THEORY OF ATOMIC FRAGMENTATION PROCESSES

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Processes whereby atomic or molecular systems break up into three or more pieces are termed fragmentation processes. When the fragments are charged, as they often are, they are difficult to describe theoretically, owing to the long range of the electrostatic interaction. The low-energy regime is particularly difficult since dynamical processes are typically described using an adiabatic basis. Such a basis accurately describes the initial two-body channels but fails for the fragmentation channels. We have developed a method[3] that employs a version of an adiabatic basis even for fragmentation channels.[4]

The essence of our method is illustrated in Fig. 1. Figure 1(a) is a schematic plot of the quantity $E(R)R^2$ *vs.* R for a model of negative ion impact on neutral atoms. The several adiabatic potential curves show an infinite sequence of avoided crossings leading to the continuum representing the breakup of the system into two neutral atoms and an electron.

The usual adiabatic representation requires all of the adiabatic states $\varphi_n(R(t);\mathbf{q})$ to accurately represent the fragmentation process. In this case the wavefunction is written as the generally infinite sum

$$\psi(t,\mathbf{q}) = \sum_n \varphi_n(R(t);\mathbf{q})a_n(t) \tag{1}$$

in the time-dependent representation or as the sum

$$\psi(R,\mathbf{q}) = \sum_n \varphi_n(R;\hat{\mathbf{R}},\mathbf{q})F_n(R) \tag{2}$$

in a wave treatment. The sum must include all states to describe the transition from bound continuum levels; thus the representation is impractical, yet the adiabatic states are appropriate for the energetically lower channels including initial, excitation, or electron capture channels. The need for adiabatic states for the lower channels, but not for the fragmentation channels, presents significant impediments to computations at low energy.

The way around this problem is seen by rotating Fig. 1(a) by 90° to obtain the plot of R vs. $\omega = E(R)R^2$ in Fig. 1(b) representing the inverse function $\rho(\omega)$. In this case there is just one single-valued function $\rho(\omega)$ which spans the same function space as the adiabatic functions. With this single basis function we can write the wave function for the system as an integral

$$\phi(t,\mathbf{q}) = \int_{-\infty}^{\infty} C(\omega)\varphi(\rho(\omega);\mathbf{q})\exp[-i\omega\tau(t)] \tag{3}$$

or in a wave treatment with $\omega \to \nu^2$ as

$$\psi(R;\mathbf{q},\hat{\mathbf{R}}) = \int_{-\infty}^{\infty} C(\nu)\varphi(\rho(\nu);,\mathbf{q},\hat{\mathbf{R}})J_\nu(KR)d\nu^2, \tag{4}$$

where the coefficients $C(\omega)$ or $C(\nu)$ are determined from a relatively simple recurrence relation and $J_\nu(KR)$ is a Bessel function. The infinite set $\varphi_n(R;\hat{\mathbf{R}},q)$ is thereby replaced by a single function $\varphi(\rho(\omega);\hat{\mathbf{R}},q)$ for this model system. In this case just one "inverse adiabatic" basis function gives a complete solution.

To extend this picture to interacting charged particles, we note that $\rho(\omega)$ is a solution of the equation $E(\rho)\rho^2 = \omega$. It can be shown that this solution is a Sturmian eigenvalue, i. e. $\rho(\omega)$ is the coefficient of the potential in the Schrödinger equation for both the model problem and charged particles. In the latter case $E(\rho)\rho^2 = \omega$ has many roots and one must employ sums over Sturmian eigenfunctions. Even so, a single term describes all processes approximately. In our computations it appears that the sum over Sturmians converges rapidly.

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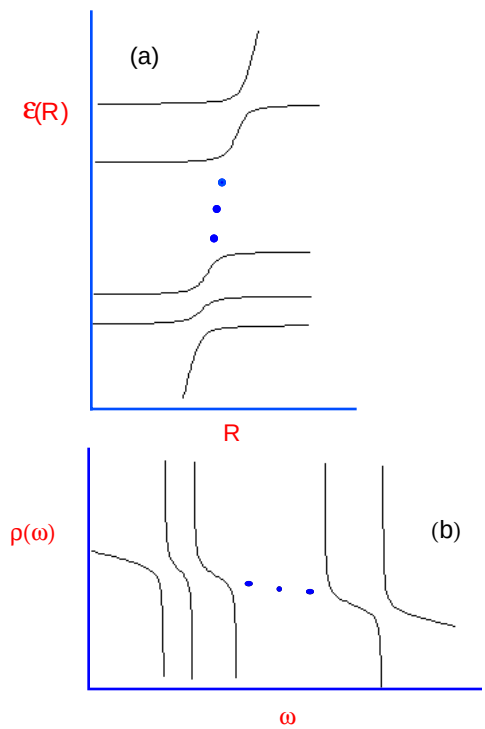

Figure 1: (a) Schematic plot of adiabatic energy levels $E(R)R^2$ *vs.* R showing a sequence of avoided crossings, and (b) plot of the inverse function $\rho(\omega)$ *vs* ω representing a single Sturmian eigenvalue.