Convergence of bound-electron–positron pair production calculations for relativistic heavy-ion collisions

A. J. Baltz,[1] M. J. Rhoades-Brown,[2,*] and J. Weneser[1]
[1]*Physics Department, Brookhaven National Laboratory, Upton, New York 11973*
[2]*Relativistic Heavy-Ion Collider Project, Brookhaven National Laboratory, Upton, New York 11973*
(Received 9 June 1994)

Large-basis coupled-channel Dirac-equation calculations of bound-electron–positron pair production in relativistic heavy-ion collisions are presented. The relative importance of the enhancement of the coupled-channel calculations over corresponding calculations performed in perturbation theory is shown to decrease with increasing basis size, indicating a systematic reduction of this effect of nonperturbative enhancement with improving convergence of the calculations. The total nonperturbative enhancement of the cross section is shown to be about 7 b for Pb^{82+} on Pb^{82+} at the Brookhaven Relativistic Heavy-Ion Collider, only some 6% over perturbation theory.

PACS number(s): 34.90.+q, 25.75.+r

I. INTRODUCTION

In a previous series of papers [1–3], we have addressed the problem of reliably calculating the probability for bound-electron–positron pair production in relativistic heavy-ion collisions. Apart from the intrinsic physics interest of this problem, there is a practical reason to be interested in these calculations: pair production with the electron captured into a bound state of one of the pair of fully stripped ions in a collider such as the Brookhaven Relativistic Heavy-Ion Collider (RHIC) provides an important limit on the beam lifetime; change of the charge of an ion leads to the loss of that ion from the beam. We were originally led to examine this problem by results [4] of nonperturbative coupled-channel calculations in a limited basis that found, at beam kinetic energies of 1.2 and 2.6 GeV/nucleon for the smallest impact parameter, bound-electron–positron production probabilities that exceeded corresponding probabilities obtained in first-order perturbation theory by about two orders of magnitude.

We were faced with several formidable challenges at the time we began to attack this problem. One was that the previous nonperturbative calculations were performed at relatively low relativistic energies (e.g., $\gamma=2.3$) using techniques appropriate for those energies, while we had to consider ultrarelativistic energies ($\gamma=23\,000$) of one ion viewed from the rest frame of the other in RHIC. A second major challenge was that we really had no measure of how large a Hilbert space would be needed to obtain meaningful nonperturbative calculations at such large energies. Nevertheless, the problem was pursued because there was not even a crude estimate of the magnitude of the nonperturbative bound-electron–positron pair production at RHIC.

Our first significant result [1] was establishing that the cross section for very high energies (high equivalent fixed target γ) was of the form

$$\sigma = A \ln\gamma + B \ , \tag{1}$$

where A and B are independent of energy (γ) and we neglect small terms of order $\ln\gamma/\gamma^2$. The $A\ln\gamma$ term comes from the large impact region of the interaction, with A entirely determined by perturbation theory and $\ln\gamma$ expressing the increasing impact parameter cutoff with increasing γ. The energy independent B expresses both the perturbative and nonperturbative contributions at smaller impact parameters; there is no dependence on γ for nonperturbative impact parameters.

En route to obtaining the result expressed in Eq. (1), we had first obtained closed forms for the multipole decomposition of the interaction in the asymptotic (large-γ) limit. We then showed that the γ dependence of the asymptotic form could be removed by a gauge transformation.

We have already presented a Brief Report [2] of the use of the asymptotic forms of the interaction to perform coupled-channel calculations in bases extended to $\kappa\rightarrow\pm5$, $E\rightarrow14.4m_ec^2$. In that work, we also showed the gauge nonindependence of calculations done in a truncated basis space for both asymptotic (high-γ) interactions and an exact interaction at $\gamma=2.3$; for the impact parameter $b\approx0$, we showed that the subtraction of a gauge invariant $\ln\gamma$ term caused great changes in computed cross sections for the limited basis of Ref. [4]. The paper of Rumrich and Greiner [5] had previously examined in a formal way how invariance is spoiled by an incomplete basis.

Since our calculations in the larger basis of the preliminary report indicated that the nonperturbative contributions were only on the order of 10% of the total cross section for bound-electron–positron pair production, we next decided that it would be a worthwhile effort to bring the uncertainty in the calculated perturbative cross sec-

*Present address: Renaissance Tech Corporation, 25 East Loop Road, Stony Brook, NY 11790.

tion in the large impact-parameter region below the estimated nonperturbative contribution to the cross section [3].

The present paper comprises an updated description of the convergence of the bound-electron–positron production in ultrarelativistic heavy-ion reactions. Following this Introduction, we describe in Sec. II the specific details of the interaction and of our solution of the coupled-channel Dirac-equation calculations. Section III presents our latest numerical results; we show the continuing improved convergence with the basis expanded to $E\rightarrow\pm 16m_e c^2$, $\kappa\rightarrow\pm 8$ (7936 channels). Since our calcualtions have concentrated on only the lowest bound-state K electron plus any continuum positron pair production, we discuss in Sec. IV the small contribution of non-K electron-positron pair production. We return to the relatively low-energy $\gamma=2.3$ zero impact parameter case in Sec. V; we demonstrate that by a straightforward expansion of the number of basis states, one finds that the enhancement over perturbation theory has been reduced to a factor of 9 from the "about 2 orders of magnitude enhancement" reported with a more severely truncated basis [4]. In the last section of the main text, we show the unimportance of the projectile form factor along with estimates of screening effects at fixed target energies. Appendix A provides the derivation of the exact multipole decomposition of the interaction for $b=0$ valid for any γ, which was utilized in Sec. V. Appendix B provides a comparison of the interaction form of Appendix A with the large-γ forms.

II. COUPLED-CHANNEL CALCULATIONS: TECHNICAL DETAILS

It is evident from previous calculations of bound-electron–positron pair production with heavy ions that the process is quasiadiabatic, that is, flux is seen to flow into positron excitations and reach a maximum at about the time of ion-ion closest approach, and then much of the flux flows back out of the excitations by the time the reaction is finished. This means that in perturbation theory there is effectively a large cancellation between negative and positive time contributions to the amplitude for producing positrons. There is an analogous cancellation in the full coupled-channel calculations. The result is that, due to the inherent cancellations, one must take particular care to obtain numerical accuracy; failure in proper cancellation naturally leads to overpredicted numerical results. Consequently, in this section we not only describe the interaction and the equations that were solved, but we also lay out several computational techniques that were necessary to attain the requisite accuracy.

A. Large γ asymptotic form of the interaction

In the consideration of the electromagnetic interaction of relativistic heavy ions, one may assume straight-line trajectories, fix a coordinate system on one of the ions, and then express the interaction of the moving ion (projectile) as the Lorentz transformed Coulomb potential

$$V(\boldsymbol{\rho},z,t)=\frac{\alpha Z_p(1-v_p\alpha_z)}{\{[(\mathbf{b}-\boldsymbol{\rho})/\gamma]^2+(z-v_p t)^2\}^{1/2}} . \tag{2}$$

Here $\boldsymbol{\rho}$, z, and t are the coordinates of the moving potential source (projectile) relative to the fixed target, $\mathbf{b}$ is the impact parameter, perpendicular to the z axis along which the projectile travels, α_z is the Dirac matrix, and Z_p, v_p, and γ are the charge, velocity, and γ factor for the projectile ($\gamma=1/\sqrt{1-v_p^2}$). The γ that appears here is that appropriate to a frame in which one of the ions is at rest: $\gamma=2\gamma_{lab}^2-1$. γ_{lab}, the energy of each colliding beam in RHIC, is a little more than 100, so that $\gamma\sim 2\times 10^4$.

