \right\rangle = \sum_{k<F} \langle 0| : \hat{\beta}_k^\dagger \hat{\beta}_k : |0\rangle . \tag{24}$$

Using Eq. (23) we find that the number of antileptons created after the reaction is given by projecting the time-evolved single-particle states $\phi_k(t \to \infty)$ with negative energy ($k < F$) onto the complete set of Dirac continuum states χ_n with positive energy ($n > F$)

$$N_-(t \to \infty) = \sum_{k<F} \sum_{n>F} |\langle \chi_n | \phi_k(t \to \infty) \rangle|^2 . \tag{25}$$

For the specific case of lepton-pair creation with capture of the lepton into a given bound state ϕ_0 we only have to consider the time evolution of one bound state $\phi_0(t)$ according to the time-dependent single-particle Dirac equation.

III. ELECTROMAGNETIC FIELDS

We saw in Sec. II that the physics of pair production is defined by the electromagnetic fields of two particles in relative motion. We choose a frame in which one heavy ion, the target T, is fixed, while the other, the projectile P, moves by. These fields enter the Hamiltonian in the form defined by Eqs. (11)–(13).

In order to keep the calculation of the external fields as simple as possible, we assume a spherical and homogeneous charge density for both nuclei. Within this approximation, the static Coulomb interaction between target nucleus and muon is given by

$$-eA_T^0(r) = -(Z_T\alpha) f(r, R_T) , \tag{26}$$

where Z_T and R_T denote the charge number and root-mean-square charge radius of the target nucleus and

$$f(r,R) = \begin{cases} \frac{1}{r}, & r > R \\ \frac{1}{2R}\left(3 - \frac{r^2}{R^2}\right), & r < R . \end{cases} \tag{27}$$

In the fixed-target frame of reference, the projectile moves with constant velocity β_f along a straight-line trajectory in the z direction, with impact parameter b. If the reaction plane is chosen to be the y-z plane, the classical trajectory of the projectile is given by

$$x_P(t) = 0, \quad y_P(t) = b, \quad z_P(t) = z_P^0 + \beta_f t . \tag{28}$$

The time-dependent em interaction between projectile nucleus and muon can be generated by a Lorentz boost of the static field. This results in

$$\begin{aligned} -eA_P^0(r'(t)) &= -(Z_P\alpha)\gamma_f f(r'(t), R_P) , \\ A_P^x &= A_P^y = 0 , \\ A_P^z(r'(t)) &= \beta_f A_P^0(r'(t)) , \end{aligned} \tag{29}$$

where Z_P and R_P are the atomic number and mean square radius of the projectile. The quantity $r'(t)$ is the distance between the muon and the center of mass of the moving projectile

$$r'(t) = \{x^2 + (y-b)^2 + \gamma_f^2[z - z_P(t)]^2\}^{1/2} . \tag{30}$$

The beam energy in the collider frame of reference is given by

$$(E_{\text{kin}})_c = m_0 c^2(\gamma_c - 1) , \tag{31}$$

where γ_c denotes the Lorentz factor. As stated above, our calculations are carried out in the fixed-target frame in which the kinetic energy of the projectile is given by

$$(E_{\text{kin}})_f = m_0 c^2(\gamma_f - 1), \quad \gamma_f = (1 - \beta_f^2)^{-1/2} . \tag{32}$$

The Lorentz factors in the two reference frames are related by

$$\gamma_f = 2\gamma_c^2 - 1 . \tag{33}$$

IV. NUMERICAL IMPLEMENTATION

In the course of Sec. II, we reduced the problem of pair production with capture to that of solving a time-dependent single-particle Dirac equation

$$H\psi(t) = i\frac{\partial\psi}{\partial t} \tag{34}$$

where

$$H = \boldsymbol{\alpha} \cdot (-i\boldsymbol{\nabla} - e\mathbf{A}) - eA_0 + \beta . \tag{35}$$

The subscript on ψ is now suppressed for clarity. We shall solve (34) on a collocation lattice, formed by discretizing space in three Cartesian coordinates. The use of Cartesian coordinates avoids the pathologies of rotating frames and the complicated metrics of spherical coordinate systems. The relativistic electromagnetic fields exhibit no usable symmetry in any case. The resulting algorithms have a pleasing conceptual and logical simplicity, which far outweighs any loss of efficiency because the representation is suboptimal with regard to the spatial distribution of lattice points. Time is treated on a different footing as we shall explain below.

