Positron production in heavy-ion collisions. I. Analytical description of the resonance in the positron continuum for supercritical atoms

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With increasing nuclear charge Z (and finite nuclear size), the lowest bound-state solution of the Dirac equation changes into a resonance located in the positron continuum (supercritical atom). We develop a formalism which enables us to treat this resonance explicitly in the manner of a quasibound state. The processes of electron and positron production in heavy-ion collisions of total charge $Z_1+Z_2 \gtrsim 170$ can then be formulated analytically in such a way that all the rapid energy dependence due to this resonance is made explicit. The definition of the resonance wave function involves some ambiguity. As a consequence, the decomposition of the transition amplitude for positron production into a "spontaneous" and an "induced" part cannot be given unambiguously. The coupled time-dependent equations for the occupation amplitudes of the adiabatic single-particle states contain matrix elements which are smooth functions of the energy, and which can be calculated easily. The application of this formalism to positron production in supercritical atoms is presented in the following article by one of us (T.T.).

I. INTRODUCTION

Much experimental[1] and theoretical[2] work has recently been devoted to atomic electron- and positron-production processes in heavy-ion collisions. Particular attention has been paid to reactions in which the total nuclear charge Z_1+Z_2 of the two ions is so large ($\gtrsim 170$) that, with decreasing internuclear distance, the energy of the lowest bound state of the Dirac equation of the combined system passes the value -1 (in natural atomic units) ("critical" atom), so that this state "dives" into the positron continuum and manifests itself there mathematically as a resonance ("supercritical" atom).

The theoretical description of this process[2] has for some time used an expansion in terms of solutions of the Dirac equation for the critical atom. Unless the resonance energy is very close to -1, this expansion has turned out to be not very satisfactory.[3] To achieve a more satisfactory description, Reinhardt *et al.*[3] have therefore recently adopted a formalism[4] developed originally in the context of nuclear physics. Their scheme is essentially numerical in character, and has been used in numerical calculations of electron and positron production cross sections.[3]

It is our aim in the present paper to carry this development one step further, and to present a treatment of the resonance which is fully analytical. In this way we hope not only to expedite the numerical calculations, but, more importantly, to gain further physical insight into the detailed mechanism of positron production in heavy-ion collisions. We achieve this aim (the analytical treatment of the resonance phenomenon) by a modification of the Wang-Shakin formalism[4] which is different from the one used by Reinhardt *et al.* We succeed in making all the strong energy dependence associated with the resonance explicit, in setting up coupled equations for the occupation amplitudes of the adiabatic wave functions which are nearly identical in form to the undercritical case, and in giving analytical formulas for the coupling matrix elements in these equations. Moreover, the coupling matrix elements are smooth functions of energy and internuclear distance aside from a principal value singularity, which does not contribute to the observable quantities.

The present paper contains the formalism. Applications are deferred to the following paper by one of the authors (T.T.). In Sec. II we define the formalism; in Sec. III we recall the procedure of Wang and Shakin[4]; in Sec. IV we present our definition of the resonance wave function φ_r (a square-integrable function); in Sec. V we construct the modified con-

tinuum wave functions (which are orthogonal to φ_r); in Sec. VI we derive the coupled differential equations for the occupation amplitudes in the supercritical case, and we establish the connection with observable quantities; in Sec. VII we present analytical formulas for the coupling matrix elements. Section VIII contains a brief summary.

II. FORMALISM

We assume that the nuclear orbital motion is classical so that the relative coordinate of two colliding nuclei is a function of time which we write as $\vec{R}(t)$. We also assume that the electron-electron interaction can be neglected. Then the whole information on electrons and positrons can be deduced[3,5,6] from an initial condition on the many-electron system and the solutions of the single-electron Dirac equation

$$\left[i\frac{\partial}{\partial t}-H(\vec{R}(t))\right]\psi(\vec{r},t)=0\ , \tag{2.1}$$

where $H(\vec{R}(t))$ is a Dirac Hamiltonian

$$H(\vec{R}(t))=-i\vec{\alpha}\cdot\frac{\partial}{\partial\vec{r}}+\beta+V(\vec{r},\vec{R}(t))\ , \tag{2.2}$$

and where we put $\hbar=c=m_e=1$.

The potential is given by

$$V(\vec{r},\vec{R})=-\int d\vec{r}\,'_1\frac{\alpha\rho_1(\vec{r}\,'_1-\vec{R}_1)}{|\vec{r}-\vec{r}\,'_1|}-\int d\vec{r}\,'_2\frac{\alpha\rho_2(\vec{r}\,'_2-\vec{R}_2)}{|\vec{r}-\vec{r}\,'_2|}\ , \tag{2.3}$$

where ρ_i is the charge density and $\vec{R}_i$ the position of nucleus i ($i=1,2$):

$$\vec{R}_1=\frac{A_2}{A_1+A_2}\vec{R}\ ,\qquad \vec{R}_2=-\frac{A_1}{A_1+A_2}\vec{R}\ . \tag{2.4}$$

We assume for ρ_i a uniformly charged sphere of a radius $R_{ni}=r_0A_i^{1/3}$ with $r_0=1.2$ fm. When R is less than several hundred fm, this potential can be well approximated by its monopole part[3]

$$V(r,R)=V_1(r,R_1)+V_2(r,R_2)\ , \tag{2.5a}$$

with

$$V_i(r,R_i)=\begin{cases}\dfrac{-Z_i\alpha}{R_i} & (r\le R_{i-}),\\[2ex] -\dfrac{Z_i\alpha}{16R_{ni}^3R_ir}[r^4-4R_ir^3+6R_{i-}R_{i+}r^2-4R_{i+}^2(R_i-2R_{ni})r+R_{i-}^3(R_i+3R_{ni})] & (R_{i-}\le r\le R_{i+}),\\[2ex] -\dfrac{Z_i\alpha}{r} & (R_{i+}\le r)\ ,\end{cases} \tag{2.5b}$$

where $R_{i\pm}=R_i\pm R_{ni}$.

We use the monopole approximation throughout. It is necessary if one wishes to obtain a simple analytical representation for the resonance wave function. The neglect of higher multipoles is, however, not essential for the success of our formal scheme. Such multipoles can be included explicitly in the coupled equations (2.10).

