

Advanced Plasma and Laser Science プラズマ・レーザー特論E

Quick review of quantum mechanics and Rabi oscillation 量子力学の復習とラビ振動

Kenichi Ishikawa

downloadable from ITC-LMS and

<http://ishiken.free.fr/english/lecture.html>

ishiken@n.t.u-tokyo.ac.jp



Hydrogen atom 水素原子の波動関数

Atomic unit 原子単位

Rabi oscillation ラビ振動

Hydrogen-like atom

水素原子の波動関数

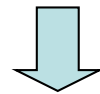
Schrödinger equation シュレーディンガー方程式

Particle of mass m moving in a potential $V(\mathbf{r})$

ポテンシャル $V(\mathbf{r})$ 中の質量 m の電子

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi(\mathbf{r}, t) + V(\mathbf{r})\psi(\mathbf{r}, t)$$

$\psi(\mathbf{r}, t)$: Wave function
: 波動関数



$\psi(\mathbf{r}, t) = \varphi(\mathbf{r})e^{-i\omega t}$ steady state 定常状態

$$-\frac{\hbar^2}{2m} \nabla^2 \varphi(\mathbf{r}) + V(\mathbf{r})\varphi(\mathbf{r}) = \varepsilon \varphi(\mathbf{r})$$

Eigenvalue problem 固有値問題

$\varepsilon = \hbar\omega$: Energy eigenvalue エネルギー固有値 (エネルギー準位)

$\varphi(\mathbf{r})$: Eigen function 固有波動関数

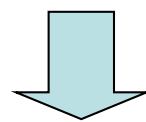
Hydrogen-like atom 水素様原子

Bare Coulomb potential from the nucleus

原子核のクーロンポテンシャル $V(\mathbf{r}) = V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r}$

(Time-independent Schrödinger equation) シュレーディンガー方程式

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{r}) - \frac{Ze^2}{4\pi\epsilon_0 r}\varphi(\mathbf{r}) = \epsilon\varphi(\mathbf{r})$$



cumbersome coefficients
係数が煩雑

Introduction of **atomic unit (a.u.)** 原子単位の導入

$$-\frac{1}{2}\nabla^2\varphi(\mathbf{r}) - \frac{Z}{r}\varphi(\mathbf{r}) = \epsilon\varphi(\mathbf{r})$$

Atomic unit 原子単位

Electron 電子

Unit system in which $\hbar = m = e = \frac{e^2}{4\pi\epsilon_0} = 1$ となるような単位系

Length
長さ

$$a_0 = \frac{\hbar^2}{m \left(\frac{e^2}{4\pi\epsilon_0} \right)} = \frac{4\pi\epsilon_0 \hbar^2}{me^2} = 5.292 \times 10^{-11} \text{ m}$$

Bohr radius
ボーア半径

Energy
エネルギー

$$\frac{e^2}{4\pi\epsilon_0 a_0} = 27.21 \text{ eV} \quad \text{2} \times (\text{ionization potential of H})$$

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

Time
時間

$$\frac{\hbar^3}{m \left(\frac{e^2}{4\pi\epsilon_0} \right)^2} = \frac{a_0}{\alpha c} = 0.0242 \text{ fs}$$

fine structure constant

$$\alpha = \frac{e^2}{4\pi\epsilon_0 c \hbar} = 7.297 \times 10^{-3} = \frac{1}{137.0} \quad \text{微細構造定数}$$

Velocity
速度

$$a_0 \div \frac{a_0}{\alpha c} = \alpha c$$

Atomic scale of length,
energy, and time

Atomic unit is closely related to Bohr hydrogen atom

Dimension	Expression	Value	Meaning
length	$a_0 = 4\pi\epsilon_0\hbar^2/me^2$	5.29×10^{-11} m	Bohr radius
energy	$E_h = \frac{me^4}{(4\pi\epsilon_0\hbar)^2} = \frac{e^2}{4\pi\epsilon_0 a_0}$	27.2 eV	Coulomb potential energy at the Bohr radius
velocity	$v = \frac{e^2}{4\pi\epsilon_0\hbar} = c\alpha$	2.19×10^6 m/s	electron orbital velocity
time	$\frac{\hbar}{E_h} = \frac{a_0}{v}$	24.2 attoseconds	time during which the electron proceeds 1 radian
electric field	$F = \frac{e}{4\pi\epsilon_0 a_0^2}$	5.14×10^{11} V/m	field at the Bohr radius
laser intensity	$\frac{1}{2}c\epsilon_0 F^2$	3.51×10^{16} W/cm ²	laser field = electric field at the Bohr radius

Hydrogen-like atom 水素様原子

Bare Coulomb potential from the nucleus

原子核のクーロンポテンシャル $V(\mathbf{r}) = V(r) = -\frac{Ze^2}{4\pi\epsilon_0 r} = -\frac{Z}{r}$

(Time-independent Schrödinger equation) シュレーディンガー方程式

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{r}) - \frac{Ze^2}{4\pi\epsilon_0 r}\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r}) \quad -\frac{1}{2}\nabla^2\varphi(\mathbf{r}) - \frac{Z}{r}\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r})$$

Polar coordinate 極座標系 $\mathbf{r} = (r, \theta, \phi)$

Bound state 束縛状態 $\varepsilon < 0$

Energy eigenvalue
エネルギー固有値

$$\varepsilon_n = -\frac{Z^2 m e^4}{(4\pi\epsilon_0)^2 2\hbar^2} \frac{1}{n^2} = -\frac{Z^2}{2n^2} \quad n = 1, 2, 3, \dots$$

Eigen function
固有波動関数

$$\varphi(\mathbf{r}) = R_{nl}(r)Y_{lm}(\theta, \phi) \quad 0 \leq l \leq n-1 \quad -l \leq m \leq l$$

