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QUANTUM MECHANICAL THEORY OF POSITRON PRODUCTION
IN HEAVY ION COLLISIONS WITH NUCLEAR CONTACT

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ABSTRACT

The interplay between atomic and nuclear interactions in heavy ion collisions with nuclear contact is studied. The general theoretical description is outlined and analyzed in a number of different limits (semiclassical approximation, DWBA, fully quantal description). The two most important physical mechanisms for generating atomic-nuclear interference, i.e., energy conservation and the introduction of additional phase shifts by nuclear reactions, are extracted. The resulting typical coupling matrix elements are analyzed for their relative importance in atomic and nuclear excitations. The description of nuclear influence on atomic excitations in terms of a classical time delay caused by nuclear reactions is reviewed, and its relationship to the underlying quantal character of the nuclear reaction is discussed.

The theory is applied to spontaneous positron emission in supercritical heavy-ion collisions ($Z_{\text{tot}} \geq 173$). It is shown that nuclear contact can lead to line structures in the positron energy spectra if the probability distribution for nuclear delay times caused by the contact has contributions for $T \geq 10^{-19}$ sec. We explicitly evaluate a model where a pocket in the internuclear potential near the touching configuration leads to formation of nuclear molecules, and predict a resonance-like excitation function for the positron peak.

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The theory is applied to spontaneous positron emission in supercritical heavy-ion collisions ($Z_{\text{tot}} \gtrsim 173$). It is shown that nuclear contact can lead to line structures in the positron energy spectra if the probability distribution for nuclear delay times caused by the contact has contributions for $T \gtrsim 10^{-19}$ sec. We explicitly evaluate a model where a pocket in the internuclear potential near the touching configuration leads to formation of nuclear molecules, and predict a resonance-like excitation function for the positron peak.

INTRODUCTION

Heavy ion collisions with nuclear contact recently have developed into an increasingly effective tool to study phenomena in a regime where nuclear and atomic excitations occur simultaneously and therefore interfere with each other. One example for this type of phenomena which has recently been the subject of particularly intensive investigations is the emission of spontaneously created positrons in supercritical ($Z_1 + Z_2 > 173$) heavy ion collisions at energies close to the Coulomb barrier. When the first peak structures were found in positron spectra from U+U, U+Th and U+Cm collisions (Schweppe et al. 1983, Clemente et al. 1984), it was attempted to interpret them as spontaneous positrons emitted from a longlived nuclear composite formed in the nuclear collision as a consequence of nuclear interactions at contact (Rafelski et al. 1978, Reinhardt et al. 1981b, U. Müller et al. 1983, Heinz et al. 1983a, 1984). Although this explanation has subsequently been excluded by the non-observance of the predicted shift with the combined

nuclear charge of the energy at which the positron line occurs (Cowan et al. 1985, Tsertos et al. 1985), there is still some evidence that the appearance of the line structures (which now have been observed in many more, even subcritical systems, see talks at this conference by Bokemeyer, Cowan, Kienle, König, and Kozhuharov) is connected in a sensitive way with the ion beam energy which has to be chosen close to the Coulomb barrier to see the peaks. A likely explanation is that nuclear contact or nuclear interactions play at least some role in the excitation mechanism for these peak structures.

This has implications for the theoretical description, because the usual picture of two ions moving on classical trajectories, and thereby providing a time-dependent Coulomb field leading to atomic excitations, is only valid for well separated nuclei; it generally breaks down if the nuclei touch, allowing the short-range nuclear interactions to modify the nuclear scattering process. In the semiclassical framework their effects may be accounted for heuristically by introducing by hand a classical time delay supposed to be caused by the nuclear interaction; but the validity of this procedure is not obvious, and the value of the time delay to be chosen is an essentially free parameter, where, in principle, it should be determined by the character of the nuclear interactions.

For this reason I will review in this lecture the general quantum mechanical treatment of heavy-ion collisions and the relation to the semiclassical picture. In a strict sense this is the formalism underlying all theoretical calculations shown at this conference. I will show that under a factorization assumption for the atomic and nuclear excitations, which in many practically relevant cases can be justified, the simple semiclassical theory can be used even when nuclear contact occurs; one only has to ensure that a probability distribution for classical nuclear delay times is used which is consistent with the underlying quantum mechanical nuclear scattering amplitude. I will show how to generally derive this classical delay time distribution from the nuclear S-matrix, and present a specific model where this relationship between quantum mechanics and the semiclassical approximation can be worked out semi-analytically. The model describes nuclear scattering through molecular resonances which are supported by a pocket in the internuclear potential at touching distance; the resulting probability distribution of classical delay times has contributions for large times $T \geq 10^{-19}$ sec which lead to formation of a pronounced peak in the positron energy spectrum in supercritical collisions due to spontaneous positron emission. Although I do no longer propose this model as an explanation for the observed line structures, it is instructive to see the basic mechanisms at work, particularly since nuclear interactions may still have some role in the occurrence of these experimentally discovered peaks.

In my presentation I will mostly follow the treatment given in Heinz et al. (1983a, 1984). The field is also reviewed in Heinz (1986), where a more complete set of references can be found.

THE THEORETICAL FRAMEWORK

This chapter lays out the general theoretical description of ion-atom or ion-ion scattering events, starting from a completely quantum mechanical treatment of both nuclear and atomic degrees of freedom. Subsequently, different approximation schemes to the full theory are discussed, recovering the known results for several limiting cases, particularly the semiclassical theory which uses classical time-dependent nuclear trajectories.

Nuclear and atomic excitations will be treated on the same footing as far as possible. However, the nuclear dynamics will always be treated non-relativistically, and the theory is not second quantized, i.e., we work with

wavefunctions instead of Fock states. The second quantized descriptor, although conceptually preferable and possible in the semiclassical theory (Reinhardt and Greiner 1977), has not yet been extended to include nuclear excitations.

The Scattering Problem

We face the following problem of stationary scattering theory: our total system is an eigenstate with eigenvalue E of the total energy:

$$H_{\text{tot}} \Psi_E(\vec{R}, \vec{r}, \vec{x}, \vec{\xi}) = E \Psi_E(\vec{R}, \vec{r}, \vec{x}, \vec{\xi}). \quad (1)$$

$\vec{R}$ is the internuclear distance, $\vec{r}$ ($\vec{x}$) is the set of electronic (photon) coordinates in the nuclear center of mass (CMN) system, and $\vec{\xi}$ are internal nuclear coordinates (possibly collective coordinates) (Fig.1). The Hamiltonian of the total energy is given by

$$\begin{aligned} H_{\text{tot}} = & \frac{\vec{P}^2}{2\mu} + V_C(R) + V_N(R) \\ & + \sum_{i=1}^Z H_{\text{TCD}}^{(i)}(\vec{r}, \vec{R}) + \frac{1}{2M_N} \left(\sum_{i=1}^Z \vec{p}_i \right)^2 + \frac{1}{2} \sum_{i \neq j}^Z v^{ee}(r_{ij}) \\ & + \sum_{m=1}^A H_{\text{int}}^{(m)}(\vec{\xi}, \vec{R}) + H_{\text{rad}}(\vec{x}, \vec{\xi}, \vec{r}, \vec{R}). \end{aligned} \quad (2)$$

$\vec{P}$ is the relative momentum of the two nuclei; μ (M_N) is their reduced (combined) mass; $V_C(R)$ is the Coulomb potential between the nuclei; $V_N(R)$ is some nuclear optical potential to be specified later; $H_{\text{TCD}}^{(i)}$ is the two-center Dirac Hamiltonian for a single electron i containing the electron kinetic energy and the interaction with the two nuclei; the next term is the energy contained in a possible collective motion of the complete electron cloud with respect to the CMN; $v^{ee}(r_{ij})$ is the interaction between electron i and j ($r_{ij} = |\vec{r}_i - \vec{r}_j|$). The second to last term is the internal nuclear Hamiltonian, summed over all degrees of freedom for internal motion. The last term, H_{rad} , is the Hamiltonian for electromagnetic radiation; it depends on nuclear and electronic coordinates since it contains coupling terms of the electromagnetic potential to the nuclear and electronic currents. H_{rad} has to be taken into account for the calculation of X-ray spectra, nuclear bremsstrahlung and internal conversion of nuclear into electron excitations.