In order to solve the Dirac equation, Eq. (2.1), we expand the wave function $\psi(\vec{r},t)$ in terms of a set of basis states. Since we are considering the cases in which $|\dot{R}|\lesssim 0.1c$ and the potential is so strong that the binding energy of the lowest bound state is about 2, it is appropriate to use adiabatic basis states which are defined as the eigenfunctions of $H(R(t))$:

$$[H(R)-E]\varphi_E(\vec{r},R)=0\ . \tag{2.6}$$

When it is necessary, we also use notations E_n ($n=0,1,2,\ldots$), E_+, and E_- in order to distinguish bound states, positive, and negative energy continuum states:

$$E_-<-1\le E_0<E_1<\cdots<1<E_+\ .$$

The bound state energies E_n depend on R.

We normalize the wave functions[7] as

$$\langle \varphi_E \mid \varphi_{E'} \rangle = \delta(E - E') \text{ for continuum states,}$$
$$\langle \varphi_n \mid \varphi_m \rangle = \delta_{nm} \text{ for bound states,} \tag{2.7}$$

where φ_n means φ_{E_n}.

For the undercritical case, we expand the wave function $\psi(\vec{r},t)$ in Eq. (2.1) in terms of the adiabatic basis as

$$\begin{aligned}\psi(\vec{r},t) &= \int_1^{\infty} dE_+ c_{E_+}(t)\exp[-i\theta_{E_+}(t)]\varphi_{E_+}(\vec{r},R(t)) + \sum_{n\geq o} c_n(t)\exp[-i\theta_n(t)]\varphi_n(\vec{r},R(t)) \\ &\quad + \int_{-\infty}^{-1} dE_- c_{E_-}(t)\exp[-i\theta_{E_-}(t)]\varphi_{E_-}(\vec{r},R(t)) \\ &\equiv \mathop{\mathscr{S}}_{E=-\infty}^{+\infty} c_E(t)\exp[-i\theta_E(t)]\varphi_E(\vec{r},R(t)) ,\end{aligned} \tag{2.8}$$

where the phase functions $\theta_E(t)$ are defined as

$$\begin{aligned}\theta_{E_\pm}(t) &= E_\pm t , \\ \theta_n(t) &= \int_0^t dt' E_n(R(t')) .\end{aligned} \tag{2.9}$$

The symbol $\mathscr{S}$ denotes summation over bound states and integration over continuum states. Putting the expression for $\psi(\vec{r},t)$, Eq. (2.8), into the Dirac equation (2.1), we obtain a set of coupled differential equations for the expansion coefficients $c_E(t)$:

$$\begin{aligned}\dot{c}_E &= -\mathop{\mathscr{S}}_{E'\geq E_1} \langle \varphi_E \mid \dot{\varphi}_{E'} \rangle \exp[i(\theta_E - \theta_{E'}]c_{E'} - \langle \varphi_E \mid \dot{\varphi}_0 \rangle \exp[i(\theta_E - \theta_0)]c_0 \\ &\quad - \int_{-\infty}^{-1} dE'_- \langle \varphi_E \mid \dot{\varphi}_{E'_-} \rangle \exp[i(\theta_E - \theta_{E'_-})]c_{E'_-} \quad (E \geq E_1) , \\ \dot{c}_0 &= -\mathop{\mathscr{S}}_{E'\geq E_1} \langle \varphi_0 \mid \dot{\varphi}_{E'} \rangle \exp[i(\theta_0 - \theta_{E'})]c_{E'} - \int_{-\infty}^{-1} dE'_- \langle \varphi_0 \mid \dot{\varphi}_{E'_-} \rangle \exp[i(\theta_0 - \theta_{E'_-})]c_{E'_-} , \\ \dot{c}_{E_-} &= -\mathop{\mathscr{S}}_{E'\geq E_1} \langle \varphi_{E_-} \mid \dot{\varphi}_{E'} \rangle \exp[i(\theta_{E_-} - \theta_{E'})]c_{E'} - \langle \varphi_{E_-} \mid \dot{\varphi}_0 \rangle \exp[i(\theta_{E_-} - \theta_0)]c_0 \\ &\quad - \int_{-\infty}^{-1} dE'_- \langle \varphi_{E_-} \mid \dot{\varphi}_{E'_-} \rangle \exp[i(\theta_{E_-} - \theta_{E'_-})]c_{E'_-} .\end{aligned} \tag{2.10}$$

III. THE SUPERCRITICAL CASE: APPEARANCE OF A RESONANCE

Inasmuch as the energy of the lowest bound state $E_0(R)$ does not reach the threshold of the negative energy continuum -1 the Dirac equation (2.1) can always be reduced to the coupled equations (2.10). For very heavy projectile-target combinations, however, there exists a critical internuclear distance R_{cr} at which E_0 becomes -1. In the case of a U + U collision, for example, R_{cr} is about 30 fm for a $1s\sigma$ state. If we decrease R further, the lowest bound state disappears and instead there appears a resonance in the negative energy continuum. Under such circumstances a one-to-one correspondence between the eigenfunctions of $H(R)$ for $R > R_{cr}$ and those for $R < R_{cr}$ cannot be established in an obvious fashion, so that the framework of Sec. II cannot be applied as it stands.

The most natural way to overcome this difficulty is to introduce a normalizable resonance state $\varphi_r(\vec{r},R)$ which tends to the lowest bound state as R tends to R_{cr}:

$$\lim_{R\to R_{cr}-0} \varphi_r(\vec{r},R) = \lim_{R\to R_{cr}+0} \varphi_0(\vec{r},R) . \tag{3.1}$$

We defer the explicit construction of φ_r to the next section and assume that φ_r has already been determined. Since for $R < R_{cr}$ the set of states $\{\varphi_{E_-}(E_- < -1)\}$ is already complete for the negative energy continuum space, a new set of states $\{\varphi_r, \varphi_{E_-}(E_- < -1)\}$ would become overcomplete. Therefore, we modify[3,4] the negative energy states φ_{E_-} by removing from them the resonance wave

function. In other words, we construct new continuum wave functions χ_{E_-} which are orthogonal to φ_r. We then diagonalize the Hamiltonian in a space orthogonal to φ_r, i.e.,

$$Q\chi_{E_-}=0\ , \tag{3.2}$$

and

$$[E_- -PH(R)P]\chi_{E_-}=0\ , \tag{3.3}$$

where

$$\begin{aligned} Q&=|\varphi_r\rangle\langle\varphi_r|\ , \\ P&=1-Q\ . \end{aligned} \tag{3.4}$$

