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Non-Perturbative Momentum-Space Approach to Relativistic Heavy Ion Collisions

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New non-perturbative numerical calculations have been set up to study atomic processes in relativistic heavy ion collisions. The approach is a direct integration of the one-electron Dirac equation in momentum space. The method has been applied for 0.24 - 10 GeV/u Au^{79+} and U^{92+} impinging on U^{91+} and probabilities have been obtained for bound-free pair production, charge transfer, ionization and excitation. For bound-free pair production at small impact parameters, our results confirm the break down of perturbation theory but the excess over the perturbative result is much smaller than reported by others.

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During the last decade, a very large effort has been devoted to the study and understanding of atomic physics processes in relativistic heavy-ion collisions, such as excitation, charge transfer, ionization and pair production (see [1,2,3] and references therein). To a large part investigations have been motivated by the practical importance of these processes at relativistic energies [4]. Of particular interest is the QED-effect of electron-positron pair creation with the electron directly produced in a bound state of one of the ions and the positron being emitted free, in the following denoted as "bound-free pair production". This effect, observed recently at the Bevalac at the Lawrence Berkeley Laboratory (LBL) [5-6], is expected to become the dominant mechanism for beam loss and luminosity limitations for Relativistic Heavy Ion Colliders [7].

While many of these collision processes and QED-effects can be computed successfully by perturbation theory, its applicability becomes uncertain in the field of relativistic collisions of high-Z ions. With the electromagnetic coupling constant $Z\alpha$ being close to one and furthermore the electromagnetic field being enhanced by the Lorentz-factor γ, perturbation theory fails to describe ionization [2,8,9], transfer [1,10], production of free electron-positron pairs [3] and, especially, bound-free pair production [11,12]. For free pair production, ionization and bound free pair production, this failure has been ascribed to unitarity [3] and a combination of unitarity and binding effects [13].

For the bound-free pair production process Rumrich et al. [12] predicted an enhancement of the probabilities at small impact parameters by up to two orders of magnitude compared to perturbative results . Their non-perturbative calculation which is confined to moderate relativistic energies, is carried out in the framework of the coupled-channels formalism with an expansion of the electron wave function in a truncated atomic basis set. However, due to the incompleteness of the basis set, this calculation has been criticized recently by Baltz et. al. [14] for being gauge dependent.

Additionally, two grid methods in configuration space have been applied to the problem of bound-free pair production. Thiel et al. used a 2-dimensional finite differences method [15] and Wells et al. used a 3-dimensional basis-spline collocation method [16] to solve the time-dependent Dirac equation in a direct numerical approach. However, the first method was limited to impact parameter zero and the second to the production of muons. Furthermore, since the continuum wave functions in configuration space spread over the entire grid, the above methods have a common problem of non-zero values of the electron-spinor at the boundaries [15]. This latter problem can be overcome by moving to momentum space, since the wave function in momentum space stays localized around the origin at all times and is practically equal to zero at the boundaries.

In this letter, we present a new computational approach to atomic processes in relativistic heavy ion collisions that is based on a direct integration of the time-dependent one-electron Dirac equation in momentum space. In addition to the localization properties in momentum space, which have been exploited in some nuclear collision theory (see, e.g. [17]), our formalism has various unique features: i) it provides a closed-form description of a wealth of atomic processes (electron transfer, excitation, ionization and bound-free pair production), for which we will also present numerical results. ii) we can treat a very wide range in collision energy. iii) we can cover a wider range in the electron/positron energy and angular momentum than in a comparable coupled-channels treatment. iv) the projection of the time evolved state onto the highly localized continuum states is simple [18].

We assume a point-like projectile of charge $Z_P e$ traveling with constant relativistic velocity v and impact parameter b along the z-axis in the rest frame of a hydrogen-like target of nuclear charge $Z_T e$. With the latter centered at the origin, the projectile path is given by: $\mathbf{R}(t) = vt\mathbf{e_z} + b\mathbf{e_x}$. Within the Lorentz gauge, the Dirac equation for the electron spinor $\psi(\mathbf{r},t)$ takes the following form in configuration space [1] ($\hbar$=m=c=1):

$$i\frac{\partial}{\partial t}\psi(\mathbf{r},t)=\left(-i\underline{\alpha}\cdot\nabla+\underline{\beta}-\frac{Z_T e^2}{r}-\frac{\gamma Z_P e^2\,(1-\underline{\alpha}\cdot\mathbf{v})}{[(x-b)^2+y^2+\gamma^2(z-vt)^2]^{1/2}}\right)\psi(\mathbf{r},t) \qquad (1)$$

