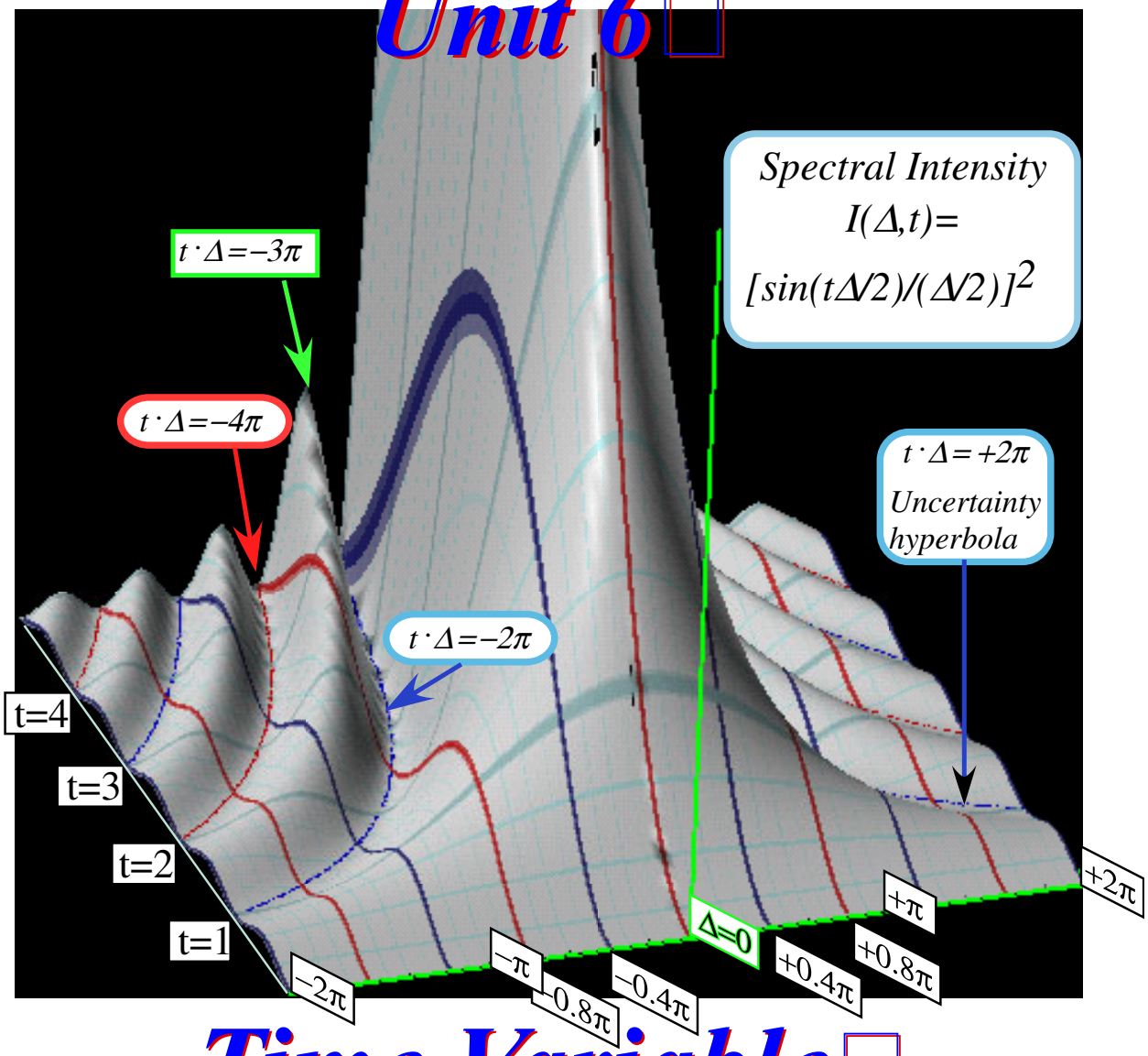
Quantum Theory for the Computer Age

Unit 6



Time Variable Perturbation and Transition

Unit 6
Time-Variable
Perturbation and Transition

In preceding Units 3-5 quantum motion is generated by a constant Hamiltonian *H*-matrix or operator **H**. This Unit 6 introduces Hamiltonian operators **H**(t) with explicit time dependence. For classical Hamiltonians, explicit time dependence requires some care, and for quantum Hamiltonians, time dependence requires extreme care. The first examples of time varying quantum perturbations are electromagnetic ones, and they are compared to corresponding classical Lorentz resonance and oscillator strength. Some shortcomings of perturbation theoretic approximations are noted and some more exacting remedies are introduced for two-state systems introduced in Chapter 10 of Unit 4. Two kinds of oscillatory perturbation introduced in Chapter 17, additive or linear and multiplicative or parametric, are discussed and compared.

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A Resonance Hero – Ken Evenson (1932-2002)

When US soldiers punch up their GPS coordinates they may owe there lives to an under sung hero who, alongside his colleagues and students, often toiled 18 hour days deep inside labs lit only by the purest light in the universe.

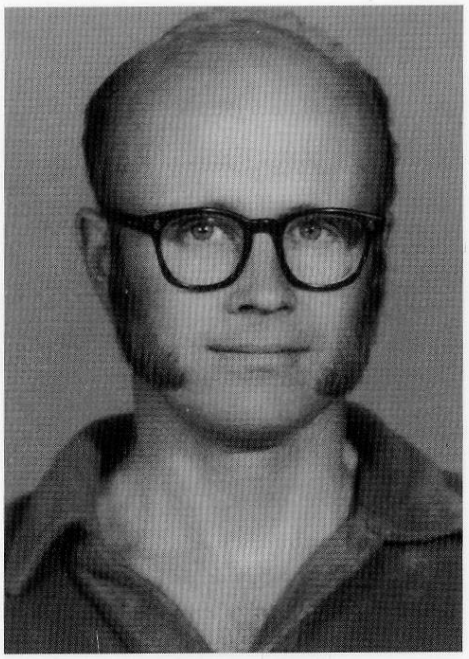
Let me introduce an "Indiana Jones" of modern physics. While he may never have been called "Montana Ken," such a name would describe a real life hero from Bozeman, Montana, whose accomplishments in many ways surpass the fictional character in *Raiders of the Lost Arc* and other cinematic thrillers.