Equation (3.3) can be rewritten as

$$[E_- -H(R)]\chi_{E_-}=-QH(R)\chi_{E_-}\ . \tag{3.5}$$

Using the Green's function for $H(R)$:

$$G^{(+)}_{E_-}=[E_- -H(R)-i\epsilon]^{-1}\ \ (\epsilon\to 0+)\ , \tag{3.6}$$

we obtain an integral equation for χ_{E_-}:

$$\chi^{(+)}_{E_-}=\varphi^{(+)}_{E_-}-G^{(+)}_{E_-}QH(R)\chi^{(+)}_{E_-}\ , \tag{3.7}$$

where $\chi^{(+)}_{E_-}$ and $\varphi^{(+)}_{E_-}$ satisfy an outgoing boundary condition.[8]

Equation (3.7) can be solved as

$$\chi^{(+)}_{E_-}=(1-\langle\varphi_r|G^{(+)}_{E_-}|\varphi_r\rangle^{-1}G^{(+)}_{E_-}Q)\varphi^{(+)}_{E_-}\ , \tag{3.8}$$

with the normalization

$$\langle\chi^{(+)}_{E_-}|\chi^{(+)}_{E'_-}\rangle=\delta(E_- -E'_-)\ , \tag{3.9}$$

and the diagonal property

$$\langle\chi^{(+)}_{E_-}|H(R)|\chi^{(+)}_{E'_-}=E_-\delta(E_- E'_-)\ . \tag{3.10}$$

We shall also request a continuity property of χ_{E_-}, similar in character to Eq. (3.1), namely

$$\lim_{R\to R_{cr}-0}\chi_{E_-}(\vec{r},R)=\lim_{R\to R_{cr}+0}\varphi_{E_-}(\vec{r},R)\ . \tag{3.11}$$

The formal constructions in this section cast the problem into the form where a quasibound state φ_r is coupled to the modified positron continuum χ_{E_-}, with coupling matrix element

$$V_{E_-}=\langle\varphi_r|H(R)|\chi_{E_-}\rangle\ , \tag{3.12}$$

and diagonal element

$$E_r=\langle\varphi_r|H(R)|\varphi_r\rangle\ . \tag{3.13}$$

The solution of the stationary equations of motion of this problem[9] yields explicitly the resonance behavior.

IV. CONSTRUCTION OF THE RESONANCE WAVE FUNCTION φ_r

A possible candidate for the resonance wave function φ_r is a continuum wave function φ_{E_0} at the resonance energy E_0 with its tail part cut off at some point in the barrier region. It we cut off the radial wave function sharply, however, the difficulty arises that the energy expectation value of φ_r becomes infinite, and that surface terms must be included in the formalism. Reinhardt *et al.*[3] avoided these problems by adding an exponential tail to the cut-off wave function. In this scheme, various matrix elements which involve φ_r or χ_{E_-} can be calculated only numerically, however. We construct φ_r in a different way, aiming at a full analytical treatment of the resonance. To this end we first note that the continuum wave function φ_{E_-} behaves inside the barrier and near the resonance energy as

$$\varphi_{E_-}\approx A_{E_-}\varphi_r\ , \tag{4.1}$$

where

$$A_{E_-}=\left[\frac{\Gamma(E_-,E_0)}{2\pi}\right]^{1/2}\{(E_- -E_0)^2+\tfrac{1}{2}\Gamma(E_-,E_0)]^2\}^{-1/2}\ , \tag{4.2}$$

and where $\Gamma(E_-,E_0)$ is the width to be discussed below. We accordingly *define the resonance wave function* φ_r by

$$\varphi_r=\int_{E_c}^{-1}dE_-A_{E_-}\varphi_{E_-}\ . \tag{4.3}$$

The cutoff energy E_c in the integral of Eq. (4.3) must be introduced because of the slow falloff of the weight function A_{E_-} with $E_- -E_0$. Without cutoff, the integral (4.3) would sample contributions from positron wave functions penetrating the barrier which have nothing to do with the resonance. We keep E_c fixed and choose it smaller than the minimum value of E_0 attained during the collision. Our formalism is obviously restricted to reactions for which E_c can be chosen such that the penetrability $P^{(0)}(E_c)$ defined below is small enough compared with 1 and that the difference E_0-E_c remains considerably larger than $\Gamma(E_c,E_0)$. These

are fortunately the only ones of any practical interest.

The width $\Gamma(E_-,E_0)$ is obviously well defined at and near the resonance energy E_0. For energies $|E_- - E_0| \gg \Gamma(E_-,E_0)$, on the other hand, the choice of $\Gamma(E_-,E_0)$ is somewhat arbitrary. We utilize this fact to impose the condition

$$\left| \frac{d\Gamma(E_-,E_0)}{dE_-} \right| \ll 1 . \tag{4.4}$$

With the help of this inequality, we can approximate $\Gamma(E_-,E_0)$ under the integral (4.3) by $\Gamma(E_0,E_0)$,

$$\langle \varphi_r | \varphi_r \rangle \approx 1 . \tag{4.5}$$

Similarly, the expectation value of the Hamiltonian is equal to E_0,

$$E_r = \langle \varphi_r | H(R) | \varphi_r \rangle \approx E_0 . \tag{4.6}$$

The error in Eqs. (4.5) and (4.6) can be estimated for the choices of $\Gamma(E_-,E_0)$ introduced below; it does not exceed 1% for any one of them.

We now turn to a practical choice of the dependence of $\Gamma(E_-,E_0)$ on E_-, writing Γ as the product of a reduced width $\gamma(E_0)$ and of a penetration factor $P(E_-)$,

$$\Gamma(E_-,E_0) = P(E_-)\gamma(E_0) . \tag{4.7}$$

The decomposition (4.7) must be chosen in such a way that it meets the following conditions:

(i) At $E_- = E_0$, the width $\Gamma(E_-,E_0)$ must equal the actual width of the resonance (twice the imaginary part of the pole of the Green's function).

(ii) Condition (4.4) must be fulfilled in order to facilitate the evaluation of various matrix elements; see also Secs. V and VII.