In the collocation approach, the wave function is expanded in basis splines, and the residual error set equal to zero at each collocation point. When the coefficients of the basis expansion are eliminated in favor of the values of the solutions at the collocation points, Eq. (34) is replaced by a matrix equation

$$\underline{H}\,\underline{\psi}(t) = i\frac{\partial \underline{\psi}}{\partial t} , \tag{36}$$

where we use an underline for matrices and an arrow for vectors in collocation space. The wave vector $\underline{\psi}$ has components $\psi^{(s)}(\xi_\alpha;t)$ labeled by the spinor index and the collocation point, and $\underline{H}$ is given by

$$\underline{H} = \vec{\underline{\alpha}}\cdot(-i\vec{\underline{\mathrm{D}}} - e\vec{\underline{\mathrm{A}}}) - e\underline{A}_0 + \underline{\beta} . \tag{37}$$

The structure of the matrices $\underline{D}_\mu$ and $\underline{A}_\mu$ will be explained shortly. The same equations can be derived from a discretized action principle, in which integrals over space are replaced by matrix products,

$$\int d^3r\, \varphi(\mathbf{r})^* \Omega \psi(\mathbf{r}) \to \underline{\varphi}^\dagger \underline{\Omega}\,\underline{\psi} . \tag{38}$$

In general, (36) is not self-adjoint, so that wave functions in the adjoint space satisfy a transposed equation

$$\underline{H}^\dagger \underline{\varphi}(t) = i\frac{\partial \underline{\varphi}}{\partial t} . \tag{39}$$

It is easy to see that (36) and (39) together guarantee such results as the conservation of inner products, $\underline{\varphi}(t)^\dagger \underline{\psi}(t)$=const.

The operator Eq. (37) has the appearance of the usual Dirac Hamiltonian with electromagnetic interactions, except that the differential operators are replaced by matrices in collocation space. However, the construction of these matrices is moderately delicate. For simplicity, we outline this procedure in one dimension. The spinor $\psi(\xi,t)$ is expanded on a set of M, Nth-order basis splines, $u_j^N(x)$,

$$\psi(x,t) = \sum_{j=1}^{M} u_j^N(x)\psi^j(t) . \tag{40}$$

The spline function $u_j^N(x)$ is made up of a series of piecewise continuous polynomials of degree $N-1$ joined at support points x_j. The calculations in this paper are all carried out with periodic boundary conditions, which are easily imposed by wrapping around the last $N-1$ splines. We choose to work with odd order splines, for which the collocation points are taken as

$$\xi_\alpha = \frac{x_{\alpha+\mu} + x_{\alpha+\mu+1}}{2}, \quad \mu = \frac{N-1}{2} . \tag{41}$$

This prescription for the collocation points is optimal for equally spaced support points and adequate for most applications. The spinor evaluated at the collocation points is obtained from the expansion coefficients by the matrix transformation,

$$\psi_\alpha = \sum_j B_{\alpha j}\psi^j , \qquad B_{\alpha j} = u_j(\xi_\alpha) . \tag{42}$$

In our application, we always fix the number of collocation points equal to the number of support points. All operators can be obtained in collocation space as simple matrices; for example, the nonrelativistic kinetic energy operator in one dimension is given by

$$T^\alpha_\beta = -\tfrac{1}{2}B''_{\beta j}B^{j\alpha} , \qquad B''_{\beta j} = \left.\frac{d^2u_j}{dx^2}\right|_{x=\xi_\beta} , \tag{43}$$

where the raised indices on the matrix B are used to denote the inverse operation. Local operators, like the fields A^μ, are diagonal matrices in this representation. In summary, the collocation points define a lattice on which the calculations are performed; neither the splines nor their support points appear explicitly again, once the derivative operators have been calculated.