Indeed, there were some exciting real life moments shared by his wife Vera, one together with Ken in a canoe literally inches from the hundred-foot drop-off of Brazil's largest waterfall. But, such outdoor exploits, of which Ken had many, pale in the light of an in-the-lab brilliance and courage that profoundly enriched the world.

Ken is one of few researchers and perhaps the only physicist to be listed twice in the *Guinness Book of Records*. The listing is not for jungle exploits but for his lab's highest frequency measurement and their speed of light determination that made it many times more precise. Then the meter-kilogram-second (mks) system of units underwent a redefinition largely because of Ken's efforts. Thereafter, the speed of light c was defined as $299,792,458 ms^{-1}$. The meter was defined in terms of c, instead of the other way around since the time precision had thoroughly trumped that of distance. Without such resonance precision, the Global Positioning System (GPS), the first large-scale wave space-time coordinate system, would have been impossible.

Ken's courage and persistence at the Time and Frequency Division of the Boulder Laboratories in the National Bureau of Standards (now the National Institute of Standards and Technology or NIST) are legendary as are his railings against boneheaded administrators who seemed bent on thwarting his best efforts. Undaunted, Ken's lab painstakingly exploited the resonance properties of metal-insulator diodes, and succeeded in literally counting the waves of near-infrared radiation and eventually visible light itself.