(iii) The reduced width $\gamma(E_0)$ must obey

$$\lim_{E_0 \to -1-0} \gamma(E_0) = 0 . \tag{4.8}$$

This ensures the continuity of the basis wave functions χ_{E_-} and φ_{E_-} at $R = R_{cr}$, Eq. (3.11), as shown in Sec. V. Moreover, the condition,

$$\lim_{E_0 \to -1-0} \left| \frac{\partial}{\partial E_0} [\gamma(E_0)]^{1/2} \right| \neq \infty \tag{4.9}$$

must be met, as otherwise the matrix element $\langle \chi_{E_-} | \dot{\varphi}_r \rangle$ diverges as $R \to R_{cr} - 0$.

Popov *et al.*[10] have introduced the WKB penetrability $P^{(0)}(E_-)$:

$$\begin{aligned} P^{(0)}(E_-) &= \exp\left[-2 \int_{r_{min}}^{r_{max}} dr [1 + \kappa^2 r^{-2} - (E_- + \zeta_u r^{-1})^2]^{1/2} \right] , \\ &= \exp\{ 2\pi \zeta_u [E_- (E_-^2 - 1)^{-1/2} + (1 - \kappa^2 \zeta_u^{-2})^{1/2}] \} . \end{aligned} \tag{4.10}$$

Here $\kappa = \mp(j + \frac{1}{2})$, $\zeta_u = (Z_1 + Z_2)\alpha$, and r_{min}, r_{max} are the zeros of the integrand. This suggests writing

$$\Gamma(E_-,E_0) = P^{(0)}(E_-)\gamma^{(0)}(E_0) . \tag{4.11}$$

The definition (4.11) is not satsifactory, however, since $\gamma^{(0)}(E_0)$ has a finite nonzero limit as $E_0 \to -1-0$, in violation of condition (4.8).

This defect can be remedied by writing the factors on the right-hand side of Eq. (4.7) in the form

$$P(E_-) = P^{(0)}(E_-)(-E_- - 1)^{-n} , \tag{4.12a}$$

$$\gamma(E_0) = \gamma^{(0)}(E_0)(-E_0 - 1)^n , \tag{4.12b}$$

where $n \geq 2$. This choice is consistent with the conditions (i)–(iii) given above if $2 \leq n \lesssim 4$.

We are thus led to the conclusion that the construction of φ_r is possible in more than one way (we note that the construction carried through in Ref. 3 offers yet another possibility). It is shown in the following paper that the ambiguity inherent in the choice of φ_r, while of course not affecting the actual calculated positron production cross section, affects the decomposition of this cross section into contributions labeled[3] "spontaneous" and "induced" positron production.

V. THE MODIFIED CONTINUUM WAVE FUNCTION χ_{E_-}

It is convenient for the following discussion to define a wave function ϕ_{E_-} which includes the resonant phase δ_{E_-}:

$$\phi_{E_-} = \exp(i\delta_{E_-})\varphi_{E_-} , \tag{5.1}$$

where

$$\delta_{E_-} = \arg\left[\left[E_0 + \frac{i}{2}\Gamma(E_-,E_0) - E_- \right]^{-1} \right] . \tag{5.2}$$

The resonance wave function φ_r can be written in terms of ϕ_{E_-} as

$$\varphi_r = \int_{E_c}^{-1} dE_- a_{E_-} \phi_{E_-} , \tag{5.3}$$

where

$$a_{E_-} = \exp(-i\delta_{E_-}) A_{E_-} = \left[\frac{\Gamma(E_-,E_0)}{2\pi}\right]^{1/2} \left[E_0 - \frac{i}{2}\Gamma(E_-,E_0) - E_-\right]^{-1} . \tag{5.4}$$

Putting

$$\chi_{E_-} = \int_{E_c}^{-1} dE'_- b_{E_-,E'_-} \phi_{E'_-} , \tag{5.5}$$

we obtain the coefficient b_{E_-,E'_-} from Eq. (3.7):

$$b_{E_-,E_-E'} = \delta(E_- - E'_-) - \frac{a_{E'_-}}{E_- - E'_- - i\epsilon} V_{E_-} \tag{5.6}$$

where

$$V_{E_-} = \langle \varphi_r | H(R) | \chi_{E_-} \rangle \tag{5.7a}$$

$$= \begin{cases} a^*_{E_-} \Big/ \int_{E_c}^{-1} dE'_- \dfrac{|a_{E'_-}|^2}{E_- - E'_- - i\epsilon} \approx -\left[\dfrac{\Gamma(E_-,E_0)}{2\pi}\right]^{1/2} & (E_c < E_- < -1) , \quad (5.7b) \\ 0 \quad (E_- < E_c) . & (5.7c) \end{cases}$$

In calculating the coefficient b_{E_-,E'_-} [Eq. (5.6)], we replaced $\varphi^{(+)}_{E_-}$ in Eq. (3.7) by ϕ_{E_-}. However, since the relation between $\chi^{(+)}_{E_-}$ and $\varphi^{(+)}_{E_-}$ is linear, χ_{E_-} determined by Eqs. (5.5) and (5.6) differs from $\chi^{(+)}_{E_-}$ only by a phase factor. The radial wave function of χ_{E_-} is (approximately) real as can be seen from Eq. (5.7b).

In obtaining Eq. (5.7b), we used approximations under the integral such as

$$\begin{aligned} & f(\Gamma(E'_-,E_0))(E_- - E'_- - i\epsilon)^{-1} \approx f(\Gamma(E_-,E_0))(E_- - E'_- - i\epsilon)^{-1} , \\ & f(\Gamma(E'_-,E_0)) \left[E_0 - \frac{i}{2}\Gamma(E'_-,E_0) - E'_-\right]^{-1} \approx f(\Gamma(E_0,E_0)) \left[E_0 - \frac{i}{2}\Gamma(E'_-,E_0) - E'_-\right]^{-1} , \end{aligned} \tag{5.8}$$

where $f(\Gamma)$ is a function of Γ, and we extended the range of the integral to infinity. The first approximation preserves the threshold behavior of V_{E_-}, i.e., $V_{E_-} \to 0$ for $E_- \to -1-0$. The error associated with the increase of the integration range is less than 1% if the energy E_- remains in the interval $E_c + 0.01 < E_- < -1.01$, i.e., E_- is not very close to the boundaries of the integral. We also neglected

$$\left| \frac{\Gamma(E_-,E_0) - \Gamma(E_0,E_0)}{E_0 - \frac{i}{2}\Gamma(E_-,E_0) - E_-} \right|$$

compared with 1. All these approximations are justified if condition (4.4) is met.

