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

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Hydrogen atom 水素原子の波動関数

Atomic unit 原子単位

Rabi oscillation ラビ振動

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Hydrogen-like atom
水素原子の波動関数

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Schrödinger equation
シュレーディンガー方程式

Particle of mass *m* moving in a potential *V*(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

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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

$$V(\mathbf{r}) = V(r) = -\frac{Ze^2}{4\pi\varepsilon_0 r}$$

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

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{r}) - \frac{Ze^2}{4\pi\varepsilon_0 r}\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r})$$

cumbersome coefficients
係数が煩雑

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

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

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Atomic unit 原子単位

Electron 電子

Unit system in which $\hbar = m = e = \dfrac{e^2}{4\pi\varepsilon_0} = 1$ となるような単位系

Length 長さ

$$a_0 = \frac{\hbar^2}{m\left(\dfrac{e^2}{4\pi\varepsilon_0}\right)} = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 5.292\times10^{-11}\,\mathrm{m}$$

Bohr radius ボーア半径

Energy エネルギー

$$\frac{e^2}{4\pi\varepsilon_0 a_0} = 27.21\ \mathrm{eV}$$

2×(ionization potential of H)

$1\ \mathrm{eV} = 1.602\times10^{-19}\ \mathrm{J}$

Time 時間

$$\frac{\hbar^3}{m\left(\dfrac{e^2}{4\pi\varepsilon_0}\right)^2} = \frac{a_0}{\alpha c} = 0.0242\ \mathrm{fs}$$

fine structure constant 微細構造定数

$$\alpha = \frac{e^2}{4\pi\varepsilon_0 c\hbar} = 7.297\times10^{-3} = \frac{1}{137.0}$$

Velocity 速度

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

Atomic scale of length, energy, and time

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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

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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 $V(\mathbf{r}) = V(r) = -\dfrac{Ze^2}{4\pi\varepsilon_0 r} = -\dfrac{Z}{r}$

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

$$-\frac{\hbar^2}{2m}\nabla^2\varphi(\mathbf{r}) - \frac{Ze^2}{4\pi\varepsilon_0 r}\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r}) \qquad -\frac{1}{2}\nabla^2\varphi(\mathbf{r}) - \frac{Z}{r}\varphi(\mathbf{r}) = \varepsilon\varphi(\mathbf{r})$$

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 $\varepsilon_n = -\dfrac{Z^2 me^4}{(4\pi\varepsilon_0)^2 2\hbar^2}\dfrac{1}{n^2} = -\dfrac{Z^2}{2n^2}$ $n = 1,2,3\cdots$

Eigen function
固有波動関数 $\varphi(\mathbf{r}) = R_{nl}(r)Y_{lm}(\theta,\phi)$ $0 \le l \le n-1$ $-l \le n \le l$

Radial wave function
動径波動関数

Spherical harmonics 球面調和関数

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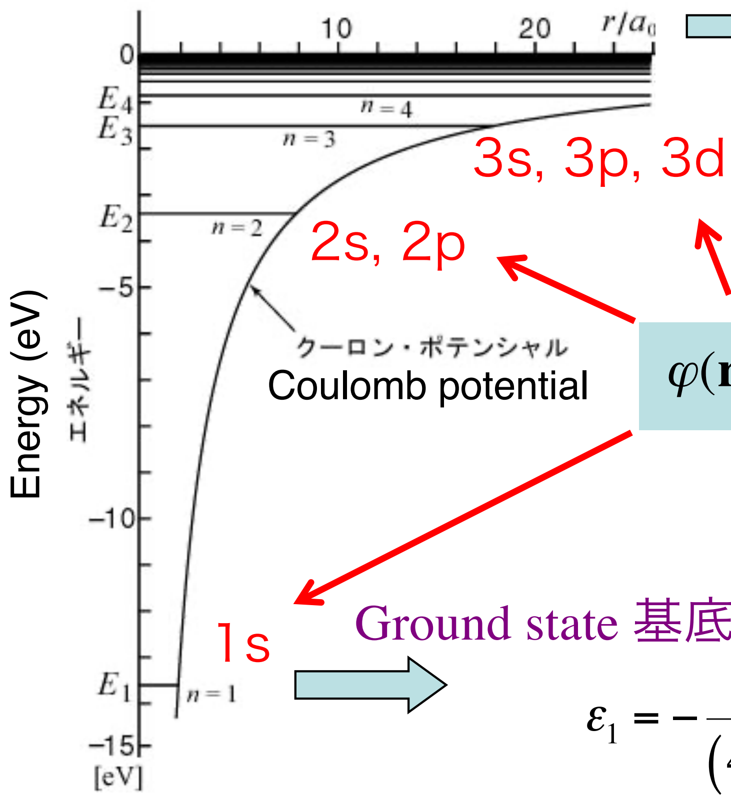
Bound states 束縛状態