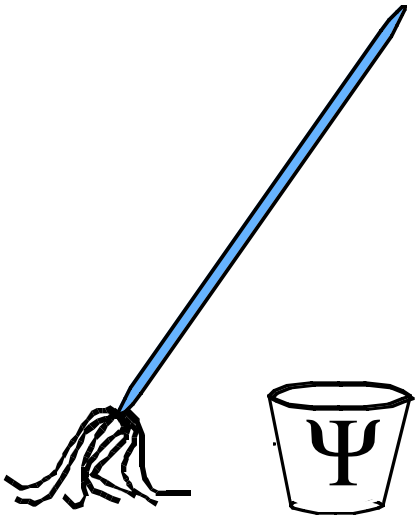
Those who knew him will always miss Ken. But, his indelible legacy of persistence lives on as ultra-precision atomic and molecular wave and pulse quantum optics continue to advance and provide mankind with heretofore-unimaginable capability.



PAULINIA, BRASIL 1976

THE SPEED OF LIGHT IS
299,792,458 METERS PER SECOND!

Kenneth M. Evenson – 1932-2002



QM for AMOP

Chapter 17

Classical Electromagnetic Perturbation

W. G. Harter

The most common perturbation is the electromagnetic field that is a practically ubiquitous occupant of spacetime. In spite of its overt or covert prevalence in virtually every experiment in physics, there are important aspects that often are misunderstood or not even discussed at all. This Chapter 17 introduces classical and semi-classical aspects of electromagnetic perturbations so they may be properly applied to quantum theory of atomic transitions in Chapters 18 and 19 and to quantum field theory in later Chapter 22. This includes the tricky problem of “gauge-boost” transformations and discussions of how linear additive Lorentz resonant perturbation differs from multiplicative or parametric resonance that underlies time-dependent quantum theory.

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Unit 5 Time-Variable Perturbation and Transition

Chapter 17 Classical Electromagnetic Perturbation

"Let there be light!" There is no single piece of physics that appears to be more significant than appearance itself. Without light and optics we are quite literally in total darkness. The same might be said for our understanding of quantum theory; the most elementary and visualizable quantum waves are electromagnetic waves. Light waves are indispensable to the development in the first two chapters of this book. So also have they been since Planck and Einstein wrote the energy-frequency equivalence relation $E=\hbar\omega$ and applied it to black-body radiation, photo-electric effects, or optical spectroscopy in general.

Just as classical electrodynamics (CED) of Maxwell, Lorentz, Gibbs, and others is one of the most significant achievements of the 19-th century, so must also be, for the 20-th century, the development of quantum electrodynamics (QED) by Feynman, Schwinger, Tomonaga and many others. A prerequisite to discussing perturbations of quantum systems by light is basic classical and quantum electro-magnetic interactions. However, such basics are far from trivial, and right away we run into complications!

17.1 Classical Mechanics of Electromagnetic Theory

(a) Classical electromagnetic Lagrangian

Newton's equations combined with Maxwell's definitions for electromagnetic fields **E** and **B** are first cast into a *Lagrangian* form, admittedly an unfamiliar one for many modern students. It starts with a familiar Lorentz *pondermotive* form for Newton's $\mathbf{F}=M\mathbf{a}= M\dot{\mathbf{v}} = M\ddot{\mathbf{R}}$ equation for a mass M of charge e.

$$M\frac{d\mathbf{v}}{dt} = \mathbf{F} = e(\mathbf{E} + \mathbf{v}\times\mathbf{B}) \tag{17.1.1}$$

Velocity is $\mathbf{v} = \dot{\mathbf{R}}$. First, the electric field **E** and the magnetic field **B** are expressed in terms of *scalar potential field* $\Phi=\Phi(\mathbf{R},t)$ and a *vector potential field* $\mathbf{A}=\mathbf{A}(\mathbf{R},t)$ using conventional Maxwell's definitions.

$$\mathbf{E} = -\nabla\Phi - \frac{\partial\mathbf{A}}{\partial t}, \qquad \mathbf{B} = \nabla\times\mathbf{A} \tag{17.1.2}$$

Combining the preceding two equations gives

$$M\frac{d\mathbf{v}}{dt} = \mathbf{F} = e\left[-\nabla\Phi - \frac{\partial\mathbf{A}}{\partial t} + \mathbf{v}\times(\nabla\times\mathbf{A})\right] = e\left[-\nabla\Phi - \frac{\partial\mathbf{A}}{\partial t} + \nabla(\mathbf{v}\bullet\mathbf{A}) - (\mathbf{v}\bullet\nabla)\mathbf{A}\right]. \tag{17.1.3}$$