In (1), (2) the electron and photon coordinates are measured in the nuclear center of mass frame. For increasing mass asymmetry between the colliding nuclei the CMN moves closer and closer to the heavier collision partner ("target"). Therefore in this case often a coordinate system with origin in the target is used to define the electron coordinates. Since the target frame is not an inertial frame, the transformation from the CMN to this frame gives rise to an additional coupling term describing the target recoil, which for non-relativistic electrons takes the form

$$H_R = \frac{m}{M_T} \vec{r} \cdot \vec{\nabla}_R (V_C(R) + V_N(R)). \quad (3)$$

The generalization to relativistic electrons is discussed by Amundsen (1978).

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FIG. 1. Definition of the coordinates used in (2). A,B denote the two nuclei, CMN their combined center of mass. (X,Y,Z) denote the laboratory-fixed coordinate system. The distance vector $\vec{R}$ between the two nuclei defines the z-axis of the rotating coordinate system. Its orientation with respect to the laboratory system is given by angles θ, ϕ . $\vec{r}_i$ denotes the location of electron i with respect to the nuclear center of mass CMN. The photon coordinates $\vec{x}$ and the internal coordinates $\vec{\xi}$ of the nuclei are not shown in this figure.

Basis Expansion

Of course, nobody wants to numerically integrate the multidimensional Schrödinger equation (1) directly. By choosing basis sets for the photons, electrons, internal nuclear degrees of freedom, and the angular part of the nuclear relative motion, and projecting equation (1) into this basis, a set of coupled differential equations in the internuclear distance R only can be derived. The trick lies in selecting the basis states in such a way that the resulting set of coupled channel equations can be truncated, and that a good approximation is obtained by taking into account only a tractable number of different channels. This implies that for different physical situations different basis sets will prove convenient. This will now be discussed in some detail.

Since photons, once emitted by the system, generally escape without final state interaction, a natural basis for them is provided by plane waves for the electromagnetic vector potential:

$$A_\mu(x) = \sum_{\lambda} \int \frac{d^3k}{(2\pi)^3} \frac{1}{\sqrt{2\omega}} \epsilon_{\mu\lambda}(\vec{k}) e^{-ikx} \equiv \sum_{\lambda} \int \frac{d^3k}{(2\pi)^3} a_{\mu\lambda}(k). \quad (4)$$

Here $x = (t, \vec{x})$ and $k = (\omega, \vec{k})$. $\lambda = 1, 2$ denotes the two transverse polarization directions, and $\epsilon_{\mu\lambda}(\vec{k})$ is the polarization unit vector.

For the nuclear internal degrees of freedom it seems natural to use eigenstates of $\sum_{m=1}^A H_{int}^{(m)}(\vec{\xi}, \vec{R})$. Except for a trivial rotation defined by the orientation of the nuclear distance vector $\vec{R} = (R, \theta, \phi)$, these states only depend on the magnitude of R . The trivial rotation is conveniently disposed of by first rotating the nuclear Hamiltonian by the angle (θ, ϕ) . Let us call the Hamiltonian in the rotating frame $H_{nuc}(\vec{\xi}, \vec{R})$; a set of nuclear basis states is then defined by

$$H_{nuc}(\vec{\xi}, \vec{R}) \chi_N(\vec{\xi}, R) = \epsilon_N(R) \chi_N(\vec{\xi}, R). \quad (5)$$

Examples for possible choices for H_{nuc} are, among many others, the two-center shell model or collective models. The index N of the wavefunction summarizes all the good quantum numbers of the respective model; among these is the projection of the nuclear intrinsic angular momentum on the vector $\vec{R}$; the total intrinsic angular momentum, however, is not a good quantum number for finite separation R .

The choice of the electron basis depends on the mass asymmetry of the scattering system and on the beam energy. For very asymmetric systems (e.g., proton-induced collisions) an atomic basis centered at the target or a superposition of atomic bases centered at both the target and the projectile have been used.

Such an approach is expected to work if the projectile can be considered as a (time-dependent) perturbation on the target and vice versa, and if sharing of electrons between target and projectile can be assumed to be small. This is particularly true at high collision energies. For larger, more symmetric systems and/or low collision energies (i.e. below the Coulomb barrier), the collision happens adiabatically enough that molecular orbitals can be established, at least by the fast moving inner shell electrons, and a molecular basis will be more appropriate.

It is defined by using eigenfunctions of the two-center Hamiltonian given in the second line of (2). If heavy ions ($Z_1 + Z_2 > 100$) are used, relativistic effects are important, and one solves the two-center Dirac equation (Müller et al. 1973, Müller and Greiner 1976). (The small term corresponding to a collective motion of the electron cloud relative to the CMN has so far always been neglected.) Again, like for the nuclear eigenstates, the basis is most conveniently determined in the rotating frame where the states (let us call them $\phi_n(\vec{r}, R)$) only depend on the absolute value of the nuclear distance.

For overcritical systems ($Z_1 + Z_2 > 173$) the negative energy continuum contains one or more resonances from dived electronic bound states. These make the use of exact two-center eigenstates awkward for practical computations. It is then more convenient (Reinhardt et al. 1981a) to project a quasibound state $\tilde{\phi}_R(\vec{r}, R)$, which approximates the resonance due to the dived state, out of the positron energy continuum and to orthogonalize this continuum with respect to this quasibound state, yielding modified positron states $\tilde{\phi}_E(\vec{r}, R)$. Instead of the two-center eigenstates, one then uses this projected basis for negative electron energies. The coupling matrix element $\langle \tilde{\phi}_R | H_{e1} | \tilde{\phi}_E \rangle$, which is now non-zero since the projected basis states are not eigenstates of H_{e1} , is interpreted as the matrix element for the spontaneous decay of a hole in the quasibound state into a continuum positron with energy E_p (Reinhardt et al. 1981a).

Finally, we may also separate the dependence on the direction of $\vec{R}$ by finding the eigenstates of the angular part of $\vec{p}^2/2\mu$ in the rotating

frame. They are found to be given by

$$\mathcal{H}_{M\Lambda}^J(\theta, \phi) = (-1)^\Lambda \sqrt{\frac{2J+1}{4\pi}} d_{M\Lambda}^J(\theta) e^{iM\phi} = (-1)^\Lambda \sqrt{\frac{2J+1}{4\pi}} D_{M\Lambda}^J(0, \theta, \phi), \quad (6)$$

where θ and ϕ are the angles of $\vec{R}$ in the laboratory frame. The rotation matrices in (6) are interpreted as those responsible for a rotation of a state of total angular momentum J and projection Λ onto the internuclear axis $\vec{R}$ (the latter is given by the sum of the projections on $\vec{R}$ of the intrinsic electron, photon, and nuclear angular momenta) into the laboratory frame, where the total angular momentum has projection M onto the beam axis.

Consider now having chosen such a set of basis states:

$$|\alpha\rangle \equiv |J M n \mu k \Lambda\rangle \equiv \mathcal{H}_{M\Lambda}^J(\theta, \phi) [\phi_n(\vec{r}, R) \chi_N(\vec{\xi}, R) a_\mu(k)]_\Lambda. \quad (7)$$

[Λ is the total projection of all intrinsic angular momenta (nuclei, electrons, and photons) on $\vec{R}$.]

The total wavefunction Ψ_E in (1) is then expanded into this basis as

$$\Psi_E(\vec{R}, \vec{r}, \vec{x}, \vec{\xi}) = \sum_{\beta} C_{\beta} \frac{F_{\beta}(R)}{R} |\beta\rangle. \quad (8)$$

The functions $F_{\beta}(R)$ describe the dynamics of the internuclear distance R in the different channels β . The constants C_{β} reflect the initial boundary conditions for the relative motion: a detailed derivation of C_{β} is given in Blair and Anholt (1982) for an atomic basis and in Heinz et al. (1983a) for a molecular electron basis.

