Molecular Dynamics Simulation of Relativistic Kinetic Energies

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We will describe molecular dynamics of high-temperature and MeV energies with Coulombic and electromagnetic fields. With high accuracy and a minimally small approximation for short periods, the electrostatic Coulomb field is solved together with the electromagnetic Maxwell equations. The Courant condition is satisfied so that dx/dt > c, the speed of light.

1. Relativistic and electromagnetic molecular dynamics simulations for a carbon-gold nanotube accelerator, M.Tanaka and M.Murakami, Computer Physics Communications,vol.241, 56-63, 2019.

2. "Physics of High Temperature Plasmas", M. Tanana and K. Nishikawa, Maruzen Publication, 1991,1996 (Japanese)。

相対論的運動エネルギーの電磁波分子動力学

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　相対論的な運動エネルギーを持ち，クーロン場と電磁波で解く分子動力学法を述べる。近似が少なく高精度であるクーロン場，そしてマクスウェル方程式で電磁波動を用いることで粒子を運動させる。なお，クーラン条件はすべての体積で満たされることが必要である：Dx/Dt> c（光速）．以下は英語で述べる。

文献

1. Relativistic and electromagnetic molecular dynamics simulations for a carbon-gold nanotube accelerator, M.Tanaka and M.Murakami, Computer Physics Communications,vol.241, 56-63, 2019.

2.「金イオンによる炭素ナノチューブ爆発過程の分子動力学」，田中基彦（「超高強度レーザーとプラズマの相互作用に関する物理」，村上匡且，田中基彦共著，プラズマ・核融合学会誌，2017 年 9 月）

3.「高温プラズマの物理学」 田中基彦，西川恭治，丸善，1991,1996。

$*$ *Molecular Dynamics Simulation of High – Energy Particles with Coulomb Field and Maxwell Equations Comp.Phys.Comm., 2019. Dr.Motohiko Tanaka, Chubu University*

a. Maxwell equations are solved,

$$(1/c)\partial \mathbf{B}/\partial t = -\nabla \times \mathbf{E}, \qquad (1)$$

$$(1/c)\partial \mathbf{E}/\partial t = \nabla \times \mathbf{B} - (4\pi/c)\sum_{i=1}^{N} q_i \mathbf{v}_i S(\mathbf{r}-\mathbf{r}_i), \qquad (2)$$

$$\nabla \cdot \mathbf{B} = 0, \qquad (3)$$

c is the speed of light, $\mathrm{B} = \mathbf{H}$ *in the CGS system*, q_i *is charge*, v_i *is velocity, and S is a shape function of particles.*

b. Coulomb field is a correction to the electric fiild, The true electric field (5) *is,*

$$-\nabla^2 \delta\varphi(\mathbf{r}) = 4\pi\rho(\mathbf{r}) - \nabla \cdot \breve{\mathbf{E}}(\mathbf{r}, t), \text{ RHS is not zero} \qquad (4)$$

$$\mathbf{E}(\mathbf{r}, t) = \breve{\mathbf{E}}(\mathbf{r}, t) - \nabla \delta\varphi(\mathbf{r}), \qquad (5)$$

c. The transverse electric field (7) *is separated from the longitudinal electric field* (6),

$$\nabla \cdot \mathbf{E}_L(\mathbf{r}) = 4\pi\rho(\mathbf{r}) = 4\pi\sum_{i=1}^{N} q_i S(\mathbf{r}-\mathbf{r}_i), \qquad (6)$$

$$\mathbf{E}_T(\mathbf{r},\ t) = \mathbf{E}(\mathbf{r},\ t) - \mathbf{E}_L(\mathbf{r}). \qquad (7)$$

d. Relativistic equations of motion $(\mathbf{r}_i, \mathbf{p}_i)$ *are solved for time advance of particles,*

$$d\mathbf{p}_i / dt = -\nabla\sum_{j=1}^{N} \left[q_i q_j / r_{ij} + \Phi(r_i, r_j) \right]$$

$$+ q_i \left[\mathbf{E}_T(\mathbf{r}_i, t) + (1/c)\mathbf{v}_i \times \mathbf{B}(\mathbf{r}_i, t) \right], \qquad (8)$$

$$d\mathbf{r}_i / dt = \mathbf{v}_i\ ,\ \mathbf{p}_i = m_i \mathbf{v}_i / \sqrt{1-(\mathbf{v}_i/c)^2} \qquad (9)$$

$\Phi(r_i, r_j)$ *is the LJ potential. Go to the step* (a) *for the next time step.*
The EM effects are set in for relativistic particles.