# Convergence of a lattice calculation for bound-free muon-pair production in peripheral relativistic heavy-ion collisions

J. C. Wells,[1,2] V. E. Oberacker,[2,3] M. R. Strayer,[2] and A. S. Umar[2,3]
[1]*Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge, Massachusetts 02138*
[2]*Center for Computationally Intensive Physics, Physics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6373*
[3]*Department of Physics and Astronomy, Vanderbilt University, Nashville, Tennessee 37235*
(Received 25 October 1995)

We have developed a nonperturbative treatment of bound-free lepton-pair production caused by the strong and sharply pulsed electromagnetic fields generated by heavy ions in peripheral, relativistic collisions based on the solution of the time-dependent Dirac equation using lattice techniques. In this paper, we discuss refinements and extensions of our numerical methods for this problem and demonstrate convergent calculations, with respect to the parameters of the lattice, for bound-free muon-pair production in collisions near grazing incidence of $^{238}U^{92+}+^{238}U^{92+}$ and beam kinetic energies of 30 GeV per nucleon in the fixed-target frame.

PACS number(s): 34.90.+q, 25.75.−q, 12.20.Ds, 02.70.Jn

## I. INTRODUCTION

The new colliding-beam heavy-ion accelerators—most notably the Relativistic Heavy-Ion Collider (RHIC) project at Brookhaven National Laboratory (BNL), designed to investigate nuclear matter at high temperatures and densities—have motivated great interest concerning possible new electromagnetic phenomena [1]. The phenomena considered are pervasive, having relevance for atomic, nuclear, and particle physics, and the design of accelerators and detectors. One of the most interesting of these processes, from the perspective of both fundamental and practical importance, is the production from the vacuum of lepton-antilepton pairs. Of particular interest is the process of bound-free electron-positron production, also called electron capture from pair production, in which the produced electron emerges from the collision bound to a participant ion, as this is a principal beam-loss mechanism for highly charged relativistic ions in a storage ring [2]. This electron capture process is unique in relativistic atomic collision physics in that its cross section increases with the collision energy [3] and no real electrons need be present in the initial state of the collision.

From a fundamental perspective, pair production in peripheral relativistic heavy-ion collisions provides an opportunity to study nonperturbative quantum electrodynamics (QED) in an entirely new and continuously varying energy regime using an interaction which is completely known, due to the combination of very high collision energies and electric charges. Low-order perturbative calculations for bound-free electron-positron pair production have been used as input into design models for RHIC [4,5], and are consistent with a 14-h beam lifetime for gold ions in a storage ring at RHIC energies [6], i.e., approximately 20 TeV per nucleon in the fixed-target frame. Since significantly larger cross sections at these extreme energies would severely limit the beam lifetime for very heavy ions, the size of nonperturbative enhancements has been a matter of great interest. Recent coupled-channel Dirac equation calculations predict nonperturbative effects to be less than 10% for very heavy ions at RHIC energies [7,8]. However, the size of these enhancements for the bound-free electron-positron pair cross section at lower energies near 1–10 GeV per nucleon has been a matter of some controversy [7,9–11].

The first direct measurement of the bound-free electron-positron pair production process was performed at Lawrence Berkeley Laboratory's Bevalac accelerator using $^{238}U^{92+}$ beams at a kinetic energy of approximately 1 GeV per nucleon on targets as heavy as gold [12]. Various perturbative and nonperturbative predictions for the cross section are within a factor of 2 or 3, but no published theoretical calculation reproduces these measurements more accurately [12]. Recently, experiments have been performed using 160 GeV per nucleon $^{208}Pb^{82+}$ beams with gold targets at the European Organization for Nuclear Research (CERN) [13]. With the results from new experiments at 10 GeV per nucleon [14], the measured cross sections will span more than two orders of magnitude in the target-frame collision energy. As such, a reasonable extrapolation of these measurements to RHIC energies should be possible, due to the moderate energy dependence of the cross section in the high-energy regime [15].

Our goal of providing a calculable, nonperturbative description of bound-free lepton-pair production valid over a wide energy range has been limited to varying degrees by the available computer performance. To ease this constraint initially, we have applied our numerical techniques for the time-dependent Dirac equation in three dimensions to the calculation of bound-free muon-antimuon pair production probabilities, as the range of natural length scales for this problem is smaller than for bound-free electron-positron pair production [17,18]. Even so, varying the parameters of our lattice to obtain numerically converged results was not practical in our previous work [17–19].

The main purpose of this paper is to present recent calculations for bound-free muon-pair production at a single impact parameter which are converged with respect to the parameters of the lattice used. That is, we demonstrate that the computed bound-free muon-pair probability does not change appreciably as the lattice spacing is decreased and the computational volume is increased. In accomplishing this, we have made two important improvements in our methods. We now use high-order basis-spline or Fourier collocation representations [20,21] for the momentum operators, rather than the lower order and factored basis-spline-collocation representations used previously [16–18]. This results in a more accurate representation of the kinetic-energy operator and an improved treatment for the lattice fermion-doubling problem [20]. Second, we have implemented our numerical methods on very powerful parallel computers [22], enabling the use of much larger lattice sizes for performing convergence tests. Following an outline of the theory of bound-free lepton-pair production in Sec. II, this paper gives an overview of lattice methods for the solution of the time-dependent Dirac equation in Sec. III. In Sec. IV, we briefly discuss our previous bound-free muon-pair production calculations and present results from our present calculations at an impact parameter of $8\lambdabar_\mu$ for a collision of fully stripped uranium ions at a fixed-target frame kinetic energy of 30 GeV per nucleon. We provide a summary and discussion of this work in Sec. V.