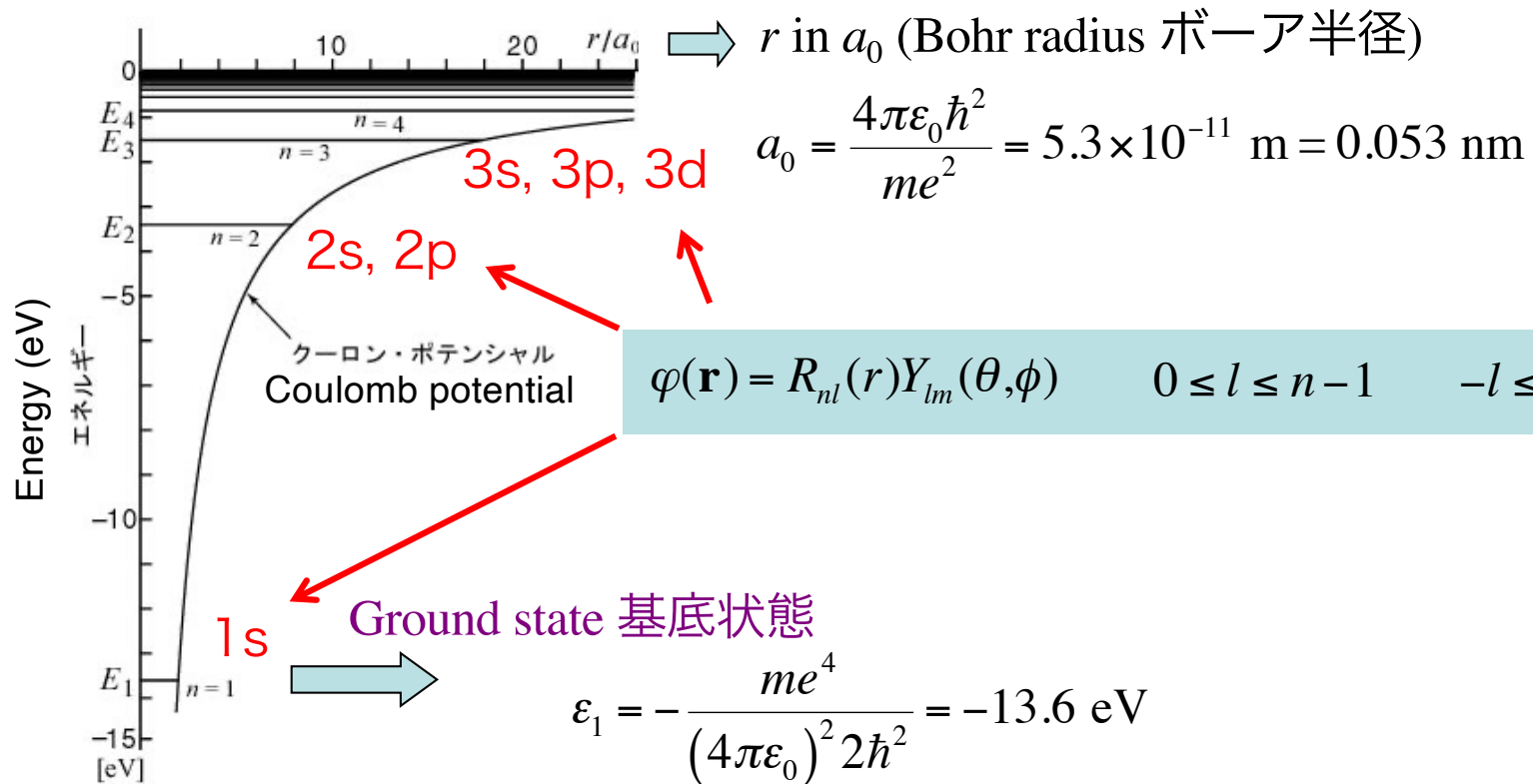
Radial wave function
動径波動関数

Spherical harmonics 球面調和関数

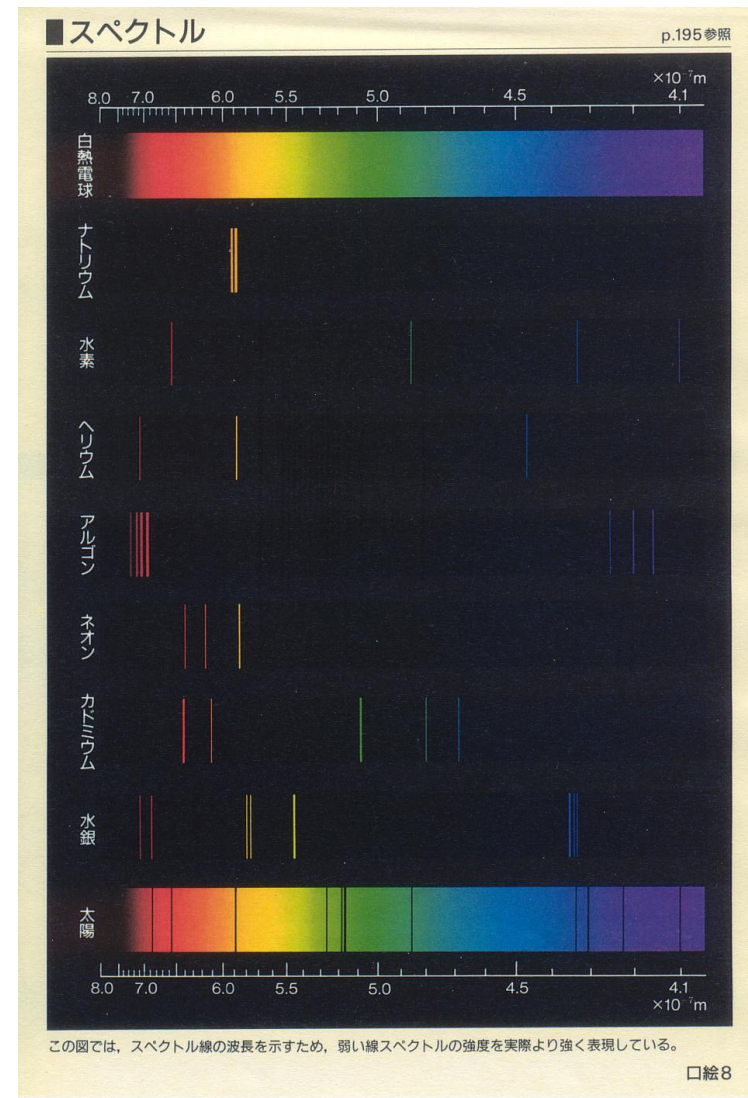
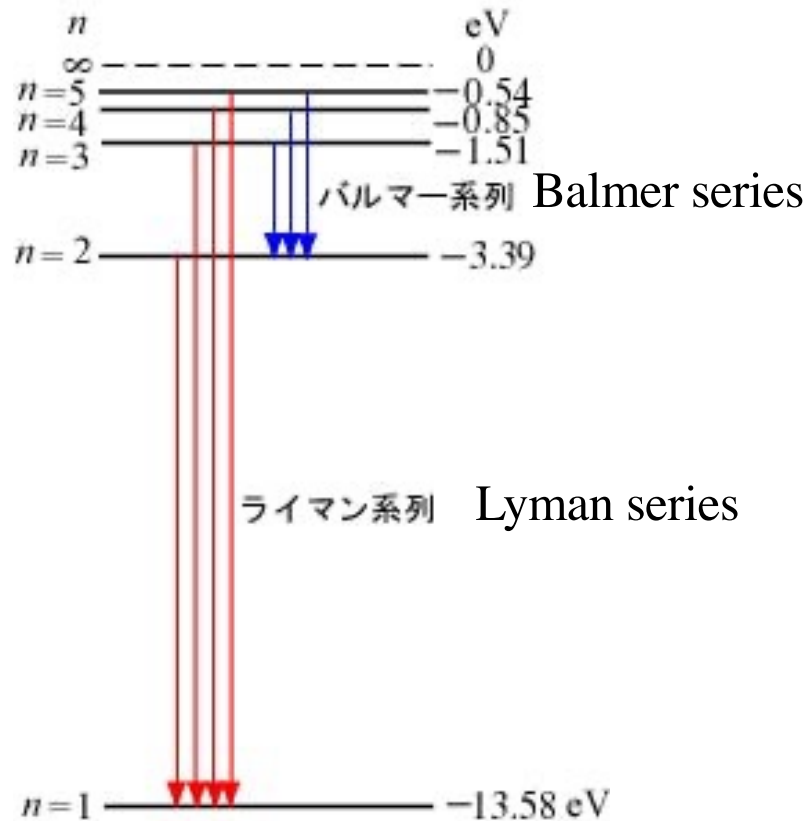
Bound states 束縛状態