Energy eigenvalue
エネルギー固有値

$$\varepsilon_n = -\frac{Z^2 me^4}{(4\pi\varepsilon_0)^2 2\hbar^2}\frac{1}{n^2} = -\frac{Z^2}{2n^2} \qquad n = 1,2,3\cdots$$



r in a_0 (Bohr radius ボーア半径)

$$a_0 = \frac{4\pi\varepsilon_0\hbar^2}{me^2} = 5.3\times10^{-11}\ \text{m} = 0.053\ \text{nm}$$

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

Ground state 基底状態

$$\varepsilon_1 = -\frac{me^4}{(4\pi\varepsilon_0)^2 2\hbar^2} = -13.6\ \text{eV}$$

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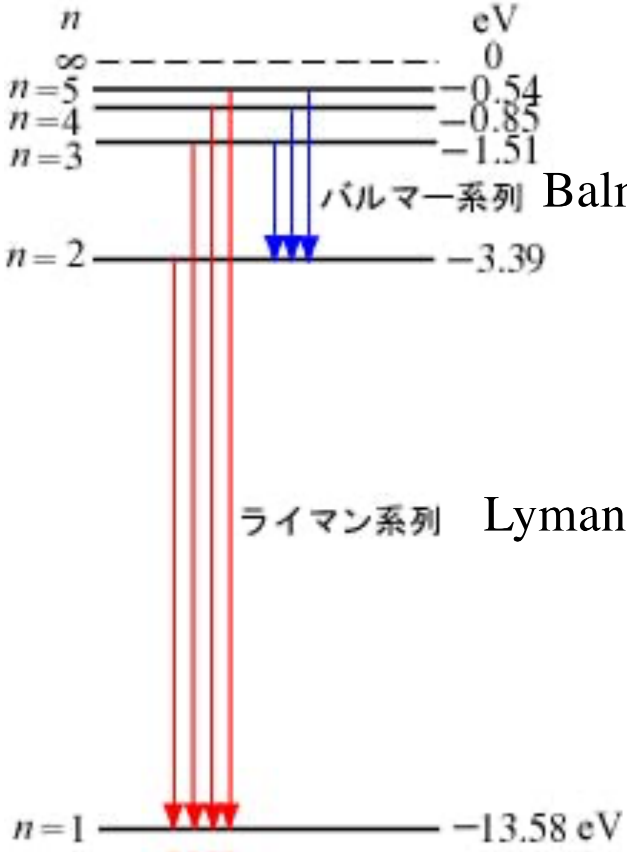
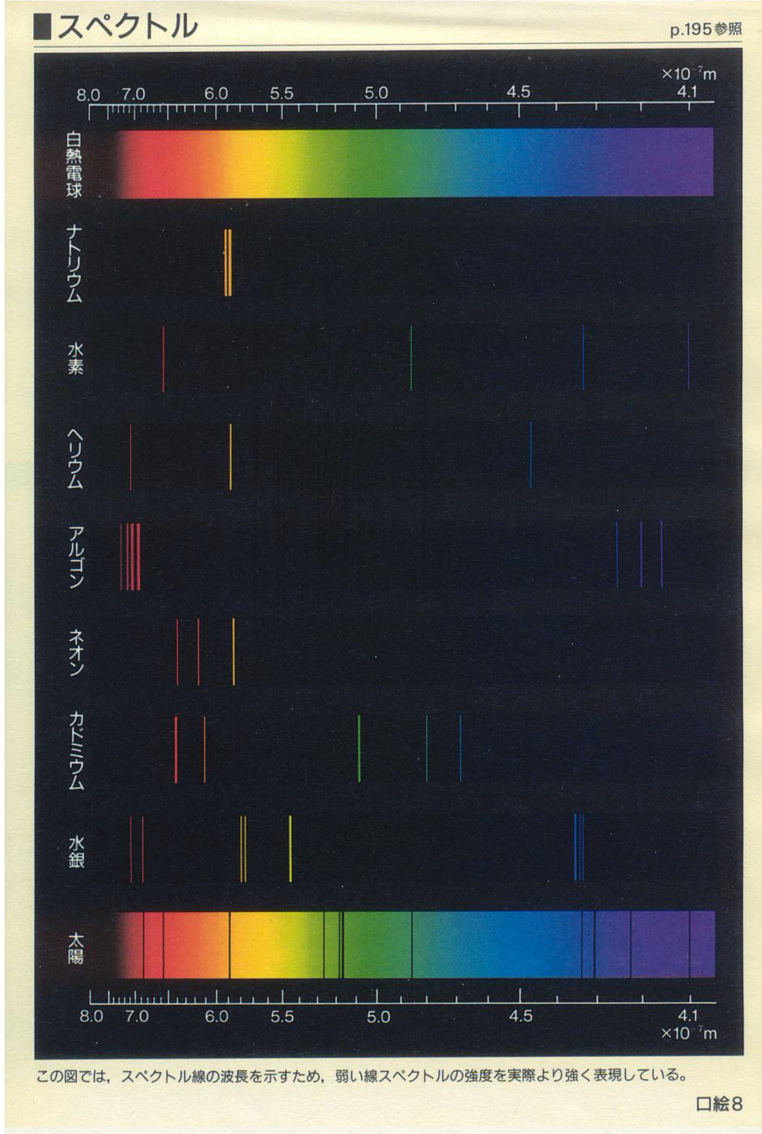
Energy eigenvalue