In the limit of large γ and impact parameter not too large, there are closed forms [1] for the multipole decomposition of the potential Eq. (2),

$$M_l^m(r,t)=\int d\Omega\, Y_l^m\frac{1}{\{[(\mathbf{b}-\boldsymbol{\rho})/\gamma]^2+(z-v_p t)^2\}^{1/2}} , \tag{3}$$

$$V(\boldsymbol{\rho},z,t)=\alpha Z_p(1-v_p\alpha_z)\sum_{l,m} M_l^m(r,t)Y_l^{m\,*}(\theta,\phi)$$

$$=\alpha Z_p(1-v_p\alpha_z)\sum_{l,m} V_l^m(\mathbf{r},t) .$$

For $m>0$, the asymptotic form is

$$M_l^m(r,t)=\frac{Y_l^m\left[\frac{t}{r},0\right]}{r}\times\begin{cases}0, & r<t\\ \frac{2\pi}{m}\left[\frac{r^2-t^2}{b^2}\right]^{m/2}, & t<r<\sqrt{b^2+t^2}\\ \frac{2\pi}{m}\left[\frac{b^2}{r^2-t^2}\right]^{m/2}, & \sqrt{b^2+t^2}<r .\end{cases} \tag{4}$$

This expression is valid for positive m and t. Negative m and t expressions are given by symmetry.

For $m=0$, the asymptotic form is

$$M_l^0(r,t)=\frac{\sqrt{\pi(2l+1)}}{r}\times\begin{cases}2Q_l\left[\frac{t}{r}\right], & r<t\\ P_l\left[\frac{t}{r}\right]\left[2\ln 2\gamma+\ln\frac{r^2-t^2}{b^2}-2\sum_{m=1}^{l}\frac{1}{m}\right], & t<r<\sqrt{b^2+t^2}\\ P_l\left[\frac{t}{r}\right]\left[2\ln 2\gamma-2\sum_{m=1}^{l}\frac{1}{m}\right], & \sqrt{b^2+t^2}<r\ ,\end{cases}\tag{5}$$

valid for positive t, with the negative t form again to be obtained from symmetry.

B. Gauge transformations of the interaction

If one makes a gauge transformation on the wave function,

$$\psi=e^{-i\chi(\mathbf{r},t)}\psi'\ ,\tag{6}$$

then the Hamiltonian is modified by the addition of the two terms to give

$$\frac{i\partial\psi'}{\partial t}=\left[H(t)-\frac{\partial\chi(\mathbf{r},t)}{\partial t}-\boldsymbol{\alpha}\cdot\nabla\chi(\mathbf{r},t)\right]\psi'\ .\tag{7}$$

The use of

$$\chi_1=2\ln 2\gamma\alpha Z_p\theta(z-t)\tag{8}$$

removes the γ-dependent part of the asymptotic (large-γ) form Eq. (5) of the interaction, $(2\ln 2\gamma)\alpha Z_p(1-\alpha_z)\delta(z-t)$.

However, one can do better and find a gauge transformation that removes both the γ dependence and the $\ln b$ dependence of the interaction. The use of

$$\chi_2'=\frac{\alpha Z_p}{v_p}\ln[\gamma(z-v_pt)+\sqrt{\gamma^2(z-v_pt)^2+b^2}]\tag{9}$$

adds to the interaction $V(\boldsymbol{\rho},z,t)$,

$$-\frac{\alpha Z_p\left[1-\frac{1}{v_p}\alpha_z\right]}{\sqrt{(z-v_pt)^2+b^2/\gamma^2}}\ .$$

The large-γ expression for the $m=0$ gauge transformed interaction then becomes

$$M_l^0(r,t)=\frac{\sqrt{\pi(2l+1)}}{r}P_l\left[\frac{t}{r}\right]\times\begin{cases}0, & r<\sqrt{b^2+t^2}\\ -\ln\frac{r^2-t^2}{b^2}, & \sqrt{b^2+t^2}<r\ .\end{cases}\tag{10}$$

Note that both these transformations affect the $m=0$ part of the interaction only.

An additional computational advantage of the form Eq. (10) is that the large positive and negative time contributions inherent in the term $Q_l(t/r)$ of Eq. (5) have been removed. Instead of needing to solve the equation beginning at $t=-100$ up to $t=+100$, as is necessary with the untransformed interaction, we now find it sufficient to begin at $t=-16$ and go to $t=16$. (Units of time are the Compton wavelength of the electron, $\lambda\!\!\!^{-}_c=\hbar/m_ec=386$ fm, divided by the speed of light c.) The paper of Toshima and Eichler [6] previously utilized a similar transform to solve the difficulty in calculations with interactions that drop off as slowly as $1/t$. It is the gauge expressed in Eq. (10) that we utilize in the extended calculations reported in Sec. III; the results displayed in Tables I and II were calculated in this gauge.

C. Dirac equation and its solution

We wish to solve the time-dependent Dirac equation

$$i\frac{\partial\psi(\mathbf{r},t)}{dt}=[H_0+V(\boldsymbol{\rho},z,t)]\psi(\mathbf{r},t)\tag{11}$$

for a single electron.

$$H_0=\boldsymbol{\alpha}\cdot\mathbf{p}+\beta-Z_Te^2/r$$

is the Hamiltonian of an electron in the rest frame of one of the completely stripped ion. $V(\boldsymbol{\rho},z,t)$ given above is the time-dependent classical field due to the other colliding ion.

We expand the solutions [4] of the Dirac equation $\psi^j(\mathbf{r},t)$ in a time-independent basis of eigenfunctions of H_0.

$$\psi^j(\mathbf{r},t)=\sum_k a_k^j(t)\phi_k(r)e^{iE_kt}\ .\tag{12}$$

ϕ_k includes the bound electron states, continuum electron states, and states in the negative energy continuum. The Dirac equation then becomes a set of coupled equations in the time-dependent amplitudes of the basis set:

$$\frac{da_f^j(t)}{dt}=-i\sum_k a_k^j(t)\langle\phi_f|V(\boldsymbol{\rho},z,t)|\phi_k\rangle e^{i(E_f-E_k)t}\ ,\tag{13}$$

where the bracket indicates integration over the three spatial coordinates. Continuing to follow Ref. [4], we represent the positive and negative continuum states as wave packets:

$$\phi_{E_k}(r)=\frac{1}{\sqrt{\Delta E}}\int_{E_k-\Delta E/2}^{E_k+\Delta E/2}\phi_E(r)dE\ .\tag{14}$$

TABLE I. Results of coupled-channel calculations (Pb+Pb case) for bound-electron–positron cross-section contributions at various impact parameters b and basis truncations. The cross-section contribution (in barns) at each impact parameter is obtained by Eq. (19), except at $b=0$ where it obtained from Eq. (20). Below each listed number of barns for the coupled-channel result is the corresponding result (in parentheses) calculated in perturbation theory.

$\lvert\kappa_{\max}\rvert$	2	4	5	6	7	8
$\lvert E_{\max}\rvert$	3.6	12.0	14.4	14.4	16.8	16.8
Channels	334	1700	3040	4312	6272	7936
b						
0	0.25	0.14	0.12	0.12		
	(0.01)	(0.03)	(0.03)	(0.04)	(0.04)	(0.04)
$0.162\lambda\!\!\!^{-}_C$	1.78	0.91	0.60	0.43		
62.5 fm	(0.03)	(0.13)	(0.20)	(0.21)	(0.23)	(0.24)
$0.324\lambda\!\!\!^{-}_C$	2.81	2.26	1.66	1.33	1.29	
125 fm	(0.13)	(0.52)	(0.62)	(0.67)	(0.76)	(0.80)
$0.648\lambda\!\!\!^{-}_C$	2.78	4.49	3.67	3.32	3.24	
250 fm	(0.55)	(1.80)	(2.10)	(2.26)	(2.51)	(2.63)
$1.295\lambda\!\!\!^{-}_C$	2.18	6.59	6.12	5.98	6.08	6.12
500 fm	(1.36)	(3.54)	(4.07)	(4.41)	(4.82)	(5.08)
$2.59\lambda\!\!\!^{-}_C$	3.93	7.75	8.49	8.62	9.15	9.49
1000 fm	(1.77)	(4.32)	(5.05)	(5.57)	(6.14)	(6.58)
$5.18\lambda\!\!\!^{-}_C$	2.68	6.70	8.04	7.80	8.48	8.73
2000 fm	(1.78)	(4.34)	(5.07)	(5.59)	(6.18)	(6.64)
$10.36\lambda\!\!\!^{-}_C$	2.01	4.99	6.01	6.22	6.89	7.18
4000 fm	(1.78)	(4.29)	(4.99)	(5.50)	(6.07)	(6.50)
$20.72\lambda\!\!\!^{-}_C$	1.83	4.46	5.24	5.66	6.24	6.63
8000 fm	(1.77)	(4.29)	(5.01)	(5.49)	(6.04)	(6.47)

In our calculations utilizing the limited basis of Ref. [4], we kept the width of the wave packets the same at $0.2m_ec^2$. In the larger bases, we set the widths of the wave packets at $0.2m_ec^2$ for $|E|<2m_ec^2$, at $0.4m_c^2$ for $2m_ec^2<|E|<4m_ec^2$, and at $0.8m_ec^2$ for $|E|>4m_ec^2$.

