¨o
ö

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t) = \big[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x},t)\big]\Psi(\mathbf{x},t)$$
(1)

$\Psi(\mathbf{x},t)$
$|\Psi(\mathbf{x},t)|^2$
t
$\mathbf{x}$
$-\frac{\hbar^2}{2m}\nabla^2$
m
$V(\mathbf{x},t)$
$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{x},t)$
V

$$E\Psi(\mathbf{x},t) = \big[-\frac{\hbar^2}{2m}\nabla^2+V(\mathbf{x})\big]\Psi(\mathbf{x},t) = H\Psi(\mathbf{x},t)$$
(2)

$\Psi(\mathbf{x},t)$
i
e

$$H = T_n+T_e+V_{n-n}+V_{n_e}+V_{e-e}$$
(3)

T_n
T_e
$V_{n-n}, V_{n-e}, V_{e-e}$

$$V_{n-n} = \sum_{i>j}\frac{q_e^2 z_i z_j}{|\mathbf{R}_i-\mathbf{R}_j|}, V_{n-e} = \sum_{i,l}\frac{q_e^2 z_i}{|\mathbf{r}_l-\mathbf{R}_i|}, V_{e-e} = \sum_{l>k}\frac{q_e^2}{|\mathbf{r}_l-\mathbf{r}_k|}$$
(4)

z_i
i
q_e
R_i
r_l

$$T_n = -\sum_i\frac{\hbar^2}{2M_i}\nabla_i^2, T_e = -\sum_l\frac{\hbar^2}{2m_l}\nabla_l^2$$
(5)

i M_i
m_l
l
i
l
M_i
$\nabla^2 =$
$\frac{\partial^2}{\partial x^2}+$
$\frac{\partial^2}{\partial y^2}+$
$\frac{\partial^2}{\partial z^2}$
?
i
T_e
U_{n-e}
U_{e-e}

$$\Psi(R_i,t) = \psi_e(r_l,R_i)\psi_n(R_i,t)$$
(6)

U_{LJ}

$$U_{CHARMM} = \underbrace{U_{LJ}+U_{Coulomb}}_{U_{non-bonded}}+\underbrace{U_{bonds}+U_{angles}+U_{dihedrals}+U_{impropers}}_{U_{bonded}}$$
(7)

$$U_{bonded} = \sum_{bonds}k_b(b-b_0)^2+\sum_{angles}k_\theta(\theta-\theta_0)^2+\sum_{Urey-Bradley}k_u(r_{UB}-r_{UB_0})^2+\sum_{dihedrals}k_\phi(1+\cos(n\psi-\delta))+\sum_{improper-dihedrals}$$
(8)

k_i
0
??
$_i$*nteractions.pdf*
The Bonded In- ter- ac- tions Ap- prox- i- mated In Clas-