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



Balmer series

Lyman series



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Radial wave function and spherical harmonics
動径波動関数と球面調和関数

$Z = 1$の場合

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

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

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

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

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

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

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

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

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

Orthonormality 規格直交性

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

Orthonormality 規格直交性

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

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

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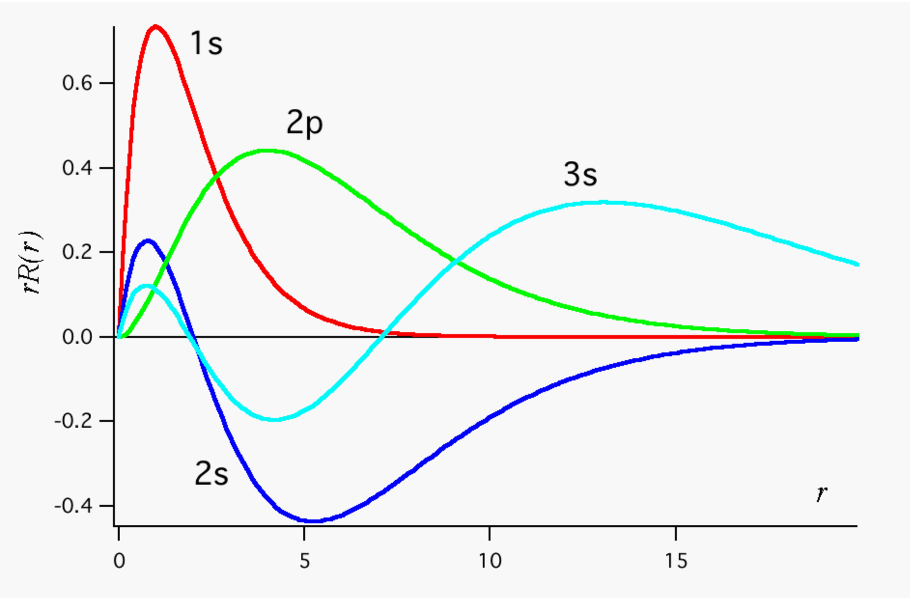
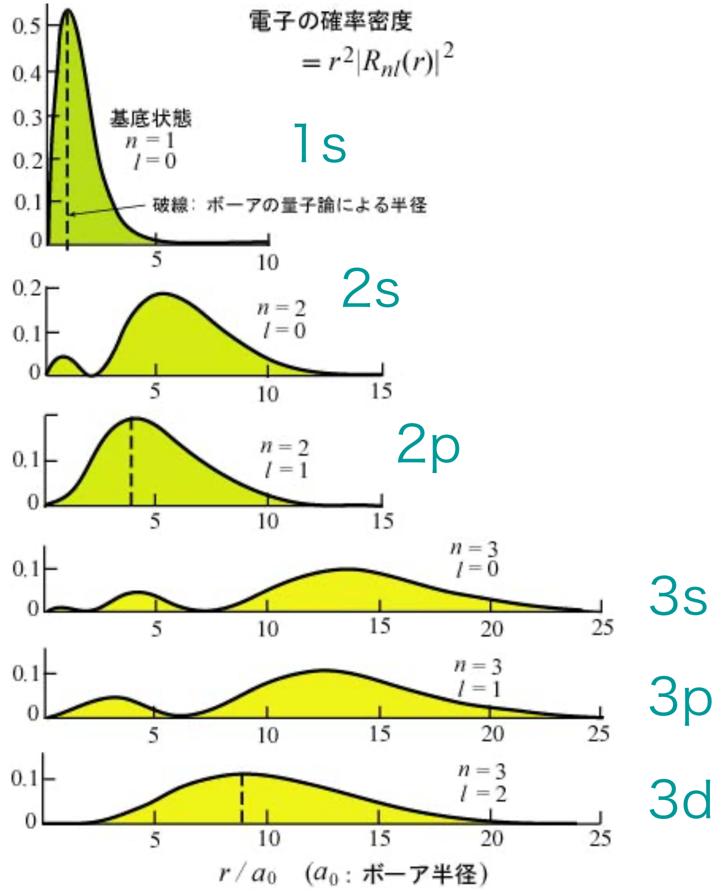
Radial wave function 動径波動関数