The difficulties of extending this approach to the first derivative operators appearing in the Dirac equation are manifested in the problem of "fermion doubling." The problem of the doubled spectrum for lattice fermions occurs in all numerical formulations of the Dirac equation in coordinate space.[15,16] In dynamical problems, high-momentum components appear in the wave function more or less at random, and grow exponentially. In a stationary problem the spurious solutions can be avoided by eliminating the lower component and discretizing an effective Schrödinger equation. This is usually not practical for dynamical problems, and in any case, restricts the types of observables which can be considered with the method. The general procedure which resolves this is obtained from a Cholesky decomposition of the kinetic energy collocation matrix,

$$\underline{T} = -\tfrac{1}{2}\underline{D}^-\underline{D}^+ . \tag{44}$$

This decomposition uniquely defines the matrices $\underline{D}^\pm$, and is a generalization of elementary forward and backward difference formulas corresponding to left and right differentiation on the lattice.

In our basis-spline-collocation approach, the Hamiltonian is replaced by a matrix (37) whose structure is sparse and blocked. Overall, $\underline{H}$ has a 4×4 spinor structure, within which the elements are matrices in collocation space. The wave functions have four spinor components, each of which is a vector in collocation space $\psi^{(s)}_{ijk}$, having indices i,j,k corresponding to the spatial coordinates x,y,z. The potentials $\underline{A}_\mu$ are diagonal matrices

$$[\underline{A}_\mu]_{ijk}\delta(i'j'k',ijk) . \tag{45}$$

Each component of $\boldsymbol{\alpha}\cdot\vec{\mathrm{D}}$, say $\alpha_x\underline{D}_x$, is a 4×4 supermatrix with two nonzero blocks symmetrically placed about the diagonal. These blocks contain the L- and U-decomposed matrices explained above. Thus $\alpha_x \underline{D}_x$ contains $\underline{D}_x^+$ and $\underline{D}_x^-$, where $\underline{D}_x^- \underline{D}_x^+$ is a representation of d^2/dx^2,

$$\alpha_x \underline{D}_x = \begin{bmatrix} 0 & \sigma_1 \underline{D}^+ \\ -\sigma_1 \underline{D}^- & 0 \end{bmatrix} . \tag{46}$$

Matrices such as $\underline{D}_x^+$ are diagonal in the other two space indices

$$[\underline{D}_x^+]_{i'i}\delta(j'k', jk) , \tag{47}$$

while σ_1 denotes the usual 2×2 Pauli matrix. In summary, all of our numerical procedures reduce to a series of *matrix times vector* operations

$$\psi_{\text{out}} = \underline{H}\psi_{\text{in}} = \sum_{\text{blocks}} \underline{H}_{\text{block}}\psi_{\text{in}} , \tag{48}$$

which can be implemented with high efficiency on a vector or parallel supercomputer. A complete analysis of pair production proceeds in three steps.

(1) *Definition of initial state.* A stationary eigenstate of the matrix Dirac equation is constructed

$$\underline{H}\,\underline{\psi}_0 = E_0 \underline{\psi}_0 \tag{49}$$

using a damped relaxation algorithm

$$\begin{aligned} \underline{\psi}^{(i+1)} &= \underline{\psi}^{(i)} + \mathcal{D}(\underline{H} - E^{(i)})\underline{\psi}^{(i)} , \\ E^{(i)} &= \underline{\varphi}^{\dagger} \underline{H}\, \underline{\psi} , \end{aligned} \tag{50}$$

where the damping operator $\mathcal{D}$ is given by (in matrix form)

$$\underline{\mathcal{D}} = \Delta t \left(\nu \underline{I} + \underline{\beta} + \frac{\vec{\underline{\alpha}} \cdot \vec{\text{p}}}{\mu} \right)^{-1} . \tag{51}$$

