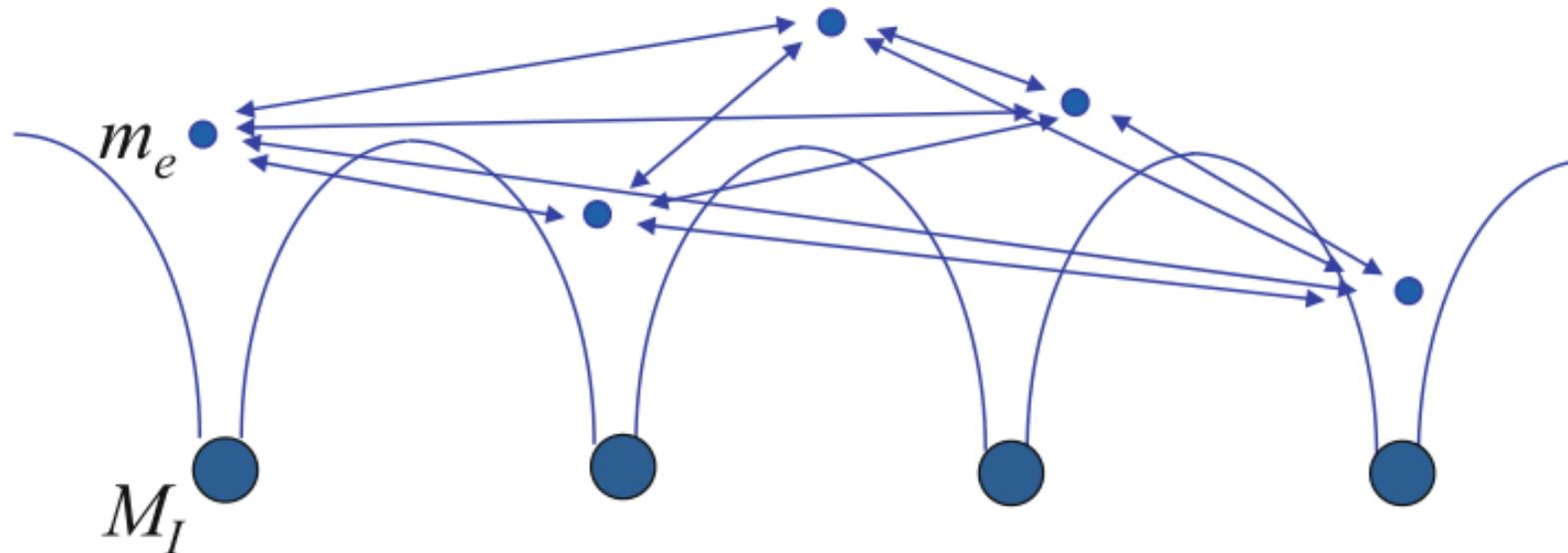# Many-body problem

(Sistema de muitas partículas interagentes)

$$\mathcal{H} = \sum_i \frac{\mathbf{p}_i^2}{2m_e} - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_I \frac{\mathbf{P}_I^2}{2M_I} + \frac{1}{2} \sum_{I,J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}$$

Sistema de múltiplas partículas interagentes (*i.e.*, acopladas p/ interação)

$$\mathscr{H} = \sum_i \frac{\mathbf{p}_i^2}{2m_e} - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \sum_I \frac{\mathbf{P}_I^2}{2M_I} + \frac{1}{2} \sum_{I,J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}$$
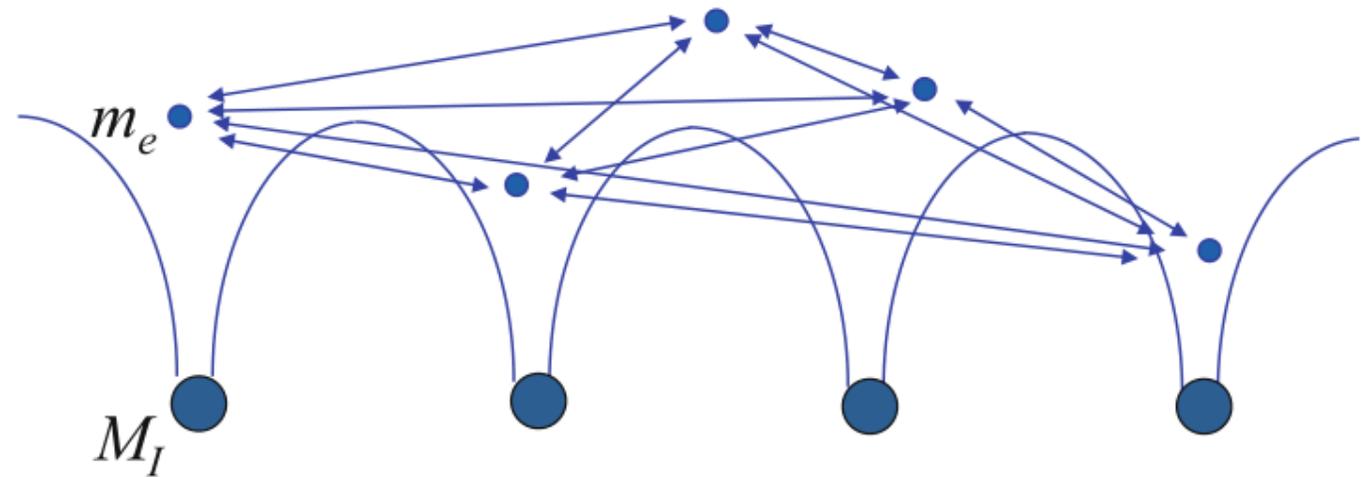
$$\mathscr{H} = -\sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \qquad \mathbf{p}_i = \frac{\hbar}{i} \nabla_i \ \text{ and } \ \mathbf{P}_I = \frac{\hbar}{i} \nabla_I$$

