量子電磁力学に基づく時間空間分解シミュレーション方法の研究

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量子化学・分子科学　　時間依存Schrödinger(Dirac)方程式

+ 古典Maxwell方程式

Heisenberg描像で場の量子論(QED)を解く。　　cf.) 阿部・中西(1992)

量子場の運動方程式

Dirac方程式

$$i\hbar\frac{\partial}{\partial t}\hat{\psi}(x) = \left\{-i\hbar c\gamma^0\gamma^k\partial_k - (Z_e e)\sum_{k=1}^{3}\gamma^0\gamma^k\hat{A}^k(x) + m_e c^2\gamma^0 + (Z_e e)\hat{A}_0(x)\right\}\hat{\psi}(x)$$

Maxwell方程式

$$-\nabla^2\hat{A}_0(x) = 4\pi\hat{\rho}_e(x),$$

$$\frac{1}{c}\frac{\partial}{\partial t}\vec{\nabla}\hat{A}_0(x) + \left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \nabla^2\right)\hat{\vec{A}}(x) = \frac{4\pi}{c}\hat{\vec{j}}_e(x),$$

電荷密度演算子

$$\hat{\rho}_e(x) = Z_e e\hat{\bar{\psi}}(x)\gamma^0\hat{\psi}(x)$$

電流密度演算子

$$\hat{\vec{j}}_e(x) = Z_e\, e\, c\,\hat{\bar{\psi}}(x)\vec{\gamma}\hat{\psi}(x)$$

$$\left\{\hat{\psi}_\alpha(ct,\vec{r}), \hat{\psi}^\dagger_\beta(ct,\vec{s})\right\} = \delta^{(3)}(\vec{r}-\vec{s})\delta_{\alpha\beta}$$

$$\left\{\hat{\psi}_\alpha(ct,\vec{r}), \hat{\psi}_\beta(ct,\vec{s})\right\} = 0$$

$$\left\{\hat{\psi}^\dagger_\alpha(ct,\vec{r}), \hat{\psi}^\dagger_\beta(ct,\vec{s})\right\} = 0$$

$$\left[\hat{A}^i(ct,\vec{r}), \hat{A}^j(ct,\vec{s})\right] = 0,$$

$$\left[\hat{E}^i_T(ct,\vec{r}), \hat{E}^j_T(ct,\vec{s})\right] = 0,$$

$$\frac{1}{4\pi c}\left[\hat{A}^i(ct,\vec{r}), \hat{E}^j_T(ct,\vec{s})\right] = i\hbar\eta^{ij}\delta^{(3)}(\vec{r}-\vec{s}) + i\hbar\frac{\partial}{\partial r^i}\frac{\partial}{\partial r^j}\left(-\frac{1}{4\pi}\cdot\frac{1}{|\vec{r}-\vec{s}|}\right)$$

クーロンゲージを採用： $\mathrm{div}\hat{\vec{A}}(x) = 0$

$$\hat{\vec{E}}_T(x) = -\frac{1}{c}\frac{\partial\hat{\vec{A}}(x)}{\partial t}$$