## II. THEORETICAL APPROACH

A semiclassical approximation is appropriate for the pair production problem assuming a classical electromagnetic field generated by the heavy ions, and neglecting lepton-lepton interactions [23]. In this formalism, strong-field quantum electrodynamics is reduced to solving the time-dependent Dirac equation coupled to a classical electromagnetic field while maintaining the quantum-field-theoretic description, which is the correct language for expressing particle production [18]. We use natural units, i.e., $\hbar = c = m_\mu = 1$, throughout this discussion. These definitions imply that energies are measured in units of the muon's rest mass, $m_\mu c^2 = 105.7$ MeV, and length and time in units of the muon's Compton wavelength, $\lambdabar_\mu = \hbar / m_\mu c = 1.87$ fm, and Compton time, $\tau_\mu = \lambdabar_\mu / c = 6.2 \times 10^{-24}$ sec, respectively.

### A. Dirac equation

We study the electromagnetic production of bound-free lepton pairs in a reference frame in which one of the nuclei, i.e., the target, is at rest, since recoil may be neglected. The target nucleus and the lepton interact via the static Coulomb field, $A_T^0$. The time-dependent interaction, $A_P^\mu(t)$, arises from the classical motion of the projectile. Splitting the Dirac Hamiltonian into static and time-dependent parts, we write the Dirac equation for a lepton described by a spinor $\phi(\vec{r},t)$ coupled to an external, time-dependent electromagnetic field

$$[H_F + H_P(t)]\phi(\vec{r},t) = i\frac{\partial}{\partial t}\phi(\vec{r},t), \tag{2.1}$$

where the static Furry Hamiltonian, $H_F$, is given by

$$H_F = -i\vec{\alpha}\cdot\vec{\nabla} + \beta - eA_T^0, \tag{2.2}$$

and the time-dependent interaction of the lepton with the projectile is

$$H_P(t) = e\vec{\alpha}\cdot\vec{A}_P(t) - eA_P^0(t). \tag{2.3}$$

The stationary eigenstates of the Furry Hamiltonian, $H_F$ [Eq. (2.2)], are defined in configuration space by

$$H_F\chi_k(\vec{r}) = E_k\chi_k(\vec{r}). \tag{2.4}$$

The Furry states are proper in and out states for asymptotic times $|t| \to \infty$, where the interaction $H_P(t)$ is zero, and thus serve as the initial states for the time evolution

$$\lim_{t\to-\infty}\phi_j(\vec{r},t) \to \chi_j(\vec{r})\exp(-iE_jt). \tag{2.5}$$

In Ref. [18], the inclusive time-dependent probability for vacuum production of leptons with capture into a bound state, $p$, is determined by computing the expectation value of the lepton number operator, $\hat{n}_p \equiv \hat{a}^\dagger\hat{a}$, for the bound state with respect to the time-evolved QED vacuum, $|\Phi_0(t)\rangle$, i.e.,

$$\begin{aligned} P_p(t) &= \langle\Phi_0(t)|\hat{n}_p|\Phi_0(t)\rangle \\ &= \sum_{r<F} |\langle\chi_p^{(+)}|\phi_r^{(-)}(t)\rangle|^2, \quad p > F, \end{aligned} \tag{2.6}$$

where $F$ denotes the Fermi surface of the initial QED vacuum state. From Eq. (2.6), it is clear that to compute probabilities for lepton-pair production, one could first project time-evolved single-particle states from the negative-energy continuum onto static Furry states, i.e., compute the squares of single-particle transition amplitudes from all states $r < F$ to the state $p$. Alternatively, one may apply the time-reversal invariance of the Dirac equation to obtain an expression where only one time-dependent solution of the Dirac equation is required [18],

$$P_p(t) = \sum_{r<F} |\langle\chi_r^{(-)}|\phi_p^{(+)}(t)\rangle|^2, \quad p > F, \tag{2.7}$$

and it is this more economical expression which we directly compute. Written in this way, bound-free pair production has the form of an ionization process to negative-energy final states.

### B. Electromagnetic interaction

The physics of lepton-pair production is defined by the electromagnetic fields of two charged particles in relative motion, and these fields enter the Hamiltonian via the dimensionless interaction energy, $\bar{A}^\mu \equiv -eA^\mu$, between the lepton and the colliding nuclei in Eqs. (2.2) and (2.3). For simplicity of discussion, we assume a pointlike charge for both the projectile and the target. However, finite-size effects are important when considering heavy leptons, and are included in our muon-pair production calculations by considering the nuclei to be uniformly charged spheres [18]. In the target frame, we choose the projectile to move with constant speed, $\beta_f$, in the $z$ direction, neglecting recoil, and the reaction to occur in the $y$-$z$ plane with impact parameter $b$. The time-dependent electromagnetic potentials between the projectile and the lepton can be generated by a Lorentz-boost of the static Coulomb field. This gives the following Lorentz-gauge interaction:

$$\bar{A}_P^0(r'(t)) = \frac{-Z_P \alpha \gamma_f}{r'(t)},$$

$$\bar{A}_P^1 = \bar{A}_P^2 = 0, \tag{2.8}$$

$$\bar{A}_P^3(r'(t)) = \beta_f \bar{A}_P^0(r'(t)),$$

where $Z_P$ is the atomic number of the projectile, $\alpha$ is the fine-structure constant, and

$$r'(t) = \sqrt{x^2 + (y-b)^2 + \gamma_f^2 (z - \beta_f t)^2} \tag{2.9}$$

is the distance between the projectile and the lepton observed in the rest frame of the target.

