New calculations for heavy-ion collisions with super-critical fields

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Abstract. An adaptation of the mapped Fourier grid method for the Dirac equation is applied to the problem of positron production in quasi-molecular collisions between fully stripped heavy ions with super-critical Coulomb fields. The resonance parameters for the 1Sσ vacancy which dives into the filled negative-energy continuum are calculated on the basis of the two similar analytic continuation methods of smooth exterior scaling and complex absorbing potential with Padé extrapolation. Previous results in monopole approximation for the U-Cf system as a function of internuclear separation are extended to a coupled-channel approximation to investigate resonance broadening. Calculations for dynamical positron production on the basis of the time-dependent Dirac equation for U-U collisions with artificially delayed nuclear trajectories are also presented, and explanations for the observed positron spectrum are provided.

1. Introduction

The phenomenon of Dirac energy levels diving into the filled negative-energy continuum received considerable attention some time ago both theoretically [1, 2], and experimentally [4, 5]. As explained in Ref. [1] the phenomenon of QED vacuum decay can be understood within Dirac hole theory, and follows in the simplest case from resonant coupling of an 1Sσ vacancy to the filled sea of negative-energy electron states. For super-critical fields the vacancy is bound so deeply that spontaneous electron-positron pair creation becomes possible: the electron fills the vacant level (and emerges as a bound electron after the collision), while a free positron is emitted.

The super-critical field experiments at GSI Darmstadt were performed with highly charged Uranium impinging on foils (e.g., Curium providing a combined charge of 188). No compelling case for the spontaneous decay of the QED vacuum could be made, as the production of dynamical positrons competes with the resonant process: the lifetimes are of the order of 10^{-19} s, while the collision times are much shorter, namely about 2 \times 10^{-21} s. The time scale for dynamical positron production is of the order of 10^{-20} s. The effect from the spontaneous decay was found to yield an enhancement, but without definite signature in the emitted positron energy spectrum. The situation changed somewhat when collisions between fully stripped nuclei were considered, particularly for the hypothetical case of sticking nuclear collisions, for which the spontaneous decay contributions would be enhanced [3]. The predicted order-of-magnitude enhancement for spontaneous decay is the result of a fully vacant K shell diving, as well as additional vacant levels getting close to the negative continuum and ‘capturing’ electrons from it. Furthermore, the system has a strengthened electric field in the absence of outer screening.

Another manifestation of the resonant behaviour would be in the scattering channel of positrons colliding with super-critical atoms (provided such atoms existed in nature). To realize
such a set-up in the context of U-U quasi-molecules with nuclei almost in contact at least for some time would be formidable, but perhaps not impossible in a facility of merged beams of fully stripped U nuclei. The trapping of highly charged uranium nuclei at sufficiently short internuclear distances could be facilitated by the addition of $\tau^-$ or $\mu^-$ particles. The SPARC collaboration at the FAIR facility (GSI Darmstadt) is proposing to perform crossed-beam experiments of fully stripped uranium nuclei in the near future with the possibility of exploring the super-critical field regime. Thus, it is timely to re-investigate some of the predictions of Ref. [3] using computational methods with enhanced energy resolution in the negative-energy continuum. In Section 2 we present converged calculations for the resonance parameters as a function of internuclear separation, and as a function of channel coupling beyond the monopole approximation. In Section 3 we show pilot calculations for positron spectra obtained with the Fourier Grid Method.

2. Super-critical Resonance Calculations

The analytic continuation method of adding a complex absorbing potential (CAP) to the Dirac equation was contrasted with the more established complex scaling (CS) approach in Ref. [7] using stabilization of the complex eigenvalue in order to find the best approximation to the resonance position and width. A matrix representation of the Dirac equation was obtained using an adaptation of the Fourier Grid Method (FGM) which was tested previously for ordinary Dirac eigenstates [6]. The CAP method was shown to be superior to CS, since it produced more stable results when basis parameters were varied. Recently we implemented the method of smooth exterior scaling (SES) and showed that it is competitive as a stabilization method with CAP [8]. We have also applied a Padé extrapolation method [9] to minimize the effect of the analytic continuation, and demonstrated that the extrapolated resonance parameters from both techniques are remarkably consistent.