Coupled Channel Equations for the Nuclear Relative Motion

Inserting the expansion (8) into (1) and projecting onto the basis states $\langle\alpha|$, a set of coupled differential equations for the radial functions $R_{\alpha}(r) \equiv C_{\alpha} F_{\alpha}(R)$ is derived:

$$\begin{aligned} & \left\{ \frac{d^2}{dR^2} - \frac{J(J+1) - \Lambda^2}{R^2} + \frac{2\mu}{\hbar^2} [E - V_C(R) - V_N(R) - \epsilon_{\alpha}(R)] \right\} R_{\alpha}(R) = \\ & = -2 \sum_{\beta \neq \alpha} \langle \alpha | \partial / \partial R | \beta \rangle \frac{dR_{\beta}(R)}{dR} + \frac{2\mu}{\hbar^2} \sum_{\beta \neq \alpha} \langle \alpha | H_{e1} + H_{nuc} + H_{rad} | \beta \rangle R_{\beta}(R) \\ & + \frac{2\mu}{\hbar^2} \sum_{\beta \neq \alpha} Q_{\alpha\beta} R_{\beta}(R). \end{aligned} \quad (9)$$

Since the diagonal contribution

$$\epsilon_{\alpha}(R) \equiv \langle \alpha | H_{e1} + H_{nuc} + H_{rad} | \alpha \rangle \equiv \epsilon_n(R) + \epsilon_N(R) + \epsilon_{rad}(R) \quad (10)$$

has been included as an additional, channel- and R -dependent potential on the left hand side, the sum on the right hand side is over all states $|\beta\rangle$, for which at least one of the quantum numbers is different from $|\alpha\rangle$ (see 7). The total angular momentum J and its projection M on the beam axis are conserved quantum numbers, hence the equations are diagonal in J, M . The $\epsilon_{\alpha}(R)$ are computed in the rotating frame (H_{e1} and $H_{nuc} + H_{rad}$, respectively, are

given by the second and third line of (2) expressed in the frame rotating with R); hence they depend only on the length and not on the orientation of R . The channel-dependent contribution of the intrinsic angular momenta to the total angular momentum barrier (which arises when the electron, photon and nuclear wavefunctions are rotated back into the lab frame) is recognized in the term $-\Lambda^2/R^2$ on the left side of eq. (9).

The coupling terms on the r.h.s. have the following origins:

$D_{\alpha\beta} \equiv \langle \alpha | \partial/\partial R | \beta \rangle$ is the so-called "radial coupling." It acts between any kind of molecular-type wavefunctions, and it is the most important mechanism for inner shell ionization in relativistic systems.

$H_{\alpha\beta} \equiv \langle \alpha | H_{e1} | \beta \rangle$ acts between the electronic basis states whenever they are not eigenstates to H_{e1} . This applies if, e.g., in supercritical systems ($Z_1 + Z_2 > 173$) a modified two-center basis is employed as discussed above; $H_{\alpha\beta}$ then describes the spontaneous positron emission.

$U_{\alpha\beta} = \langle \alpha | H_{nuc} | \beta \rangle$ describes the intrinsic nuclear excitations. $V_{\alpha\beta} \equiv \langle \alpha | H_{rad} | \beta \rangle$ describes radiative transitions and internal conversion of nuclear transitions. $Q_{\alpha\beta}$ finally summarizes all further effects, like Coriolis coupling (stemming from the use of a rotating coordinate system), and nucleon and electron translation effects (if a molecular basis is used). The corresponding matrix elements are known and can be easily included (Heinz et al. 1981).

The set of equations (9) is the practical basis of a theoretical description of heavy-ion collisions. No approximation is involved as long as there is no restriction on the number of basis states. Its practical usefulness relies on a convenient selection of basis states and on the availability of approximation schemes to further simplify the structure of the equations (9), such that the number of channels to be retained can be reduced as much as possible. The question of basis states was already discussed. In the remainder of this chapter we will occupy ourselves with the different available approximation schemes to solve equations (9).

Starting from (9), a major theoretical branching point involves a decision whether to continue with a quantum mechanical description of the nuclear relative motion, or whether to replace it by a classical trajectory. In the latter case, one substitutes the nuclear distance R by a time parameter which automatically distinguishes the ingoing ($t < 0$) and outgoing ($t > 0$) part of the collision, thereby considerably simplifying the formalism. The full quantum theory, however, is necessary for a deeper understanding, e.g., of the real meaning of the delay time T introduced in the semiclassical picture in order to describe nuclear contact (see below). After this point, the theoretical development is quite parallel in both approaches, and one can derive coupled channel equations for excitation amplitudes, solve them in perturbation theory or nonperturbatively, etc., as we will show below.

Most results obtained from (9) one way or the other involve the assumption that atomic and nuclear excitations occur in different spatial regions, $R > R_m$ and $R < R_m$ respectively. [Only recently has progress been made in describing on the basis of (9) simultaneous nuclear and atomic transitions during the nuclear sticking process (see Schramm's talk and Schramm et al. 1986).] If spontaneous decay processes like united atom X-ray emission or spontaneous positron production are involved, the corresponding matrix elements are assumed to be constant in the nuclear region $R < R_m$; this allows to factorize the atomic processes from those nuclear ones leading to sticking.

In this simplified picture, atomic-nuclear interference occurs because a given atomic excitation $\alpha \rightarrow \beta$ may happen before or after the nuclear scattering, which happens at different effective energies in the two cases. For an isolated nuclear resonance, the nuclear scattering thus may be on or off resonance, depending on whether the atomic excitation occurs before or afterwards. This results in different contributions to the cross section from the in- and outgoing parts of the collision. The difference between the two nuclear scattering amplitudes can be interpreted as a relative phase which is proportional to the energy derivative of the nuclear scattering phase shift or, classically, to the nuclear sticking time. This is the physics contained in the Blair-Anholt formula and its semiclassical analog, the Ciocchetti-Molinari formula (see below). As the beam energy scans the nuclear resonance, this relative phase between the in- and outgoing transition amplitudes changes, often leading to a characteristic interference pattern in the cross section. If the nuclear resonance is too wide, the change in phase is too small, and the interference is lost. If the nuclear resonance is very narrow compared to the atomic excitation energy, the in- and outgoing amplitudes become incoherent; then one obtains effectively two nuclear resonances, one corresponding to atomic excitations before and one to excitations after the nuclear scattering (see Heinz 1986).

For a nuclear reaction proceeding through a compound nucleus, the same principles apply, but the nuclear scattering amplitude can no longer be parametrized by a single resonance. Rather, the cross section is determined by the nuclear autocorrelation function, i.e. the beam energy average of the product of two scattering amplitudes at different energies. Still, it can be related to a distribution of classical delay times, thus allowing match-up with the semiclassical picture as I will show. These considerations play a role for the process of spontaneous positron production in very heavy ion collisions.

The Semiclassical Approximation - Collisions with Classical Time Delay

It is instructive to rewrite (9) in a more compact form:

$$\left\{ \frac{d^2}{dR^2} - U_\alpha(R) \right\} R_\alpha(R) = X_\alpha(R). \quad (11)$$

U_α comprises all nonderivative terms on the l.h.s. of (9), and $X_\alpha(R)$ summarizes all interchannel couplings. Asymptotically (for $R \rightarrow \infty$), the latter vanish, and $U_\alpha(R) \rightarrow [2\mu/\hbar^2](E - \epsilon_\alpha(\infty))$ becomes very large due to the huge kinetic energy contained in the nuclear relative motion. Therefore, at large R the functions R_α have to be rapidly oscillating (with wavelengths of order 0.1 fm). We can make use of the asymptotic dominance of the total energy (plus corrections from the long-range Coulomb repulsion between the two nuclei and from the angular momentum barrier) to guess and extract the rapidly oscillating part of the functions R_α , leaving a set of differential equations for the remaining "modulation amplitudes" which has much more slowly varying solutions and is easier to handle numerically.

In this subsection we discuss the semiclassical approach, in which the rapidly oscillating part of the R_α is assumed to be given by JWKB-solutions of (11) neglecting the couplings X_α between channels. Within this scheme it is possible to define a classical nuclear trajectory $R(t)$ parametrized by a time variable $-\infty < t < \infty$. This approximation usually breaks down if nuclear reactions are involved; however, one can simulate nuclear reactions by introducing a classical contact or delay time and by appropriately modifying the classical trajectory $R(t)$ during this time interval, as you have seen in other talks at this meeting.