Energy eigenvalue
エネルギー固有値

$$\varepsilon_n = -\frac{Z^2 m e^4}{(4\pi\epsilon_0)^2 2\hbar^2} \frac{1}{n^2} = -\frac{Z^2}{2n^2} \quad n=1,2,3\ldots$$



Energy eigenvalue
エネルギー固有値 $\varepsilon_n = -\frac{Z}{2n^2} \quad n = 1, 2, 3 \dots$



Radial wave function and spherical harmonics

動径波動関数と球面調和関数

$Z = 1$ の場合

$$R_{1s} = \left(\frac{1}{a_0}\right)^{3/2} 2e^{-r/a_0}$$

$$R_{2s} = \left(\frac{1}{a_0}\right)^{3/2} \frac{1}{\sqrt{2}} e^{-r/2a_0} \left(1 - \frac{r}{2a_0}\right)$$

$$R_{2p} = \left(\frac{1}{a_0}\right)^{3/2} \frac{1}{2\sqrt{6}} e^{-r/2a_0} \frac{r}{a_0}$$

$$R_{3s} = \left(\frac{1}{a_0}\right)^{3/2} \frac{2}{3\sqrt{3}} e^{-r/3a_0} \left[1 - \frac{2}{3} \frac{r}{a_0} + \frac{2}{27} \left(\frac{r}{a_0}\right)^2\right]$$

Orthonormality 規格直交性

$$\int_0^\infty R_{nl}^*(r) R_{n'l'}(r) r^2 dr = \delta_{nn'}$$

$$\int \varphi_{nlm}^* \varphi_{n'l'm'} r^2 \sin\theta dr d\theta d\phi = \delta_{nn'} \delta_{ll'} \delta_{mm'}$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta \quad Y_{1,\pm 1} = \mp \sqrt{\frac{3}{8\pi}} \sin\theta e^{\pm i\phi}$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$$

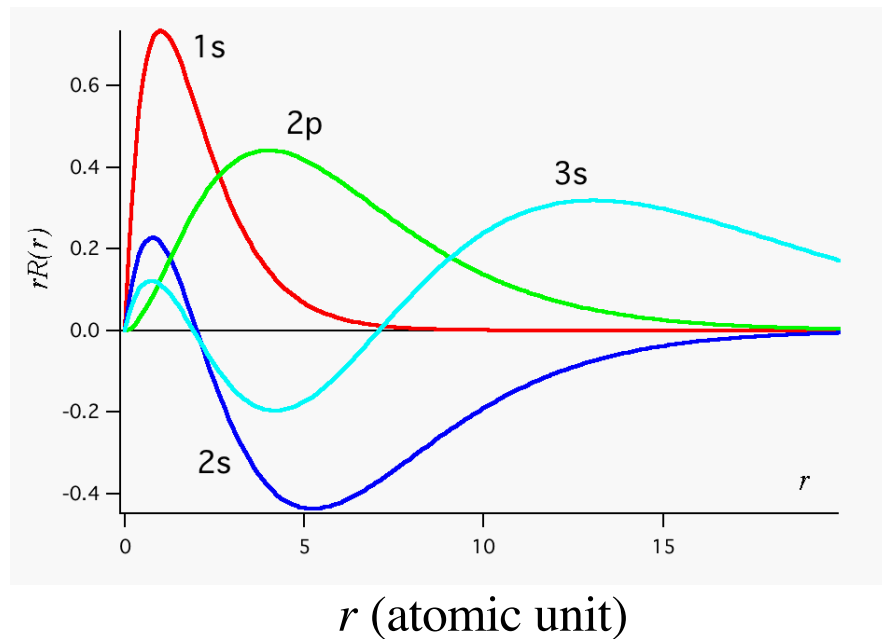
$$Y_{2,\pm 1} = \mp \sqrt{\frac{15}{8\pi}} \sin\theta \cos\theta e^{\pm i\phi}$$