It should be noted that while the "spontaneous coupling" matrix element Eq. (5.7) has the definite value $-[\Gamma^{(0)}(E_0,E_0)/2\pi]^{1/2}$ at the resonance energy, the off-resonance value is to some extent arbitrary, depending on the choice made for $P(E_-)$ in Eqs. (4.12). This arbitrariness in the off-resonance continuation of V_{E_-} is the reason why an unambiguous decomposition of the transition amplitude into a "spontaneous" and an "induced" part is not possible. It can also be seen that, because of Eqs. (4.12), V_{E_-} tends to zero as $E_0 \to -1-0$. Equation (5.4) shows that a_{E_-} has a vanishing limit, too. Hence, b_{E_-,E'_-} tends to $\delta(E_- - E'_-)$, and we obtain a continuity relation, using Eqs. (5.1), (5.2), and (5.5),

$$\lim_{R\to R_{\rm cr}-0}\chi_{E_-}(\vec{r},R)=\lim_{R\to R_{\rm cr}+0}\varphi_{E_-}(\vec{r},R)\ . \quad (5.9)$$

The functions χ_{E_-} obviously do not contain the resonance. We expect that the matrix elements involving these functions will depend smoothly on energy. This expectation is borne out by Eq. (5.7b) and the equations given in Sec. VII.

VI. THE COUPLED EQUATIONS FOR THE OCCUPATION AMPLITUDES. CALCUATION OF OBSERVABLES

We expand the wave function $\psi(\vec{r},t)$ in Eq. (2.1) as Eq. (2.8) but replace for $R(t)<R_{\rm cr}$ the lowest bound state φ_0 by the resonance state φ_r, and φ_{E_-} by χ_{E_-}:

$$\psi(\vec{r},t)=\int_1^\infty dE_+ c_{E_+}(t)\exp[-i\theta_{E_+}(t)]\varphi_{E_+}(\vec{r},R(t))+\sum_{n\geq 1}c_n(t)\exp[-i\theta_n(t)]\varphi_n(\vec{r},R(t))$$
$$+c_0(t)\exp[-i\theta_0(t)]\varphi_r(\vec{r},R(t))+\int_{-\infty}^{-1}dE_- c_{E_-}(t)\exp[-i\theta_{E_-}(t)]\chi_{E_-}(\vec{r},R(t))\ . \quad (6.1)$$

Because of the continuity of the basis states at $R(t)=R_{\rm cr}$, Eqs. (3.1) and (5.9), the expansion coefficients in Eq. (6.1) are also continuous at $R_{\rm cr}$. Putting the expression for $\psi(\vec{r},t)$ of Eq. (6.1) into the Dirac equation, Eq. (2.1), we obtain a set of coupled differential equations for $R(t)<R_{\rm cr}$:

$$\dot{c}_E=-\mathop{\mathcal{S}}_{E'\geq E_1}\langle\varphi_E\,|\,\dot{\varphi}_{E'}\rangle\exp[i(\theta_E-\theta_{E'})]c_{E'}-\langle\varphi_E\,|\,\dot{\varphi}_r\rangle\exp[i(\theta_E-\theta_0)]c_0$$
$$-\int_{-\infty}^{-1}dE'_-\langle\varphi_E\,|\,\dot{\chi}_{E'_-}\rangle\exp[i(\theta_E-\theta_{E'_-})]c_{E'_-}\quad(E\geq E_1)\ ,$$
$$\dot{c}_0=-\mathop{\mathcal{S}}_{E'\geq E_1}\langle\varphi_r\,|\,\dot{\varphi}_{E'}\rangle\exp[i(\theta_0-\theta_{E'})c_{E'}-\int_{-\infty}^{-1}dE'_-(\langle\varphi_r\,|\,\dot{\chi}_{E'_-}\rangle+iV_{E'_-})\exp[i(\theta_0-\theta_{E'_-})]c_{E'_-}\ , \quad (6.2)$$
$$\dot{c}_{E_-}=-\mathop{\mathcal{S}}_{E'\geq E_1}\langle\chi_{E_-}\,|\,\dot{\varphi}_{E'}\rangle\exp[i(\theta_{E_-}-\theta_{E'})]c_{E'}-(\langle\chi_{E_-}\,|\,\dot{\varphi}_r\rangle+iV^*_{E_-})\exp[i(\theta_{E_-}-\theta_0)]c_0$$
$$-\int_{-\infty}^{-1}dE'_-\langle\chi_{E_-}\,|\,\dot{\chi}_{E'_-}\rangle\exp[i(\theta_{E_-}-\theta_{E'_-})]c_{E'_-}\ .$$

Comparing Eqs. (6.2) with Eqs. (2.10), we observe that the only difference between the two sets resides—aside from the actual *value* of E_0—in the occurrence of the matrix element V_{E_-} defined in Eq. (5.7). This matrix element describes the spontaneous decay of the resonance φ_r into the positron continuum which happens without external field. Whether or not the "diving" of the state into the positron continuum makes a qualitative difference for positron production will depend on the relative importance of the matrix elements $\langle\varphi_r\,|\,\dot{\chi}_{E_-}\rangle$ and V_{E_-}.