Here $\underline{\alpha}$ and $\underline{\beta}$ are the Dirac matrices and $\gamma=(1-v^2)^{-1/2}$ is the Lorentz factor. The Fourier transformation of the Dirac-Spinor to momentum space is given by:

$$\psi(\mathbf{k},t)=\frac{1}{(2\pi)^{3/2}}\int d^3r\,\psi(\mathbf{r},t)\,e^{-i\mathbf{k}\cdot\mathbf{r}} \qquad (2)$$

With this prescription the Dirac equation in momentum-space takes the form:

$$i\frac{\partial}{\partial t}\psi(\mathbf{k},t)=(\underline{\alpha}\cdot\mathbf{k}+\underline{\beta})\psi(\mathbf{k},t)$$

$$-\frac{e^2}{2\pi^2}\int d^3k'\left(\frac{Z_T}{q^2}+\frac{Z_P\,(1-\underline{\alpha}\cdot\mathbf{v})}{q_x^2+q_y^2+q_z^2/\gamma^2}\,e^{i\mathbf{q}\cdot\mathbf{R}(t)}\right)\psi(\mathbf{k}',t) \qquad (3)$$

where $\mathbf{q}=\mathbf{k}'-\mathbf{k}$. Note that in momentum space the Dirac equation turns into an integro-differential equation; to get the time derivative at a given value of $\mathbf{k}$ an integration over all of momentum space is required.

In order to perform the time integration, Eq. (3) is rewritten as a linear system of coupled equations, which we integrate by a fourth order Adams-Bashfort predictor-corrector method [19]. In a first stage of this work, the time-dependent momentum wave function

$\psi(\mathbf{k},t)$ is defined in spherical coordinates k, θ and φ on a three dimensional (13 x 7 x 10) grid. We choose an equidistant distribution of the angular grid points and a logarithmic distribution in the radial variable. The maximum radius in the k-variable is typically k_{max} = 10. The $\psi(\mathbf{k}',t)$ values required for the $\mathbf{k}'$-integration of Eq. (3) are obtained using a 2-dimensional spline interpolation for the k and θ variables and a quadratic interpolation for the φ variable. The latter interpolation is found to be sufficiently accurate for the φ variable due to the nearly axial symmetry of the collision. For the $\mathbf{k}'$-integration we slice the spherical integration volume into cells and integrate each cell by Gauss-Legendre quadrature.

Most of the results presented here have been obtained on a farm of ten Sparc10/410 workstations at LBL which offer a maximum performance of 170 Mflops, using the PVM ("Parallel Virtual Machine") software package. As a test of the quality of the calculation we have checked the normalization of the spinor $\psi(\mathbf{k},t)$ throughout the collision. Its value changed by less than 2% over the entire time-interval. This shift from unity builds up monotonically over time and is due to small inaccuracies of the wavefunction at large k-values which carry a substantial weight in the computation of the normalization. A systematic computation using various grids and numerical accuracy shows that this error translates in the main into a similar relative error of the calculated probabilities. However, processes that involve large momenta are affected more than those involving small momenta only. On a later stage of this project, we moved our code to a massively parallel computer (MasPar MP-2) with 4096 processors and a total performance of 1.6 Gflops. The grid was refined to (25 x 13 x 14) points in cylindrical coordinates k_z, ρ and φ, respectively. This refinement of the grid and change to cylindrical coordinates did result in only minor changes of the calculated probabilities. It takes approximately 20-30 CPU hours to run one impact parameter.

We applied the method to a bare Au^{79+} projectile impinging with γ=2 on a hydrogen-like U^{91+} ion at rest in laboratory. We start the time integration of Eq. (3) with the electron in the 1s spin-up state of the uranium. The starting time for the numerical integration is set to t_{start}=-30. We checked that a change of t_{start} to an earlier negative time did not change the results presented here.