Derivation of Time-dependent Coupled Channel Equations

We consider the equation

$$\left\{ \frac{d^2}{dR^2} - \frac{J(J+1)}{R^2} + \frac{2\mu}{\hbar^2} [E - V_C(R) - V_N(R) - \bar{\epsilon}(R)] \right\} r_J(R) = 0. \quad (12)$$

It is obtained from (11) by neglecting the coupling terms $X_\alpha(R)$ and the channel dependent contribution to the angular momentum barrier, and by replacing the channel dependent binding energies $\epsilon_\alpha(R)$ by a channel independent "average" $\bar{\epsilon}(R)$. Different choices of $\bar{\epsilon}(R)$ will lead to slightly different nuclear trajectories, but in general (within the domain of applicability of the JWKB approximation) these effects are small and can be neglected. The purpose of these manipulations is that

$$\bar{P}_J^2(R) = 2\mu [E - V_N(R) - V_C(R) - \bar{\epsilon}(R)] - \frac{J(J+1)\hbar^2}{R^2} \quad (13)$$

defines a channel independent classical nuclear trajectory (see below) which only depends on the total energy and the total angular momentum (classically related to the impact parameter). Its zero defines a channel independent classical turning point R_0 . (There may be more than one R_0 , e.g. in a potential with pockets.) The in- and outgoing JWKB-solutions to (12) are given by

$$r_J^\pm(R) = [\bar{P}_J(R)]^{-1/2} \exp(\pm i S_J(R)/\hbar \pm i \pi/4) \quad (14)$$

with

$$S_J(R) = \int_{R_0}^R \bar{P}_J(R') dR'. \quad (15)$$

The radial functions R_α in (11) are now expanded into these semiclassical solutions:

$$R_\alpha(R) = a_\alpha^+(R) r_J^+(R) e^{i\gamma_\alpha(R)/\hbar} - a_\alpha^-(R) r_J^-(R) e^{-i\gamma_\alpha(R)/\hbar}. \quad (16)$$

$\gamma_\alpha(R)$ is the additional channel dependent phase shift due to the binding energies $\epsilon_\alpha(R)$ and the term $-\Lambda_\alpha^2/R^2$:

$$\gamma_\alpha(R) = \int_{R_0}^R P_\alpha(R') dR' - S_J(R) = \int_{R_0}^R [\bar{\epsilon}(R') - \epsilon_\alpha(R') + \Lambda_\alpha^2 \hbar^2 / 2\mu R'^2] \frac{\mu dR'}{\bar{P}_J(R')} \quad (17)$$

with

$$P_\alpha^2(R) = 2\mu [E - V_N(R) - V_C(R) - \epsilon_\alpha(R)] - \frac{[J(J+1) - \Lambda_\alpha^2] \hbar^2}{R^2}. \quad (18)$$

Extracting these phases from the expansion amplitudes $a_\alpha^\pm$ in (16) has the advantage of removing all diagonal coupling terms from the equations governing their dynamics. Furthermore all second derivatives $a_\alpha^\pm$ can be eliminated by the constraint on (16),

$$r_J^+(R) \frac{da_\alpha^+}{dR} = r_J^-(R) \frac{da_\alpha^-}{dR}, \quad (19)$$

which leaves us with the proper number of independent functions, namely one

independent modulation amplitude for every channel wavefunction $R_\alpha(R)$.

One now proceeds to insert the ansatz (16) into (11) and to expand in powers of $\hbar$. The next step involves neglecting all terms containing strongly oscillating factors; it is crucial for defining a classical nuclear trajectory (see below) since it decouples the ingoing amplitudes a_α^- from the outgoing ones, a_α^+ . It is only allowed outside of the largest classical turning point R_0 ; in the case where the internuclear "potential" U_α in (11) contains pockets, resonance scattering is possible, invalidating the concept of a channel independent classical trajectory (different channels may be on or off resonance, depending on $\epsilon_\alpha(R)$). Still, it may be possible to use JWKB wavefunctions inside the pocket; in matching them to the outside solution, coupling of in- and outgoing amplitudes will, however, be unavoidable (Schramm et al. 1986).

In the final step one defines a time variable through

$$dt = \pm \frac{\mu}{P_J(R)} dR \quad (20)$$

with the + (-) sign for the outgoing (ingoing) amplitudes. Matching these amplitudes at the classical turning point ($t = t_0$) by the regularity condition,

$$a_\alpha^+(R_0) = a_\alpha^-(R_0), \quad (21)$$

one finally obtains the time dependent coupled channel equations

$$\frac{da_\alpha}{dt} = - \sum_{\beta \neq \alpha} [\dot{R}(t) D_{\alpha\beta}(t) + \frac{i}{\hbar} (H_{\alpha\beta} + U_{\alpha\beta} + V_{\alpha\beta} + Q_{\alpha\beta})] e^{i\chi_{\alpha\beta}(t)} a_\beta(t). \quad (22)$$

The phases $\chi_{\alpha\beta}(t)$ are given by

$$\chi_{\alpha\beta}(t) = \frac{1}{\hbar} \int_{t_0}^t \left(\epsilon_\alpha - \epsilon_\beta - \frac{(\Lambda_\alpha^2 - \Lambda_\beta^2)\hbar^2}{2\mu R^2} \right) dt' \equiv \chi_\alpha(t) - \chi_\beta(t). \quad (23)$$

(The last term in the integral is usually neglected as being small.)

Fully Quantum Mechanical Treatment

A quantum mechanical set of coupled channel equations for the occupation amplitudes can be derived very much along the same lines as in the semiclassical case. The basic improvement lies in a more accurate choice for the rapidly oscillating part of the nuclear relative motion wavefunction which allows one also to go outside the region where the JWKB approximation is applicable. On account of the dominance of the internuclear Coulomb potential at large distances, a natural candidate for the rapidly oscillating part of the nuclear relative wavefunctions R_α is given by in- and outgoing Coulomb waves, i.e. solutions of

$$\left\{ \frac{d^2}{dR^2} - \frac{J(J+1) - \Lambda_\alpha^2}{R^2} + \frac{2\mu}{\hbar^2} [E - V_C(R) - \epsilon_\alpha(\infty)] \right\} H_{L_\alpha}^\pm(K_\alpha R) = 0. \quad (24)$$

Here $K_\alpha^2 \hbar^2 \equiv 2\mu[E - \epsilon_\alpha(\infty)]$, and L_α is defined by $L_\alpha(L_\alpha+1) = J(J+1) - \Lambda_\alpha^2$. The analog of the semiclassical expansion (16) reads:

$$R_{\alpha}(R) = b_{\alpha}^{+}(R) H_{\alpha}^{+}(R) - b_{\alpha}^{-}(R) H_{\alpha}^{-}(R), \quad (25)$$

where $H_{\alpha}^{\pm}(R) \equiv H_{L_{\alpha}}^{\pm}(K_{\alpha}R)/\sqrt{K_{\alpha}}$, and the auxiliary condition (19) is replaced by

$$H_{\alpha}^{-} b_{\alpha'}^{-} = H_{\alpha}^{+} b_{\alpha'}^{+} \quad (26)$$

(primes denote d/dR). The wavefunction (25) is regular at the origin if

$$b_{\alpha}^{+}(R=0) = b_{\alpha}^{-}(R=0). \quad (27)$$

After insertion into (11) one obtains without approximations the coupled channel equations

$$b_{\alpha}^{\pm'} = \pm i \sum_{\beta} \{ (D_{\alpha\beta} H_{\alpha}^{\mp} H_{\beta}^{\pm'} - \tilde{H}_{\alpha\beta} H_{\alpha}^{\mp} H_{\beta}^{\pm}) b_{\beta}^{\pm} - (D_{\alpha\beta} H_{\alpha}^{\mp} H_{\beta}^{\mp} - \tilde{H}_{\alpha\beta} H_{\alpha}^{\mp} H_{\beta}^{\mp}) b_{\beta}^{\mp} \} \quad (28)$$

Here we defined for $\alpha \neq \beta$

$$\tilde{H}_{\alpha\beta} = \frac{\mu}{\hbar^2} (H_{\alpha\beta} + U_{\alpha\beta} + V_{\alpha\beta} + Q_{\alpha\beta}), \quad (29)$$

whereas the diagonal matrix element

$$\tilde{H}_{\alpha\alpha} \equiv \Delta V_{\alpha} = \frac{\mu}{\hbar^2} [V_N(R) + \epsilon_{\alpha}(R) - \epsilon_{\alpha}(\infty)] \quad (30)$$

contains all potential couplings not taken into account in the Coulomb wavefunctions.