We have found that the following parametrization: μ=3.0, $\nu = -0.74$, Δt=4.5 is satisfactory for the calculations described in this paper. The operator $\mathcal{D}$ is constructed to remove the high-frequency components of the residual. This method does not depend on the spectrum of $\underline{H}$ being bounded from below. Once more, the implementation reduces to a series of matrix times vector operations. Further details, including a rationale for the choice of parameters and methods for constructing $\mathcal{D}$ in three dimensions can be found elsewhere.[17]

(2) *Propagation in time.* Time is discretized in the sense that the interactions are taken as constant in each of a series of successive small intervals $(t, t+\tau)$. In each interval, the solution of the time-dependent single-particle Dirac equation is obtained exactly from the Taylor series expansion of the time development operator $\underline{U}(t+\tau, t)$

$$\begin{aligned} \underline{\psi}(t+\tau) &= \underline{U}(t+\tau, t)\underline{\psi}(t) \\ &= \exp(-i\tau \underline{H})\underline{\psi}(t) \\ &= \left(1 + \sum_{n=1}^{N} \frac{(-i\tau \underline{H})^n}{n!} \right) \underline{\psi}(t) \end{aligned} \tag{52}$$

which can be implemented numerically by a series of matrix times vector operations.

(3) *Projection of the final state $\psi(\infty)$ on a complete set of continuum eigenvectors χ_q.* In particular, the antilepton energy distribution is given by the projections on the eigenvectors of the negative energy continuum. The free Dirac continuum states

$$H_0|\chi_{ns}\rangle = (-i\boldsymbol{\alpha} \cdot \boldsymbol{\nabla} + \beta)|\chi_{ns}\rangle = E_n|\chi_{ns}\rangle \tag{53}$$

are known analytically; the quantum numbers n and s denote the energy and spin, respectively. However, it would be inconsistent simply to evaluate these functions at the lattice points; rather, we must generate the continuum states directly on the lattice. Our numerical procedure is to generate the relativistic continuum eigenvectors $\underline{\chi}_{ns}$ from the corresponding nonrelativistic continuum states $\underline{\zeta}_n$ defined by

$$\underline{T}\,\underline{\zeta}_n = \tau_n \underline{\zeta}_n \tag{54}$$

which can easily be obtained on the collocation lattice. One finds the following connection:

$$[\underline{\chi}_{n\uparrow}, \underline{\chi}_{n\downarrow}] = \mathcal{N}(1 + \underline{H}_0/E_n) \begin{bmatrix} \underline{\zeta}_n & 0 \\ 0 & \underline{\zeta}_n \end{bmatrix} \tag{55}$$

where $\mathcal{N}$ is a normalization factor, and $E_n = \pm\sqrt{1+2\tau_n}$. Note that, even though we use the free Dirac Hamiltonian, the above procedure incorporates some of the Coulomb distortion effects by generating continuum states that are orthogonal to the exact Coulomb bound states on the collocation lattice.

V. RESULTS

A complete solution of the lepton-pair production problem requires the propagation in time of a large number of single-particle Dirac continuum states. We have deferred a direct attack on this problem for the present, though we are pursuing simplified approaches. Rather, we shall focus on the more tractable problem of muon-pair production with capture of the negative muon into the $1s_{1/2}$ ground state of the target muonic atom. This requires that *only one* bound state be propagated backwards in time [see Eq. (25)].

The first step is the calculation of the eigenstates of the static Hamiltonian. For the specific case discussed here, we need only the ground state of the muonic atom $^{197}_{79}$Au. The static Coulomb interaction between target nucleus and muon is evaluated from Eq. (26) for a homogeneous nuclear charge distribution with a radius $R = 1.40 \times A^{1/3}$ fm. Using the damped relaxation method discussed in the preceding section, we have varied the size of the lattice to test the convergence of our results. At first we employed a uniform cubic lattice with $N = N_x N_y N_z = 20^3$ lattice points using third-order splines. The collocation points were placed at $-19.0\lambda_c, -17.0\lambda_c, \ldots, +19.0\lambda_c$, where λ_c denotes the muon Compton wavelength. We find a total ground-state energy of $E_{\text{tot}} = 0.8975 m_\mu c^2$ which corresponds to a binding energy $E_b = -10.8$ MeV. (For comparison, a point nucleus would have a much larger binding energy of -19.3 MeV.) The rms radius of the ground-state wave function is found to be $4.79\lambda_c$.