Let $c_{E_i,E}(t)$ denote the coefficients $c_E(t)$ which satisfy Eq. (2.10) for $R(t)\geq R_{\rm cr}$ and Eq. (6.2) for $R(t)<R_{\rm cr}$ [joined smoothly at $R(t)=R_{\rm cr}$], and the initial condition

$$c_{E_i,E}(-\infty)=\delta_{E_i,E}\ , \quad (6.3)$$

where $\delta_{E_i,E}$ should be interpreted as $\delta(E_i-E)$ if $|E_i|>1$. The coefficients $c_{E_i,E}(t)$ $(-\infty<E_i,E<+\infty)$ provide a complete description of the solution of the one-body Dirac equation, Eq. (2.1). If the initial condition of a many-electron system is such that all the states below a Fermi level E_F are occupied, then the probability density to find a positron of energy E_- at time $t\to+\infty$ is given by[3,5,6]

$$\frac{dP_{e^+}}{dE_-}=\mathop{\mathcal{S}}_{E_i>E_F}|c_{E_i,E_-}(+\infty)|^2\ , \quad (6.4)$$

which can be rewritten in the case of a symmetric trajectory $R(t)=R(-t)$ as

$$\frac{dP_{e^+}}{dE_-}=\mathop{\mathcal{S}}_{E_f>E_F}|c_{E_-,E_f}(+\infty)|^2\ . \quad (6.5)$$

The evaluation of the positron probability dP_{e^+}/dE_- given in Eq. (6.4) can be simplified even if the trajectory is not symmetric. Let $\tilde{c}_{E,E_f}(t)$ denote the coefficients $c_E(t)$ which satisfy Eq. (2.10) for $R(t)\geq R_{\rm cr}$ and Eq. (6.2) for $R(t)<R_{\rm cr}$ [joined smoothly at $R(t)=R_{\rm cr}$] and the "final" condition

$$\tilde{c}_{E,E_f}(+\infty)=\delta_{E,E_f}\ . \quad (6.6)$$

Then the following relation holds:

$$c_{E_i,E_f}(+\infty)=\tilde{c}^{*}_{E_i,E_f}(-\infty)\ , \tag{6.7}$$

because both terms are equal to

$$\lim_{\substack{t\to-\infty\\ t'\to+\infty}} \langle \exp[-i\theta_{E_f}(t')]\varphi_{E_f}(R(t'))\,|\,U(t',t)\,| \times\exp[-i\theta_{E_i}(t)]\varphi_{E_i}(R(t))\rangle\ , \tag{6.8}$$

where $U(t',t)$ is a time evolution operator in the Schrödinger picture:

$$U(t',t)=T\int_t^{t'} dt''\exp[-iH(R(t''))] \tag{6.9}$$

with T denoting a time ordering. Using the new coefficients $\tilde{c}$, we can rewrite Eq. (6.4) as

$$\frac{dP_{e^+}}{dE_-}=\sum_{E_i>E_f} |\tilde{c}_{E_i,E_-}(-\infty)|^2\ . \tag{6.10}$$

In order to obtain $c_{E_-,E_f}(+\infty)$ [or $\tilde{c}_{E_i,E_-}(-\infty)$] for a given E_-, we have to solve the coupled differential equations forward (or backward) in time only once because E_- in these coefficients can be viewed as specifying the initial (or "final") condition. Intuitively speaking, we solve the Dirac equation backward in time because we ask: If there is a positron at energy E_- and at $t=+\infty$, from which levels could it have come? Summing up the answer over those levels which were empty at time $t=-\infty$ we find the desired result. Equations (6.5) or (6.10) are obviously useful for practical calculations.

VII. ANALYTICAL EVALUATION OF THE MATRIX ELEMENTS

In this section we express the matrix elements of the radial derivative operator $\partial/\partial R$ in terms of those of $\partial H/\partial R$ between unmodified basis states.

The matrix elements of the time derivative operator $\partial/\partial t$ which appear in Eqs. (2.10) and (6.2) are obtained by multiplying them by $\partial R(t)/\partial t$. Taking the matrix element of the commutator $[\partial/\partial R,H(R)]$ between the states φ_E and $\varphi_{E'}$, one finds

$$\left\langle\varphi_E\left|\frac{\partial}{\partial R}\right|\varphi_{E'}\right\rangle=\frac{\mathscr{P}}{E'-E}\left\langle\varphi_E\left|\frac{\partial H}{\partial R}\right|\varphi_{E'}\right\rangle\ , \tag{7.1}$$

where $\mathscr{P}$ indicates that a principal part should be taken upon integration. A possible additional term proportional to $\delta(E-E')$ does not arise because the radial wave function in φ_E was chosen to be real. If the wave function ϕ_{E_-} defined by Eq. (5.1) is used, the term $i(\partial\delta_{E_-}/\partial R)\delta(E_--E'_-)$ should be added to the right-hand side of Eq. (7.1). The matrix element of $\partial H/\partial R$ is easily calculated in the monopole approximation:

$$\left\langle\varphi_E\left|\frac{\partial H}{\partial R}\right|\varphi_{E'}\right\rangle=\int_0^{r_{\max}} dr\frac{\partial V(r,R)}{\partial R}(F_EF_{E'}+G_EG_{E'})\ , \tag{7.2}$$

where F_E and G_E are radial wave functions of φ_E multiplied by r, and $r_{\max}$ equals R_{1+} or R_{2+}, whichever is larger.

Matrix elements of $\partial/\partial R$ which involve the resonance wave function φ_r and/or the modified negative energy continuum wave functions χ_{E_-} are obtained in the Secs. VII A–VII C. We use the approximation of omitting terms which are relatively small of order $P(E_-)$, $E_c\le E_-\le -1$. We also use the fact that φ_r has real radial wave functions. This implies

$$\left\langle\varphi_r\left|\frac{\partial}{\partial R}\right|\varphi_r\right\rangle=0\ . \tag{7.3}$$

A. $\left\langle\chi_{E_-}\left|\frac{\partial}{\partial R}\right|\chi_{E'_-}\right\rangle$ and $\left\langle\chi_{E_-}\left|\frac{\partial}{\partial R}\right|\varphi_r\right\rangle (E_c<E_-,E'_-<-1)$

Using the steps which lead to Eq. (7.1), we find

$$\left\langle\chi_{E_-}\left|\frac{\partial H}{\partial R}\right|\chi_{E'_-}\right\rangle=(E'_--E_-)\left\langle\chi_{E_-}\left|\frac{\partial}{\partial R}\right|\chi_{E'_-}\right\rangle+V_{E'_-}\left\langle\chi_{E_-}\left|\frac{\partial}{\partial R}\right|\varphi_r\right\rangle-V^{*}_{E_-}\left\langle\varphi_r\left|\frac{\partial}{\partial R}\right|\chi_{E'_-}\right\rangle\ , \tag{7.4}$$

$$\left\langle\chi_{E_-}\left|\frac{\partial H}{\partial R}\right|\varphi_r\right\rangle=(E_0-E_-)\left\langle\chi_{E_-}\left|\frac{\partial}{\partial R}\right|\varphi_r\right\rangle+\frac{\partial V^{*}_{E_-}}{\partial R}+\int_{E_c}^{-1} dE'_-V^{*}_{E'_-}\left\langle\chi_{E_-}\left|\frac{\partial}{\partial R}\right|\chi_{E'_-}\right\rangle\ . \tag{7.5}$$