For large projectile velocities, i.e., $\beta_f \to 1$, large cancellations occur between scalar and vector amplitudes arising from the time and spatial components, respectively, of the Lorentz-gauge interaction [24], which are troublesome for many numerical approaches [15,18]. To avoid this difficulty, we have explored the use of noncovariant gauges, as have other authors [7,15]. We have found that the axial gauge avoids these severe cancellations and, in addition, other difficulties associated with the use of the sharply peaked Lorentz-gauge interaction with lattice techniques [18]. Specifically, in the axial-gauge interaction, we require the $z$ component of the interaction to be zero, i.e.,

$$\bar{A}_P^3(r'(t)) \to \tilde{A}_P^3(r'(t)) = \bar{A}_P^3(r'(t)) + \partial_z \Lambda(r'(t)) \equiv 0. \tag{2.10}$$

Integrating this equation to obtain the axial-gauge function for pointlike interactions, one obtains

$$\Lambda(r'(t); z_0) = Z \alpha \beta_f \ln \frac{\zeta(t) + \sqrt{\zeta^2(t) + \rho'^2}}{\zeta_0(t) + \sqrt{\zeta_0^2(t) + \rho'^2}}, \tag{2.11}$$

where $z_0$ is an arbitrary integration constant typically set to zero in practice, $\zeta(t) \equiv \gamma_f(z - \beta_f t)$, $\zeta_0(t) \equiv \gamma_f(z_0 - \beta_f t)$, and $\rho'^2 = x^2 + (y-b)^2$. One obtains the axial-gauge interaction for a pointlike projectile by performing a gauge transformation on the Lorentz-gauge interaction in Eq. (2.8) using the gauge function in Eq. (2.11).

## III. NUMERICAL SOLUTION

The solution of the Dirac equation coupled to such an external field is a difficult numerical task. In heavy-ion collisions with relative velocities up to approximately $0.3c$, it is reasonable to expand the projectile and target interactions with the lepton about some point on the internuclear axis and retain only the monopole term, since pair production is dominated by the rapid collapse of the $K$ shell when the nuclei are very close [25]. However, for extreme relativistic velocities, the retarded electromagnetic interaction breaks the approximate monopole symmetry and indeed all symmetries of three-dimensional space. As a result, multipole expansions of the time-dependent interaction converge slowly. However, progress has been made with the coupled-channels approach by considering the high-energy limit of the multipole components of the interaction represented in a noncovariant gauge [8,26]. Compounding the computational difficulties resulting from a lack of spatial symmetry is the fact that accurate calculations depend on the interaction being well represented over multiple physical length scales. For bound-free electron-pair production, the relevant length scales are the nuclear radius of the heavy ion ($R_{\rm nuc} \approx 8$ fm), the Compton wavelength of the electron ($\lambda\!\!\!^{-}_e \approx 400$ fm), the spatial extent of the bound electron's probability density ($10\lambda\!\!\!^{-}_e$), and the width of the electromagnetic pulse generated by the projectile, $b/\gamma_f$.

Largely in response to these numerical challenges, basis-spline-collocation methods have been developed as accurate, stable, and flexible methods for solving partial-differential equations [16,20,27], and applied to the solution of the time-dependent Dirac equation [16,18]. More recently, we have also implemented the similar, but more widely used, Fourier-collocation, i.e., pseudospectral, methods [21]. In such grid-based methods, one represents an approximate solution to a differential equation with a basis of functions complete in a finite-dimensional space. A set of linear equations for the expansion coefficients are defined by an application of the collocation method to the residual of the differential equation. One eliminates the expansion coefficients from the linear equations in favor of the approximate solution evaluated at the collocation points. We note that the memory requirement of many large three-dimensional problems is dominated by storage for the solution vector, not the Hamiltonian matrix, because of the separability of the kinetic-energy operator represented in orthogonal coordinates. Therefore, high-order methods, with their improved accuracy, which reduce the total number of lattice points required have an advantage when memory capacity is a constraint, as is the case for these calculations of bound-free lepton-pair production.

As a result of representing the Dirac operator on a configuration-space lattice, one must manage the fermion-doubling, or spectral-doubling, problem [28,30]. Fermion doubling is manifested by energy-momentum dispersion relations for which, as a function of increasing momentum, the energy decreases associating low-energy eigenvalues with large momenta [16]. For a lattice with an even number of points, one has the extreme situation of a degenerate zero kinetic-energy state associated with the maximum momentum $k = k_{\rm max} = \pi/\Delta x$, where $\Delta x$ is the lattice spacing [20]. In dynamical problems, this spectral doubling causes unphysical, high-momentum components to dominate the evolution [16].