To evaluate the time-dependent matrix elements, we of course need the Dirac wave functions of the basis. We obtain these following the conventions of Rose [7]. The continuum radial wave functions can be expressed in terms of confluent hypergeometric functions, and these are evaluated using the code [8] WCLBES distributed by CERNLIB.

The coupled-channel equations are integrated with initial conditions specified by the index j,

$$a_f^j(t=-\infty)=\delta_{fj} \ . \tag{15}$$

TABLE II. Nonperturbative enhancement of bound-electron–positron pair production (Pb+Pb case). Differences between coupled-channel calculations and perturbation-theory calculations of Table I tabulated for the convenience of the reader.

$\lvert\kappa_{\max}\rvert$	2	4	5	6	7	8
Fraction	18%	43%	50%	55%	61%	65%
b						
0	0.24	0.11	0.09	0.08		
$0.162\lambda\!\!\!^{-}_C$	1.75	0.78	0.40	0.22		
$0.324\lambda\!\!\!^{-}_C$	2.68	1.84	1.04	0.66	0.53	
$0.648\lambda\!\!\!^{-}_C$	2.22	2.69	1.57	1.06	0.73	
$1.295\lambda\!\!\!^{-}_C$	0.82	3.04	2.05	1.57	1.26	1.04
$2.59\lambda\!\!\!^{-}_C$	2.15	3.43	3.44	3.05	3.00	2.91
$5.18\lambda\!\!\!^{-}_C$	0.90	2.36	2.97	2.21	2.30	2.09
$10.36\lambda\!\!\!^{-}_C$	0.23	0.70	1.02	0.72	0.82	0.68
$20.72\lambda\!\!\!^{-}_C$	0.06	0.17	0.23	0.17	0.20	0.16
Sum	11.05	15.12	12.81	9.74	<9.14	<8.44

The $a_f^j(t)$ determine a single electron during the collision. Since we neglect the electron-electron interaction, their only influence on each other is through the Pauli principle. Then we are solving a one-particle equation, and the final state is constructed as a Slater determinant of these one-particle solutions. However, one can show [9] that the number of negative sea electrons N_g excited into a vacant level g may be expressed

$$N_g = \sum_{j<F} |a_g^j|^2, \quad g > F \ , \tag{16}$$

where F is the Fermi level, $E_F = -m_e c^2$. Each of the a_g^j corresponds to a coupled-channel calculation with the electron in one particular negative sea initial state (and the rest of the negative sea vacant). Thus one should do j coupled-channel calculations where j is the number of positron states in the model space. If one is interested in only the population of one final state for the electron (e.g., the $1s$ bound state), then one can use time reversal to write

$$N_{1s} = \sum_{j<F} |a_j^{1s}|^2 \ . \tag{17}$$

Thus our initial condition is an electron in the K orbit for the calculations here reported. The actual numerical solutions of the equations for the coupled amplitudes Eq. (13) are carried out using the Bashforth-Adams-Milne predictor-corrector method [10].

D. Large negative and positive time corrections to numerical calculations in the untransformed gauge

Our large basis, high-γ calculations (presented in Sec. III) were performed in the gauge of Eq. (10) where the large negative and positive time contributions inherent in the untransformed interaction have been removed. Nevertheless, we would like to discuss the effect of large time contributions of the untransformed gauge since that gauge was utilized in exploratory calculations previously reported [2] as well as in the low-γ calculations reported here in Sec. V. In the untransformed interaction, Eq. (5), the large negative and positive time interaction is dominated by the $m=0$ interaction for $t > r$,

$$V_l^0(\mathbf{r},t) = Y_l^0(\theta) 2\sqrt{\pi} \frac{\sqrt{2l+1}}{r} Q_l(t/r) \ .$$

(Recall that there is no $t > r$ interaction for $m \neq 0$.) There is a similar $Q_l(t/r)$ dependence in the exact $b=0$ expression of Sec. V. The problem here is that even in calculations that go from very large negative time to very large positive time (e.g., $t=-100$ to $t=+100$), one must carefully approximate contributions from even larger negative and positive times to obtain calculations of sufficient accuracy. For the monopole interaction,

$$V_0^0(r,t) = \frac{1}{2r} \ln \left| \frac{1+t/r}{1-t/r} \right| = \frac{1}{t} + \frac{r^2}{3t^3} + \frac{r^4}{5t^5} + \cdots \ .$$

Thus the self-coupling matrix element has a long-range part equal to $\alpha Z_p/t$. By analyzing $Q_l(t/r)$ for $l \neq 0$, one finds that other $m=0$ interactions, $V_l^0(r,t)$, have terms of longest range going as $1/t^{l+1}$. Therefore, one can show, in general, that for large t and $m=0$ transfer, the time-dependent coupling in Eq. (13) goes as

$$\exp[i(E_i - E_0)t] \sum_l \frac{C_l}{t^{l+1}} \ ,$$

where l represents the angular momentum transfer components contributing.

We write the coupling matrix element

$$\langle \phi_i | V(\rho,z,t) | \phi_0 \rangle = U_{0i}(t) \ ,$$

where $U_{0i}(t)$ is a slowly decreasing function of t. For a given state i, the amplitude at large negative time is coupled importantly only to the initial state; then

$$\frac{da_i(t)}{dt} \cong -iU_{0i}(t) e^{i(E_i - E_0)t} a_0(t) \ . \tag{18}$$

To lowest order, the largest interaction contribution to $a_0(t)$ is the self-coupling, and we can write

$$\frac{da_0(t)}{dt} = -i \frac{\alpha Z_p}{t} a_0(t) \ .$$

Near some large negative-t starting point $t_{\min}$, $|a_0(t_{\min})| = 1$, we can arbitrarily choose the background phase, and the sole effect of the self-coupling is to produce a phase that varies as $\alpha Z_P \ln t$,

$$a_0(t) = e^{-i\alpha Z_p (\ln t - \ln t_{\min})} \ .$$

From Eq. (18),

$$a_i(t_{\min}) = -i \int_{-\infty}^{t_{\min}} U_{0i}(t) e^{i(E_i - E_0)t} a_0(t) dt \ .$$

The rapidly changing factor is $e^{i(E_i - E_0)t}$, while $U_{0i}(t)$ and $a_0(t)$ are rather flat. For a Pb target $\alpha Z_p \approx 0.6$, and the derivative of a_0 at $t_{\min} = -100$ is $-0.006i$. In contrast, the smallest value of the derivative of $e^{i(E_i - E_0)t}$ (when E_i is the first excited bound-electron state) is $0.15i$ for Pb. Then, integrating by parts and neglecting $dU_{0i}/dt(t)$ and da_0/dt,

$$a_i(t_{\min}) = -\frac{U_{0i}(t) e^{i(E_i - E_0)t} a_0(t)}{(E_i - E_0)} \Bigg|_{-\infty}^{t_{\min}}$$

$$= \frac{U_{0i}(t_{\min}) e^{i(E_i - E_0)t_{\min}}}{(E_i - E_0)} \ ,$$

since $U_{0i}(-\infty)$ vanishes sufficiently quickly. This formula provides the initial value for all a_i (except $i=0$) at the $t_{\min}$ when we begin the numerical solution of the coupled equations. In a similar way, we may obtain a form that permits the continuation of $a_i(t)$ from $t_{\max}$ to ∞ in terms of the numerical solutions at $t_{\max}$. We have

$$\frac{da_i(t)}{dt} = -i \sum_{j \neq i} U_{ji}(t) e^{i(E_i - E_j)t} a_j(t) \ .$$

If we assume $U_{ji}(t)$ and $a_j(t)$ are slowly varying, then

$$a_i(\infty)-a_i(t_{\max})=+\sum_j \frac{U_{ji}(t_{\max})e^{i(E_i-E_j)t_{\max}}a_j(t_{\max})}{(E_i-E_j)} .$$

These connecting forms have been tested by direct numerical calculations.