In contrast to the semiclassical coupled channel equations (22), in (28) in- and outgoing amplitudes are coupled to each other. The coupling terms contain products of two in- or outgoing Coulomb functions, which outside the nuclear Coulomb barrier are rapidly oscillating and whose semiclassical analog is argued to be negligible. If, however, important physics happens near or inside the Coulomb barrier, where these coupling terms between in- and outgoing amplitudes are no longer rapidly oscillating, they become essential. For example, they generate the proper resonance behavior of the nuclear relative motion wavefunction in collisions which proceed through, say, longlived molecular or compound states, thus giving rise to a large probability density at small internuclear distances. In such a scenario, the occupation amplitudes $b_{\alpha}^{\pm}(\infty)$ are also rapidly dependent on the total angular momentum J , because channels with nearby values of J may be on or off resonance. This invalidates a saddle point approximation for the partial wave sum in the expression for the cross section, and one has to explicitly evaluate

$$\frac{d\sigma_{\alpha\beta}}{d\Omega}(\theta) = \frac{1}{4K_{\alpha}^2} \left| \sum_J (2J+1) e^{i(\sigma_J^{\alpha} + \sigma_J^{\beta})} a_{\alpha\beta}^J d_{\Lambda_{\alpha}\Lambda_{\beta}}^J(\theta) \right|^2. \quad (31)$$

rather than being able to use the simple semiclassical formula

$$\frac{d\sigma_{\alpha\beta}}{d\Omega}(\theta) = \left| a_{\alpha\beta}^{J_0} \right|^2 \cdot \frac{d\sigma_R}{d\Omega}(\theta). \quad (32)$$

In (31) $K_{\alpha} = \frac{1}{\hbar} \sqrt{2\mu(E - \epsilon_{\alpha}(\infty))}$, and the asymptotic phase shifts σ_J^{α} are semiclassically defined by

$$\sigma_J^\alpha = \frac{1}{\hbar} \lim_{R \rightarrow \infty} \left(\int_{R_0}^R P_\alpha(R') dR' - P_\alpha(R) \cdot R + \frac{J\hbar\pi}{2} \right). \quad (33)$$

The saddle point J_s in (32) in the case of Rutherford scattering is related to the impact parameter and the scattering angle by ($P = \mu v$ is the asymptotic relative momentum)

$$J_s = bP/\hbar = \frac{Z_1 Z_2 e^2}{\hbar v} \cot \theta/2. \quad (34)$$

The Factorization Ansatz

As we discussed, sufficiently far away from the nuclear interaction region the collision can be treated semiclassically, i.e., the rapidly oscillating terms in (28) can be neglected. Since the semiclassical equations (22) are so much easier to solve than (28), due to the decoupling of in- and outgoing solutions, we would like to define a matching distance R_m as close as possible to the nuclear interaction regime, such that for $R > R_m$ it is sufficient to solve (22). (Fig. 2) Inside R_m , we will generally have to solve the full set of equations (28) with boundary conditions at R_m determined by the semiclassical solution outside R_m . It is obvious that the solution of (28) would be trivial if inside R_m all couplings would vanish. This is in general not achievable. But even if for $R < R_m$ only the atomic excitations vanish, things simplify because now the solution of (28) inside R_m just determines the nuclear transition S-matrix, and the total excitation amplitude factorizes into a nuclear part from inside R_m and an atomic part

Fig. 2. A schematic picture of radial vs. spontaneous coupling in a semiclassical model. R is the two-center distance $R > R_0$, where R_0 is the classical turning point (semiclassically associated with time $t=0$). R_d is the diving point, R_m the matching radius defined in the text. For the radial excitation the semiclassically relevant combination $\dot{R} \langle \alpha | \partial / \partial R | 0 \rangle$ is drawn which shows explicitly that, semiclassically at least, most of the radial coupling occurs at distances $R \gg R_0$. This semiclassical picture is the motivation for our choice of R_m in the text.

from outside R_m . Such an approximation is often justified: the radial coupling vanishes near the point of closest approach due to the vanishing nuclear relative velocity; spontaneous transitions, if their intensity is not very sensitive on the exact nuclear configuration after contact but can be reasonably assumed to be constant inside R_m , can be eliminated by transforming at the matching point R_m to an eigenstate basis in which the spontaneous coupling $H_{\alpha\beta}$ is absent by construction. Under these conditions the asymptotic transition amplitude in angular momentum channel β can be written as:

$$a_{i \rightarrow f}^{\ell}(\infty, \infty) = - \int_{n_1 n_2 j} a_{i \rightarrow n_1}^{-\ell}(\infty, R_m) U_{j n_1}^{\ell}(R_m) S_{i \rightarrow f}^{\ell}(E - \epsilon_j(R_m)) U_{j n_2}^{\ell}(R_m) a_{n_2 \rightarrow f}^{+\ell}(R_m, \infty) \quad (35)$$

This formula was first given by Tomoda and Weidenmüller (1983); its semiclassical analogue had been derived earlier by Müller and Oberacker (1980). $a^{\pm}$ denote the in- and outgoing semiclassical amplitudes from (22) outside R_m ; U denotes the transformation matrix to eigenstates at R_m ; $S_{i \rightarrow f}^{\ell}$ is the nuclear transition matrix element in particle wave ℓ , evaluated at the available scattering energy at R_m , $E - \epsilon_j(R_m)$. For elastic nuclear scattering this simplifies to

$$a_{i \rightarrow f}^{\ell}(\infty, \infty) = - \int A_{i \rightarrow j}^{-\ell}(\infty, R_m) \exp(2i\delta_{\ell}(E - \epsilon_j)) A_{j \rightarrow f}^{+\ell}(R_m, \infty), \quad (36)$$

where $A^{-} \equiv a^{-} \cdot U$ etc., and the nuclear S-matrix has been parametrized by a phase shift depending on the available nuclear scattering energy.

Perturbative Expansion

If all the transition amplitudes are small, one can solve (22) or (28) in perturbation theory, i.e., neglecting multistep processes $i \rightarrow n_1 \rightarrow \dots \rightarrow f$. Based on (28), this results in replacing the outside amplitudes $a_{\alpha \rightarrow \beta}^{-}(\infty, R_m)$ by

$$B_{\beta\alpha} = \sqrt{\frac{K_{\alpha}}{K_{\beta}}} \int_{R_m}^{\infty} (D_{\beta\alpha} + i\tilde{H}_{\beta\alpha}/K_{\alpha}) \exp(i\bar{q}(R) \cdot R) dR \quad (37)$$

where

$$\bar{q}(R) \cdot R \approx (K_{\alpha} - K_{\beta})R + \frac{Z_1 Z_2 e^2}{2E} (K_{\alpha} - K_{\beta}) \ln 2K_{\alpha} R. \quad (38)$$

The contribution from the (constant) spontaneous coupling $H_{\beta\alpha}^{\text{spont}}$ inside R_m can be evaluated analytically (Blair and Anholt 1982, Heinz et al. 1983a). One obtains the following expression for the cross section to excite channel β :

$$\frac{d\sigma_{\beta}}{d\Omega}(\theta) = \left| f(\theta, E - \epsilon_{\beta}) \right|^2 \sum_{\alpha} \left| B_{\beta\alpha} - \frac{K_{\alpha}}{K_{\beta}} \frac{f(\theta, E - \epsilon_{\alpha})}{f(\theta, E - \epsilon_{\beta})} B_{\beta\alpha}^{*} - \frac{K_{\alpha} + K_{\beta}}{2\sqrt{K_{\alpha}K_{\beta}}} \frac{H_{\beta\alpha}^{\text{spont}}}{\epsilon_{\beta\alpha}} \left(\frac{f(\theta, E - \epsilon_{\alpha})}{f(\theta, E - \epsilon_{\beta})} - 1 \right) \right|^2. \quad (39)$$

The factor $|f(\theta, E - \epsilon_{\beta})|^2$ is the nuclear cross section in channel β . The ratios of nuclear scattering amplitudes under the sum over initial channels α can be brought into a more intuitive form by using the quantum mechanical definition of a nuclear delay time as the energy derivative of the scattering phase shift:

$$\frac{f(\theta, E - \epsilon_{\alpha})}{f(\theta, E - \epsilon_{\beta})} \approx 1 + \epsilon_{\beta\alpha} \frac{\partial}{\partial E} \ln f(\theta, E - \epsilon_{\alpha}) = 1 + i\epsilon_{\beta\alpha} \tau_{\alpha}^{\text{QM}}/\hbar \approx \exp(i\epsilon_{\beta\alpha} \tau_{\alpha}^{\text{QM}}/\hbar). \quad (40)$$

Inserting this into (39) reproduces the semiclassical formula in terms of a classical nuclear delay time τ , as it was derived years ago by Ciocchetti et al. (1963) and used by Gerd Soff in his talk at this meeting.