In the second set of calculations, we increased the number of lattice points to $N = 30^3$ resulting in $E_{\rm tot} = 0.9045 m_\mu c^2$ and $E_b = -10.1$ MeV, respectively, with a rms radius of $5.35\lambda_c$ for the ground state of the muonic atom. For these static calculations, we used two convergence criteria: the relative change in energy $(E^{n+1} - E^n)/E^{n+1}$ was always less than 10^{-12} and the energy fluctuation $\eta = (\langle H^2\rangle - \langle H\rangle^2)^{1/2}$ was required to be less than 10^{-6}. The latter requirement turns out to be more stringent. On the 30^3 lattice the damped relaxation method required about 100 iterations to converge.

The time-dependent single-particle Dirac equation is solved on the same lattice using the Taylor series expansion of the time development operator, Eq. (52); we consider a maximum number of 15 terms in the series expansion of the exponential operator. In practice, about 8 terms in the Taylor expansion suffice to preserve unitarity at the 1 part in 10^{10} level.

Because of limited computational resources we were not able to solve the infinite-range dynamical Coulomb problem which would have required a substantially larger lattice size. Therefore, we carried out model calculations for a *screened* Lorentz-boosted Coulomb interaction between projectile nucleus and muon, i.e., the interaction given in Eq. (29) was multiplied by a factor

$$\exp\{-[r'(t)/r_s]^2\} \tag{56}$$

with $r_s = 20\lambda_c$.

Initially, the projectile nucleus is located at a distance of $-25\lambda_c$ giving rise to a negligible interaction potential at the position of the target nucleus which is fixed at the center of the cubic lattice. Calculations were performed for a straight-line trajectory and uniform velocity; the beam energy was varied between 0.2 and 2.0 GeV/nucleon in the collider frame of reference, and impact parameters between 2 and $30\lambda_c$ were considered. The dynamical calculations required typically about 600 time steps. The norm conservation of the wave function is an important indicator for the numerical accuracy of the dynamical calculations. We found that the norm was generally conserved with an accuracy of about 1 part in 10^6. Figure 1 shows the time dependence of the probability for capture into the ground state of the muonic atom following pair creation from the QED vacuum. We see that the probability $P(t)$ rises sharply as the nuclei reach their distance of closest approach; at large distances, $P(t)$ reaches a constant value, an indication for the numerical convergence of our calculation. The bump in $P(t)$ shortly after the distance of closest approach is caused by the nonadiabaticity of the process and is typical for Coulomb excitation processes.

The dependence of the muon capture probability on impact parameter at three energies is shown in Fig. 2. For the system ^{197}Au+^{197}Au at collider energies of 0.2, 1.0 and 2.0 GeV/nucleon we obtain probabilities for dilepton production with capture between 1.0×10^{-3} and 7.0×10^{-2} at the grazing impact parameter $b = 8.8\lambda_c$. These capture probabilities are several orders of magni-