E. Singularity at $r=t$ for $m=0$

The asymptotic formulas for the $m=0$ potential contain an integrable singularity that goes as $-\ln(t-r)$ for $r<t$ and as $\ln(r-t)$ for $r>t$ (where, as we previously noted, we need only consider positive t, using symmetry and the same forms for negative t). If we consider the analytic integration of $\ln(t-r)$ over r from the singularity at $t-r$ to the limit of one mesh point Δr, we have

$$I_A=-\int_{t-\Delta}^{t}\ln(t-r)dr=-\Delta\ln\Delta+\Delta .$$

On the other hand, the simple midpoint formula used numerically gives

$$I_N=-\Delta\ln\frac{\Delta}{2} .$$

To improve accuracy in the numerical calculations, we want to effectively use the average value of $-\ln(t-r)$ over the mesh point, which has the singularity at one end (I_A/Δ), rather than the midponit prescription (I_N/Δ). In practice, we correct this first mesh point for the error in $\ln(t-r)$ by adding in the difference:

$$\delta_{\ln}=(I_A-I_N)/\Delta=-\ln2+1=0.307 .$$

Note that the correction of the mesh point value is independent of the mesh, and that this error goes linearly with mesh size if it is not removed.

For $r<t$ we must consider $Q_l(t/r)$, which has a piece equal to $-\ln(t-r)$, and the correction is made in the same way. Likewise, for $t<r<\sqrt{b^2+t^2}$, we must consider

$$\ln\frac{(r^2-t^2)}{b^2}=\ln\left[\frac{r+t}{b^2}\right]+\ln(r-t) ,$$

and the corresponding correction

$$\delta_{\ln}=\ln2-1=-0.307$$

is equally easily made.

III. COUPLED-CHANNEL CALCULATIONS: NUMERICAL CONVERGENCE AND THE JOINING TO PERTURBATION CALCULATIONS AT LARGE IMPACT PARAMETERS

The total cross section for bound-electron–positron pair production is given by the classical expression

$$\sigma=2\pi\int_0^{b_{\max}}P(b)b\,db ,$$

where $P(b)$ is equal to N_{1s} of Eq. (17) obtained in a coupled-channel calculation for the straight-line trajectory of the particular impact parameter b. We have shown [1–3] that for those trajectories for which perturbation theory applies, $P(b)\sim 1/b^2$. In order to match up with the perturbational results most smoothly, we have chosen a rough logarithmic scale (except near $b=0$) to perform our coupled-channel calculations, with the impact parameter b being doubled for each mesh point over the region of interest. Then the contribution to the total σ of the mesh point at some b_0 should be weighted by $(2\pi b_0^2\ln2)$, since

$$\Delta\sigma(b_0)=2\pi\int_{b_0/\sqrt{2}}^{\sqrt{2}b_0}P(b)b\,db\approx 2\pi b_0^2P(b_0)\int_{b_0/\sqrt{2}}^{\sqrt{2}b_0}\frac{db}{b} ,$$

$$\Delta\sigma(b_0)\approx 2\pi b_0^2P(b_0)\ln2 . \tag{19}$$

In the perturbative region, where $P(b_0)\sim 1/b_0^2$, the mesh of successively doubled values of b_0 gives uniform contributions $\Delta\sigma(b)$ to the cross section σ. For the region near $b=0$, $P(b)$ is more nearly constant and we take a weighting of $\pi/2b_{0\min}^2$, since

$$\begin{aligned}\Delta\sigma(b=0)&=2\pi\int_0^{b_{0\min}/\sqrt{2}}P(b)b\,db\\&\approx 2\pi P(b=0)\int_0^{b_{\rho\min}/\sqrt{2}}b\,db\\&\approx\frac{\pi}{2}P(b=0)b_{0\min}^2 .\end{aligned} \tag{20}$$

Perturbative and coupled-channel calculations were carried out at $b_0=0$, 62.5, 125, 250, 500, 1000, 2000, 4000, and 8000 fm for various truncations of basis. We utilized the manifestly beam-energy-independent gauge of Eq. (10) for the $m=0$ part of the interaction. Perturbative calculations at these small impact parameters were carried out using techniques identical to those used for the coupled-channel calculations, but with all but lowest order couplings appropriately suppressed. We discuss below the joining of these low impact-parameter calculations with perturbation-theory calculations [3] that extend to the largest appropriate impact parameters, energies, and angular momenta.

We have previously presented a preliminary report [2] of results that include bases up to $\kappa=\pm5$, $E=\pm14.4m_ec^2$. In order to further investigate the degree of convergence of our calculations, we have extended the basis to $\kappa=\pm6$, $E=\pm14.4$ for all impact parameters and to $\kappa=\pm8$, $E=\pm16.8$ for $b\geq250$ fm.

Table I summarizes the results of the impact-parameter coupled-channel calculations. Especially at the lowest impact parameters, one sees that the enormous ratio of the results with coupled channels to those based on perturbation theory obtained at the smallest basis is greatly reduced with increase of basis. The approximate constancy as a function of impact parameter of the perturbative results for $b\geq1000$ fm indicates the onset of the region where the perturbative $P(b)\sim1/b^2$ is valid. The smallest basis shown ($\kappa\rightarrow\pm2$, $E\rightarrow\pm3.6m_ec^2$) is the same basis as used by Rumrich *et al.* [4] for their Pb+Pb calculations at $\gamma=2.3$. These authors investigated the impact-parameter dependence of the coupled-channel calculations and perturbation-theory calculations out to about $b=500$ fm. (At such a small γ the impact parame-

ters contributing to the process are limited to the small-b region, since the inherent exponential cutoff is at $b \sim \gamma \lambda\!\!\!^{-}_C$.) They found that the total cross section calculated in coupled channels was five times that calculated in perturbation theory. From this they inferred: "Thus, the total cross section is underestimated in perturbation theory by a factor of 5." It is interesting to note that for their small basis and in the same impact-parameter region out to $b \approx 500$ fm, we find that our high-γ coupled-channel cross section also exceeds the corresponding perturbation-theory cross section by about a factor of 5. On the other hand, in the most complete basis for which we have complete calculations for the small impact parameters $\kappa \rightarrow \pm 6$, $E \rightarrow \pm 14.4 m_e c^2$, the coupled-channel cross section exceeds that of perturbation theory by only a factor of ~ 1.5 for this impact-parameter region.