r (atomic unit)

Probability density

存在確率密度



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Continuum states 自由状態、連続状態

$\varepsilon > 0$ Necessary when ionization is considered イオン化を考えるときに必要

$\varepsilon > 0$ Arbitrary positive number 任意の正の実数

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

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 $k = \sqrt{2mE}/\hbar = \sqrt{2E}$ $\qquad n' = \dfrac{Z}{k}$

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

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

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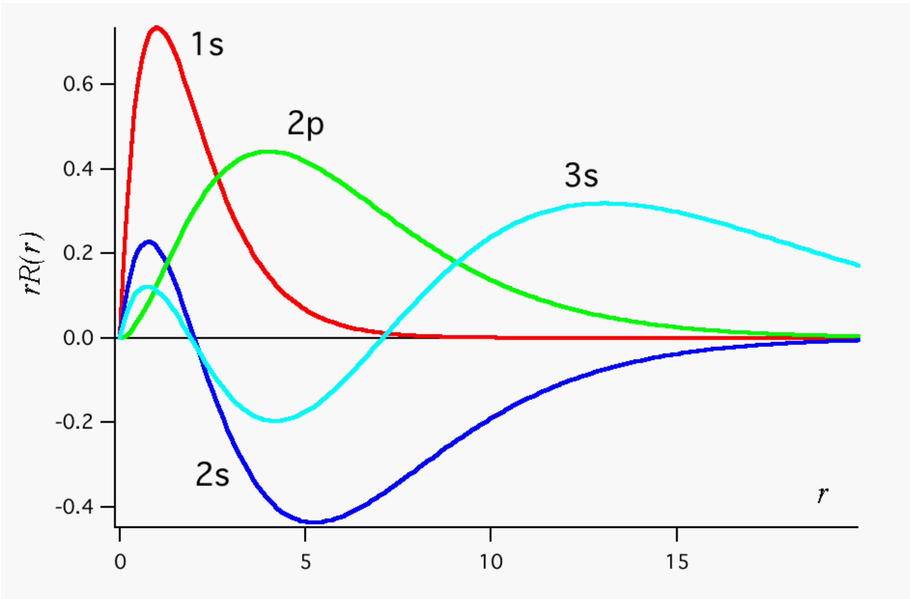
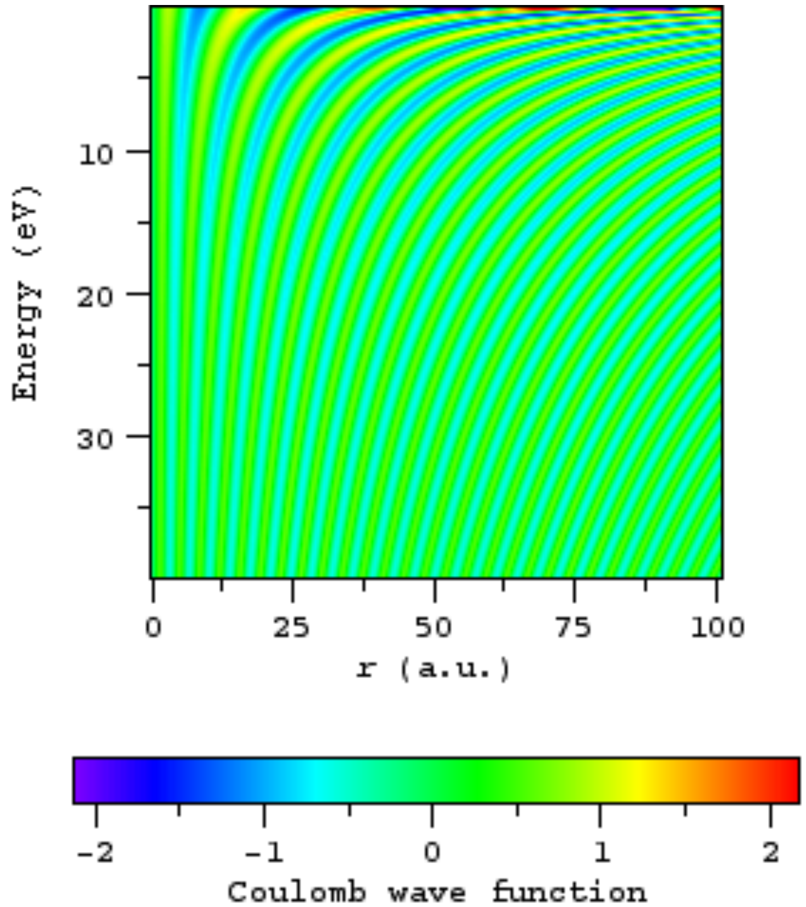
Radial wave function 動径波動関数