One method for avoiding the doubling is to represent the upper- and lower-Dirac components using two distinct grids, shifted with respect to each other [29]. For the case of finite-difference operators, these shifted grids are equivalent to the use of two-point forward and backward derivatives to discretize the lower and upper components of the Dirac spinor, respectively. This idea was generalized to the lattice-collocation method by factoring the second derivative matrix with Cholesky decomposition to obtain upper- and lower-triangular representations of the first-order derivative [16]. However, we discovered that, when used in the context of a large three-dimensional solution, this generalization introduced errors into the imposed boundary conditions which were too significant to overcome by simply increasing the size and extent of the numerical lattice [17,18]. These errors were especially troublesome for the bound-free pair produc-

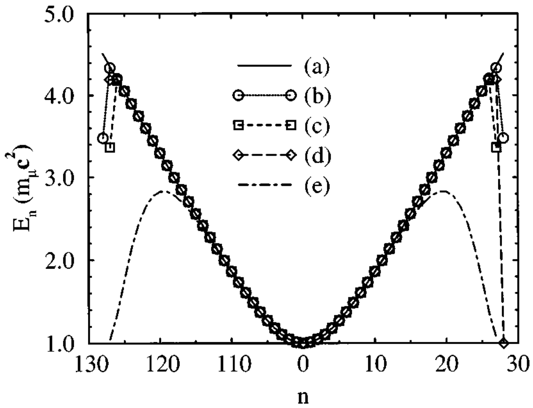


FIG. 1. The positive branch of the Dirac energy spectrum for a free particle in one dimension versus the eigenvalue index using (a) the Fourier-collocation method with 57 points, and the basis-spline-collocation method with (b) 57th-order splines and 57 points, (c) 55th-order splines and 55 points, (d) 55th-order splines and 56 points, and (e) 5th-order splines and 55 points. The energy spectrum in example (a) reproduces the physical dispersion relation, while all other examples given show some departure from the physical relation. The spectra in examples (b) and (c) show a departure from the physical relation at large energy, while the spectra in examples (d) and (e) show very significant errors.

tion problem as it is the small, negative-energy-continuum components of the Dirac spinor which are of interest.

Therefore, we have abandoned the use of the upper- and lower-triangular representations of the first-derivative operator in favor of an (anti)symmetric representation of the first derivative using Fourier or very high-order basis-spline collocation representations [20,30]. Figure 1 demonstrates for the case of the one-dimensional free Dirac equation that these representations avoid the doubled energy spectrum for a finite, but odd, number of lattice points. The Fourier derivative provides a completely accurate energy dispersion relation up to the maximum energy contained on the lattice. Using the maximal-order spline representation, only the energy states with the largest wave number have an appreciable error, and this error does not constitute a complete doubling of the spectra, but does reduce by approximately 20% the range of wave numbers for which a physical dispersion relation is well represented [20].

Once the lattice representation of the Dirac Hamiltonian is obtained, the solution of the time-dependent Dirac equation proceeds in three general steps: (i) partial eigensolution for the initial state, (ii) evolution of this state in time, and (iii) spectral analysis, i.e., projection, of the time-evolved solution to obtain the probabilities. Efficient algorithms used in our present work for each of these three steps are described in detail in Refs. [18,22]. These algorithms are iterative in nature and reduce to a series of generalized matrix-matrix operations which may be implemented efficiently using vector or parallel computers. Current calculations for this paper were performed on the Intel Paragon-MP distributed memory computer achieving a sustained floating-point performance of 12 Gflop/s on 256 nodes.

## IV. THREE-DIMENSIONAL CALCULATIONS

Because of the muon's comparatively large mass, its Compton wavelength and the nuclear radius are of similar size, i.e., $R_{\rm nuc}\approx 4\lambda\!\!\!^{-}_{\mu}$. As a result, the spatial extent of the $K$-shell muon's probability density is very compact, being on the order of $10\lambda\!\!\!^{-}_{\mu}$, with a significant probability for the muon to be found inside the nucleus. As a result, accurately representing the Coulomb cusp in the atomic wave function, which is an issue for the electron-pair production problem, is not a concern for the muon production problem. Moreover, the range of length scales found in the muon-pair production problem is smaller than that found in the electron-positron pair production problem. For these reasons, our nonperturbative, three-dimensional calculations for bound-free pair production have been performed to date only for muon pairs as this calculation is expected to be less difficult.

