Semiconductor Bloch Equation (SBE)

内容

1. multi-band SBEの導出
2. SBEを用いたHHGの計算(Huberらの手法)

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Semiconductor Hamiltonian

$$\hat{H} = \sum_{\lambda,k} \epsilon_k^\lambda \hat{a}^\dagger_{\lambda,k}\hat{a}_{\lambda,k} - E(t) \sum_{\lambda,\lambda',k} d_{\lambda,\lambda'}(k)\hat{a}^\dagger_{\lambda,k}\hat{a}_{\lambda',k} + i|e|E(t)\sum_{\lambda,k}\hat{a}^\dagger_{\lambda,k}\nabla_k\hat{a}_{\lambda,k} + \hat{V},$$

λはバンド指数、kは結晶運動量、aは生成演算子、E(t)は電場

ϵ_k^λ はエネルギー、dはdipole matrix $\boldsymbol{d}_{\lambda\lambda'} \equiv \frac{1}{\Omega}\int_\Omega \mathrm{d}r^3 \phi^*_\lambda(\boldsymbol{r}) e\boldsymbol{r}\phi_{\lambda'}(\boldsymbol{r})$

運動項

電場と電子の相互作用

$$\mathcal{H}_I = \int d^3r\, \hat{\psi}^\dagger(\mathbf{r})(-e\mathbf{r})\cdot\mathcal{E}(\mathbf{r},t)\hat{\psi}(\mathbf{r})$$

クーロン相互作用

$$\mathcal{H}_C = \frac{1}{2}\sum_{\alpha,\alpha'}\int d^3r\, d^3r'\, \rho_\alpha(\mathbf{r})\,\rho_{\alpha'}(\mathbf{r}')\,W(\mathbf{r}-\mathbf{r}')$$

$$= \frac{1}{2}\sum_{\substack{\mathbf{k},\mathbf{k}' \\ \mathbf{q}\neq 0 \\ s,s'}} \hat{a}^\dagger_{\mathbf{k}+\mathbf{q},s}\hat{a}^\dagger_{\mathbf{k}'-\mathbf{q},s'}\hat{a}_{\mathbf{k}',s'}\hat{a}_{\mathbf{k},s}V_{\mathbf{q}}$$

SBE の導出

①Heisenbergの方程式 $\frac{db}{dt} = \frac{i}{\hbar}[\mathcal{H}, b]$ を以下の演算子に適用する。

$\hat{a}^{\dagger}_{\lambda,k}\hat{a}_{\lambda',k}$ (λ≠λ') … 還元密度演算子の非対角成分

$\hat{a}^{\dagger}_{\lambda,k}\hat{a}_{\lambda,k}$ … 電子の個数演算子　　$a_{\lambda',\mathbf{k}}a^{\dagger}_{\lambda',\mathbf{k}}$ … 正孔の個数演算子

②得られた方程式の(アンサンブル平均?)をとる。以下の量を定義する。

$P^{\lambda,\lambda'}_{\mathbf{k}} \equiv \langle a^{\dagger}_{\lambda,\mathbf{k}}a_{\lambda',\mathbf{k}}\rangle$ …微視的な分極(microscopic polarization, pair function)

$f^{e,\lambda}_{\mathbf{k}} \equiv P^{\lambda,\lambda}_{\mathbf{k}} = \langle a^{\dagger}_{\lambda,\mathbf{k}}a_{\lambda,\mathbf{k}}\rangle$ … 伝導帯電子の占有数(occupation number)

$f^{h,\lambda'}_{\mathbf{k}} = \langle a_{\lambda',\mathbf{k}}a^{\dagger}_{\lambda',\mathbf{k}}\rangle = 1 - \langle a^{\dagger}_{\lambda',\mathbf{k}}a_{\lambda',\mathbf{k}}\rangle = 1 - P^{\lambda',\lambda'}_{\mathbf{k}}$ … 価電子帯正孔の占有数

③ fについてエネルギー緩和(relaxation)を導入し、pについて位相緩和(dephasing)を導入する。

[HHG電場] $E_{\mathrm{HHG}}(t) \propto \frac{\partial}{\partial t}P(t) + J(t)$　　[分極] $P_j = \sum_{\lambda,\lambda',k} d^{\lambda\lambda'}_{k}\, p^{\lambda\lambda'}_{k,j},$

