Dmitri Babikov,[a)] Robert B. Walker, and Russell T Pack
Theoretical Chemistry and Molecular Physics Group (T-12, MS B268), Theoretical Division of Los Alamos National Laboratory, Los Alamos, New Mexico 87545

( )

+

( )

( )

is

$v =$ $j =$

(

and

$$\dot{\gamma}_n = \mathbf{p}_n$$

[( )]

j

$\mathbf{p}_n$

( ) ( )

($j>$ $\mathbf{r}_n$

$\mathbf{p}_n$

( ) ( )

$\mathbf{r}_n$

$\mathbf{p}_n$ ( ) ( )

$j=$

$j>$ +

( )

(

)

$$\nabla_{\mathbf{r}} V\ \mathbf{r}^{+}\ = -\nabla_{\mathbf{r}} V\ \mathbf{r}^{-}$$

nonsymmetric

[( )]

+

−

symmetric [( )]

R *t*

[( ) ( )]

+

$$\mathbf{r}^{+}(t) = \mathbf{r}\ + \int^{t} \frac{\mathbf{p}^{+}(t)}{\mu} dt \qquad (\quad)$$

$$\mathbf{p}^{+}(t) = \mathbf{p}\ - \int^{t} \nabla_{\mathbf{r}} V(\mathbf{r}^{+}\ t) d$$

$\langle b$

$$S_{ba}^{(\ )} = S_{ba}^{(\ )} - S_{bb}^{(\ )} \frac{\langle b|\phi_a\rangle}{\langle a|\phi_a\rangle} = \frac{\langle b|\psi_a\rangle}{\langle a|\phi_a\rangle} - S_{bb}^{(\ )} \frac{\langle b|\phi_a\rangle}{\langle a|\phi_a\rangle} \quad b \neq a$$

(