A matrix representation of the Dirac equation using the FGM is obtained as follows. First we define the radial channels by decomposing the state using spinor spherical harmonics $\chi_{\kappa,\mu}$:

$$\Psi_\mu(r, \theta, \phi) = \sum_{\kappa} \left( \frac{G_\kappa(r)}{iF_\kappa(r)} \chi_{\kappa,\mu}(\theta, \phi) \right),$$

(1)

where $\kappa = \pm(j + 1/2)$ is related to the total angular momentum label $j$, and $\mu$ is the magnetic quantum number. The Dirac equation for radial functions ($f(r) = rF(r), g(r) = rG(r)$, $\hbar = c = m_e = 1$ units) becomes

$$\frac{df_\kappa}{dr} - \frac{\kappa}{r} f_\kappa = - (E - 1) g_\kappa + \sum_{\bar{\kappa} = \pm 1}^{\pm \infty} \langle \chi_{\kappa,\mu} | V(r, R) | \chi_{\bar{\kappa},\mu} \rangle g_{\bar{\kappa}} ,$$

(2)

$$\frac{dg_\kappa}{dr} + \frac{\kappa}{r} g_\kappa = (E + 1) f_\kappa - \sum_{\bar{\kappa} = \pm 1}^{\pm \infty} \langle \chi_{-\kappa,\mu} | V(r, R) | \chi_{-\bar{\kappa},\mu} \rangle f_{\bar{\kappa}},$$

(3)

where the multipole-expanded potential of two homogeneous spheres separated by distance $R$, i.e., $V(r, R) = \sum_{l=0}^{\infty} V_l(r, R) P_l(\cos \theta)$ provides coupling between the $\kappa$ channels. The $\kappa$ criticality is foremost related to the monopole part ($l = 0$), most prior calculations are truncated at this level. For the present work we concentrate on the $\kappa = -1$ channel, and consider couplings to the nearest neighbours $\bar{\kappa} = 1, -2$ which represent the $P_{1/2}$ and $P_{3/2}$ states, as well as $\bar{\kappa} = 2, -3$ for the $D_{3/2}$ and $D_{5/2}$ states. The dipole and quadrupole parts of the interaction play a role at those separations $R$ where diving of the ground state into the negative continuum begins.

The FGM generates a matrix representation on the basis of a collocation mesh that can be tailored for the problem at hand. Details are given in Ref. [6, 7]. The mesh is very fine at small
$r$, and steps out in bigger increments at large $r$ with an adjustable scale parameter such that the dependence of final results on the chosen mesh can be tested. The matrix elements for the derivative operators are calculated exactly, as the method is based upon a Fourier-sine series representation of the large- and small-component radial functions.

Smooth exterior scaling (SES) is defined by scaling the radial coordinate past some value $r_s$ (which is chosen in the tunneling region, i.e., in the region where the bound part of the resonance state is about to connect with the oscillatory part; in natural units $r_s = 2 \approx 770 \text{ fm}$):

$$r \rightarrow \begin{cases} r & \text{for } r < r_s \\ (r - r_s) e^{i \theta} + r_s & \text{for } r_s \leq r. \end{cases}$$

The scaling angle $\theta$ is chosen where the eigenvalue is least sensitive to it (stabilization method).

The method of adding a CAP of scalar type to the Dirac Hamiltonian has strong similarities to the SES method. In our case a quadratic CAP over a linear one is demonstrated. The complex eigenenergies yield resonance position and full width according to

$$\hat{H} \to \hat{H} - i \eta \hat{\Theta}(r - r_c)(r - r_c)^2.$$  

The distance $r_c$ is again chosen to be within the gap region, which can be defined as the region between the crossings of the resonance energy with the curves $V(r, R) - mc^2$ and $V(r, R) + mc^2$. The strength parameter $\eta$ plays the same role as $\theta$ in the SES method. In principle, for a sufficiently large basis set the complex eigenenergies should be independent of $\eta$. In practice, for a finite-size basis one computes a complex energy trajectory as a function of $\theta$ or $\eta$ and looks for stability in either $|E_{\text{res}}|$ or in the real and imaginary parts (SES often does not lead to stability in all three quantities). In Ref. [7] some dependence of stabilized resonance parameters on $r_c$ is shown, and the advantage of a quadratic CAP over a linear one is demonstrated. The complex eigenenergies yield resonance position and full width according to $E = E_{\text{res}} + i \Gamma/2$; note the change in sign for the imaginary part as compared to the Schrödinger case, as the resonance position is negative ($E_{\text{res}} < -mc^2$).