It is in Table II that the increasing convergence with increasing basis size is most evident. We display in Table II the difference between the coupled channels and the perturbational cross sections of Table I. For each basis labeled by $|\kappa_{\max}|$ there is also listed the fraction of the total perturbative cross section [3] contained within the particular truncation of basis; this serves as a measure of the effective completeness of the basis, and therefore as an indicator of validity. For the expansion of basis from $|\kappa_{\max}|=5$ (50%) to $|\kappa_{\max}|=6$ (55%), the nonperturbative enhancement decreases for every impact parameter. The decreasing cross-section enhancement up to the $|\kappa_{\max}|=8$ (65%) basis indicates a probable upper limit of about 9 b for the nonperturbative enhancement. The fact that the enhancement is decreasing very slowly for $b \geq 2.59$ allows us to put a probable lower limit of about 5 b for this case. Thus for all practical purposes we have achieved convergence, the nonperturbative enhancement for ultrarelativistic Pb+Pb K-electron–positron pair production is 7 ± 2 b. Since we have shown that the cross section is of the form $A \ln\gamma + B$ in the large-γ limit, with all nonperturbative contributions energy independent and contained in B, this result of 7 ± 2 b nonperturbative enhancement is applicable to both RHIC and the Large Hadron Collider (LHC).

At this point, we would like to put the 7-b enhancement in perspective by evaluating the total perturbation-theory cross section for ultrarelativistic Pb^{82+} on Pb^{82+} K-electron–positron pair production. We follow the method of joining perturbation-theory results presented previously [3].

If one examines the results of the last column in Table I, one finds that the perturbational cross section corresponding to integration over impact parameters from 0 to $b_{\max}$ is approximately given by

$$\sigma(b_{\max}) \simeq 9.4 \ln b_{\max} + 3.2 \text{ barns} , \quad (21)$$

for $b_{\max} \gtrsim 2.5 \lambda\!\!\!^{-}_C$. On the other hand, we have the perturbation-theory results [3], including the highest energy and angular momentum states for Au^{79+} on Au^{79+} and U^{92+} on U^{92+} that are appropriate for large values of b, $b > b_{\min}$. Making use of the approximate $Z^{6.6}$ dependence that we found in the cross sections, we can translate the published results to the case of Pb^{82+} on Pb^{82+}; the cross section integrated over all impact parameters greater than $b_{\min}$ is

$$\sigma(b_{\min}) \simeq 14.3 \ln(\gamma / b_{\min}) - 36.2 \text{ barns} . \quad (22)$$

The incompleteness of the basis in Eq. (21) is now evident by a comparison of the coefficient of the $\ln b$ term with that of Eq. (22); the incomplete basis corresponds to 65% of the perturbative cross section in the large-b region. We therefore scale Eq. (21) upwards to obtain

$$\tilde{\sigma}(b_{\max}) \simeq 14.3 \ln b_{\max} + 4.9 \text{ barns} ,$$

and the whole perturbative cross section is just the sum,

$$\sigma_{\text{pert}} \simeq \tilde{\sigma}(b_{\max}) + \sigma(b_{\min}), \quad b_{\max} = b_{\min} = b ,$$

for all b values of overlapping validity. Then,

$$\sigma_{\text{pert}} \simeq 14.3 \ln\gamma - 31 \text{ barns} . \quad (23)$$

Thus at the γ of RHIC, we have a perturbative cross section of 112 b for Pb^{82+} on Pb^{82+}; the 7-b nonperturbative enhancement amounts to only a 6% correction. From Eq. (23), we may also obtain the corresponding perturbative cross section for LHC of 209 b and the 7-b nonperturbative enhancement is only a 3% correction.

Implicit in our treatment is the assumption that the large energy and angular momentum positrons calculated only in perturbation theory [3], Eq. (22), are effectively decoupled from the smaller energy and angular momentum positrons of the present coupled-channel calculations. One indication of the validity of the decoupling assumption is the slowly decreasing nonperturbative enhancement exhibited in Table II.

A second indication comes from a more detailed examination of computer results for the impact parameter of largest nonperturbative enhancement, $b = 2.59$. If one considers positron states of energy one unit removed from the edge of the basis ($E = -15.6 m_e c^2$), then one finds that the sum of the probabilities for all the angular momentum states $|\kappa| \leq 7$ in coupled channels is only 1% greater than the corresponding sum in perturbation theory. Individual states differ a bit more in coupled channels and perturbation theory, but none by as much as 10%. Somewhat greater discrepancies appear at the edge of the basis ($E = -16.4$ for all κ; $|\kappa| = 8$ for $E = -15.6$), presumably due to truncation edge effects. The bulk of the nonperturbative enhancement comes at the lower energies, away from the larger energy boundary of the basis set.

IV. ESTIMATES OF CONTRIBUTIONS FROM OCCUPATION OF HIGHER LYING BOUND-ELECTRON STATES

We have limited our coupled-channel calculations to the problem of pair production with the electron resident in the K orbit. This bound-electron state is the $N=1$, $\kappa=-1$ (nonrelativistically $1s$) state. The practical and usual assumption was that this is the dominant contribution to bound-electron–positron pair production. For example, the RHIC design parameters assumed an additional 20% contribution to bound-electron–positron pair production with non-ground-state electron population.

In order to verify that such an assumption is roughly valid, we have performed several perturbative calculations for non-ground-state electrons.

Our previously reported extensive investigation of the perturbational cross sections [3] was limited to K-orbit ($\kappa=-1$, $N=1$) electron-positron pair production. Using the same approximation to the perturbational sum used in Ref. [3] (caption to Fig. 2), we have now computed the perturbational ($\kappa=-1$, $N=2$) electron-positron pair production cross section for continuum positron states up to $\kappa=\pm 40$, $E=-60m_ec^2$ for Au^{79+} on Au^{79+}. The ratio of the $\kappa=-1$, $N=2$ cross section to the corresponding $\kappa=-1$, $N=1$ cross section is 0.17 for the above summed energy and κ positron range.

Exploratory perturbative calculations were also carried out for all the $N=2$ electron states for the smaller space of the present paper (in this case, $\kappa\rightarrow\pm 7$, $E\rightarrow 16.8m_ec^2$). We find that the ratio of the $\kappa=-1$, $N=2$ electron-positron cross section to the ground-state–electron-positron cross section is 0.13 for this basis. Corresponding ratios of $\kappa=+1$, $N=2$ and $\kappa=-2$, $N=2$ cross sections to the ground-state are 0.04 and 0.02, respectively.

V. CALCULATION FOR THE $b=0$, $\gamma=2.3$ CASE IN AN EXPANDED BASIS

For the calculation of electron-positron pair production in heavy-ion reactions, the situation as $b\rightarrow 0$ is of particular interest because it is in this lowest impact regime that the failure of perturbation theory is greatest. Since the scale at which nuclear effects contribute for two interacting large nuclei ($b\lesssim 15$ fm) is much smaller than the atomic scale for electrons and positrons ($\hbar/m_ec=386$ fm), the $b=0$ solution should be of interest as closely approximating the situation at the smallest impact parameter for which nuclear effects are not applicable.

For $b=0$, the asymptotic interaction Eq. (5) takes on the simple form, good up to order $\ln\gamma/\gamma^2$:

$$M_l^m(r,t)=\delta_{m,0}\frac{\sqrt{\pi(2l+1)}}{r}\times\begin{cases}2Q_l(t/r) & \text{if } r<t\\ 2P_l(t/r)\left[\ln 2\gamma-\sum_{n=1}^{l}1/n\right] & \text{if } r>t\ .\end{cases}\tag{24}$$

Our analogous but exact expression for the $b=0$ case is

$$M_l^m(r,t)=\delta_{m,0}\frac{\sqrt{\pi(2l+1)}}{rv_p}\times\begin{cases}2P_l(1/v_p)Q_l(t/r) & \text{if } r<v_pt\\ 2Q_l(1/v_p)P_l(t/r) & \text{if } r>v_pt\ .\end{cases}\tag{25}$$

This simple and striking result is proved in Appendix A. In Appendix B, we show how Eq. (24) approximates Eq. (25) in the large-γ limit. It was use of this simple and exact form for $b=0$ that facilitated our comparison [2] with the calculations of Rumrich *et al.* [4] for small γ.