The objective is to recast $\mathbf{F}=M\mathbf{a}$ to a *canonical* form involving a *Lagrangian function* $L=T-V$, *canonical momentum* $\mathbf{P}=\partial L/\partial\mathbf{v}$, and *Lagrange equations* $\dot{\mathbf{P}} = \partial L/\partial\mathbf{R}$. (Gradient ∇ is just $\partial/\partial\mathbf{R}$.)

$$\frac{d}{dt}\frac{\partial L}{\partial\mathbf{v}} = \frac{\partial L}{\partial\mathbf{R}}, \text{ or: } \dot{\mathbf{P}} = \nabla L, \text{ where: } L = T - V = \frac{1}{2}mv^2 - V, \text{ and: } \mathbf{P} = \frac{\partial L}{\partial\mathbf{v}} \tag{17.1.4}$$

A chain rule expansion of vector potential derivative is needed. Note "convection" $(\mathbf{v}\bullet\nabla)\mathbf{A}$ term.

$$\frac{d\mathbf{A}}{dt}=\frac{\partial\mathbf{A}}{\partial x}\dot{x}+\frac{\partial\mathbf{A}}{\partial y}\dot{y}+\frac{\partial\mathbf{A}}{\partial z}\dot{z}+\frac{\partial\mathbf{A}}{\partial t}=\frac{\partial\mathbf{A}}{\partial t}+(\mathbf{v}\bullet\nabla)\mathbf{A}$$

Combining this with the pondermotive equation (17.1.1) simplifies the $\mathbf{F}=M\mathbf{a}$ equation (17.1.3).

$$M\frac{d\mathbf{v}}{dt}=e\left[-\nabla\Phi+\nabla(\mathbf{v}\bullet\mathbf{A})-\frac{\partial\mathbf{A}}{\partial t}-(\mathbf{v}\bullet\nabla)\mathbf{A}\right]=e\left[-\nabla(\Phi-\mathbf{v}\bullet\mathbf{A})-\frac{d\mathbf{A}}{dt}\right]\qquad(17.1.5a)$$

The trick is to let -**A** be $\frac{\partial}{\partial\mathbf{v}}(\Phi-\mathbf{v}\bullet\mathbf{A})$. (**A** and Φ are velocity independent.) Also, let $M\mathbf{v}$ be $\frac{\partial}{\partial\mathbf{v}}\frac{M\mathbf{v}\bullet\mathbf{v}}{2}$.

$$\frac{d}{dt}\frac{\partial}{\partial\mathbf{v}}\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}=\frac{d}{dt}\frac{\partial}{\partial\mathbf{v}}(e\Phi-\mathbf{v}\bullet e\mathbf{A})-\nabla(e\Phi-\mathbf{v}\bullet e\mathbf{A})\qquad(17.1.5b)$$

In this way the *canonical electromagnetic Lagrange equations* emerge.

$$\frac{d}{dt}\frac{\partial L}{\partial\mathbf{v}}=\frac{d}{dt}\frac{\partial}{\partial\mathbf{v}}\left(\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-(e\Phi-\mathbf{v}\bullet e\mathbf{A})\right)=\nabla(e\Phi-\mathbf{v}\bullet e\mathbf{A})=\frac{\partial L}{\partial\mathbf{R}}\qquad(17.1.5c)$$

Here the *electromagnetic Lagrangian* is

$$L=L(\mathbf{R},\mathbf{v},t)=\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-\left(e\Phi(\mathbf{R},t)-\mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\right)\qquad(17.1.5d)$$

The *canonical electromagnetic momentum* is defined according to (17.1.4).

$$\mathbf{P}=\frac{\partial L}{\partial\mathbf{v}}=\frac{\partial}{\partial\mathbf{v}}\left(\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-\left(e\Phi(\mathbf{R},t)-\mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\right)\right)=M\mathbf{v}+e\mathbf{A}(\mathbf{R},t)\qquad(17.1.5e)$$

Without the magnetic vector potential $\mathbf{A}=\mathbf{A}(\mathbf{R},t)$ the Lagrangian has the usual form $L=T-V$ with a electric (scalar) potential $V=e\Phi(\mathbf{R},t)$ and momentum $\mathbf{P}$ reduces to the usual $M\mathbf{v}$.