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）



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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

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

In a free space

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

Spherical Bessel function

Coulomb wave function

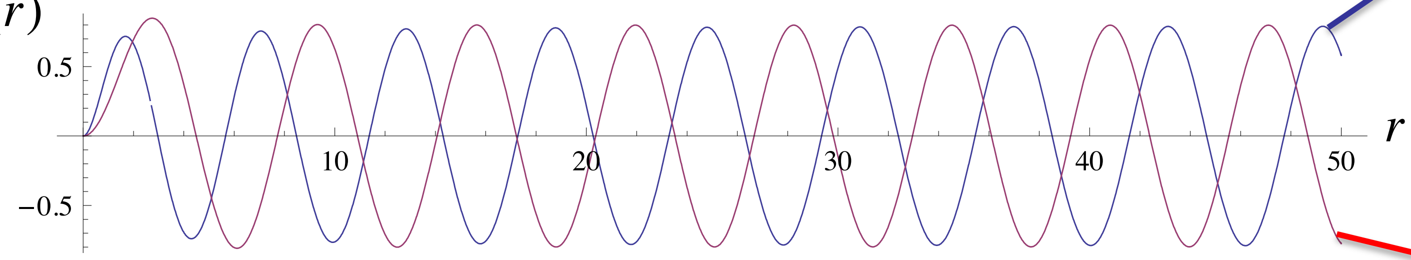
$$R_{El}(r)\xrightarrow[r\to\infty]{}\sqrt{\frac{2}{\pi k}}\frac{1}{r}\cos\left[kr+\frac{Z}{k}\log 2kr-\frac{\pi}{2}(l+1)-\sigma_l\right]$$

Phase shift 位相シフト（位相のずれ）$\sigma_l=\arg\Gamma(l+1+iZ/k)$

$rR_{El}(r)$

$l=1$
(p-wave)

$E = 13.6$ eV



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

短距離ポテンシャル

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

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

Spherical Bessel function

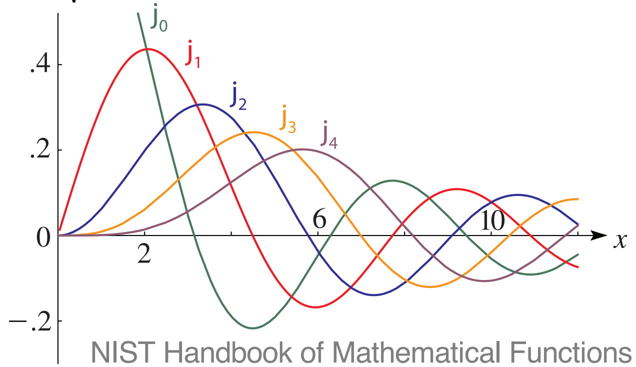

Figure 10.48.1: $j_n(x), n=0(1)4,\ 0\le x\le 12$.