$$Y_{2,\pm 2} = \sqrt{\frac{15}{32\pi}} \sin^2\theta e^{\pm 2i\phi}$$

Orthonormality 規格直交性

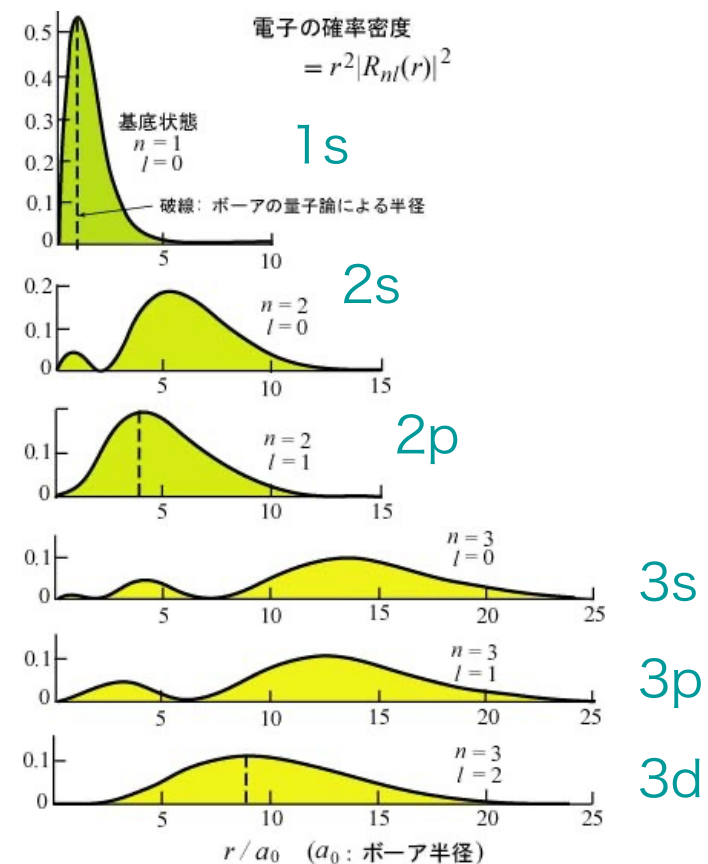
$$\int Y_{lm}^*(\theta, \phi) Y_{l'm'}(\theta, \phi) \sin\theta d\theta d\phi = \delta_{ll'} \delta_{mm'}$$

Radial wave function 動径波動関数



Probability density

存在確率密度



Continuum states 自由状態、連続状態

$$\varepsilon > 0$$

Necessary when ionization is considered イオン化を考慮するときが必要

$$\varepsilon > 0$$

Arbitrary positive number 任意の正の実数

$$\varphi(\mathbf{r}) = R_{\varepsilon l}(r) Y_{lm}(\theta, \phi) \quad l \geq 0 \quad -l \leq n \leq l$$

Radial wave function 動径波動関数 → Coulomb wave function クーロン波動関数

$$R_{\varepsilon l}(r) = \frac{2\sqrt{Z}}{\sqrt{1 - e^{-2\pi n'}}} \prod_{s=1}^l \sqrt{s^2 + n'^2} \frac{(2kr)^l}{(2l+1)!} e^{-ikr} F(in' + l + 1, 2l + 2, 2ikr)$$

confluent hypergeometric function
合流型超幾何関数

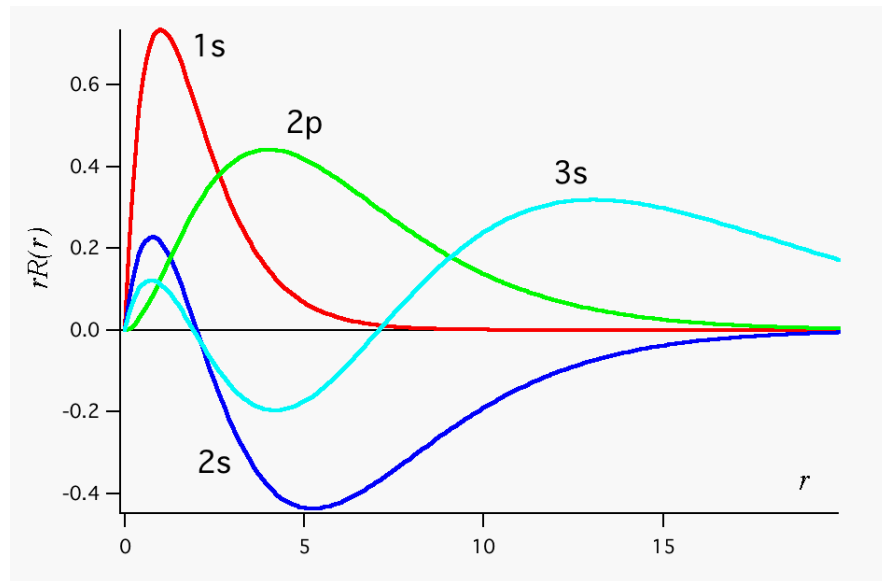
wave number 波数 $k = \sqrt{2mE}/\hbar = \sqrt{2E}$ $n' = \frac{Z}{k}$

$$\varepsilon \neq \varepsilon' \Rightarrow \int_0^\infty R_{\varepsilon l}^*(r) R_{\varepsilon' l}(r) r^2 dr = 0$$

$$\int_0^\infty |R_{\varepsilon l}(r)|^2 r^2 dr > 0 \Rightarrow \text{Density of states 状態密度}$$

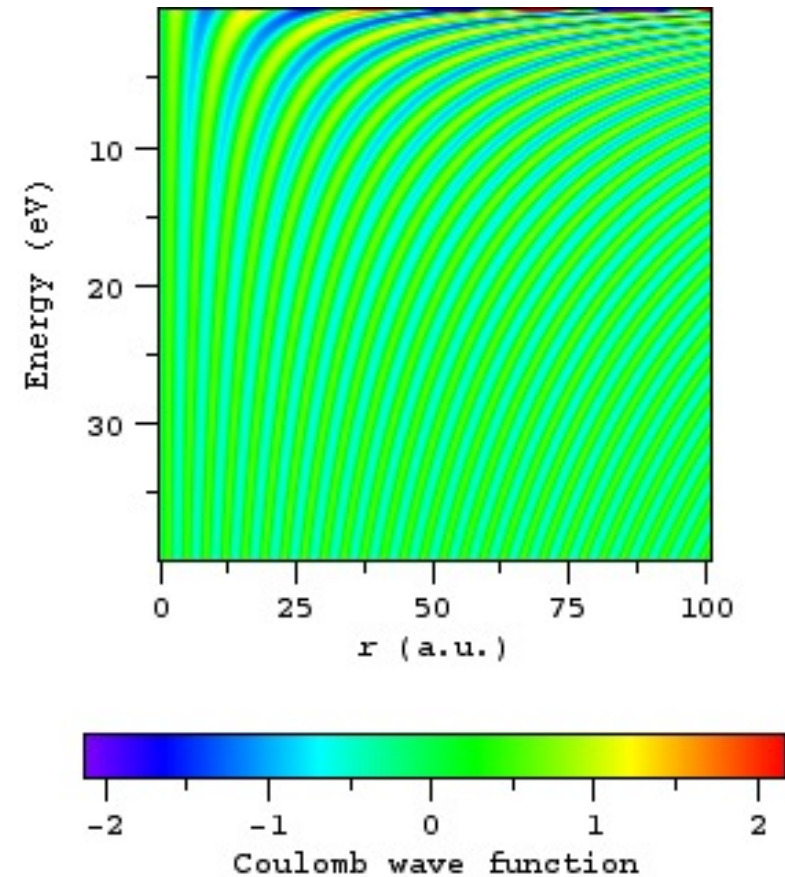
Radial wave function 動径波動関数

Bound states 束縛状態



r の単位は a_0 (ボーア半径)