In Fig. 1 we show the complex $1S_{\sigma}$ energy trajectories from both CAP and SES methods using three coupled channels, and indicate the stabilized values by crosses. Note that the axes defining the complex energy plane have a fine scale, and are labeled in different units for the $E_{\text{res}}$ and $\Gamma$. The SES results follow a curved trajectory computed for an equidistant fine $\theta$ mesh: starting at finite $\theta$ at the bottom of the graph they stabilize as $\theta$ is reduced, and then move away in an abrupt fashion. The CAP data behave similarly as a function of $\eta$: starting at the top right for some intermediate $\eta$-value they follow a linear trajectory as $\eta$ is reduced. Stabilization occurs at some small value of $\eta$, and then the trajectory moves away abruptly. The almost erratic behaviour in both calculations for very small parameters $\theta$ or $\eta$ is related to the fact that the basis set is not able to represent the wave function at large values of $r$. In the naive limit of $\theta = 0$ or $\eta = 0$ the Hamiltonian becomes hermitean, and the information of the resonance is spread over a number of continuum channels as demonstrated in Ref. [7] in the monopole approximation.

The main idea behind the extrapolation method is as follows [9]: complex eigenvalues as a function of stabilization parameter are meaningful only above some critical value (which happens to be close to the stabilized value). We can use a number of points from the trajectory (e.g., $N_p = 4$) to construct a rational function approximation for the true complex-energy path as a function of stabilization parameter. We can then seek the limiting value for zero parameter. This is done on the basis of points marked by the squares, and the trajectory is drawn as a curve for either method. Both extrapolations ($\theta = 0$ and $\eta = 0$) lead to very consistent values for $E_{\text{res}} + i \Gamma/2$. The extrapolation method yields an order-of-magnitude improvement in the answer over stabilization, and thus permits computations with smaller basis size.

A few extrapolated coupled-channel resonance positions and width as a function of internuclear separation $R$ are given in Table 1 for the Uranium-Californium system ($Z_1 = \ldots$)
Figure 1. (Colour online) U-Cf at $R = 20$ fm: complex $1S_{\sigma}$ eigenenergy trajectories from the SES (blue) and CAP (red) methods with stabilized values indicated by large crosses. Lines represent Padé fits with meaningful extrapolations to $\theta = 0$ and $\eta = 0$ respectively. Squares indicate the first and last data point used for the $N_p = 8$ Padé fit.

When comparing different coupled-channel results one notices a small change when going from pure S-state calculations (monopole approximation) to coupled S-P channels [8]. This is the result of the nearly charge-symmetric U-Cf system having a small dipole potential. The broadening of the widths due to the added interaction increases with internuclear separation $R$. A more substantial increase in the $\Gamma$ values is obtained when the quadrupole coupling between S and D states is included. These results are reported here for the first time.

Table 1. (Colour online) Position and width for the $1S_{\sigma}$ resonance in the U-Cf system as a function of internuclear separation $R$ using S, S-P, and S-P-D channel couplings. Energies are given in keV, the coupled-channel resonance positions are given in the monopole approximation (first column), and in the S-P-D approximation (last column). The positron kinetic energy is given by $|E_{\text{res}} + 511.0|$ keV.

| $R$[fm] | $E_{\text{res}}$(S) | $\Gamma$(S) | $\Gamma$(S-P) | $\Gamma$(S-P-D) | $E_{\text{res}}$(S-P-D) |
|---------|---------------------|-------------|---------------|-----------------|---------------------|
| 16      | -1025.3             | 8.1482      | 8.1502        | 8.6810          | -1040.3             |
| 20      | -898.3              | 4.0848      | 4.0874        | 4.6509          | -918.1              |
| 24      | -797.7              | 1.6967      | 1.6989        | 2.1502          | -820.4              |
| 28      | -717.4              | 0.5222      | 0.5235        | 0.79425         | -741.2              |
| 32      | -651.5              | 0.0931      | 0.0936        | 0.20107         | -675.8              |

Table 1 gives an indication of how narrow the resonances are: for vacuum decay under sticking conditions for the two nuclei positrons of about 514 keV would be emitted with an uncertainty in the one-percent range. Some further broadening of $\Gamma$ can be expected from couplings to higher angular-momentum states; a more significant effect in this regard is expected at larger values of $R$, but the computed widths are substantially smaller in those cases.
To explain these results we show in Fig. 2 the multipole decomposition of the potential due to two homogeneously charged spheres at a separation of $R = 20$ fm, which corresponds to 0.052 Compton wavelengths. The $l = 0$ monopole contribution has a long-range tail and clearly dominates at all distances. The $l = 1$ dipole contribution is weak due to the near-symmetry in the U-Cf system. The $l = 2$ quadrupole potential is more pronounced and leads to the results reported in the final two columns of Table 1. Note that the $l = 2,4$ multipole contributions are significant for distances in the $r < R$ range only. The bound part of the resonance wave function exhibits a peak in this region, i.e., it samples the multipole contributions efficiently. The potentials enter the coupled-channel equations via radial matrix elements, multiplied by angular integrals which depend on the value of $j$. Within a given orbital angular momentum sector (such as $\{2P_{1/2},2P_{3/2}\}$, or $\{3D_{3/2},3D_{5/2}\}$) the sublevels have similar couplings to the dominant $1S_{1/2}$ channel.