However, for non-zero vector potential the $-e\mathbf{v}\cdot\mathbf{A}$ term acts as a velocity dependent "potential" to give a screwy canonical momentum $\mathbf{P}$ in (17.1.5e). The particle momentum $M\mathbf{v}$ is related to $\mathbf{P}$ as follows.

$$M\mathbf{v}=\mathbf{P}-e\mathbf{A}(\mathbf{R},t)\qquad(17.1.6)$$

Canonical momentum $\mathbf{P}=\partial L/\partial\mathbf{v}$ boggles Newtonian intuition. But it makes quantum sense! Phase S of a wave $\psi(x,t)=e^{iS/\hbar}|\psi(0)|$ is *Hamilton's Principle Action* $S=S_P=\int L dt$ and integral of *Poincare's invariant* dS.

$$dS=L\,dt=\mathbf{P}\bullet d\mathbf{R}-H\,dt\qquad(17.1.7a)$$

H is the *Hamiltonian*. The chain rule implies that $\mathbf{P}$ is the gradient of S and H its $(-t)$-derivative.

$$\mathbf{P}=\partial S/\partial\mathbf{R}\quad,\quad H=-\partial S/\partial t\qquad(17.1.7b)$$

These are the Hamilton-Jacobi equations (5.3.3); a classical "derivation" of quantum operator relations:

$\boldsymbol{P}=(\hbar/i)\partial/\partial\mathbf{R}$ gives: $\boldsymbol{P}\psi=(\mathbf{P})\psi=(\partial S/\partial\mathbf{R})\psi$, $\quad\mathbf{H}=(\hbar\, i)\partial/\partial t$ gives: $\mathbf{H}\psi=(H)\psi=(-\partial S/\partial t)\psi$.

(b) Classical electromagnetic Hamiltonian

The Hamiltonian function is defined by inverting Poincare's phase invariant as in the following:

$$H\,dt = \mathbf{P}\bullet d\mathbf{R} - L\,dt \quad \text{or:} \quad H = \mathbf{P}\bullet\mathbf{v} - L\,, \tag{17.1.8a}$$

As before, velocity is $\mathbf{v} = \dot{\mathbf{R}}$. Inserting the Lagrangian L from (17.1.5d) gives the Hamiltonian H.

$$\begin{aligned} H = \mathbf{P}\bullet\mathbf{v} - L &= \left(m\mathbf{v} + e\mathbf{A}(\mathbf{R},t)\right)\bullet\mathbf{v} - \left(\frac{m}{2}\mathbf{v}\bullet\mathbf{v} - \left(e\Phi(\mathbf{R},t) - \mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\right)\right) \\ &= \frac{m}{2}\mathbf{v}\bullet\mathbf{v} + e\Phi(\mathbf{R},t) \qquad \begin{pmatrix}\text{Numerically}\\ \text{correct}\end{pmatrix} \end{aligned} \tag{17.1.8b}$$

The vector potential $e\mathbf{A}$ cancels leaving a familiar $H=T+V$ where V is just a scalar potential $e\Phi$. But, H is an explicit function $H(\mathbf{P},\mathbf{R})$ of canonical *momentum* $\mathbf{P}$, not of velocity $\mathbf{v}$ like a Lagrangian $L(\mathbf{v},\mathbf{R})$. This formality is needed to rewrite Lagrange (and Newton) equations as *Hamilton's equations* by (17.1.8a).