Continuum states 自由状態 (連続状態)



Coulomb wave function vs. electron in a free space $V(r)=0$ クーロン波動関数と自由空間の電子波動関数のとの比較

$$V(r)=0 \quad \longrightarrow \quad -\frac{1}{2}\nabla^2\varphi(\mathbf{r})=\varepsilon\varphi(\mathbf{r}) \quad \longrightarrow \quad -\frac{1}{2}\left[\frac{d^2}{dr^2}+\frac{2}{r}\frac{d}{dr}-\frac{l(l+1)}{r^2}\right]R(r)=\varepsilon R(\mathbf{r})$$

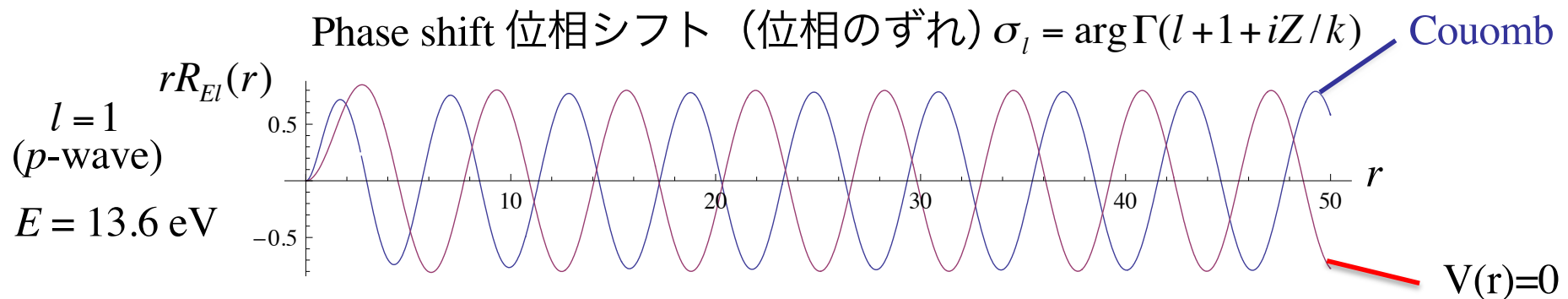
In a free space

$$R_{El}(r)=\sqrt{\frac{2k}{\pi}}j_l(kr)\xrightarrow{r\rightarrow\infty}\sqrt{\frac{2}{\pi k}}\frac{1}{r}\cos\left[kr-\frac{\pi}{2}(l+1)\right]$$

Spherical Bessel function

Coulomb wave function

$$R_{El}(r)\xrightarrow{r\rightarrow\infty}\sqrt{\frac{2}{\pi k}}\frac{1}{r}\cos\left[kr+\frac{Z}{k}\log 2kr-\frac{\pi}{2}(l+1)-\sigma_l\right]$$



Short-range potential $V(r) = 0$ at $r > r_0$

短距離ポテンシャル

$$V(r) = 0 \quad r > r_0 \quad \Rightarrow \quad -\frac{1}{2}\nabla^2\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r}) \quad \Rightarrow \quad -\frac{1}{2}\left[\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2}\right]R(r) = \varepsilon R(r)$$

$$R_{El}(r) = \sqrt{\frac{2k}{\pi}} (c_j j_l(kr) + c_y y_l(kr))$$

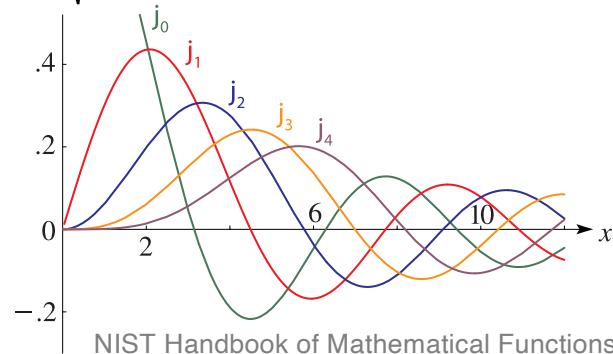


Figure 10.48.1: $j_n(x)$, $n = 0(1)4$, $0 \leq x \leq 12$.

Spherical Bessel function

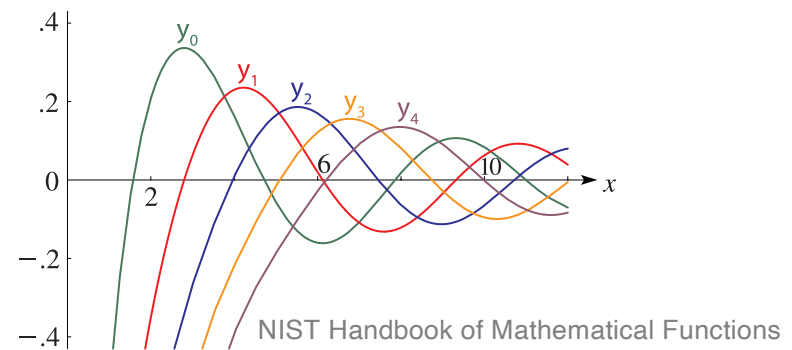


Figure 10.48.2: $y_n(x)$, $n = 0(1)4$, $0 < x \leq 12$.

$$j_l(kr) \xrightarrow{r \rightarrow 0} \frac{(kr)^l}{(2l+1)!!} \xrightarrow{r \rightarrow \infty} \frac{1}{kr} \cos\left[kr - \frac{\pi}{2}(l+1)\right]$$

$$y_l(kr) \xrightarrow{r \rightarrow 0} -\frac{(2l-1)!!}{(kr)^{l+1}} \xrightarrow{r \rightarrow \infty} \frac{1}{kr} \sin\left[kr - \frac{\pi}{2}(l+1)\right]$$

Phase shift 位相シフト (位相のずれ)