THE GENERAL RELATIONSHIP BETWEEN THE NUCLEAR S-MATRIX AND A CLASSICAL DELAY TIME DISTRIBUTION

Let us return to the cross section formula (31); in most cases the influence on the intrinsic spins $\Lambda_\alpha, \Lambda_\beta$ is small, and we can replace the d-matrix by $P_\ell(\cos\theta)$, summing over relative orbital momenta ℓ instead of J . Since the amplitudes $a_{\alpha+\beta}^\ell$ are defined by expanding the relative motion into Coulomb waves, the σ_ℓ in are the Coulomb phaseshifts. Their channel dependence is through the Sommerfeld parameter and small enough to be neglected. In most cases which involve nuclear contact and compound nucleus formation, the nuclear S-matrix hidden in the amplitudes $a_{\alpha+\beta}^\ell$ (see 35/36) is a very rapidly varying function of energy, due to a huge number of closely spaced compound states. An experiment with a finite beam energy resolution therefore can only measure S averaged over some finite energy interval, rather than resolve individual compound nucleus states. Let us therefore perform an energy average over the cross section, using the fact that compared to the nuclear S-matrix the energy variation of the atomic amplitudes $a_{\alpha+\beta}^\ell$ and of the Coulomb phases is very slow. To further simplify the calculation, we realise that also the angular momentum dependence of the atomic amplitudes outside the matching radius R_m is slow compared to the Legendre polynomials; they can be extracted from the sum over partial waves and are replaced by their average value evaluated at an appropriate "effective angular momentum". One finds

$$\begin{aligned} \left\langle \frac{d\sigma_{I \rightarrow F}}{d\Omega} \right\rangle &= \frac{1}{4K^2} \sum_{nm} a_{I+n}^- a_{n+f}^+ a_{I+m}^{-*} a_{m+f}^{+*} \cdot \\ &\cdot \sum_{\ell\ell'} (2\ell+1)(2\ell'+1) P_\ell P_{\ell'} e^{2i(\sigma_\ell - \sigma_{\ell'})} \\ &\cdot \left\langle S_{\ell', I \rightarrow F}(E - \epsilon_n) S_{\ell, I \rightarrow F}^*(E - \epsilon_m) \right\rangle, \end{aligned} \quad (41)$$

The brackets $\langle \dots \rangle$ denote the beam energy average over an interval ΔE as defined, e.g., by the prescription

$$\langle f(E) \rangle = \frac{\Delta E}{\pi} \int_{-\infty}^{\infty} \frac{f(\epsilon) d\epsilon}{(\epsilon - E)^2 + \Delta E^2}. \quad (42)$$

Equation (41) contains the nuclear autocorrelation function

$$A_{\ell\ell'}^{I \rightarrow F}(E_{nm}, \omega) \equiv \left\langle S_{\ell', I \rightarrow F}(E_{nm} - \hbar\omega/2) S_{\ell, I \rightarrow F}^*(E_{nm} + \hbar\omega/2) \right\rangle, \quad (43)$$

where

$$E_{nm} \equiv E - \frac{1}{2}(\epsilon_n + \epsilon_m); \quad \hbar\omega \equiv \epsilon_n - \epsilon_m. \quad (44)$$

Neglecting the slight channel dependence of $E_{nm} \approx E$, the Fourier transform $f_{E, \ell\ell'}^{I \rightarrow F}(T)$ of the autocorrelation function,

$$A_{\ell\ell'}^{I \rightarrow F}(E, \omega) = \int_{-\infty}^{\infty} dT e^{-i\omega T} f_{E, \ell\ell'}^{I \rightarrow F}(T), \quad (45)$$

can be used to bring the cross section into the following form (Reinhardt et al. 1983):

$$\left\langle \frac{d\sigma_{I \rightarrow F}}{d\Omega}(\theta) \right\rangle = \int_{-\infty}^{\infty} dT \left| \sum_n a_{I \rightarrow n}^- e^{-i\epsilon_n T/\hbar} a_{n \rightarrow F}^+ \right|^2 \cdot \frac{1}{4K^2} \sum_{\ell\ell'} (2\ell+1)(2\ell'+1) P_{\ell} P_{\ell'} e^{2i(\sigma_{\ell}' - \sigma_{\ell})} f_{E,\ell\ell'}^{I \rightarrow F}(T). \quad (46)$$

The sum over n is recognized as the semiclassical atomic excitation amplitude for a collision with a classical time delay T . This suggests the interpretation of the variable T as a nuclear delay time. The partial wave sum then defines a different nuclear cross section for every delay time T ; the probability of the latter to occur in a collision where the nuclei go from state I to F is given by $f_{E,\ell\ell'}^{I \rightarrow F}(T)$:

$$\left\langle \frac{d\sigma_{I \rightarrow F}}{d\Omega} \right\rangle = \int_{-\infty}^{\infty} dT \left| a_{I \rightarrow F}(T) \right|^2 \frac{d\sigma_{I \rightarrow F}^{\text{nuc}}}{d\Omega}(\theta, T) \quad (47)$$

with

$$\frac{d\sigma_{I \rightarrow F}^{\text{nuc}}}{d\Omega}(\theta, T) = \frac{1}{4K^2} \sum_{\ell\ell'} (2\ell+1)(2\ell'+1) P_{\ell} P_{\ell'} e^{2i(\sigma_{\ell}' - \sigma_{\ell})} f_{E,\ell\ell'}^{I \rightarrow F}(T). \quad (48)$$

In the models so far discussed in the literature (see below), the nuclear autocorrelation function (43) does not have any poles in the lower half of the complex ω -plane; in that case, the probability distribution $f_{\ell\ell'}(T)$ in (45) vanishes identically for negative T , and the cross section (47) receives contributions only from positive (and real) delay times. This provides additional support for the interpretation of the variable T as a classical delay time.

The formula (47) is very important in practice because it essentially extends the range where semiclassical methods can be used into a domain where one naively would have assumed it to break down. We realize that even for collisions with nuclear contact where complicated nuclear processes can happen the use of classical trajectories and classical delay times can be possible. Of course, quantum mechanics enters through the back door in that the distribution function of classical delay times $f_{\ell\ell'}(T)$ (which determines the nuclear cross section for the delayed events) has to be chosen consistent with the properties of the underlying quantum mechanical nuclear scattering amplitude; i.e., it has to be the Fourier transform of the appropriate nuclear autocorrelation function. This can become a technically very hard task. Two rather simple examples will be discussed in the following section.

Equations (45), (47) and (48) can, however, also be viewed differently: detailed measurement of atomic excitation cross sections in coincidence with the scattered nuclei (which in general will be in an excited state or have gained or lost a few particles) can be used in an attempt to draw conclusions on the shape of the probability distribution $f_{\ell\ell'}(T)$ for nuclear delay times, and hence to infer characteristic properties of the nuclear S -matrix. In particular, it should be possible to decide whether the distribution of delay times is peaked at $T=0$ with rather small contributions from finite T , or has a nonvanishing mean value T larger than the typical Rutherford collision time of about 10^{-21} sec (see the talks by Soff and Senger). The implications for the nuclear autocorrelation function would

be quite drastic (see below), pointing to a more stochastic nuclear S-matrix with rather short-range correlations in energy and angular momentum in the first case, versus long-range nuclear correlations in energy and/or angular momentum in the second case (Reinhardt et al. 1983).