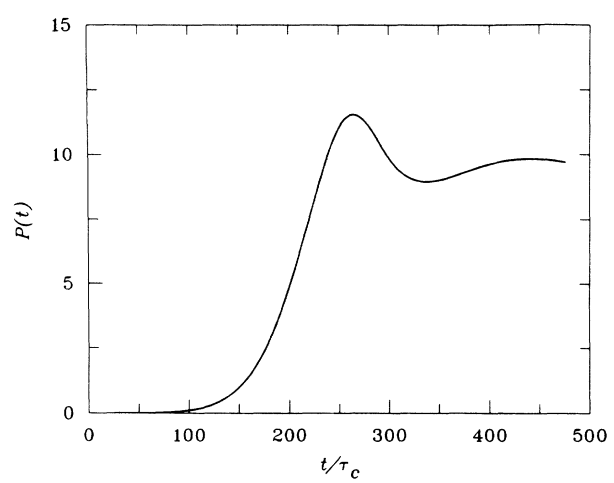

FIG. 1. Muon capture probability into the $1s_{1/2}$ ground state as a function of time (in units of the muon Compton time). The muon pairs are produced electromagnetically from the QED vacuum in collisions of ^{197}Au+^{197}Au at a collider energy of 0.2 GeV/nucleon. The impact parameter amounts to ten muon Compton wavelengths, i.e., 18.7 fm. The calculations are performed on a uniform cubic lattice with 30^3 collocation points.

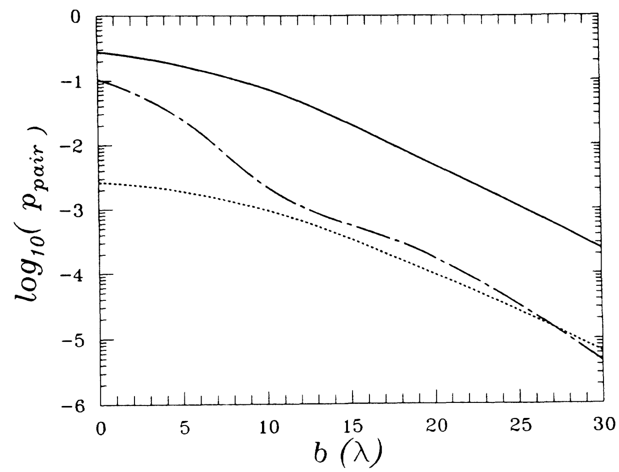

FIG. 2. Muon capture probability as a function of the impact parameter (in units of the muon Compton wavelength) for ^{197}Au+^{197}Au collisions. Depicted is the probability of muon capture into the $1s_{1/2}$ ground state of one of the ions following electromagnetic pair creation from the QED vacuum at three different collider energies: solid curve, E=2 GeV/nucleon, 20^3 lattice; dot-dashed curve, E=1 GeV/nucleon, 20^3 lattice; dotted curve, E=0.2 GeV/nucleon, 30^3 lattice.

TABLE I. Results for electromagnetic muon-pair production from the QED vacuum in ^{197}Au+^{197}Au collisions at a collider energy of 0.2 GeV/nucleon. The numerical calculations are performed with B splines of order 3 and a collocation lattice with 30^3 lattice points. Listed is the probability for capture of the μ^- into the $1s_{1/2}$ ground state, P^-, and the corresponding positive continuum excitation probability, P^+, as a function of the impact parameter b (in units of the muon Compton wavelength).

b	P^-	P^+
2.0	2.391×10^{-3}	3.139×10^{-1}
10.0	9.704×10^{-4}	1.582×10^{-1}
20.0	9.779×10^{-5}	2.518×10^{-2}
30.0	6.397×10^{-6}	2.189×10^{-3}

tude larger than those calculated in first-order perturbation theory by Momberger *et al.*,[18] who find a total capture cross section of $\sigma = 3.7 \times 10^{-9}$ barn in U+U collisions at $E_{\rm lab} = 10$ GeV/nucleon. This confirms our expectation that em lepton-pair production is strongly nonperturbative in relativistic collisions of very heavy ions. Table I summarizes the muon capture probability and the positive continuum excitation probability at different impact parameters.

VI. CONCLUSIONS

The primary goal of our program is to solve nonperturbatively the equations for the evolution of the QED vacuum perturbed by strong, time-dependent electromagnetic fields. In this paper, we have presented for the first time *three-dimensional lattice* calculations for dilepton production by the strong transient electromagnetic fields that are generated in relativistic heavy-ion collisions.