Temporal evolution by an external field

外場との相互作用による時間発展

$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi(\mathbf{r},t) - \frac{Z}{r}\psi(\mathbf{r},t) + \underline{V_I(\mathbf{r},t)\psi(\mathbf{r},t)}$$

相互作用 Interaction

$$i\frac{\partial\psi}{\partial t} = (H_0 + H_I)\psi(\mathbf{r},t) \quad H_0 = -\frac{1}{2}\nabla^2 - \frac{Z}{r} \quad H_I = V_I(\mathbf{r},t)$$

Without the external field 相互作用項がない場合

$$H_0\varphi_n(\mathbf{r}) = \varepsilon_n\varphi_n(\mathbf{r}) \quad \psi_n(\mathbf{r},t) = \varphi_n(\mathbf{r})e^{-i\omega_nt} \quad \omega_n = \frac{\varepsilon_n}{\hbar} \quad \text{Eigen state 固有状態}$$

With the external field 相互作用項がある場合

$$\psi(\mathbf{r},t) = \sum_n c_n \varphi_n(\mathbf{r}) e^{-i\omega_nt} \quad c_n = e^{i\omega_nt} \int \varphi_n^*(\mathbf{r}) \psi(\mathbf{r},t) dV = e^{i\omega_nt} \langle n | \psi \rangle$$

$$H_0 |n\rangle = \omega_n |n\rangle \quad (\text{atomic unit})$$

$$i\frac{\partial}{\partial t}|\psi\rangle = (H_0 + H_I)|\psi\rangle \qquad \langle n|\psi\rangle = c_n e^{-i\omega_n t}$$

$$\Rightarrow i\frac{\partial}{\partial t}\langle n|\psi\rangle = \langle n|H_0 + H_I|\psi\rangle = \langle n|H_0|\psi\rangle + \langle n|H_I|\psi\rangle = \omega_n \langle n|\psi\rangle + \langle n|H_I|\psi\rangle$$

$$\Rightarrow i\dot{c}_n = \langle n|H_I|\psi\rangle e^{i\omega_n t} \qquad \sum_m |m\rangle\langle m| = I \quad \text{Identity operator 単位演算子 can be inserted anywhere}$$

$$\Rightarrow i\dot{c}_n = \sum_m \langle n|H_I|m\rangle\langle m|\psi\rangle e^{i\omega_n t} = \sum_m \langle n|H_I|m\rangle c_m e^{i(\omega_n - \omega_m)t}$$

$$i\dot{c}_n = \sum_m \langle n|H_I|m\rangle c_m e^{i(\omega_n - \omega_m)t}$$

$\langle n|H_I|m\rangle$ **Transition matrix element 遷移行列要素**

Image イメージ

Transition from m to n due to the interaction H_I
 状態 m が相互作用 H_I によって状態 n に遷移する
 The interaction H_I couples m to n .

Important example: Rabi oscillation

重要な例：ラビ振動

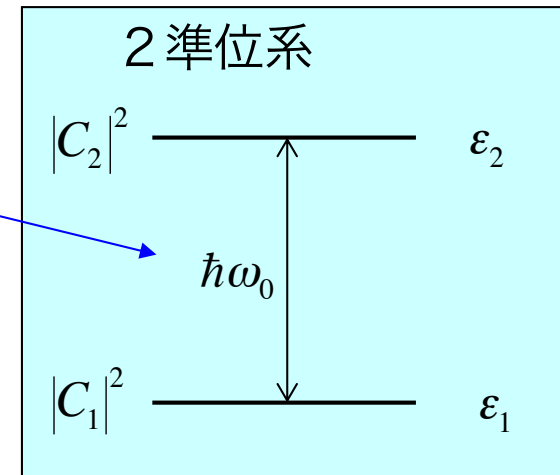
Resonance frequency 遷移振動数（共鳴振動数）

$$\hbar\omega_0 = \varepsilon_2 - \varepsilon_1$$

Two-level atom 2 準位系

If the laser frequency ω is close to ω_0 , only the two levels are relevant.

光の振動数が ω_0 に近いときは、放射過程に関与するのは選ばれた二つの原子状態のみ。



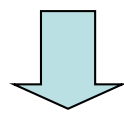
$$\psi(\mathbf{r}, t) = C_1(t)\psi_1(\mathbf{r}, t) + C_2(t)\psi_2(\mathbf{r}, t)$$

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \nabla^2 \psi(\mathbf{r}, t) - \frac{Z}{r} \psi(\mathbf{r}, t) + V_I(\mathbf{r}, t) \psi(\mathbf{r}, t)$$

$$\psi(\mathbf{r}, t) = C_1(t) \psi_1(\mathbf{r}, t) + C_2(t) \psi_2(\mathbf{r}, t)$$

$$\int |\psi(\mathbf{r}, t)|^2 d^3 \mathbf{r} = |C_1(t)|^2 + |C_2(t)|^2 = 1$$

$$V_I(C_1 \psi_1 + C_2 \psi_2) = i \left(\frac{\partial C_1}{\partial t} \psi_1 + \frac{\partial C_2}{\partial t} \psi_2 \right)$$



multiply with ψ_1^* from the left and take a volume integral

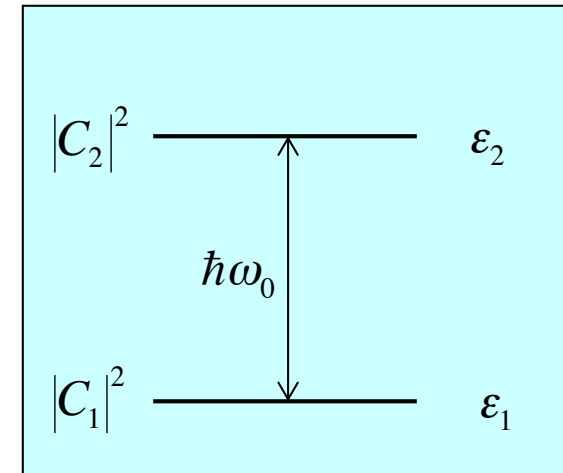
ψ_1^* を左からかけて空間積分

$$i \frac{\partial C_1}{\partial t} = C_1 V_{11} + C_2 V_{12} e^{-i\omega_0 t}$$

$$i \frac{\partial C_2}{\partial t} = C_1 e^{i\omega_0 t} V_{21} + C_2 V_{22}$$

Similarly
同様に

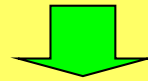
$$V_{ij} = \langle i | V_I | j \rangle = \int \varphi_i^* V_I \varphi_j d^3 \mathbf{r}$$



