

Euler-Lagrange equations of motion for ADMP

- Equations of motion for density matrix and nuclei

acceleration of density matrix, P

“Fictitious” mass of P

$$\frac{d^2\mathbf{P}}{dt^2} = -\mu^{-1/2} \left[\left. \frac{\partial \mathbf{E}}{\partial \mathbf{P}} \right|_{\mathbf{R}} + \Lambda \mathbf{P} + \mathbf{P} \Lambda - \Lambda \right] \mu^{-1/2}$$

Force on P

$$M \frac{d^2\mathbf{R}}{dt^2} = - \left. \frac{\partial \mathbf{E}}{\partial \mathbf{R}} \right|_{\mathbf{P}}$$

- **Classical dynamics in $\{(\mathbf{R}, \mathbf{V}, M), (\mathbf{P}, \mathbf{W}, \mu)\}$ phase space**
- Next few slide: Forces, propagation equations, formal error analysis

E Motion Admp

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