The duration of the projectile's electromagnetic pulse in the fixed-target frame, $\Delta t \approx b/\gamma_f c$, determines the maximum equivalent-photon frequency present in the projectile-lepton interaction, i.e., $E_{\rm max}\approx \gamma_f \hbar c/b$. To produce a lepton pair, the maximum photon energy must be at least two lepton-mass units, i.e., $\gamma_f \hbar c/b \gtrsim 2 m_0 c^2$, or equivalently, $b/\gamma_f \lesssim \lambda\!\!\!^{-}_c/2$. That is, the width of the electromagnetic pulse must be at least one-half of the lepton's Compton wavelength for the pair production process to be above threshold. For muon-pair production, this means that $b/\gamma_f \lesssim 0.5\lambda\!\!\!^{-}_{\mu} \approx 1$ fm, i.e., the width of the pulse determines the minimum length scale for collision energies above threshold. The smallest peripheral impact parameter is approximately $b_{\rm min}\approx 2R_{\rm nuc}\approx 8\lambda\!\!\!^{-}_{\mu}$ for a heavy nucleus. (Pair production in peripheral, i.e., noncentral, collisions may be distinguished experimentally by detecting a positron in time coincidence with full-energy projectile ions which have not undergone hard nuclear collisions.) We estimate the threshold target-frame Lorentz factor for muon-pair production at this impact parameter to be $\gamma_f \gtrsim 4R_{\rm nuc}/\lambda\!\!\!^{-}_{\mu}\approx 16$, or a target-frame kinetic energy of approximately 15 GeV per nucleon. In the collider frame, this corresponds to a Lorentz factor of $\gamma_c \approx 3$, or a kinetic energy of 2 GeV per nucleon.

### A. Previous calculations

Our initial three-dimensional calculations were designed to demonstrate the feasibility of our numerical methods for the Dirac equation by performing a schematic study of bound-free muon-pair production into the $K$-shell in relativistic heavy-ion collisions [17]. We considered collisions of $^{197}\mathrm{Au}^{79+} + {}^{197}\mathrm{Au}^{79+}$ at collider energies up to 2 GeV per nucleon using $20^3$ lattice points, i.e., 20 points in each of the three Cartesian directions [17]. We chose the collision energy to be near threshold to minimize the overall range of length scales in the calculation, and to perform calculations in a regime in which low-order perturbation theory would apply. Because of the limited computational resources, the calculations reported in Ref. [17] were performed using a model, screened Lorentz-boosted Coulomb interaction. These initial calculations resulted in very large bound-free muon-pair probabilities on the order of $10^{-2}$, given the fact that the chosen collision energy is relatively low.

We improved our numerical approach by successfully incorporating the realistic electromagnetic interaction into the lattice solution through the use of the noncovariant axial gauge [18]. However, our calculations were still limited to relatively small grid sizes. Using a lattice of $16^3$ points and a lattice spacing of $2.5\lambda_\mu$, we performed calculations for bound-free muon-pair production into the $K$-shell in collisions of $^{197}\mathrm{Au}^{79+}+{}^{197}\mathrm{Au}^{79+}$ near the grazing impact parameter at collider kinetic energies of 2 GeV per nucleon, resulting again in large probabilities of order $10^{-2}$.

Both the calculations in Refs. [17,18] were far from being converged partially due to the course grid spacing of 2.0–$2.5\lambda_\mu$, as our new calculations will demonstrate. However, difficulties persisted in subsequent calculations which were not resolved by increasing the size of the lattice within practical limits. The most obvious point of concern was that the calculated bound-free pair production probabilities were very large considering the relatively small collision energy, and did not easily converge to smaller numbers with increasing lattice size as anticipated. This effect was especially noticeable for large impact parameters for which the collision energy was below threshold for producing muon pairs. The major source of these problems was identified as numerical error resulting from the use of upper- and lower-triangular derivative matrices in the kinetic-energy operator in avoiding the fermion-doubling problem as discussed in Sec. III.

We implemented our current treatment of the fermion-doubling problem using the Fourier-collocation method in the calculations reported in Ref. [19] once again for our test system of $^{197}\mathrm{Au}^{79+}+{}^{197}\mathrm{Au}^{79+}$ at collider kinetic energies of 2 GeV per nucleon. Using a single processor of a Cray-C90 computer, we performed convergence tests in a computational volume of $(40\lambda_\mu)^3$ using lattice sizes ranging in six steps from $17^3$ points to $81^3$ points. The computed bound-free muon-pair probabilities were observed to decrease readily with increasing lattice size, but did not reach a converged value. Still larger lattice sizes were required for convergence. For the $81^3$ lattice, we computed bound-free muon probabilities which were much smaller than our previous calculations, being approximately $6\times10^{-5}$.

In performing this work, we were able to identify the major source of the error remaining in these calculations as an under-representation on the lattice of the width of the electromagnetic pulse resulting from too few lattice points in the beam direction. The error from this effect was large compared to the size of the bound-free muon probabilities, but was negligible for the calculation of other observables, such as the ionization probability. We were able to confirm this idea by performing calculations in the same computational volume, but using $29^2\times81$ lattice points. This calculation gave total bound-free probabilities approximately the same as the $81^3$ calculations since the same numerical error which dominated both calculations, i.e., $\Delta z$, was too large. Further exploratory calculations performed using $29^2\times161$ lattice points resulted in decreasing this error to a point where it no longer dominated the bound-free probabilities [19].