Interaction Hamiltonian

相互作用ハミルトニアン

Complete Hamiltonian for the interaction of an atom with an electromagnetic field is rather complicated. 電磁場と原子の間の相互作用に対するハミルトニアンの完全な形は複雑



Dipole approximation is often sufficient. レーザーに関しては、多くの場合、電気双極子近似で十分

Wave number 波数 $k = \frac{2\pi}{\lambda}$ — Wavelength 波長

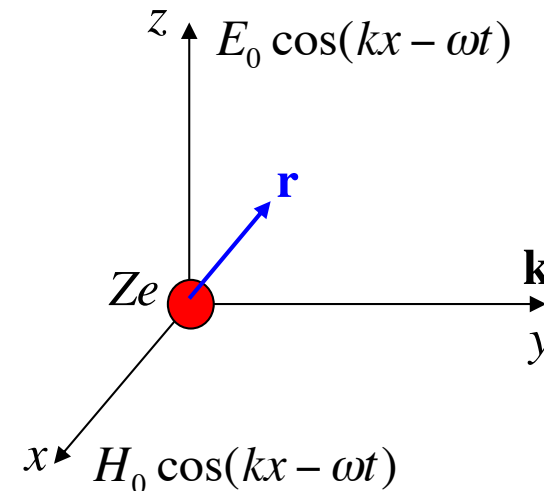
$$x \ll \lambda \Rightarrow kx \ll 1$$

$$E_0 \cos(kx - \omega t) \Rightarrow E_0 \cos \omega t$$

$$V_I = zE_0 \cos \omega t$$

(原子単位)

Dipole approximation
電気双極子近似



How V_I couples the two levels.

「 V_I のおかげで $j \rightarrow i$ に遷移する」割合

$$V_{ij} = \langle i | V_I | j \rangle = \int \varphi_i^* V_I \varphi_j d^3 \mathbf{r}$$

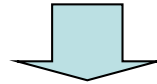
$$V_I = z E_0 \cos \omega t$$

$$i \frac{\partial C_1}{\partial t} = C_1 V_{11} + C_2 V_{12} e^{-i\omega_0 t}$$

$$i \frac{\partial C_2}{\partial t} = C_1 e^{i\omega_0 t} V_{21} + C_2 V_{22}$$

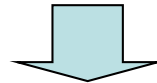
$$V_{ij} = \langle i | V_I | j \rangle = \int \varphi_i^* V_I \varphi_j d^3 \mathbf{r} = \cos \omega t \int z E_0 \varphi_i^* \varphi_j d^3 \mathbf{r} = X_{ij} \cos \omega t$$

$$X_{11} = X_{22} = 0 \quad X_{12} = X_{21} = 2\gamma \quad (\text{Real 実数})$$



$$i \frac{\partial C_1}{\partial t} = 2\gamma C_2 e^{-i\omega_0 t} \cos \omega t$$

$$i \frac{\partial C_2}{\partial t} = 2\gamma C_1 e^{i\omega_0 t} \cos \omega t$$



$$i \frac{\partial C_1}{\partial t} = \gamma C_2 \left[e^{i(\omega - \omega_0)t} + e^{-i(\omega + \omega_0)t} \right]$$

$$i \frac{\partial C_2}{\partial t} = \gamma C_1 \left[e^{i(\omega + \omega_0)t} + e^{-i(\omega - \omega_0)t} \right]$$

Rabi oscillation ラビ振動

$$i \frac{\partial C_1}{\partial t} = \gamma C_2 \left[e^{i(\omega - \omega_0)t} + e^{-i(\omega + \omega_0)t} \right]$$

$$i \frac{\partial C_2}{\partial t} = \gamma C_1 \left[e^{i(\omega + \omega_0)t} + e^{-i(\omega - \omega_0)t} \right]$$

回転波近似 $\Downarrow$ Rotating wave approximation

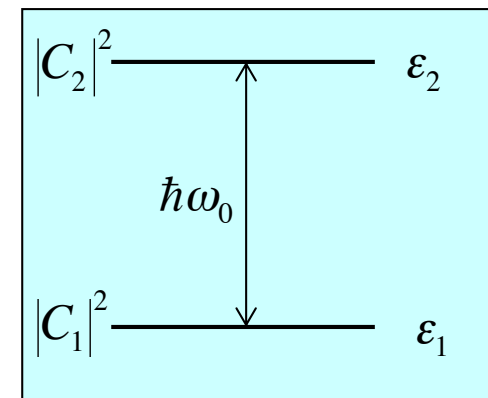
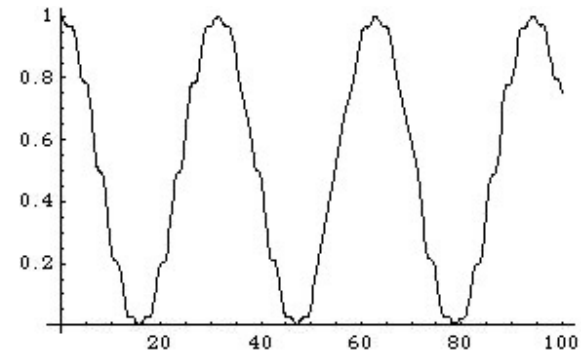
$$i \frac{\partial C_1}{\partial t} = \gamma e^{i(\omega - \omega_0)t} C_2 \quad i \frac{\partial C_2}{\partial t} = \gamma e^{-i(\omega - \omega_0)t} C_1$$

Initial condition

初期条件 $C_1 = 1, C_2 = 0$ $\Downarrow$

$$C_1(t) = \left(\cos \Omega t - \frac{i(\omega - \omega_0)}{2\Omega} \sin \Omega t \right) \exp \left[\frac{i}{2} (\omega - \omega_0) t \right]$$

$$C_2(t) = -\frac{i\gamma}{\Omega} \sin \Omega t \exp \left[-\frac{i}{2} (\omega - \omega_0) t \right] \quad \Omega = \sqrt{\gamma^2 + \frac{(\omega - \omega_0)^2}{4}}$$