Let me remind the reader that the basis of this very elegant formulation is the factorization ansatz (35,36) for the excitation amplitudes where all atomic excitations happen outside R_m (and are treated semiclassically, and all nuclear effects are confined to distances less than R_m and are contained in the S-matrix $\bar{S}_{\beta \rightarrow \alpha}(R_m)$. For processes where such a separation is impossible eq. (47) is not applicable. In some sense these would be genuine quantum mechanical nuclear-atomic interference phenomena, because there semiclassical intuition appears to fail completely. Unfortunately, the computational complexities avalanche in that case and have only recently been tackled; Schramm will show in his talk for the case of nuclear sticking caused by a pocket in the internuclear potential that by a proper matching of WKB solutions in- and outside the pocket the interplay of nuclear and atomic transitions during nuclear contact can be described theoretically.

AN EXAMPLE: ELASTIC SCATTERING OFF NUCLEAR MOLECULAR RESONANCES

To illustrate the procedure presented in the last section let us study the elastic scattering off nuclear molecular resonances supported by a pocket near the touching distance in the internuclear potential (see Fig. 3). The pocket is assumed to be sufficiently deep to contain one or more quasibound vibrational states (corresponding to radial excitations of the nuclei around the touching configuration) with energies E , $n=1, \dots, N$.

Fig. 3. Schematic picture of the internuclear potential. The parameters indicated are those used in the calculations of this talk: $V_{\max} = 725$ MeV; $V_{\max} - V_{\min} = 20$ MeV; $R_{\max} - R_{\min} = 0.1$; $R_m = 17$ fm; $E = V_{\max} - 8$ MeV; $\gamma = \hbar^2/(2\mu R_{\min}^2) = 0.7$ keV; beam energy = 6.2 MeV/n ($E_{\text{cm}} = 750$ MeV).

On top of each vibrational state one assumes a rotational band with energies

$$E_{nl} = E_n + \gamma l(l+1), \quad (49)$$

corresponding to a rotation of the nuclear molecule around its center of mass. l is the angular momentum of the rotation, and $\gamma = \hbar^2/(2\mu R_{\min}^2)$ is the rotational constant (inverse moment of inertia) of the molecule, defined by the nuclear separation $R_{\min}$ at the minimum of the potential pocket. For large nuclei γ is rather small (~ 0.7 keV for a U-U molecule (Hess et al. 1984)) which means that rotational excitations with very large angular momenta can be supported by even a rather shallow pocket $l_{\text{crit}}^{\text{U-U}} \sim 300\hbar$ if the band head state is bound by 10 MeV).

It is assumed that each molecular resonance contributes to the elastic nuclear phase shift with a Breit-Wigner form:

$$S_l(E) = \prod_{n=1}^N (E - E_{nl} - i\Gamma_{nl}/2) / (E - E_{nl} + i\Gamma_{nl}/2). \quad (50)$$

The resonance widths are determined from a simple barrier penetration formula:

$$\Gamma_{nl} = \frac{\hbar\omega_{\min}}{2\pi} \exp\left\{-\frac{2\pi}{\hbar\omega_{\max}} \left(V_{\max} + \frac{l(l+1)\hbar^2}{2\mu R_{\max}^2} - E_{nl}\right)\right\}. \quad (51)$$

$\omega_{\min}$ ($\omega_{\max}$) are the curvature of the potential at the minimum (maximum), and $V_{\max}^l \equiv V_{\max} + l(l+1)\hbar^2/2\mu R_{\max}^2$ is the energy of the effective potential barrier in partial wave l . Obviously the resonances are very narrow and long-lived far below the barrier, and become wide very rapidly close to the barrier top and above. This implies that delayed nuclear scattering will be dominated by a few resonances slightly below the barrier top, because the higher states decay too fast to yield appreciable delay, and the very narrow deep-lying states have hardly a chance to be hit by the incoming nuclei because the tunneling probability through the barrier is too small.

Using the prescription (42) for the energy average, the autocorrelation function and delay time distribution can be obtained analytically from the S-matrix (50). The technical details are given in Heinz et al. (1984a). For $N=1$ (one rotational band) one finds

$$\begin{aligned} \left\langle \frac{d\sigma_{i \rightarrow f}}{d\Omega}(\theta) \right\rangle &= \left| a_{i \rightarrow f, T=0} \right|^2 \frac{d\sigma_R}{d\Omega}(\theta) \\ &+ \int_0^\infty dT \left| a_{i \rightarrow f, T} \right|^2 \frac{d\sigma_{\text{delayed}}^{\text{nuc}}}{d\Omega}(\theta, T) + \text{interference term}, \end{aligned} \quad (52)$$

with

$$\frac{d\sigma_{\text{delayed}}^{\text{nuc}}}{d\Omega}(\theta, T) = \frac{1}{4K^2} \left| \sum_l (2l+1) e^{2i\sigma_l} P_l(\cos \theta) \alpha_l^E(T) \right|^2. \quad (53)$$

The functions $\alpha_l^E(T)$ are given by

$$\alpha_l^E(T) = \frac{\Gamma_l \sqrt{2\Delta E}}{E - E_l + i\Gamma_l/2 + i\Delta E} e^{-iE_l T - \Gamma_l T/2}. \quad (54)$$

The first term in (52) is a "background" of pure Coulomb scattering events, and contains the undelayed transition probability times the nuclear Rutherford cross section. The second term describes the additional contribution from delayed nuclear scattering events (i.e. events which proceed through the molecular resonances). The interference term is rapidly damped out for increasing T ; as $\Delta E \rightarrow \infty$, its time structure $\Delta E e^{-2\Delta E|T|} \rightarrow \delta(T)$ approaches that of the prompt contribution. It is therefore to be interpreted as the flux taken out of the prompt scattering channel due to the presence of delayed scattering events. Typically the delayed term is by three orders of magnitude smaller than the prompt contribution; hence this flux correction to the direct scattering can safely be neglected unless delay times $T < 0(1/\Delta E)$ are of interest. (Typically $\Delta E \sim 10$ MeV, and all events with delay times more than 10^{-22} sec can be treated incoherently from the prompt scattering contribution.)

In Fig. 4 we show the nuclear cross section for the delayed events, eq. (53), as a function of delay time T , for the case of a potential pocket which supports ten rotational bands of molecular resonances. Although this "distribution of delay times" looks quite chaotic, it has a distinctive feature: although peaked at small T , it contains appreciable probability for large delay times $T \geq 10^{-19}$ sec. The fall-off is much weaker than an exponential corresponding to stochastic decay of a compound nucleus; the slope of the envelope of Fig. 4 is nearly proportional to $1/T$. This means that the long-range energy correlations, introduced into the nuclear autocorrelation function through the law (49) for the energy eigenvalues of the nuclear molecule, are reflected in a delay time distribution with significantly stronger relative importance of large delay times than one obtains from the stochastic compound nucleus theory (Reinhardt et al. 1983). This illustrates very nicely the relationship between the statistical properties of the eigenstate spectrum of the combined nuclear system and the expected time delay in collisions with nuclear contact.

Fig. 4. Time distribution of the delayed nuclear cross section for two nuclear scattering angles, $\theta = 60^\circ$ and 90° , employing ten rotational bands of molecular resonances with band heads at 1, 2, ..., 10 MeV below the top of the potential barrier.