The main purpose of the present calculations is to demonstrate the feasibility of the numerical method. The present results are not yet very accurate, essentially because of the size of the collocation lattice dictated by the computational expense. For the same reason, we employed a *screened* time-dependent em interaction between projectile and muon. Therefore, the present calculations should be regarded as a feasibility study rather than a final result. We estimate that realistic calculations on e^- or μ^- capture require 70–100 points in each direction. We will also explore the use of nonlinear lattices, to which the B-spline method is well suited, for QED problems. Further refinements of the formalism will be necessary for impact parameters less than grazing, because the deceleration of the nuclei during interpenetration must be taken into account. Also, for central collisions, we can no longer describe the nuclei as homogeneously charged spheres; instead, form factors for the nucleons will be needed.

Although our calculations are somewhat schematic, it is interesting to note that we obtain pair production with capture probabilities which are several orders of magnitude larger than those obtained in first-order perturbation theory.[18] This could signal the breakdown of the first-order perturbation approach in the strong-coupling regime ($Z\alpha \approx 0.5$) or might be caused by the atomic basis expansion used in Ref. 18. These matters require further investigation.

ACKNOWLEDGMENTS

This research was sponsored in part by the U.S. Department of Energy under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy Systems, Inc. and under Contract No. DE-FG05-87ER40376 with Vanderbilt University. The numerical calculations were carried out on CRAY X-MP and CRAY-2 supercomputers at the National Center for Supercomputing Applications, Illinois, and at the National Magnetic Fusion Energy Computer Center, Livermore.

[1]K. Kajantie, M. Kataja, L. McLerran, and P. V. Ruuskanen, Phys. Rev. D **34**, 811 (1986).
[2]K. Kajantie, J. Kapusta, L. McLerran, and A. Mekjian, Phys. Rev. D **34**, 2746 (1986).
[3]C. Bottcher and M. R. Strayer, in *Physics of Strong Fields*, edited by W. Greiner (Plenum, New York, 1987), Vol. 153, p. 629.
[4]C. Bottcher and M. R. Strayer, in Proceedings of the Second Workshop on Experiments and Detectors for RHIC, Berkeley, CA, 1987 [Lawrence Berkeley Laboratory Report No. LBL-24604, 1987 (unpublished)].
[5]T. E. Cowan and J. S. Greenberg, in *Physics of Strong Fields*, edited by W. Greiner (Plenum, New York, 1987), Vol. 153, p. 111.
[6]P. Kienle, in *Atomic Physics 10*, edited by H. Narumi and I. Shimamura (North-Holland, Amsterdam, 1987), p. 105.
[7]H. Gould, in *Atomic Theory Workshop in Relativistic and QED Effects in Heavy Atoms (National Bureau of Standards in Gaithersburg, MD)*, Proceedings of the Atomic Theory Workshop on Relativistic and QED Effects in Heavy Atoms, AIP Conf. Proc. No. 136, edited by Hugh Pikelly and Yong-Ki Kim (AIP, New York, 1985).
[8]C. Itzykson and J. B. Zuber, *Quantum Field Theory* (McGraw-Hill, New York, 1980).
[9]C. Bottcher and M. R. Strayer, Ann. Phys. (N.Y.) **175**, 64 (1987).
[10]S. L. Alder and T. Piran, Rev. Mod. Phys. **56**, 1 (1984).
[11]C. Bottcher and M. R. Strayer, Nucl. Instrum. Methods **B31**, 122 (1988).
[12]C. Bottcher, M. R. Strayer, A. S. Umar and V. E. Oberacker, Phys. Rev. C **37**, 2487 (1988).
[13]J. Reinhardt, B. Müller, and W. Greiner, Phys. Rev. A **24**, 103 (1981).
[14]W. H. Furry, Phys. Rev. **81** , 115 (1951).

[15]C. M. Bender, K. A. Milton, and D. H. Sharp, Phys. Rev. D **31**, 383 (1985).
[16]C. Bottcher and M. R. Strayer, Phys. Rev. Lett. **54**, 669 (1985).
[17]C. Bottcher, M. R. Strayer, A. S. Umar, and P. G. Reinhard, Phys. Rev. A **40**, 4182 (1989).
[18]K. Momberger, N. Grün, W. Scheid, U. Becker, and G. Soff, J. Phys. B **20**, L281 (1987).