### B. Convergence tests

Now that the quality of our calculations has substantially improved, another significant difficulty in performing these bound-free lepton-pair production calculations becomes more apparent. These bound-free probabilities are orders of magnitude smaller than other observables, and very accurate numerical methods are required to compute bound-free probabilities on the order of $10^{-5}$ or $10^{-6}$ where, in comparison, the ionization probability is on the order of 0.1. Therefore, to facilitate our convergence tests, we have considered a different collision system with larger charge and collision energy for which the bound-free pair probabilities are expected to be larger, i.e., $^{238}\mathrm{U}^{92+}+{}^{238}\mathrm{U}^{92+}$ at beam kinetic energies of 30 GeV per nucleon in the fixed-target frame. The larger collision energy will decrease the width of the electromagnetic pulse, $b/\gamma_f$, and thus the necessary lattice spacing in the beam direction, by a factor of 2.

In performing the calculations for the convergence tests, we varied the size of the initial time step to insure the insensitivity of the results to this parameter of the calculation. In addition, the time step size was varied inversely to the absolute magnitude of the extremum of the electromagnetic interaction during the calculation to improve the accuracy of the evolution near the distance of closest approach in the collision [18]. We first fixed the volume of the numerical box to be $(32\lambda_\mu)^3$, and the lattice spacing for each of the three dimensions to be $0.5\lambda_\mu$, i.e., two points per muon Compton wavelength. Experience shows this spacing to be adequate for the transverse grid in computing the total bound-free muon-pair production probability. However, as we have mentioned, we expect the beam direction to require $\Delta z\approx b/2\gamma_f\approx0.13\lambda_\mu$. Using up to 128 nodes of an Intel Paragon-MP computer, we performed calculations with successively smaller $\Delta z$, until the total bound-free probability does not change more than about 1% as $\Delta z$ is increased. Calculations were performed using grids ranging in size from $63^3$ to $63^2\times319$. A calculation performed with $\Delta z=0.125$, i.e., with $63^2\times255$ lattice points, is sufficient for convergence with respect to the lattice spacing in a volume of $(32\lambda_\mu)^3$, and results in a calculated asymptotic bound-free probability of approximately $4\times10^{-6}$.

We present these convergence tests for the bound-free muon-pair probabilities in Fig. 2. This figure shows that transient probabilities on the order of $10^{-3}$ are reached in these collisions near the distance of closest approach for the projectile before the probabilities relax to much smaller values at asymptotic times. The sharp local minimum occurring at $t=0$ is a characteristic feature of performing these calculations in the axial gauge enforcing only asymptotic gauge invariance [10]. From experience, we attribute the fluctuations observed in the small asymptotic values of the larger runs in Fig. 2 to errors resulting from a numerical volume which is too small. We note that the two largest runs presented in Fig. 2 give practically identical results.

In testing the convergence with respect to the volume of the numerical box, we maintain the lattice spacing which produced converged calculations for the $(32\lambda_\mu)^3$ volume, i.e., $\Delta x=\Delta y=0.5\lambda_\mu$, and $\Delta z=0.125\lambda_\mu$, and increase this volume in two steps to $(40\lambda_\mu)^3$ and $(48\lambda_\mu)^3$. These two calculations, requiring $79^2\times319$ and $95^2\times383$ lattice points, respectively, agree with one another within 5%. The bound-free probabilities as a function of time are presented in Fig. 3. With the improved accuracy of these larger calculations, we notice a long-range, slowly relaxing tail for the time-dependent probabilities which we attribute to the small longitudinal component of the projectile-muon interaction.

As a final test, we perform a very large calculation in a rectangular volume of size $48\lambda_\mu\times72\lambda_\mu\times48\lambda_\mu$, allowing more space in the reaction plane. For this calculation, we use

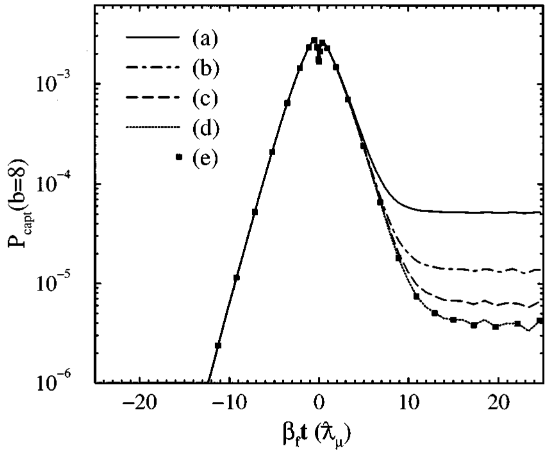


FIG. 2. Depicted are time-dependent bound-free muon-pair probabilities into the atomic $K$ shell, $P_{\mathrm{capt}}$, calculated for 30 GeV per nucleon fixed-target frame collision of $^{238}U^{+92}+^{197}U^{+92}$ at $b=8\lambda_\mu$ for various lattice sizes ranging from $63^3$ to $63^2\times319$. Convergence is achieved when the lattice spacing in the beam direction, $\Delta z$, is sufficiently small compared to the width of the electromagnetic pulse. Calculations are performed for (a) $\Delta z=0.51$, (b) $\Delta z=0.34$, (c) $\Delta z=0.25$, (d) $\Delta z=0.125$, and (e) $\Delta z=0.10$.

a lattice of $95\times143\times479$ points, resulting is a lattice spacing of $\Delta x=\Delta y=0.5\lambda_\mu$ and $\Delta z=0.10\lambda_\mu$. We allowed this calculation to proceed much longer in time until the probability decreases less than 1.5% within the last five muon Compton time units to obtain an asymptotic probability of $1.4\times10^{-6}$. Results from this calculation, presented in Fig. 3, agree well with the previous two calculations, and so we conclude that the extra space provided for the reaction plane was unnecessary.