Fig. 1 shows the time evolution of the electron density $\psi^+(\mathbf{k},t)\psi(\mathbf{k},t)$ for a collision with b=0.5 (this value corresponds to approximately one-third of the Uranium K-shell radius). As is obvious from the figure, which displays the density in the plane defined by the projectile trajectory and the target nucleus, the electron density remains localized around the origin at all times; unlike the situation in configuration space [8,15] we do not observe a

spread of the electron density over the entire grid at positive times. At t=-10 the electron density is very close to the distribution of the starting 1s state. As the projectile approaches the target the momentum distribution of the electron shifts gradually toward negative values and at the point of minimum approach (t=0) peaks at $k_z \approx -0.5$. This reflects an acceleration of the electron toward the approaching projectile. The probabilities for different processes such as bound-free pair production, K-shell excitation, ionization, and electron transfer to the projectile can be obtained by projecting the final wave function on the corresponding states (and squaring). In order to compute bound-free pair production with the electron ending in the ground state of the target ion we apply time reversal [12] and the final wave function $\psi(\mathbf{k},t)$ of the current calculation is projected on the negative continuum states of the target.

Fig.2 shows the time evolution of the occupation probabilities of different target states for b=0. The projections at intermediate times are not physically meaningful since the electron is still strongly influenced by both nuclei, but they allow for comparison with coupled-channels calculations. We observe that a substantial fraction of the density stays in the initial state throughout the collision (ending at 0.32). At the final time, the total population of excited states of the target amounts to 0.11. The curves labeled ionization and bound-free pair production shown in Fig.2 correspond to the sum of the squares of projections on continuum states of positive and negative energy (up to $|E| = 6$), respectively. The procedure for obtaining continuum waves in momentum space and for projection on these states is described in ref. [18]. We sum over angular momenta up to l=6. We checked that the contribution from higher angular momenta is negligible. Bound-free pair production ends up at a probability of 0.001 whereas the total K-shell ionization ends up at about 0.55.

Due to its low value, our probability for bound-free pair production, given above, may be somewhat uncertain. Indeed, calculations at large impact parameters seem to indicate that bound-free pair production probabilities tend to come out somewhat too high. To check and improve the accuracy of the probabilities for bound-free pair production we took advantage of the cylindrical symmetry of the collision for b=0 to further refine the grid to 128 x 32 in the z and ρ directions, respectively, for this impact parameter. This led to a probability for bound-free pair production of 4.3×10^{-4}. Within few percent the probabilities for ionization, excitation and transfer remained unchanged. It is striking that the probabilities for excitation to high excited states remained unchanged regardless of their values which can be as small as 10^{-5}. The overall change of normalization with the fine grid amounted to less than 0.1%.

The probability for bound-free pair production quoted above is about a factor of five larger than the corresponding perturbative result of 0.89×10^{-4}. With the current precision in the numerical calculations there is no doubt that the enhancement of bound-free pair production probabilities at small impact parameters is much less than reported by Rumrich et al. [12] at similar energies. It does appear that improvements in the accuracy of our calculations tend to bring the probabilities at small impact parameters much closer to perturbative results. We also performed the calculation for U^{92+} impinging on an U^{91+} at 10 GeV/u. We obtain a probability of 7.8×10^{-4} which is only a factor of two larger than the perturbative result. In contrast Thiel et al [15], using the finite-difference method for the same collision system, reported a probability of 0.16 which is more than two orders of magnitude larger than the perturbative result.

We also performed the calculation at $\gamma=5$ for the same collision system as above. For b=0 this led to a probability of 4×10^{-4} for bound free pair production, 0.11 for excitation and 0.44 for ionization. The probability for bound-free pair production is still somewhat uncertain,. nevertheless, our results at b=0, suggest that at small impact parameters it is weakly dependent on the collision energy. Here again the perturbative result is 2.2×10^{-4} which is only a factor of two smaller than our non-perturbative value. The ionization probability is found to decrease substantially with energy between $\gamma=2$ and $\gamma=5$ while the excitation probabilities to individual states are found to vary much less with energy.

We find that, for the excitation process, the population of states follows very closely the well known n^{-3} law where n is the principal quantum number. We also find that the population of states which involve a spin-flip remains small for all impact parameters considered here ($b \leq 2$). We note in particular that the population of the $1s_{1/2}$ spin down which requires only a spin flip of the initial state is found to be very small (for example 7.8×10^{-3} for b=0.5) although the two states are degenerate. This degeneracy causes special problems for coupled channels calculations since the two states are strongly coupled so that the total cross section diverges logarithmically [1].

In addition to transitions between target states, the final wave function $\psi(\mathbf{k},t)$ contains information on the electron transfer from the U^{91+} to the Au^{79+} projectile. For $\gamma=2$ and b=0, we obtain a probability of 0.025 for transfer from the ground state of the target to the ground state of the projectile. This value agrees with the transfer probability calculated by Toshima et al [10] for U^{92+} on U^{91+} at 1 GeV/u and scaled with a Z_p^5 dependence [1].