Contributions to matrix elements of $\partial H/\partial R$ come only from the region $0\le r\le r_{\max}$, and $r_{\max}$ is smaller than $\sim$25 fm for U + U when there is a resonance at all. Therefore, $\langle\chi_{E_-}\,|\,\partial H/\partial R\,|\,\varphi_r\rangle$ is of order $[P(E_{E_-})]^{1/2}$

(since $\chi_{E\_}$ by construction does not contain the resonance wave function), and Eq. (7.5) shows that $\langle \chi_{E\_} \mid \partial/\partial R \mid \varphi_r \rangle$ itself is also of order $[P(E\_)]^{1/2}$. Using this in Eq. (7.4), we see that $\langle \chi_{E\_} \mid \partial/\partial R \mid \chi_{E'\_} \rangle$ is of order $P(E\_)P(E'\_)^{1/2}$ which in turn implies that the last term in Eq. (7.5) is relatively small of order $P(E\_)$. Hence,

$$\left\langle \chi_{E\_} \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle \approx \frac{\mathscr{P}}{E_0 - E\_} \left[\left\langle \chi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle - \frac{\partial V^*_{E\_}}{\partial R} \right] . \tag{7.6}$$

Using Eqs. (5.5) and (5.6) for $\chi_{E\_}$, we obtain

$$\left\langle \chi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle = \left\langle \phi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle - V^*_{E\_} \int_{E_c}^{-1} dE'\_ \frac{a^*_{E'\_}}{E\_ - E'\_ + i\epsilon} \left\langle \phi_{E'\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle . \tag{7.7}$$

The weight function $a^*_{E'\_}$ in Eq. (7.7) is peaked at the resonance energy. Therefore, the approximation $\phi_{E'\_} \approx a^*_{E'\_} \varphi_r$ is expected to be extremely good under the integral. This yields

$$\left\langle \chi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle \approx \left\langle \phi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle - a_{E\_} \left\langle \varphi_r \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle \approx \left\langle \phi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle - a_{E\_} \frac{\partial E_0}{\partial R} . \tag{7.8}$$

The last equality is obtained in the same way as Eqs. (7.4) and (7.5). Altogether, this yields

$$\left\langle \chi_{E\_} \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle \approx \frac{\mathscr{P}}{E_0 - E\_} \left[\left\langle \phi_{E\_} - a^*_{E\_} \varphi_r \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle - \frac{\partial V^*_{E\_}}{\partial R} \right] . \tag{7.9}$$

Equation (7.9) shows explicitly that aside from a principal value singularity which does not contribute because of the slow change of the phase factors and the occupation amplitudes multiplying it in Eq. (6.2), $\langle \chi_{E\_} \mid \partial/\partial R \mid \varphi_r \rangle$ is a smooth function of energy, and is small of order $[P(E\_)]^{1/2}$. In the limit $E_0 \to -1$, we have $a_{E\_} \to 0$ and

$$\left\langle \chi_{E\_} \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle \to \frac{1}{E_0 - E\_} \left[\left\langle \varphi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_0 \right\rangle - \lim_{E_0 \to -1} \frac{\partial V^*_{E\_}}{\partial R} \right] . \tag{7.10}$$

This expression coincides with

$$\left\langle \varphi_{E\_} \left| \frac{\partial}{\partial R} \right| \varphi_0 \right\rangle = \frac{1}{E_0 - E\_} \left\langle \varphi_{E\_} \left| \frac{\partial H}{\partial R} \right| \varphi_0 \right\rangle , \tag{7.11}$$

because

$$\lim_{E_0 \to -1} \frac{\partial V^*_{E\_}}{\partial R} = 0 , \tag{7.12}$$

if the value of n defined in Eq. (4.12) is chosen to be larger than 2. When n is just equal to 2, however, the limit of $\partial V^*_{E\_}/\partial R$ does not vanish so that the two expressions (7.10) and (7.11) are discontinuous at $R = R_{cr}$. This simply means that the *derivatives* of the basis states $\chi_{E\_}(\vec{r},R)$ and $\varphi_{E\_}(\vec{r},R)$ with respect to R are discontinuous at $R = R_{cr}$ for $n = 2$ although the basis states themselves are continuous. It should be noted that such discontinuity of the derivative of basis states causes no difficulty at all.

In an analogous fashion, we obtain from Eq. (7.4)

$$\left\langle \chi_{E_-} \left| \frac{\partial}{\partial R} \right| \chi_{E'_-} \right\rangle \approx \frac{\mathscr{P}}{E'_- - E_-} \left[\left\langle \phi_{E_-} - a^*_{E_-} \varphi_r \left| \frac{\partial H}{\partial R} \right| \phi_{E'_-} - a^*_{E'_-} \varphi_r \right\rangle \right.$$
$$+ V_{E'_-} \frac{\mathscr{P}}{E_- - E_0} \left[\left\langle \phi_{E_-} - a^*_{E_-} \varphi_r \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle - \frac{\partial V^*_{E_-}}{\partial R} \right]$$
$$\left. + V^*_{E_-} \frac{\mathscr{P}}{E'_- - E_0} \left[\left\langle \varphi_r \left| \frac{\partial H}{\partial R} \right| \phi_{E'_-} - a^*_{E'_-} \varphi_r \right\rangle - \frac{\partial V_{E'_-}}{\partial R} \right] \right] . \tag{7.13}$$

It is again obvious that the matrix element is smooth in E_-, E'_-. In the limit $E_0 \to -1$, we have $a^*_{E_-} \to 0$, $V_{E_-} \to 0$, and therefore

$$\left\langle \chi_{E_-} \left| \frac{\partial}{\partial R} \right| \chi_{E'_-} \right\rangle \to \frac{\mathscr{P}}{E'_- - E_-} \left\langle \varphi_{E_-} \left| \frac{\partial H}{\partial R} \right| \varphi_{E'_-} \right\rangle , \tag{7.14}$$

as it should. We also observe that $\langle \chi_{E_-} | \partial / \partial R | \chi_{E'_-} \rangle$ is of order $[P(E_-)P(E'_-)]^{1/2}$.