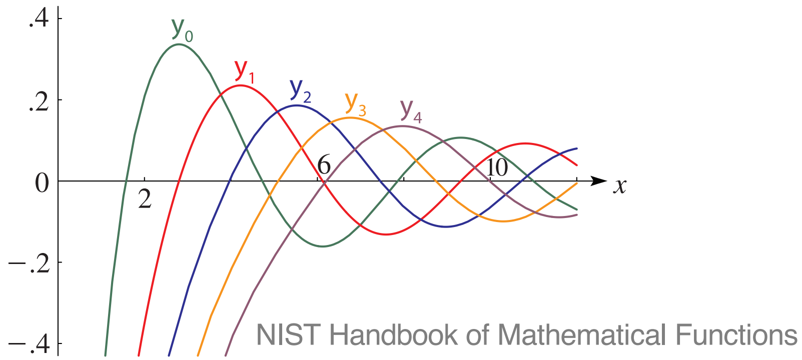

Figure 10.48.2: $y_n(x), n=0(1)4,\ 0< x\le 12$.

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

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

Phase shift 位相シフト（位相のずれ）

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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

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

Without the external field 相互作用項がない場合

$$H_0\varphi_n(\mathbf{r}) = \varepsilon_n\varphi_n(\mathbf{r}) \qquad \psi_n(\mathbf{r},t) = \varphi_n(\mathbf{r})e^{-i\omega_n t} \qquad \omega_n = \frac{\varepsilon_n}{\hbar}$$

Eigen state 固有状態

With the external field 相互作用項がある場合

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

$$H_0|n\rangle = \omega_n|n\rangle$$

(atomic unit)

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

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

$$\Rightarrow i\dot{c}_n = \langle n|H_I|\psi\rangle e^{i\omega_n t} \qquad \sum_m |m\rangle\langle m| = I$$

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.

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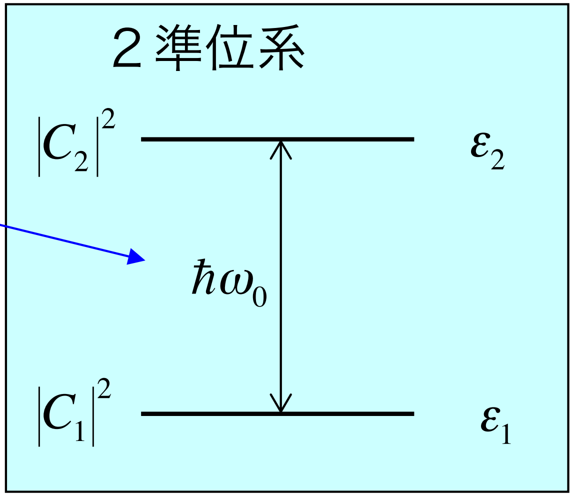
Important example: Rabi oscillation 重要な例：ラビ振動

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。

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

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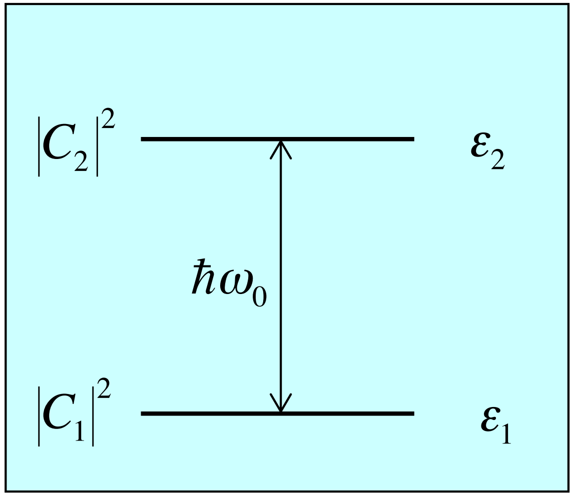
$$i\frac{\partial\psi}{\partial t} = -\frac{1}{2}\nabla^2\psi(\mathbf{r},t) - \frac{Z}{r}\psi(\mathbf{r},t) + V_I(\mathbf{r},t)\psi(\mathbf{r},t)$$



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

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

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

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

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

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

Similarly
同様に

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

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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 $k = \dfrac{2\pi}{\lambda}$