Since transfer probabilities are rather small at $\gamma=2$ we illustrate the transfer process by showing in Fig.3 the time evolution of the electron density for a lower energy collision ($\gamma=1.259$). This particular energy was chosen to be in the so-called "matching velocity"

regime [1]. The 3-D distribution is markedly different from Fig. 1. For large times ($t > 6$) a substantial fraction of the density stays localized around the k_z axis, at $k_z = 0.76$. This value of the momentum corresponds to an electron moving with the same velocity as the projectile and is thus interpreted as corresponding to the transfer of the electron from the U^{91+} target to the Au^{79+} projectile. The projection of the final distribution on the moving $1s_{1/2}$ state of the projectile amounts to a probability for electron transfer of 0.26. As expected we obtain large transfer probabilities at this energy.

In summary we showed that the numerical solution of the time dependent Dirac equation in momentum space gives a complete picture of the collision process of relativistic heavy ions. Our results confirm the break down of perturbation theory at small impact parameters for bound-free pair production. However, this break down of perturbation theory appears to be much less severe than reported by others using different non-perturbative methods.

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References:

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Figure captions:

Fig. 1: 3-D plot of the electron density $\psi^+(\mathbf{k},t)\psi(\mathbf{k},t)$ for Au^{79+} with $\gamma=2$ impinging on a stationary U^{91+} at b=0.5. The figure shows a cut in the k_X-k_Z plane for four different times. The electron is initially in the U^{91+} ground state.

Fig. 2: Time evolution of the population of different target states for the same collision system as in figure 1 at an impact parameter b=0. The data shown are obtained with a cylindrical grid of 25x13x14 in the k_Z, ρ and φ directions, respectively. A refinement of the grid lowers the final value of the probability of bound-free pair production to 4.3×10^{-4}.

Fig. 3: 3-D plot of the electron density $\psi^+(\mathbf{k},t)\psi(\mathbf{k},t)$ for Au^{79+} with $\gamma=1.259$ impinging on a stationary U^{91+} at b=0. The figure shows a cut in the k_X-k_Z plane for four different times. The electron is initially in the U^{91+} ground state.