B. $\left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle$ ($E < E_c$ or $E > -1$)

We proceed as in the derivation of Eqs. (7.4) and (7.5) and obtain

$$\left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle = (E_0 - E) \left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle + \int_{E_c}^{-1} dE'_- V^*_{E'_-} \left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \chi_{E'_-} \right\rangle . \tag{7.15}$$

It is shown below that $\langle \varphi_E | \partial / \partial R | \chi_{E'_-} \rangle$ is of order $[P(E'_-)]^{1/2}$. The last term in Eq. (7.15) is therefore relatively small of order $P(E_-)$ ($E_c < E_- < -1$) and is omitted. This gives

$$\left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \chi_{E_-} \right\rangle = \left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \phi_{E_-} \right\rangle - V_{E_-} \int_{E_c}^{-1} dE'_- \frac{a_{E'_-}}{E_- - E'_- - i\epsilon} \left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \phi_{E'_-} \right\rangle , \tag{7.18}$$

where Eqs. (5.5) and (5.6) for χ_{E_-} were used. The approximation $\phi_{E'_-} \approx a^*_{E'_-} \varphi_r$ under the integral which was used to obtain Eq. (7.8) in Sec. VII A yields

$$\left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle \approx \frac{1}{E_0 - E} \left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle . \tag{7.16}$$

The form of Eq. (7.16) is the same for a bound-state wave function φ_0. In the limit $E_0 \to -1$, it exactly coincides with this form. The neglect of the last term in Eq. (7.15) is consistent with the neglect of the level shift, i.e., the difference $E_r - E_0$ in Sec. IV, which is also relatively small of order $P(E_0)$.

C. $\left\langle \phi_E \left| \frac{\partial}{\partial R} \right| \chi_{E_-} \right\rangle$ ($E < E_c$ or $E > -1$; $E_c < E_- < -1$)

Evaluating the commutator $[\partial / \partial t, H(R(t))]$ between the states φ_E and ϕ_{E_-}, we obtain

$$\left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \chi_{E_-} \right\rangle = \frac{1}{E_- - E} \left[\left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \chi_{E_-} \right\rangle - V_{E_-} \left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \varphi_r \right\rangle \right] . \tag{7.17}$$

The matrix element of $\partial H / \partial R$ on the right-hand side is given as

$$\left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \chi_{E_-} \right\rangle \approx \left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \varphi_{E_-} \right\rangle - \left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle a^*_{E_-} . \tag{7.19}$$

Putting Eqs. (7.16) and (7.19) into Eq. (7.17), we obtain finally

$$\left\langle \varphi_E \left| \frac{\partial}{\partial R} \right| \chi_{E_-} \right\rangle \approx \frac{1}{E_0 - E} \left[\left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \phi_{E_-} - a^*_{E_-} \varphi_r \right\rangle - \frac{V_{E_-}}{E_0 - E} \left\langle \varphi_E \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle \right]. \tag{7.20}$$

The matrix element $\langle \varphi_E \mid \partial/\partial R \mid \chi_{E_-} \rangle$ is obviously of order $[P(E_-)]^{1/2}$; this fact was used in Sec. VII B. For $E_0 \to -1$, we find that

$$\langle \varphi_E \mid \partial/\partial R \mid \chi_{E_-} \rangle \to (E_- - E)^{-1} \langle \varphi_E \mid \partial H/\partial R \mid \varphi_{E_-} \rangle$$

as it should.

In order to complete the description of the present method, we finally mention how to calculate the matrix elements $\langle \varphi_r \mid \partial H/\partial R \mid \varphi_E \rangle$ and $\langle \varphi_r \mid \partial H/\partial R \mid \varphi_r \rangle$. These are evaluated by using the approximation $\phi_{E'_-} \approx a^*_{E'_-} \varphi_r$ under integration as follows:

$$\left\langle \varphi_r \left| \frac{\partial H}{\partial R} \right| \varphi_E \right\rangle \approx \int_{E_c}^{-1} dE'_- a^*_{E'_-} (a_{E'_-}/a_{E_0}) \left\langle \phi_{E_0} \left| \frac{\partial H}{\partial R} \right| \varphi_E \right\rangle ,$$

$$\approx \left\langle \phi_{E_0} \left| \frac{\partial H}{\partial R} \right| \varphi_E \right\rangle / a_{E_0} , \tag{7.21a}$$

$$\left\langle \varphi_r \left| \frac{\partial H}{\partial R} \right| \varphi_r \right\rangle \approx \left\langle \phi_{E_0} \left| \frac{\partial H}{\partial R} \right| \phi_{E_0} \right\rangle / |a_{E_0}|^2 , \tag{7.21b}$$

where in Eq. (7.21b) the approximation is used twice.

The central results of this section are the Eqs. (7.9), (7.13), (7.16), and (7.20).

VIII. SUMMARY

We have presented an analytical approach to treat the resonance which appears in the positron continuum during a collision between very heavy ions. By introducing a square-integrable resonance wave function φ_r and the modified positron continuum χ_{E_-} which does not contain the resonance, we succeeded in handling the resonance analytically and explicitly in all the formulas given. Our procedure is, in a sense, the inverse of the Dirac-Fano method[9] of handling quasibound states. In the case of the Dirac equation for supercritical atoms, we are *given* a resonance and look for the definition of a modified Hamiltonian such that φ_r appears as a quasibound state. In constructing φ_r and χ_{E_-}, we paid due attention to proper threshold behavior ($E_- \to 1$) of all relevant quantities and ascertained that the matrix elements which appear in the coupled equations (6.2) are easily calculable, and have the right limit as the resonance energy $E_0 \to -1$. Moreover, these matrix elements are smooth functions of energy and internuclear distance aside from a principal value singularity, which does not contribute to the observable quantities. Therefore, the coupled equations (6.2) can easily be solved, and the influence of the resonance on the production cross section for positrons can be studied in detail. Numerical calculations along these lines are given in the following paper by one of us (T.T.). Since the resonance width off the resonance energy involves some arbitrariness, a unique decomposition of the production amplitude for positrons into an "induced" and a "spontaneous" term cannot be given. The consequences of this ambiguity for the interpretation of positron spectra are also investigated in the following paper.

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