λ — Wavelength 波長

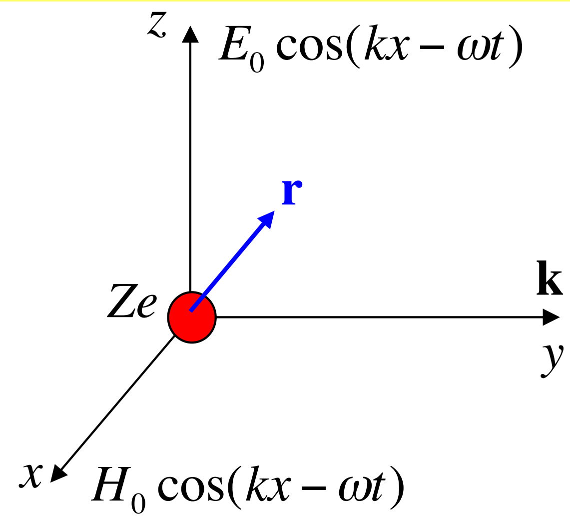
$x << \lambda$ ⇒ $kx << 1$

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

$V_I = zE_0 \cos \omega t$ （原子単位）

Dipole approximation

電気双極子近似



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

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

How V_I couples the two levels.

「V_Iのおかげで$j \to i$に遷移する」割合

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

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

$$V_{ij} = \langle i | V_I | j \rangle = \int \varphi_i^* V_I \varphi_j d^3\mathbf{r} = \cos\omega t \int zE_0 \varphi_i^* \varphi_j d^3\mathbf{r} = X_{ij} \cos\omega t$$

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

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

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

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Rabi oscillation ラビ振動

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

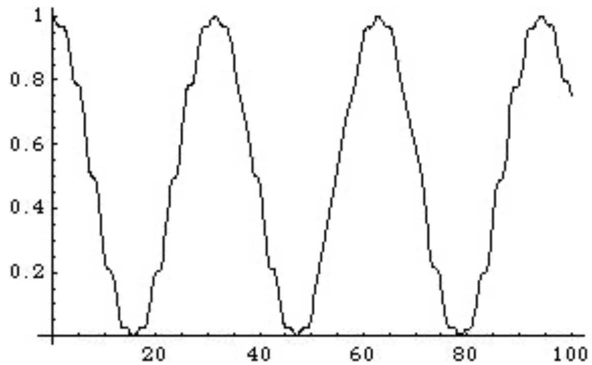
回転波近似 ⇩ Rotating wave approximation

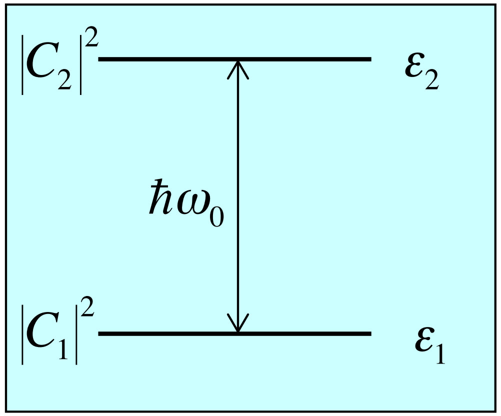
$$i\frac{\partial C_1}{\partial t} = \gamma e^{i(\omega-\omega_0)t} C_2 \qquad i\frac{\partial C_2}{\partial t} = \gamma e^{-i(\omega-\omega_0)t} C_1$$