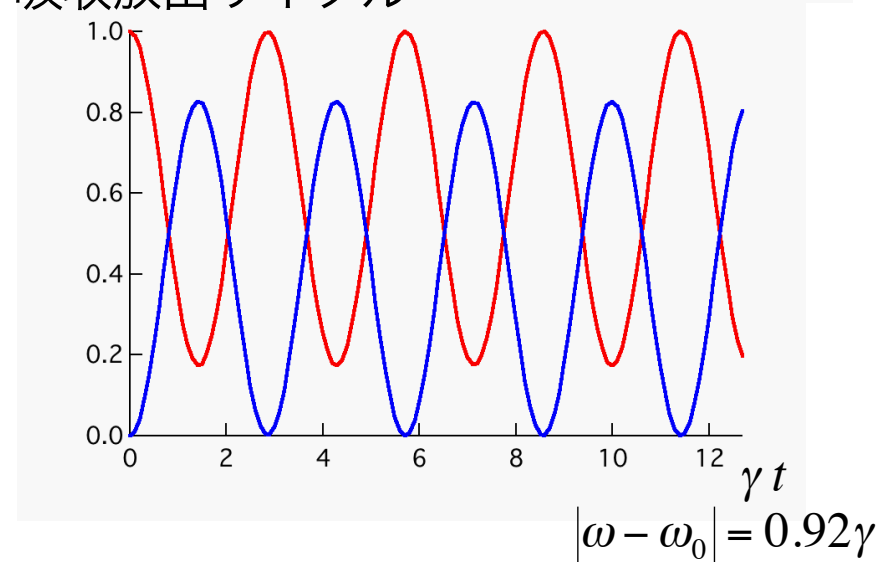
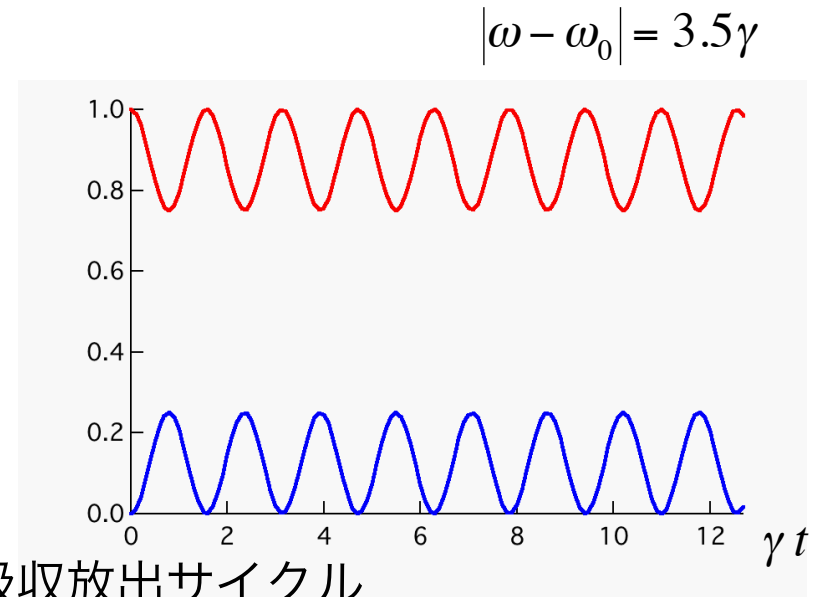
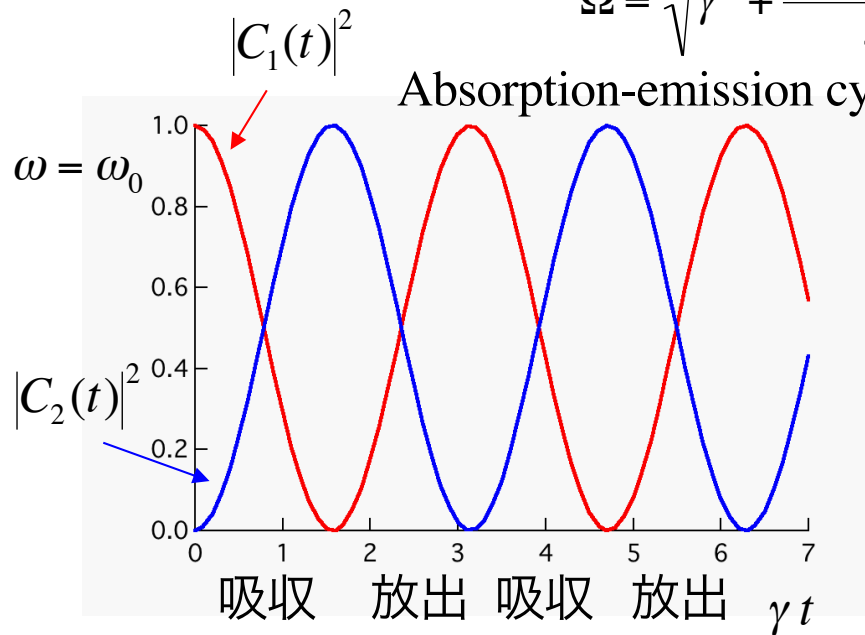
Rabi oscillation ラビ振動

Population ポピュレーション

$$|C_1(t)|^2 = 1 - |C_2(t)|^2$$

$$|C_2(t)|^2 = \frac{\gamma^2}{\Omega^2} \sin^2 \Omega t$$

$$\Omega = \sqrt{\gamma^2 + \frac{(\omega - \omega_0)^2}{4}}$$



Dipole interaction can be expressed in either the length or velocity gauge

Length gauge

velocity gauge

$$i\frac{\partial\psi_L}{\partial t} = \left[\frac{\mathbf{p}^2}{2} + V(\mathbf{r}) + \mathbf{r} \cdot \mathbf{E}(t) \right] \psi_L \quad \longleftrightarrow \quad i\frac{\partial\psi_V}{\partial t} = \left[\frac{(\mathbf{p} + \mathbf{A}(t))^2}{2} + V(\mathbf{r}) \right] \psi_V$$

gauge transformation $\psi_L = e^{i\mathbf{r} \cdot \mathbf{A}(t)} \psi_V$ $\mathbf{A}(t) = - \int \mathbf{E}(t) dt$ vector potential

All physical observables are gauge invariant.

probability density $|\psi_L|^2 = |\psi_V|^2$

projection on eigenstate i (or population of eigenstate i) depends on gauge!

$$\int \phi_i^* \psi_L d\mathbf{r}^3 \neq \int \phi_i^* \psi_V d\mathbf{r}^3$$

Level population (such as C_1 and C_2) is meaningful only if

$\mathbf{A}(t) = 0$ or after the pulse