We have now expanded the calculations from their original basis to basis sets corresponding to $|\kappa_{\max}|=4$ and $|\kappa_{\max}|=6$. Note that for this particular calculation only, we use an untransformed Lorentz gauge [Eq. (25)], and it is the same gauge as originally used by Rumrich *et al.* Table III displays the results. Our original surmise, based on gauge noninvariance of the calculations, that the two order-of-magnitude enhancement over perturbation theory would decrease with use of more complete bases, has been supported by these calculations in the original Lorentz gauge, but with expanded basis spaces: the coupled-channel results decrease with increasing basis, while the perturbation-theory results must of course increase. The enhancement for $|\kappa_{\max}|=6$ is down to a factor of 9 and apparently decreasing with increasing basis size.

VI. COHERENCE AND THE EFFECTS OF THE PROJECTILE CHARGE FORM FACTOR

In the body of this work, we have postulated that the projectile, a fully stripped nucleus, acts as a point source with Z_p units of electric charge. That is to say, the charge form factor has been taken as unity and the probability of disintegration under recoil effects as zero. In this section, these postuletes are examined and shown to be justified as applied here, also pointing to the limits of validity.

As a simple beginning point, recall that in the very large-γ limit, the perturbational expression for a target excitation, $\omega=E_f-E_0$, is written in the target rest frame as

$$\sigma=8\pi(\alpha Z_p)^2\int_{b_{\min}}^{\infty}db\,b\left|\int d\tau\,\psi_f^*\mathbf{j}\cdot\hat{\mathbf{b}}e^{i\omega z}\psi_0\right|^2\left[\frac{1}{\gamma}K_1\left(\left|\frac{\omega b}{\gamma}\right|\right)\right]^2;\tag{26}$$

$\mathbf{j}$ is the current operator ($\boldsymbol{\alpha}$ for the electron field, and the usual form for the nuclear case); b is the impact parameter of the projectile whose path is along the z axis; K_1 is the familiar modified Bessel function; $b_{\min}$ is the minimum b value for which perturbation theory is valid and such that $b_{\min}\gg$(effective internal variables of the target, ρ). We have, then, an effective photon field acting

TABLE III. Results of $\gamma=2.3$ coupled-channel calculations (Pb+Pb case) for bound-electron–positron production probability at zero impact parameter $P(0)$, and the cross-section contribution (in barns) $\Delta\sigma(b=0)$ as in Table I. Below each listed number for the coupled-channel result is the corresponding result (in parentheses) calculated in perturbation theory.

$\lvert\kappa_{\max}\rvert$	2	4	6
$\lvert E_{\max}\rvert$	3.6	12.0	14.4
Channels	112	344	636
$P(0)$	0.00347	0.00132	0.00112
	(0.00007)	(0.00011)	(0.00012)
$\Delta\sigma(b=0)$	0.213	0.081	0.069
	(0.0043)	(0.0070)	(0.0074)

on the target:

$$\sum_{\omega} e^{i(\omega z-\omega t)}\frac{1}{\gamma}K_1\left(\left|\frac{b\omega}{\gamma}\right|\right). \tag{27}$$

Had we gone further back than the very large-γ limit, we would see that the Fourier component that turns into the effective photon is of the form

$$e^{i(\omega/v_p z-\omega t)}, \tag{28}$$

where v_p is the projectile velocity as seen in the target frame. We have, then, to ask about the effects on the projectile of the emission of such "photons."

Since we know the form factor and photodisintegrability of the projectile nucleus *as given in its own rest frame,* we must transform back to that frame. Transformed back into the projectile rest frame, the corresponding "momentum" is $\omega/\gamma\beta\sim\omega/\gamma$. In the calculations of this and related papers, $\gamma\sim 2\times 10^4$, while $\omega\lesssim 100 m_e c^2$. We immediately see that such recoils are coherently contained in the ground state; since the nuclear form factor for a momentum transfer of q is approximated by $e^{-q^2R_P^2/10}=F(q)$ (R_P is the nuclear uniform-density radius), F differs from unity by less than a part in 10^{-3}.

Next we ask about the transverse effects. Since the effects we are investigating are concerned with b values much smaller than γ/ω, we can use the approximate form of the interaction

$$\frac{1}{\omega\gamma}\hat{\mathbf{j}}\cdot\hat{\mathbf{b}}K_1\left(\left|\frac{\omega b}{\gamma}\right|\right)\to\frac{\hat{\mathbf{j}}\cdot\mathbf{b}}{b} \tag{29}$$

[$K_1(x)=1/x$ for $x\ll 1$; $\sqrt{\pi/2x}\,e^{-x}$ for $x\gg 1$.]

In order to include variation over the projectile charge distribution, we change notation by $\mathbf{b}\to\mathbf{b}+\mathbf{s}$, where $\mathbf{b}$ now denotes the nuclear center and $\mathbf{s}$ ranges over its transverse dimensions. We then have to consider the interaction

$$\frac{\hat{\mathbf{j}}\cdot(\mathbf{b}-\mathbf{s})}{|\mathbf{b}-\mathbf{s}|^2}. \tag{30}$$

Averaging over the orientation of $\mathbf{s}$ results in the two-dimensional version of Gauss's law,

$$\begin{aligned}\frac{1}{2\pi}\int d\phi\frac{\hat{\mathbf{j}}\cdot(\mathbf{b}-\mathbf{s})}{(\mathbf{b}-\mathbf{s})^2}&=\frac{1}{2\pi}\int d\phi\hat{\mathbf{j}}\cdot\hat{\mathbf{b}}\frac{\hat{\mathbf{b}}\cdot(\mathbf{b}-\mathbf{s})}{(\mathbf{b}-\mathbf{s})^2},\\&=\frac{\hat{\mathbf{j}}\cdot\mathbf{b}}{2\pi}\int d\phi\frac{b-bs\cos\phi}{b^2+s^2-2bs\cos\phi},\\&=\frac{\hat{\mathbf{j}}\cdot\hat{\mathbf{b}}}{b},\quad b>s,\\&=0,\quad b<s.\end{aligned} \tag{31}$$

Since the minimum value of the impact parameter must be taken as at least $2R_P$ in order to avoid counting over the region of strong nucleon interaction, we see at once, since $b>s$, that there is no s dependence and, therefore, unit form factor for the ground state→ground state projectile transition. To evaluate the projectile excited-state contributions, we use the upper limit afforded by the closure sum. Since for any operator $\mathcal{O}$,

$$\sum_{n\neq 0}|\langle n|\mathcal{O}|0\rangle|^2=\langle 0|\mathcal{O}^+\mathcal{O}|0\rangle-|\langle 0|\mathcal{O}|0\rangle|^2, \tag{32}$$

we need only simple ground-state properties to complete the estimate. Expanding in powers of s/b,

$$\left[\frac{\hat{\mathbf{j}}\cdot(\mathbf{b}-\mathbf{s})}{(\mathbf{b}-\mathbf{s})^2}\right]^2=(\hat{\mathbf{j}}\cdot\mathbf{b}-\hat{\mathbf{j}}\cdot\mathbf{s})^2\times\left\{\frac{1}{b^4}+\frac{4sP_1}{b^5}+\frac{s^2}{b^6}(6P_1^2+4P_2)+\right\}, \tag{33}$$

the P_n are the usual Legendre polynomials, but written in terms of the polar angle appropriate to two dimensions (where they lack orthogonality). Averaging over angle,

$$\frac{1}{2\pi}\int d\phi\left[\frac{\hat{\mathbf{j}}\cdot(\mathbf{b}-\mathbf{s})}{(\mathbf{b}-\mathbf{s})^2}\right]^2=\frac{(\hat{\mathbf{j}}\cdot\hat{\mathbf{b}})^2}{b^2}+\frac{1}{2}\frac{s^2}{b^4}\cdots. \tag{34}$$

Recalling that $|\langle 0|\mathcal{O}|0\rangle|^2=(\hat{\mathbf{j}}\cdot\hat{\mathbf{b}})^2/b^2$, we immediately know that the ratio of incoherent to coherent contribution is just

$$\frac{\frac{1}{2}\langle 0|s^2|0\rangle/b^4}{(\hat{\mathbf{j}}\cdot\hat{\mathbf{b}})^2/b^2}=\frac{\frac{1}{4}R_P^2/b^4}{(\hat{\mathbf{j}}\cdot\hat{\mathbf{b}})^2/b^2}. \tag{35}$$