[電流] $J(t) = \sum_{\lambda,k} j_{\lambda}(k) f^{\lambda}_{k} = \sum_{k}\left[\sum_{e_\lambda} j_{e_\lambda}(k) f^{e_\lambda}_{k} + \sum_{h_\lambda} j_{h_\lambda}(k) f^{\lambda_\lambda}_{k}\right]$, $j_{\lambda}(k) = \frac{|e|}{\hbar}\nabla_{k}\epsilon^{\lambda}_{k}$

SBE (占有数) ...クーロン相互作用を省略したもの

[伝導帯の電子]

$\Omega_{k,j}^{\lambda\lambda'} = d_k^{\lambda\lambda'} E_j(t)$ はRabiエネルギー

$$\hbar \frac{\partial}{\partial t} f_{k,j}^{\mathrm{e}_i} = -2\mathrm{Im}\left[\sum_{e_\lambda \neq e_i} \Omega_{k,j}^{\mathrm{e}_i \mathrm{e}_\lambda} \left(p_{k,j}^{\mathrm{e}_\lambda \mathrm{e}_i}\right)^* + \sum_{h_\lambda} \Omega_{k,j}^{\mathrm{e}_i \mathrm{h}_\lambda} \left(p_{k,j}^{\mathrm{h}_\lambda \mathrm{e}_i}\right)^*\right] + |e| E_j(t) \nabla_k f_{k,j}^{\mathrm{e}_i} + \Gamma_{k,j}^{\mathrm{e}_i},$$

電場と相互作用

バンド間遷移

緩和

バンド内遷移

(電場中の電子の運動)

[価電子帯の正孔]

$$\hbar \frac{\partial}{\partial t} f_{k,j}^{\mathrm{h}_i} = -2\mathrm{Im}\left[\sum_{h_\lambda \neq h_i} \Omega_{k,j}^{\mathrm{h}_\lambda \mathrm{h}_i} \left(p_{k,j}^{\mathrm{h}_i \mathrm{h}_\lambda}\right)^* + \sum_{e_\lambda} \Omega_{k,j}^{\mathrm{e}_\lambda \mathrm{h}_i} \left(p_{k,j}^{\mathrm{h}_i \mathrm{e}_\lambda}\right)^*\right] + |e| E_j(t) \nabla_k f_{k,j}^{\mathrm{h}_i} + \Gamma_{k,j}^{\mathrm{h}_i},$$

SBE (分極)…クーロン相互作用を省略したもの

[伝導帯↔価電子帯]

バンド内遷移
(のようなもの?)

(直接)バンド間遷移

$$\mathrm{i}\hbar\frac{\partial}{\partial t}p_{k,j}^{\mathrm{h}_i\mathrm{e}_l}=\left(\mathcal{E}_k^{\mathrm{h}_i\mathrm{e}_l}+\mathrm{i}|e|E_j(t)\nabla_k\right)p_{k,j}^{\mathrm{h}_i\mathrm{e}_l}-\Omega_{k,j}^{\mathrm{e}_l\mathrm{h}_i}\left(1-f_{k,j}^{\mathrm{e}_l}-f_{k,j}^{\mathrm{h}_i}\right)+\Gamma_{k,j}^{\mathrm{h}_i\mathrm{e}_l}$$

位相緩和

$$+\sum_{e_\lambda\neq e_l}\left[\Omega_{k,j}^{\mathrm{e}_\lambda\mathrm{h}_i}p_{k,j}^{\mathrm{e}_\lambda\mathrm{e}_l}-\Omega_{k,j}^{\mathrm{e}_l\mathrm{e}_\lambda}p_{k,j}^{\mathrm{h}_i\mathrm{e}_\lambda}\right]+\sum_{h_\lambda\neq h_i}\left[\Omega_{k,j}^{\mathrm{h}_\lambda\mathrm{h}_i}p_{k,j}^{\mathrm{h}_\lambda\mathrm{e}_l}-\Omega_{k,j}^{\mathrm{e}_l\mathrm{h}_\lambda}p_{k,j}^{\mathrm{h}_i\mathrm{h}_\lambda}\right],$$