$$-\sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 + \frac{1}{2} \sum_{I,J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}.$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathscr{H} \Psi$$

$$i\hbar \frac{\partial \Psi}{\partial t} = \mathscr{H}\Psi$$

$$\Psi(\{\mathbf{r}_i\}, \{\mathbf{R}_I\}; t) = \Phi(\{\mathbf{r}_i\}, \{\mathbf{R}_I\})e^{-iEt/\hbar}$$

$$\mathscr{H}\Phi(\{\mathbf{r}_i\}, \{\mathbf{R}_I\}) = E\Phi(\{\mathbf{r}_i\}, \{\mathbf{R}_I\})$$

$$\Phi_{\alpha n}(\{\mathbf{r}_i\}, \{\mathbf{R}_I\}) = \Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\})u_{n\alpha}(\{\mathbf{R}_I\}) \qquad \Psi_\alpha(\{\mathbf{r}_i\} \; : \; \{\mathbf{R}_I\})$$

$$\left[-\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2}\sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2}\sum_{I,J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|}\right]\Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\})$$

$$= W_\alpha(\{\mathbf{R}_I\})\Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\})$$

$$\left[-\sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} + \frac{1}{2} \sum_{I,J} \frac{Z_I Z_J e^2}{|\mathbf{R}_I - \mathbf{R}_J|} \right] \Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\})$$

$$= W_\alpha(\{\mathbf{R}_I\}) \Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\}) \qquad\qquad W_\alpha(\{\mathbf{R}_I\})$$
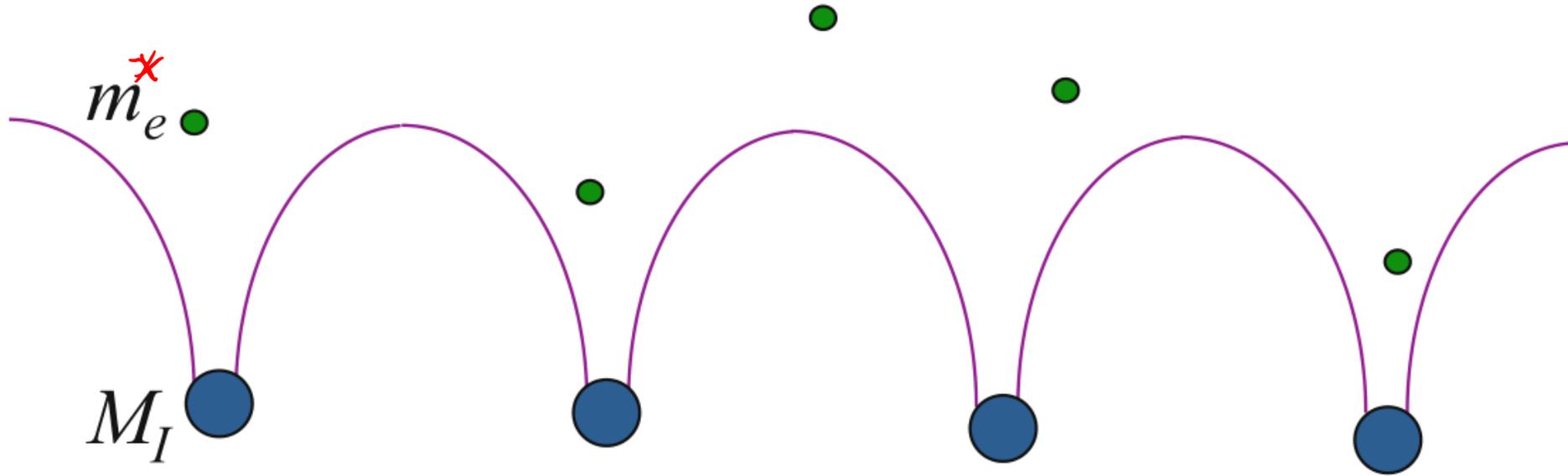
$$\left[-\sum_I \frac{\hbar^2}{2M_I} \nabla_I^2 + W_\alpha(\{\mathbf{R}_I\}) - E \right] u_{n\alpha}(\{\mathbf{R}_I\}) = 0 \qquad u_{n\alpha}(\{\mathbf{R}_I\})$$

$$\left[-\sum_i \frac{\hbar^2}{2m_e} \nabla_i^2 - \sum_{i,I} \frac{Z_I e^2}{|\mathbf{r}_i - \mathbf{R}_I|} + \frac{1}{2} \sum_{i,j} \frac{e^2}{|\mathbf{r}_i - \mathbf{r}_j|} \right] \Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\})$$

$$= E_\alpha(\{\mathbf{R}_I\}) \Psi_\alpha(\{\mathbf{r}_i\} : \{\mathbf{R}_I\})$$

$$\left[-\frac{\hbar^2}{2m_e} \nabla^2 + V_{\mathrm{KS},s}(\mathbf{r}) \right] \psi_{s,\alpha}(\mathbf{r}) = E_{s,\alpha} \psi_{s,\alpha}(\mathbf{r})$$

$$V_{\mathrm{KS},s}(\mathbf{r}) = -\sum_I \frac{Z_I e^2}{|\mathbf{r} - \mathbf{R}_I|} + \int d^3 r' \frac{e^2 n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + V_{\mathrm{xc},s}(\mathbf{r})$$

Sistema de partículas ou quasipartículas não interagentes (livres): (*i.e.,* excitações quantizadas de um campo quântico) desacopladas