## V. SUMMARY AND DISCUSSION

In summary, we have demonstrated convergence of a lattice calculation, with respect to the refinement of the lattice parameters, for bound-free muon-pair production probabilities into the $K$-shell in collisions of $^{238}U^{92+}+^{238}U^{92+}$ at beam kinetic energies of 30 GeV per nucleon in the fixed-target frame with an impact parameter of $8\lambda_\mu$. Our calculations require large lattice sizes, and converge slowly to a value of $P_{\mathrm{capt}}=1.4\times10^{-6}$. We observe that the convergence of our calculation is very sensitive to the faithful representation on the lattice of the width of the electromagnetic pulse generated by the projectile, which is the smallest physical length scale which plays a role in this problem. Other observables, such as target excitation and ionization, which can be calculated given the time-evolved spinor, converge much more easily than the bound-free pair probability primarily because other larger length scales characterize these processes.

Our previous bound-free muon-pair calculations were preliminary in nature and designed primarily to explore the feasibility of performing three-dimensional lattice calculations for bound-free pair production. These initial calculations were typically performed using only $16^3$ or $20^3$ lattice points and gave bound-free probabilities near grazing impact on the order of $10^{-2}$. The reasons for the large change in these preliminary values and the results of our current calculations are numerical in nature. Specifically, current lattice sizes are orders of magnitude larger than previously used and allow the performance of convergence tests, and our current lattice representation of the Dirac Hamiltonian is much improved with respect to accuracy as compared to that used in our previous work.

A remaining aspect of improving the present calculations is the improvement of the method for projecting the time-evolved spinor onto the negative-energy continuum states. We currently approximate these continuum states by requiring negative-energy eigenstates of the lattice representation of the free Dirac Hamiltonian to be orthogonal to the initial state of the system, and thereby approximately include Coulomb distortion effects [18]. One can improve this computationally convenient representation of the lattice Dirac continuum states by forcing orthogonalization to higher-lying bound states of the target. We are also working to relax this approximation altogether by extending the so-called *continuum-filter* techniques used with lattice representations of the Schrödinger equation to the Dirac equation to efficiently project onto exact eigenstates of the lattice representation of the Furry Hamiltonian [31,32].

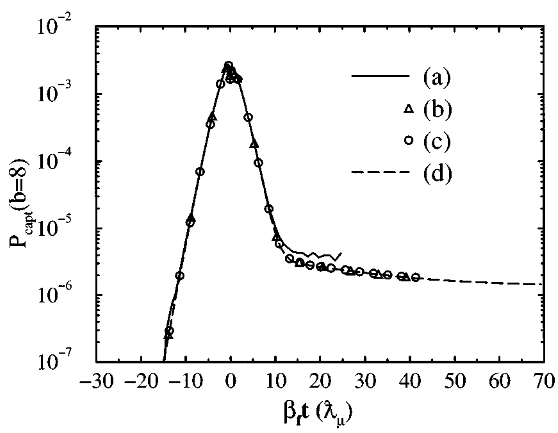


FIG. 3. Plotted are calculations of the bound-free muon-pair probabilities, as in Fig. 2, testing convergence of the lattice calculation with respect to the volume of the numerical box used. Calculations are presented for the following lattice parameters: (a) a volume of $(32\lambda_\mu)^3$ using $63^2\times255$ points, (b) a volume of $(40\lambda_\mu)^3$ using $79^2\times319$ points, (c) a volume of $(48\lambda_\mu)^3$ using $95^2\times383$ points, and (d) a volume of $48\lambda_\mu\times72\lambda_\mu\times48\lambda_\mu$ using $95\times143\times479$ points.

## ACKNOWLEDGMENTS

This research project was sponsored by the National Science Foundation through a grant for the Institute for Theoretical Atomic and Molecular Physics at Harvard University and the Smithsonian Astrophysical Observatory, and the U.S. Department of Energy under Contract No. DE-FG05-87ER40376 with Vanderbilt University, under Contract No. DE-AC05-84OR21400 with Oak Ridge National Laboratory managed by Lockheed Martin Energy Systems, Inc., and under the High Performance Computing and Communications Program (HPCC) as the "Quantum Structure of Matter Grand Challenge" Project.

[1] H. A. Gould, Lawrence Berkeley Laboratory Technical Information, Report No. LBL 18593 UC-28 (unpublished); *Atomic Theory Workshop on Relativistic and QED Effects in Heavy Atoms, Gaithersburg, Maryland, 1985*, edited by Hugh P. Kelly and Yong-Ki Kim, AIP Conf. Proc. Vol. 136 (AIP, New York, 1985).

[2] M. Fatyga, M. J. Rhoades-Brown, and M. Tannenbaum, Brookhaven National Laboratory Report No. BNL-52247 (unpublished).

[3] A. Belkacem, H. Gould, B. Feinberg, R. Bossingham, and W. E. Meyerhof, Phys. Rev. Lett. **73**, 2432 (1994).

