An Application of Eq. (21)

By way of example, we consider a three-center problem, $A + BC \longrightarrow AB + C$, proceeding via a linear collision-complex. In mass-weighted configuration space the reaction path is curved.[9,21] As mentioned earlier, this path can be matched in the local approximation by the corresponding path for a surface which permits separation of variables. The matching has been discussed previously[7] and, in the following discussion, will be regarded as having been performed.

The plane defined in mass-weighted configuration space by the tangent and principal normal to the reaction path, the osculating plane of this path, will be called the "plane of reaction". In many diagrams in the literature[9,21] one assumes for simplicity that the reaction coordinate lies in a plane determined only by the AB and BC interatomic distances, mass-weighted as in Eq. (3). The remaining degrees of freedom are taken to be dynamically uncoupled from these two in those discussions. We consider this special case first.

In terms of the properties of a suitable coordinate system for matching of the potential energy functions, the latter assumption leads to a choice of a cylindrical coordinate system (Cartesian, circular, parabolic or elliptic cylinder):[7] The Z-axis, which is normal to the plane of reaction, represents the set of all degrees of freedom but the AB and BC distances. The latter two coordinates can be used to describe any point in the plane. In Eq. (6) one has then three sets, $m = 3$. With proper choice of coordinates one can diagonalize the kinetic energy contribution of the co-