The relative contributions to the overall cross section require integration over the impact parameter; in rough approximation,

$$\frac{1}{5}R_P^2\int_{b_{\min}}^{\gamma/\omega}b\,db\frac{1}{b^4}\Big/\int_{b_{\min}}^{\gamma/\omega}b\,db\frac{(\hat{\mathbf{j}}\cdot\hat{\mathbf{b}})^2}{b^2}\cong\frac{1}{5}\frac{R_P^2/b_{\min}^2}{\ln(\gamma/\omega b_{\min})}. \tag{36}$$

(The upper limit follows from the cutoff properties of $K_1(x)$ for $x\gg 1$.) Since for the atomic problem addressed in this paper $b_{\min}\sim\lambda\!\!\!^{-}_c$, this ratio is $\sim 10^{-5}$. Were we to apply the formalism to nuclear electromagnetic excitation and exclude true nuclear collisions, we would take $b_{\min}\gtrsim 2R_P$ (ions of equal A); then for $\gamma\sim 2\times 10^4$, $\omega\sim 100$ MeV, $R_P\sim 7.5$ fm, the ratio is $\leq 10^{-2}$. The lowest-order approximation, the point source, for the projectile nucleus seems quite sufficient.

A number of experiments are underway to measure the process analyzed in this paper—production of a bound-electron plus positron pair. Since these experiments must at present use fixed targets (at $\gamma=14$ and 200) their measurements necessarily deal with an exciting source that is fully clothed in its atomic electrons (the bound-e^-–e^+ pair is to be observed attached to the fully stripped beam ion), shielding considerations are forced upon us.

To connect with the analysis outlined in the previous pages, we must take the rest frame at the beam ion, the site of the created bound e^-, and have the clothed target particle moving relative to it. Unfortunately, this leaves us with the cross association of target↔beam; the effective target is that fixed by the observer's counter system.

To obtain a qualitative feeling for the screening problem, it is useful to begin with the spatial dimensions of the excitation process. The range of impact parameters over which there are important contributions is $[\gamma/(\omega/m_ec^2)]\lambda\!\!\!^{-}_C$, $\lambda\!\!\!^{-}_C=\hbar/m_ec=386$ fm; it will be recalled that the $\ln\gamma$ dependence of the cross section comes about from small probabilities accumulated over a large impact-parameter region in increments of db/b. A very important part of the frequency spectrum is that below $\sim 3m_ec^2$, lesser but sizeable contributions up to $\sim 10m_ec^2$, and a gradual fall off, as $1/\omega^2$, so that $\sim 80\%$ of the whole cross section is accumulated below $\sim 20m_ec^2$—all from calculations on U-U collisions. At $3m_ec^2[\gamma/(\omega/m_ec^2)]\lambda\!\!\!^{-}_C=4.3\lambda\!\!\!^{-}_C$ for $\gamma=14$, and $62\lambda\!\!\!^{-}_C$ for $\gamma=200$; at $20m_ec^2$, we have to do with $0.7\lambda\!\!\!^{-}_C$ for $\gamma=14$ and $10\lambda\!\!\!^{-}_C$ for $\gamma=200$. Atomic electron orbits range from the $\lambda\!\!\!^{-}_C/\alpha Z$ of a K orbit to $n\lambda\!\!\!^{-}_C/\alpha$ (n highest principal quantum number) of an outer electron. Therefore, important parts of the impact-parameter range are sufficiently large so that the excited nucleus is seen only through a considerable density of orbital electrons. In a Thomas-Fermi atom, half the total electron charge lies within $\sim 180/Z^{1/3}\lambda\!\!\!^{-}_C - \sim 30\lambda\!\!\!^{-}_C$ for Pb—half the impact-parameter values of importance at $\gamma=200$. Were the electrons to act coherently, those at separations from the exciter nucleus smaller than the impact parameter would act as if at the nucleus and screen the nuclear charge. This is clearly much more important the larger the γ value.

Not all of the electron interactions will, however, be coherent. Recall that longitudinal momenta $\sim\omega/\gamma$ act back on the interacting electrons. The larger the ω and the smaller the γ, the more effective the recoil will be in ejecting the electrons from their stable orbits, thus rendering their response incoherent with respect to that of the inner nucleus and each other. Such an incoherent response adds a contribution proportional to the number of incoherent electrons compared to the Z_p^2 proportionality of a stripped ion. A coherent electron response would reduce the nuclear charge. On this qualitative basis, we would expect from both the impact-parameter dependence and the recoil effects roughly an order $1/Z_p$ correction for smaller γ and lower Z_p, with larger shielding effects at larger γ and larger Z_p.

APPENDIX A: EXACT MULTIPOLE DECOMPOSITION FOR $b=0$

Let us consider the $b=0$ case without any approximation in $1/\gamma$. By definition, we have

$$M_l^m(r,t)=\int d\Omega\, Y_l^m \frac{1}{\{\rho^2/\gamma^2+(z-v_pt)^2\}^{1/2}} . \tag{A1}$$

By symmetry, only $m=0$ is nonvanishing, and we immediately integrate over ϕ,

$$M_l^m(r,t)=\delta_{m,0}2\pi\int_{-1}^{1}\frac{Y_l^0(\cos\theta)d(\cos\theta)}{\{(r^2/\gamma^2)\sin^2\theta+(r\cos\theta-v_pt)^2\}^{1/2}} . \tag{A2}$$

Let us define $x=\cos\theta$, and note that $1/\gamma^2=1-v_p^2$ to rewrite

$$M_l^m(r,t)=\frac{\sqrt{2\pi(2l+1)}}{rv_p}\int_{-1}^{1}\frac{P_l(x)dx}{\{1/v_p^2+t^2/r^2-1-2xt/(v_pr)+x^2\}^{1/2}} . \tag{A3}$$

If we note that the expression is symmetric in $1/v_p$ and t/r, then it is clear that the integral over x can be carried out in closed form for each value of l, but with increasing complexity with increasing l. However, consideration of the results of integration for the first few l's suggest a simple and remarkable general result,

$$M_l^m(r,t)=\delta_{m,0}\frac{\sqrt{\pi(2l+1)}}{rv_p}\times\begin{cases}2P_l(1/v_p)Q_l(t/r) & \text{if } r<v_pt\\ 2Q_l(1/v_p)P_l(t/r) & \text{if } r>v_pt\end{cases} . \tag{A4}$$

To prove this result it is now only necessary to prove the following identity for the real parameters w and u (it is understood that one of the parameters, w, is greater than 1, to be associated with the physical value of $1/v_p$):

$$\int_{-1}^{1}\frac{P_l(x)dx}{\{w^2+u^2-1-2wux+x^2\}^{1/2}}=\begin{cases}2P_l(w)Q_l(u), & u>w,\ w>1\\ 2Q_l(w)P_l(u), & w>u,\ w>1\end{cases} . \tag{A5}$$

The proof is given in two phases: first for the restricted parameter region, $(w>1,u>1)$; then extended to $(w>1,u\le 1)$. For the first phase begin the proof by explicitly carrying out the integral over ϕ in the following expression

$$\int_{-1}^{1}dx\int_0^{2\pi}d\phi\frac{P_l(x)}{wu-x+\sqrt{w^2-1}\sqrt{u^2-1}\cos\phi}=2\pi\int_{-1}^{1}\frac{P_l(x)dx}{\sqrt{w^2+u^2-1-2wux+x^2}},\quad wu>1 . \tag{A6}$$

Now recall the identity

$$Q_l(z)=\tfrac{1}{2}\int_{-1}^{1}\frac{P_l(t)dt}{(z-t)},\quad [z \text{ off the } (1,-1) \text{ cut}] ,$$

and therefore,

$$Q_l(wu+\sqrt{w^2-1}\sqrt{u^2-1}\cos\phi)=\tfrac{1}{2}\int_{-1}^{1}\frac{P_l(x)dx}{wu-x+\sqrt{w^2-1}\sqrt{u^2-1}\cos\phi}\ . \tag{A7}$$