POSITRON SPECTRA FROM DELAYED NUCLEAR COLLISIONS

In this section we use these results for the delayed nuclear cross section to compute positron spectra in U + Cm collisions with nuclear contact. We will focus on the second term in (52) describing the positrons coming from genuinely delayed collisions. The reason for doing so is that in our model even at the position of the spontaneous positron line this last term is generally 2 to 3 orders of magnitude smaller than the "dynamical" background of positrons coming from undelayed Rutherford collisions and could be hardly recognized in the complete spectrum. Of course, this is in strong disagreement with the experimental peaks which stick out from the dynamical background by about a factor of 2. On the other hand, this discrepancy was to be expected from our restriction to elastic nuclear scattering: in order to hit nuclear resonances with sufficiently long lifetimes to produce a clear and narrow positron line, in elastic scattering the nuclei first have to penetrate the potential barrier in Fig. 3. The tunneling probability ("entrance width") in elastic scattering is the same as the subsequent decay probability of the resonance ("exit width") and is correspondingly small for the long-lived nuclear resonances we require, leading to a cross section for collisions with sufficiently long delay times that is much too small.

A possible way out of this dilemma is to let the two nuclei come in above the barrier, thereby increasing the entrance width by orders of magnitude, and subsequently let them lose relative kinetic energy due to internal nuclear excitation, thereby trapping them in one of the long-lived resonances with small exit width below the barrier. This mechanism is known in light nuclear molecules like $^{12}\text{C}-^{12}\text{C}$, $^{16}\text{O}-^{16}\text{O}$, etc., as the double resonance mechanism. Of course, the giant nuclear system, being captured in the pocket, may also decay through other channels like light-particle emission, multiple fission, etc. With our formula (51) for the widths, we estimate that in order to gain a factor 10^3 to 10^4 in the entrance width relative to the exit width, the nuclei would have to lose (with probability close to 1) 2 to 3 MeV of relative energy due to excitations. This does not appear to be a problem in any realistic model for intrinsic nuclear excitations (e.g., already nuclear Coulomb excitation along Rutherford trajectories yields an average nuclear excitation energy of 4 to 6 MeV), and such a factor would be ample to boost the absolute intensity of our spontaneous positron peak into a regime compatible with the experimental peaks. (For a cautionary comment how to not implement this idea see Tom Pinkston's talk at this meeting; with his ansatz for the nuclear S-matrix he actually finds a reduction of the peak cross section due to the presence of inelastic nuclear processes.)

As has become clear in Berndt Müller's talk, the fact that the positron lines fail to shift appreciably in energy as the combined nuclear charge is varied has excluded the spontaneous vacuum decay as a possible explanation of (all) the existing data. Therefore, we do not think that this model provides a viable explanation of the GSI experiments, and we have not performed such more elaborate calculations. We will show results based on the elastic scattering model from the last section simply to demonstrate for the case of spontaneous positron emission the basic mechanisms of nuclear contact on atomic excitations spectra.

In Fig. 5 we show positron emission probabilities from delayed nuclear collisions (53), normalized to the Rutherford cross section, for the form of the delayed nuclear cross section shown in Fig. 4. One clearly sees the line due to spontaneous positron emission; its energy is determined by the matching radius R_m through the 1s binding energy at this value for the nuclear separation (because at this point we transform to the eigenstate basis in order to eliminate the spontaneous coupling inside R_m). More

Fig. 5. Positron spectra from delayed nuclear collisions, computed from the nuclear delay time distributions shown in Fig. 4, for two nuclear scattering angles, $\theta = 60^\circ$ and 90° . The spectra are normalized to the nuclear Rutherford cross section. The "dynamical" positrons from Rutherford events are not added.

properly, the spontaneous coupling should be taken at the location of the minimum of the potential pocket, thereby increasing the peak energy by an amount depending on the location of this pocket in your model. This is clearly seen in the calculations to be presented by Stefan Schramm.

The sharpness of the line is due to its origin in the tail of the delay time distribution (Fig. 4) at large delay times $T \geq 10^{-19}$ sec; the broad bump at its base reflects the maximum of this delay time distribution at small values of T . That the peak shows so clearly above the bump demonstrates the "magnifying power" of spontaneous positron emission, allowing to see even small fractions of strongly delayed nuclear events above a large background of rather prompt nuclear collisions (Reinhardt et al. 1981b).

We conclude our study of this model with an investigation of the beam energy dependence of the positron spectra. This beam energy dependence is determined by the fact that only those resonances E_{ng} , which lie within an energy interval $\pm \Delta E$ around the mean incident energy $\bar{E}$, contribute to the delayed cross section. Therefore, at energies far below the potential barrier, resonances are too narrow to be excited, and the cross section for delayed scattering events (and thus the chance to see spontaneous positron emission) is negligible. Far above the barrier, the beam can only hit the high-lying, short-lived resonances, again leading to a very low chance for spontaneous positron emission. Only if the beam energy is barely below the barrier is there a reasonable probability to be captured by a resonance with sufficiently long lifetime to lead to enhanced production of spontaneous positrons (Heinz et al. 1983b).

This is shown in Fig. 6. Since the atomic amplitudes are only weakly energy dependent, the relevant physical parameter is $E - V_{\max}$, the c.m. energy relative to the potential energy. In our calculation we varied this parameter by varying $V_{\max}$, i.e., by shifting the whole internuclear

Fig. 6. Positron spectra for three values of $E - V_{max}$, at $\theta = 60^\circ$. Only the contribution from scattering events with delay times $0 < T \leq 6 \cdot 10^{-19}$ sec normalized to the Rutherford cross section is shown. The "background" from Rutherford events is not added.

Fig. 7. The height of the maximum in the positron spectra as in Fig. 6 is shown as a function of c.m. energy for $\theta = 60^\circ$.

potential. This certainly is a good first approximation and saves us the computation of the atomic amplitudes for several energies.

Figure 6 demonstrates that the spontaneous positron line at $E_e^+ \approx 300$ keV shows a clear resonance behavior: barely visible far below and above the barrier, it is quite prominent if E is close to the barrier. This is demonstrated in more detail in Fig. 7, which shows the "excitation function" for spontaneous positrons. The positron line is strongest if the c.m. energy is ~ 20 MeV above the top of the ($l=0$)-barrier; since typical angular momenta are of the order of $200\hbar$, then E is barely below the effective potential barrier.

Although the absolute position of the maximum in Fig. 7 as well as its width reflects to some extent the potential parameters used in the calculation, and may slightly change for different shapes of the pocket and for different values of the energy spread ΔE of the beam (we expect the peak in Fig. 7 to become narrower for smaller ΔE and shallower potential pockets), the qualitative similarity with recent experimental data is striking: as stressed again in the talks by Bokemeyer, Cowan, and Kienle, there is some (although not completely uncontroversial) evidence for a resonance-like sensitivity of the experimentally found positron peaks on the beam energy. While such a feature falls out naturally from the assumption of a nuclear potential pocket, no other model has so far given such a feature. This may be indication for some nuclear origin along the lines discussed in this talk in the excitaton mechanism for the measured positron peaks.

SUMMARY

In this talk, the formal framework for the description of atomic excitations in heavy ion collisions was based on quantum mechanical scattering theory. This resulted in a unified treatment of nuclear and atomic dynamics and excitations. Outside the nuclear reaction region the nuclear motion may be accurately described using the semiclassical approximation. Neglecting electronic transitions inside the reaction region (except for spontaneous positron creation), the nuclear interaction may be treated independently from atomic processes. Then the asymptotic excitation amplitudes can be represented by a factorization ansatz as a product of incoming and outgoing atomic amplitudes connected through the nuclear S-matrix. The resulting excitation cross section has to be averaged over the spread in beam energy. This procedure introduces the nuclear autocorrelation function. If, in a further step, a Fourier transformation is introduced, the result takes the form of an integral over a time variable T of the atomic transition probability calculated for a fixed classical time delay, multiplied by the corresponding delayed scattering cross section.

The main result of this study is a better understanding of the relationship between the classical notion of a nuclear delay time and the structure of the quantum mechanical nuclear scattering amplitude. At least for elastic nuclear scattering it was shown that from the quantum mechanical nuclear autocorrelation function a classical delay time distribution can be derived, which can be used within the semiclassical framework to consistently extend it into the region where one might have assumed it to break down due to the presence of nuclear interaction. This is of enormous practical significance.

We also pointed out the limits of applicability of this procedure which relies on the mentioned factorization of nuclear and atomic excitation processes. In absence of this property the quantum mechanical scattering framework leads to more complicated coupled channel equations for the transition amplitudes which, however, with present computer technology can be tackled and, as shown by Schramm, have been used to obtain quantitative results.

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