Initial condition
初期条件 $C_1 = 1,\ C_2 = 0$ ⇩

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

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





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Rabi oscillation ラビ振動

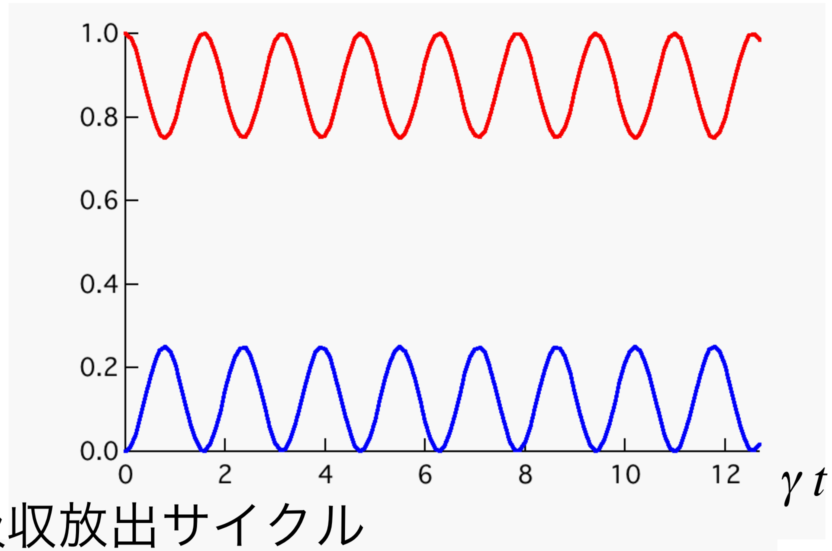
Population ポピュレーション

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

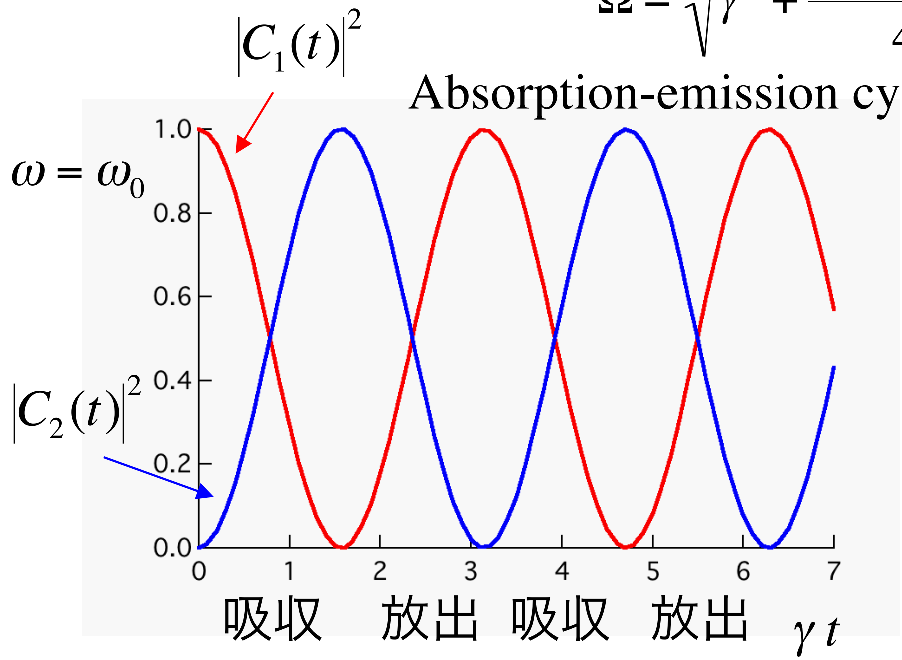
$$|C_2(t)|^2 = \frac{\gamma^2}{\Omega^2}\sin^2 \Omega t$$

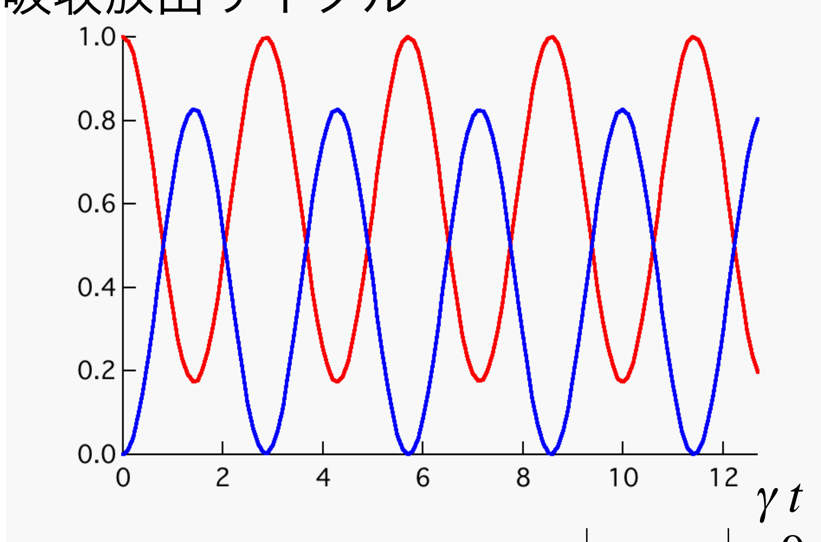
$$\Omega = \sqrt{\gamma^2 + \frac{(\omega-\omega_0)^2}{4}}$$

$|\omega - \omega_0| = 3.5\gamma$



Absorption-emission cycle 吸収放出サイクル





$|\omega - \omega_0| = 0.92\gamma$

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

Length gauge | **velocity gauge**

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

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

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