But we also have the addition theorem [11]

$$Q_l(wu+\sqrt{w^2-1}\sqrt{u^2-1}\cos\phi)=Q_l(w)P_l(u)+2\sum_{m=1}^{\infty}Q_l^m(w)P_l^{-m}(u)\cos m\phi,\quad w>u>1\ . \tag{A8}$$

Combining (A7) and (A8), we obtain

$$\int_{-1}^{1}\frac{P(x)dx}{wu-x+\sqrt{w^2-1}\sqrt{u^2-1}\cos\phi}=2Q_l(w)P_l(u)+4\sum_{m=1}^{\infty}Q_l^m(w)P_l^{-m}(u)\cos m\phi,\quad (w>u)\ . \tag{A9}$$

Integrating over ϕ, everything on the right-hand side vanishes by orthogonality except the first term,

$$\int_0^{2\pi}d\phi\int_{-1}^{1}\frac{P(x)dx}{wu-x+\sqrt{w^2-1}\sqrt{u^2-1}\cos\phi}=4\pi Q_l(w)P_l(u),\quad w>u>1\ . \tag{A10}$$

Combining (A6) and (A10) now completes the proof of (A5) for the parameter region $(w>1,\ u>1)$ if one notes that the expression is symmetric in the interchange of w and u.

The extension to the parameter region $(w>1,\ u\le 1)$ proceeds by a straightforward examination of the integral that appears in (A5). First note that the denominator is nonvanishing over the interval of integration for $w>1$ $(u\gtrless 1, u=1)$; therefore the integrated function is continuous across the boundary between $(w>1,\ u>1)$ and $(w>1,\ u\le 1)$. Since the P_l are simple polynomials, we have to do with integrals of the form $\int_{-1}^{+1}x^n/\sqrt{X}\,dx$, $X=[w^2+u^2-1-(2wu)x+x^2]$. The elementary recursion relation,

$$\begin{aligned}\int_{-1}^{+1}\frac{x^n dx}{\sqrt{X}}&=\frac{1}{n}x^{n-1}\sqrt{X}\Big|_{x=-1}^{x=1}\\&+\frac{2n-1}{n}wu\int_{-1}^{+x}\frac{x^{n-1}}{\sqrt{X}}dx\\&-\left[\frac{n-1}{n}\right](w^2+u^2-1)\int_{-1}^{+1}\frac{x^{n-2}}{\sqrt{X}}dx\ ,\end{aligned} \tag{A11}$$

gives us the general reduced form

$$\begin{aligned}\int_{-1}^{+1}\frac{x^n dx}{\sqrt{X}}=\sum_{i,j}\Big\{&A_{i,j}^{(n)}w^i u^j(x\sqrt{X}\,|_{-1}^{+1})\\&+B_{i,j}^{(n)}w^i u^j(\sqrt{X}\,|_{-1}^{+1})\\&+C_{i,j}^{(n)}w^i u^j\int_{-1}^{+1}\frac{dx}{\sqrt{X}}\Big\}\ .\end{aligned} \tag{A12}$$

Noting that in the domain ($w>1$ and $w>u$)

$$\begin{aligned}&(\sqrt{X}\,|_{-1}^{+1})=-2u\ ,\\&(x\sqrt{X}\,|_{-1}^{+1})=2w\ ,\\&\int_{-1}^{-1}\frac{dx}{\sqrt{X}}=\ln\frac{w+1}{w-1}\ ,\end{aligned} \tag{A13}$$

whether $u>1$ or $u\le 1$, allows us to write

$$\begin{aligned}\int_{-1}^{+1}\frac{x^n}{\sqrt{X}}dx=\sum_{i,j}\Big\{&2A_{i,j}^{(n)}w^{i+1}u^j-2B_{i,j}^{(n)}w^i u^{j+1}\\&+C_{i,j}^{(n)}w^i u^j\ln\frac{w+1}{w-1}\Big\}\end{aligned} \tag{A14}$$

for $w>1$, $u\gtrless 1$. But this then tells us at once that the form valid for the domain $(w>u>1)$ is just the same for $(w>1,\ w>u,\ u\le 1)$, proving (A8) for $w>1$, as desired. The main result of this Appendix, Eq. (A4), is thus established.

APPENDIX B: COMPARISON WITH LARGE-γ FORMS

The connection of the exact form, Eqs. (25) and (A4), to the asymptotic form, Eq. (24), can be easily made. Using the expansion of $P_l(z)$ in powers of $(1-z)$ (8.1.2 in Abramowitz and Stegun [11]),

$$\begin{aligned}P_l(1/v_p)&=P_l(1+1/(2\gamma^2)+\cdots)\\&\approx 1+l(l+1)/(4\gamma^2)+O(1/\gamma^4)\ .\end{aligned} \tag{B1}$$

Including the effect of the overall $1/v_p$, we find that the exact formula for $r<v_p t$ is $[1+(l^2+l+2)/(4\gamma^2)]$ times that of the asymptotic formula [in conformity with our previously estimated [1] correction of $(b^2/t^2)(l+1)(l+2)/2\gamma^2$].

For $r>v_p t$, one may make the connection in a parallel manner. In particular, since [11]

$$\begin{aligned}Q_l(1/v_p)=\Big\{&\left[\tfrac{1}{2}P_l(1/v_p)\ln\left[\frac{1/v_p+1}{1/v_p-1}\right]\right]\\&-\sum_{n=1}^{l}(1/n)P_{n-1}(1/v_p)P_{l-n}(1/v_p)\Big\}\ ,\end{aligned} \tag{B2}$$

using

$$\ln\left[\frac{1/v_p+1}{1/v_p-1}\right]=2\ln 2\gamma+2\ln\frac{1+v_p}{2}\ , \tag{B3}$$

and Eq. (B1) for the Legendre polymonials, we obtain

$$(1/v_p)Q_l(1/v_p) \approx \left[\ln 2\gamma - \sum_{n=1}^{l} (1/n)\right] \times [1+(l^2+l+2)/(4\gamma^2)] + (l^2+l-1)/(4\gamma^2) . \quad \text{(B4)}$$

Thus for $r > v_p t$ the exact formula $[1+(l^2+l+2)/(4\gamma^2)]$ times the asymptotic formula, plus a term of order $(l^2+l-1)/(4\gamma^2)$.

In the asymptotic form, the split between the two regions $r \gtrless u_p t$ has been written as $r \gtrless t$, dropping the $(1/\gamma^2)$ differences.

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

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

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

[4] Klaus Rumrich, Klaus Momberger, Gerhard Soff, Walter Greiner, Norbert Grün, and Werner Scheid, Phys. Rev. Lett. **66**, 2613 (1991).

[5] K. Rumrich and W. Greiner, Phys. Lett. A **149**, 17 (1990).

[6] N. Toshima and J. Eichler, Phys. Rev. A **42**, 3896 (1990).

[7] M. E. Rose, *Relativistic Electron Theory* (Wiley, New York, 1961).

[8] WCLBES is identical in substance to the code COULCC described in I. J. Thompson and A. R. Barnett, Comput. Phys. Commun. **36**, 363 (1985).

[9] J. G. Reading, Phys. Rev. A **8**, 3269 (1973).

[10] J. Mathews and R. L. Walker, *Mathematical Methods of Physics* (Benjamin, New York, 1965), p. 336.

[11] *Handbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun, National Bureau of Standards, Applied Math. Ser. No. 55 (U.S. GPO, Washington, DC, 1965); W. Magnus and F. Oberhettinger, *Formulas and Theorems for the Functions of Mathematical Physics* (Chelsea, New York, 1959); I. S. Gradshteyn and I. M. Ryzhik, *Tables of Integrals, Series, and Products,* corrected and enlarged ed. (Academic, New York, 1980).