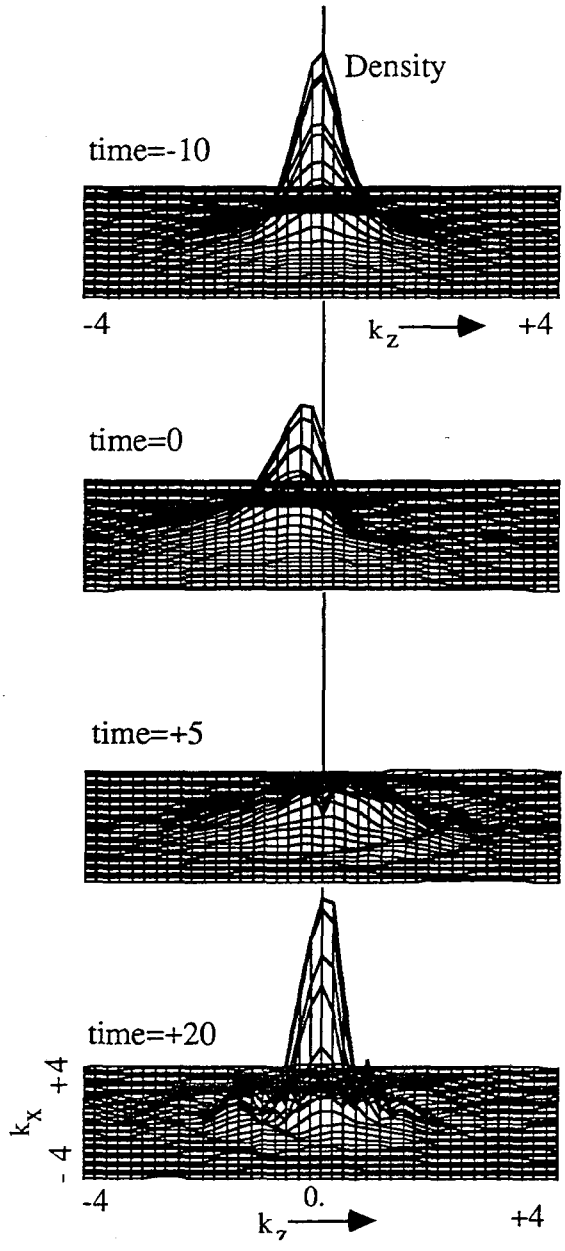

Figure 1

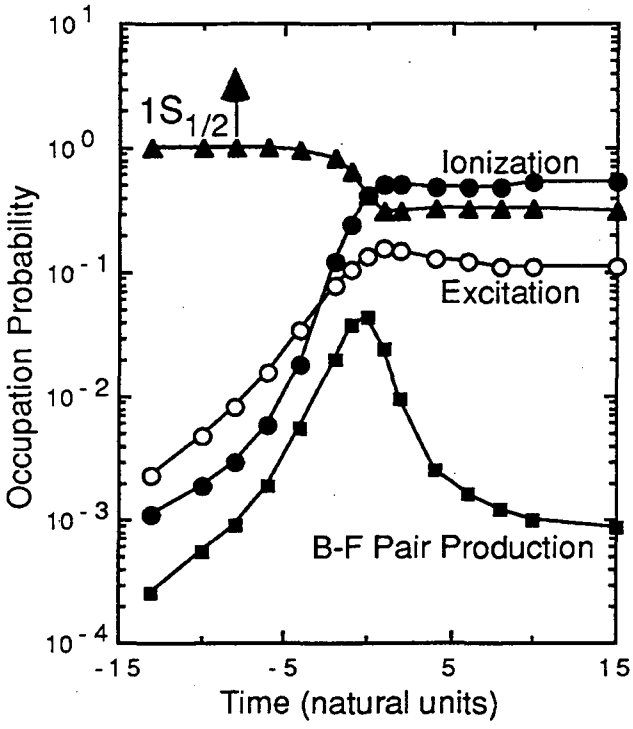
10^1
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
$1S_{1/2}$
Ionization
Excitation
B-F Pair Production
Occupation Probability
-15
-5
5
15
Time (natural units)

Figure 2

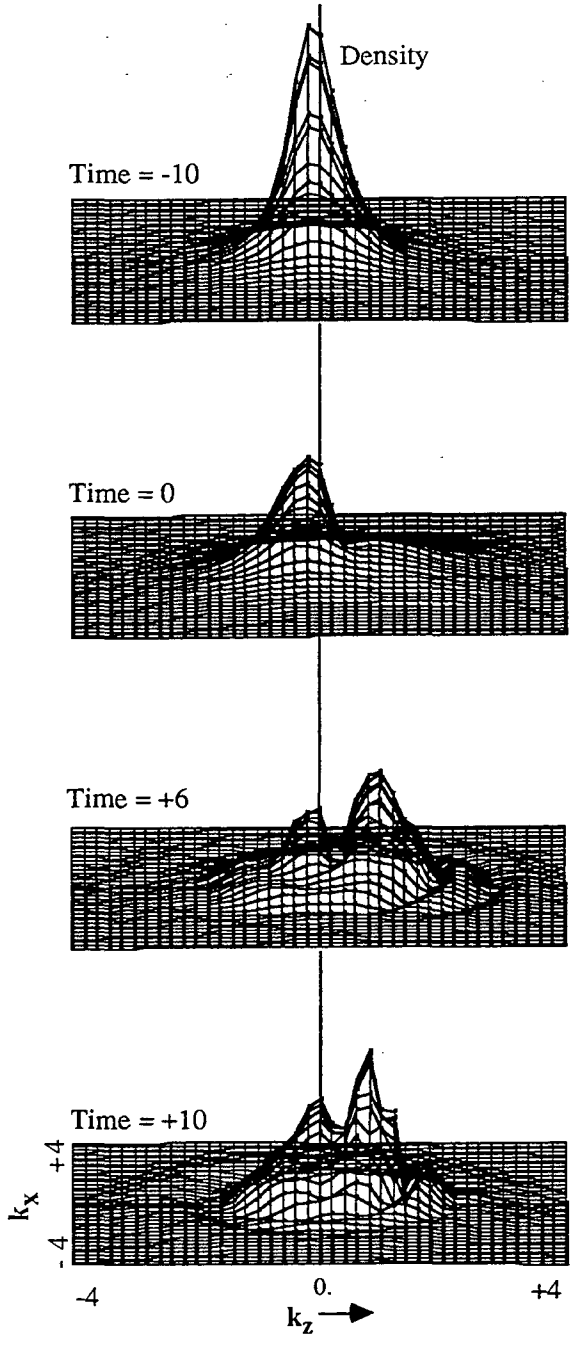

Figure 3

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