3. Dynamical Positron Production

Previous calculations of positron production in super-critical heavy-ion collisions at the Coulomb barrier [1, 2, 3] employed a method where the resonant $1S_\sigma$ state was approximated as a discrete bound state, and the negative-energy continuum was orthogonalized using the Feshbach projection formalism. The isolation of the resonance from the basis was required, as computational resources did not permit to resolve the continuum at a sufficiently fine level. Our own calculations with the FGM and hermitean Dirac-Hamiltonian were shown to have sufficient resolution to demonstrate the Breit-Wigner shape directly in the density of states [7] (when using a basis of $N = 3900$ states). It should be possible to use an analytically continued Hamiltonian in the time-dependent calculation, with the resonance represented by a single state, while the density of continuum states would be structureless. For the present work the resonance is not isolated from the continuum, and its representation is somewhat crude in a basis of, e.g., $N = 512$ states.

One of the motivations for the present work is based on the observation that the calculations of Ref. [3] produce broad structures in the positron spectra even for long sticking times $T$, i.e.,
when dynamical positron production (and the associated interference effects) should be less important. The widths of the positron energy distributions do not scale as $\hbar/T$ either. Thus, we are interested in finding out what leads to the substantial additional broadening, and also to a shift of the centre from the expected location as calculated in the previous section.

For the computation of ionization and positron production spectra we have developed a propagation scheme for the time-dependent Dirac equation within the FGM. It is based on the idea that the Coulomb repulsion slows the nuclei in the vicinity of the closest approach, which is the regime when level diving and spontaneous electron-positron pair production occurs. The electronic system is treated adiabatically, i.e., the stationary Dirac equation in matrix representation is solved by the FGM for many internuclear separations $R_{\nu}$. For the short time intervals corresponding to the inter-nuclear motion $R_{\nu} \rightarrow R_{\nu+1}$ time propagation is carried out by trivial evolution of the eigenvectors using the computed phases. At the end of the interval, i.e., at $t_{\nu+1}$ corresponding to $R_{\nu+1}$ a change of representation of the propagated solution vector is carried out by projection. The time-steps $\Delta t_{\nu} = t_{\nu+1} - t_{\nu}$ are adjusted to obtain converged results. The technique is computationally feasible, since the kinetic energy matrix is pre-computed once for a given choice of Fourier grid, the potential energy just needs to be computed on the given coordinate-space grid, and matrix diagonalization is fast.

The continuously changing Hamiltonian is approximated by a staircase defined by the time discretization. We have tested the method favourably against a finite-difference method [10] at highly relativistic impact energies, and note that a review of modern propagation techniques for the Dirac equation can be found in Ref. [11].

To demonstrate that the method can describe both dynamical positron production and positrons due to spontaneous vacuum decay we consider an artificial trajectory: for given incident energy a Coulomb trajectory for head-on collisions leads to a uniquely defined distance of closest approach $R_{ca}$. We introduce a time delay $T$ while the system is at $R_{ca}$: this results in filling of the $1S_{\nu}$ vacancy and simultaneous positron production. The positron probability is expected to grow linearly as $T/\tau$ (initially the exponential decay of the $1S_{\nu}$ vacancy follows linear behaviour). For short times $T$ of the order of the collision time the behaviour can be complicated due to the coherent addition of dynamical and spontaneous positron components [3]. For longer delay times $T$ the spontaneous positron production should dominate, and the decay rate $1/\tau$ should be related to the resonance width $\Gamma\tau = \hbar$ as computed from the stationary Dirac equation in the previous section. For incident energies such that $R_{ca}$ corresponds to a nuclear diameter, sticking for some time $T$ may, in fact, occur occasionally in nature (deep inelastic collisions, as discussed in Ref. [3]).