運動項由来

電場と相互作用

$\mathcal{E}_k^{\lambda\lambda'}$ はバンド間の遷移エネルギー

(間接)バンド間遷移

[伝導帯↔伝導帯]

$$\mathrm{i}\hbar\frac{\partial}{\partial t}p_{k,j}^{\mathrm{e}_i\mathrm{e}_l}=\left(\mathcal{E}_k^{\mathrm{e}_i\mathrm{e}_l}+\mathrm{i}|e|E_j(t)\nabla_k\right)p_{k,j}^{\mathrm{e}_i\mathrm{e}_l}+\Omega_{k,j}^{\mathrm{e}_l\mathrm{e}_i}\left(f_{k,j}^{\mathrm{e}_l}-f_{k,j}^{\mathrm{e}_i}\right)+\Gamma_{k,j}^{\mathrm{e}_i\mathrm{e}_l}+\sum_{e_\lambda\neq e_l}\Omega_{k,j}^{\mathrm{e}_\lambda\mathrm{e}_i}p_{k,j}^{\mathrm{e}_\lambda\mathrm{e}_l}$$
$$-\sum_{e_\lambda\neq e_i}\Omega_{k,j}^{\mathrm{e}_l\mathrm{e}_\lambda}p_{k,j}^{\mathrm{e}_i\mathrm{e}_\lambda}+\sum_{h_\lambda}\left[\Omega_{k,j}^{\mathrm{h}_\lambda\mathrm{e}_i}p_{k,j}^{\mathrm{h}_\lambda\mathrm{e}_l}-\Omega_{k,j}^{\mathrm{e}_l\mathrm{h}_\lambda}\left(p_{k,j}^{\mathrm{h}_\lambda\mathrm{e}_i}\right)^*\right],$$

[価電子帯↔価電子帯]

$$\mathrm{i}\hbar\frac{\partial}{\partial t}p_{k,j}^{\mathrm{h}_i\mathrm{h}_l}=\left(\mathcal{E}_k^{\mathrm{h}_i\mathrm{h}_l}+\mathrm{i}|e|E_j(t)\nabla_k\right)p_{k,j}^{\mathrm{h}_i\mathrm{h}_l}+\Omega_{k,j}^{\mathrm{h}_l\mathrm{h}_i}\left(f_{k,j}^{\mathrm{h}_i}-f_{k,j}^{\mathrm{h}_l}\right)+\Gamma_{k,j}^{\mathrm{h}_i\mathrm{h}_l}+\sum_{h_\lambda\neq h_l}\Omega_{k,j}^{\mathrm{h}_\lambda\mathrm{h}_i}p_{k,j}^{\mathrm{h}_\lambda\mathrm{h}_l}$$
$$-\sum_{h_\lambda\neq h_i}\Omega_{k,j}^{\mathrm{h}_l\mathrm{h}_\lambda}p_{k,j}^{\mathrm{h}_i\mathrm{h}_\lambda}+\sum_{e_\lambda}\left[\Omega_{k,j}^{\mathrm{e}_\lambda\mathrm{h}_i}\left(p_{k,j}^{\mathrm{h}_l\mathrm{e}_\lambda}\right)^*-\Omega_{k,j}^{\mathrm{h}_l\mathrm{e}_\lambda}p_{k,j}^{\mathrm{h}_i\mathrm{e}_\lambda}\right],$$

参考にした教科書

・Hartmut Haug, and Stephan W. Koch, “Quantum Theory of the Optical and Electronic Properties of Semiconductors”, Chap. 5, 7, 10, 12.

・Mackillo Kira, and Stephan W. Koch,“Semiconductor Quantum Optics” Chap. 18, 24 -26

参考にした論文

・F. Langer et. al., “Symmetry-controlled temporal structure of high-harmonic carrier fields from a bulk crystal,” Nature Photonics 11, 227 (2017).

・M. Hohenleutner et. al., “Real-time observation of interfering crystal electrons in high-harmonic generation”, Nature 523, 572 (2015).

multi-band SBEを用いたHHGの計算(Huberらの手法)

[dipole transition matrix]

・oscillator strength? $f_{CB} = 2|P_{CB}|^2/(m_0\hbar\omega)$.

A. Segura et al., "Strong optical nonlinearities in gallium and indium selenides related to inter-valence-band transitions induced by light pulses," PRB 56 , 15 (1997)

…GaSeでd_h1↔h2は、d_h1↔eやd_h2↔eに比べて10倍くらい大きい

・parity of single particle eigenfunctions

[バンド構造]

・refined tight binding model (1D); effective mass, band width/gap

D Golde et al., "Microscopic theory of the extremely nonlinear terahertz response of semiconductors," Phys. Status Solidi B 248, 863 (2011)

[位相/エネルギー緩和]

・constant dephasing (1.1 fs)

・constant relaxation towards distributions with even parity (6 fs)

Schuh K. et al., "Influence of many-body interactions during the ionization of gases by short intense optical pulse," Phys. Status Solidi B 248, 863 (2011)