[4] C. Bottcher and M. R. Strayer, Phys. Rev. D **39**, 1330 (1989).

[5] M. J. Rhoades-Brown, T. Ludlam, J.-S. Wu, C. Bottcher, and M. R. Strayer, Brookhaven National Laboratory Report No. BNL-52262, 1990 (unpublished), p. 325.

[6] M. J. Rhoades-Brown, C. Bottcher, and M. R. Strayer, Phys. Rev. A **40**, 2831 (1989); Nucl. Instrum. Methods B **43**, 301 (1989).

[7] A. J. Baltz, M. J. Rhoades-Brown, and J. Weneser, Phys. Rev. A **47**, 3444 (1993).

[8] A. J. Baltz, M. J. Rhoades-Brown, and J. Weneser, Phys. Rev. A **50**, 4842 (1994).

[9] K. Rumrich, K. Momberger, G. Soff, W. Greiner, N. Grün, and W. Scheid, Phys. Rev. Lett. **66**, 2613 (1991).

[10] K. Rumrich, G. Soff, and W. Greiner, Phys. Rev. A **47**, 215 (1993).

[11] K. Momberger, A. Belkacem, and A. Sorensen, LBL Report No., LBL-37101, UC-411, 1995 (unpublished).

[12] A. Belkacem, H. Gould, B. Feinberg, R. Bossingham, and W. E. Meyerhof, Phys. Rev. Lett. **71**, 1514 (1993).

[13] H. F. Krause *et al.*, in *Abstracts of Contributed Papers, Nineteenth International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC), July 1995*, edited by J. B. A. Mitchell *et al.* (World Scientific, Singapore, 1995), p. 818.

[14] Harvey Gould *et al.*, in *Abstracts of Contributed Papers, Nineteenth International Conference on the Physics of Electronic and Atomic Collisions (ICPEAC), July 1995* (Ref. [13]), p. 815.

[15] A. J. Baltz, M. J. Rhoades-Brown, and J. Weneser, Phys. Rev. A **44**, 5569 (1991).

[16] C. Bottcher and M. R. Strayer, Ann. Phys. **175**, 64 (1987).

[17] M. R. Strayer, C. Bottcher, V. E. Oberacker, and A. S. Umar, Phys. Rev. A **41**, 1399 (1990).

[18] J. C. Wells, V. E. Oberacker, A. S. Umar, C. Bottcher, M. R. Strayer, J.-S. Wu, and G. Plunien, Phys. Rev. A **45**, 6296 (1992).

[19] J. C. Wells, V. E. Oberacker, M. R. Strayer, and A. S. Umar, Nucl. Instrum. Methods Phys. Res. Sect. B **99**, 293 (1995).

[20] J. C. Wells, V. E. Oberacker, M. R. Strayer, and A. S. Umar, Int. J. Mod. Phys. **6**, 143 (1995).

[21] V. Blum, G. Lauritsch, J. A. Maruhn, and P.-G. Reinhard, J. Comput. Phys. **100**, 364 (1992).

[22] J. C. Wells, A. S. Umar, V. E. Oberacker, C. Bottcher, M. R. Strayer, J.-S. Wu, J. Drake, and R. Flanery, Int. J. Mod. Phys. C **4**, 459 (1993).

[23] J.-S. Wu, C. Bottcher, and M. R. Strayer, Phys. Lett. B **252**, 37 (1990).

[24] P. A. Amundsen and K. Aashamar, J. Phys. B. **14**, 4047 (1981).

[25] W. Greiner, B. Müller, and J. Rafelski, *Quantum Electrodynamics of Strong Fields* (Springer-Verlag, Berlin, 1985).

[26] A. J. Baltz, M. J. Rhoades-Brown, and J. Weneser, Phys. Rev. A **48**, 2002 (1993).

[27] A. S. Umar, J.-S. Wu, M. R. Strayer, and C. Bottcher, J. Comput. Phys. **93**, 426 (1991).

[28] R. Friedberg *et al.*, J. Math. Phys. **35**, 5600 (1994); A. K. Trivedi, Phys. Lett. B **230**, 113 (1989); F. Wilczek, Phys. Rev. Lett. **59**, 2397 (1987); M. Ninomiya and C. Tan, *ibid.* **53**, 1661 (1984); J. M. Rabin, Nucl. Phys. B **201**, 315 (1982); H. B. Nielsen and M. Ninomiya, Phys. Lett. **105B**, 219 (1981); J. M. Rabin, Phys. Rev. D **24**, 3218 (1981); L. H. Karsten and J. Smit, Nucl. Phys. B **183** 103 (1981); L. H. Karsten, Phys. Lett. **104B** 315 (1981).

[29] R. Stacey, Phys. Rev. D **26**, 468 (1982).

[30] S. D. Drell *et al.*, Phys. Rev. D **14**, 1627 (1976); H. R. Quinn and H. Weinstein, Phys. Rev. Lett. **57**, 2617 (1986); M. Weinstein, Phys. Rev. D **26**, 839 (1982).

[31] C. Bottcher, M. R. Strayer, A. S. Umar, and V. E. Oberacker, Phys. Rev. C. **37**, 2487 (1988).

[32] J. C. Wells, Ph.D. dissertation, Vanderbilt University, 1994 (unpublished).