We investigated the bare U-U collision system for collision energies of 610 and 740 MeV, which lead to values of $R_{ca} = 20, 16.5$ fm respectively, both of which are super-critical for the $1S_{\nu}$ state. In the former case a 200 keV positron line with a width of $\Gamma = 0.5$ keV would be expected in the limit $T \sim \tau$, while in the latter it would be at 300 keV and $\Gamma = 2$ keV. Our objective is to demonstrate the growth of the total positron production rate as a function of the artificial delay time $T$, and to investigate the positron energy spectrum. We did observe linear behavior of the positron yield for $T \geq 5 \times 10^{-21}$ s with the rate given by $R = 1/\tau$ for both collision energies. However, the rate fell behind the expected decay rate $\Gamma/\hbar$: in both cases by about one third. This result was stable when basis parameters were changed, and will need to be confirmed with calculations where the resonance is treated as an isolated state in the computational basis.

In Fig. 3 we show the final positron emission spectrum for the case of 610 MeV relative impact energy ($R_{ca} = 20$ fm) as a function of delay time $T$ at this separation. Our results for the case where the delay can be interpreted as sticking ($R_{ca} = 16.5$ fm) are close to the results of U. Müller et al. [3]. The spectra for both energies and equal time delay $T$ are more similar to each other than one would expect on the basis of the true resonance parameters.
Figure 3. (Colour online) Positron energy spectra (in $1/mc^2$) for head-on collisions in the \(U^{92+}-U^{92+}\) system at \(E = 610\) MeV with a distance of closest approach of \(R_{\text{ca}} = 20\) fm. The trajectory is delayed artificially at this separation by \(T = 5, 10, 20 \times 10^{-21}\) s. The vertical dash-dotted line indicates the resonance position for \(R = 20\) fm (\(E_{\text{res}} \approx 200\) keV, \(\Gamma \approx 0.5\) keV). The number of \(E < -mc^2\) continuum channels is 512.

What is the reason for the broadening and shift of the positron spectrum away from \([E_{\text{res}}, \Gamma]\) for delay times \(T < \tau\)? One might argue that the correct energy width for the positrons produced with stationary nuclei at \(R_{\text{ca}}\) should be \(\Gamma_{\text{eff}} = \hbar/T\): a wavepacket with a dominant wavenumber corresponding to the resonance energy would be emitted for a finite time \(T\) leading to a broadening by the envelope function. The time-varying Coulomb field on the outgoing part of the trajectory will modify the spectrum, but this should be independent of the value of \(T\). If one looks at the spectrum in Fig. 3 (or Fig. 2b in Ref. [3]) it is clear that the width of the main peak does not scale like \(1/T\) even when just comparing \(T = 10 \times 10^{-20}\) s with \(T = 2 \times 10^{-20}\) s. The corresponding shift towards higher positron kinetic energies for shorter \(T\) is also hard to explain (after all, the Coulomb repulsion decreases as the nuclei recede).

In order to understand the phenomenon we compare in Fig. 4 the negative-energy population for a few times during the collision in the case of \(T = 2 \times 10^{-20}\) s. At the end of the delay time the spectrum is narrow and centered on the resonance energy (the very high \(1S_{\sigma}\) peak is cut off in the figure). As the \(1S_{\sigma}\) resonance moves out towards the energy gap the spectrum broadens, and begins to shift towards higher energies. While the \(1S_{\sigma}\) discrete state, and other states, bound and \(E > mc^2\) (which share the vacancy by now) adapt to the weakening Coulomb field, they still capture some population from \(E < -mc^2\), the population shifts in kinetic energy (peak goes from 200 to 250 keV), while an additional smaller peak forms at about 470 keV. This second peak is low, and one is tempted to explain it as an interference effect between dynamical and spontaneous positron production. We note, however, that the nodal structure in the positron spectra is initially correlated strongly with the delay time \(T\), and shifts by a small amount during the dynamical positron production phase. The boost in positron yield during the time when the \(1S_{\sigma}\) state moves further into the gap is similar for all cases of \(T\) considered. We found that dynamical positron production on the outgoing part of the trajectory (when the
Figure 4. (Colour online) Time history of the $E < -mc^2$ population for head-on collisions in the U$^{92+}$-U$^{92+}$ system at $E = 610$ MeV with $R_{ca} = 20$ fm, and an artificial delay by $T = 2 \times 10^{-20}$ s. For the separations of $R_{ca} = 20, 25$ fm the $1S_0$ state distorts the positron spectrum. The number of $E < -mc^2$ continuum channels is 512.

4. Conclusions
We calculated resonance parameters in the supercritical heavy-ion system U-Cf beyond the monopole approximation, to include multipoles up to $l = 4$. Coupling to the D-wave introduces an appreciable increase in the resonance widths, and a small change in position. Dynamical calculations for bare U-U collisions were also performed, and reasons for the very substantial broadening and shifting even for long delay times $T$ in the nuclear trajectories were indicated.

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