$$\begin{aligned} \frac{\partial H}{\partial \mathbf{v}} &= \mathbf{P} - \frac{\partial L}{\partial \mathbf{v}}, & \frac{\partial H}{\partial \mathbf{r}} &= 0 - \frac{\partial L}{\partial \mathbf{R}}, & \frac{\partial H}{\partial \mathbf{P}} &= \mathbf{v} - \frac{\partial L}{\partial \mathbf{P}}, & \frac{dH}{dt} &= -\frac{\partial L}{\partial t}\,. \\ &= 0\,, & &= -\dot{\mathbf{P}}\,, & &= \mathbf{v} = \dot{\mathbf{R}}\,. \end{aligned} \tag{17.1.9}$$

So the H equation (17.1.8b) in $\mathbf{v}$ is correct numerically, only. Velocity $\mathbf{v}$ by (17.1.6) in terms of momentum $\mathbf{P}$ gives the formally correct *electromagnetic Hamiltonian* function for charge e of mass M.

$$H = \frac{1}{2M}\left(\mathbf{P} - e\mathbf{A}(\mathbf{R},t)\right)\bullet\left(\mathbf{P} - e\mathbf{A}(\mathbf{R},t)\right) + e\Phi(\mathbf{R},t) \qquad \begin{pmatrix}\text{Formally}\\ \text{correct}\end{pmatrix} \tag{17.1.10a}$$

The result expands into a more complicated but still formally correct Hamiltonian.

$$H = \frac{\mathbf{P}\bullet\mathbf{P}}{2M} - \frac{e}{2M}\left(\mathbf{P}\bullet\mathbf{A} + \mathbf{A}\bullet\mathbf{P}\right) + \frac{e^2}{2M}\mathbf{A}\bullet\mathbf{A} + e\Phi(\mathbf{R},t) \tag{17.1.10b}$$

Hamilton's equations (17.1.9) then follow. The $\dot{\mathbf{R}}$ equation just relates $\dot{\mathbf{R}} = \mathbf{v}$ to $\mathbf{P}$. (Recall (17.1.6).)

$$\mathbf{v} = \dot{\mathbf{R}} = \frac{\partial H}{\partial \mathbf{P}} = \frac{\mathbf{P} - e\mathbf{A}(\mathbf{R},t)}{M} \tag{17.1.10c}$$

The $\dot{\mathbf{P}}$ equation uses 3D-index notation *(μ=x,y,z)* to avoid confusing $\nabla(\mathbf{P}\bullet\mathbf{A})$ and $(\mathbf{P}\bullet\nabla)\mathbf{A}$.

$$\dot{P}_a = -\frac{\partial H}{\partial x_a} = -\sum_\mu \frac{\partial}{\partial x_a}\frac{\left(P_\mu - eA_\mu\right)^2}{2M} - e\frac{\partial\Phi}{\partial x_a} = \sum_\mu \frac{\left(P_\mu - eA_\mu\right)}{M} e\frac{\partial A_\mu}{\partial x_a} - e\frac{\partial\Phi}{\partial x_a} \tag{17.1.10d}$$

We use (17.1.2) to express Φ in terms of $\mathbf{E}$ and $\mathbf{A}$, and (17.1.4) to give $\mathbf{P}$ in terms of $\mathbf{v}$.

$$M\dot{v}_a + e\dot{A}_a = e\left(\sum_\mu v_\mu \frac{\partial A_\mu}{\partial x_a} + \frac{\partial A_a}{\partial t} + E_a\right) \tag{17.1.10e}$$

Index notation for total time derivative (17.1.4) of $\mathbf{A}$ is

$$\dot{A}_a = \sum_\mu v_\mu \frac{\partial A_a}{\partial x_\mu} + \frac{\partial A_a}{\partial t}. \qquad (17.1.4)_{\text{repeated}}$$

Finally, an equation for particle momentum is found by combining the preceding two equations.

$$M\dot{v}_a = e\left(\sum_\mu v_\mu \frac{\partial A_\mu}{\partial x_a} - v_\mu \frac{\partial A_a}{\partial x_\mu} + E_a\right) \qquad (17.1.11)$$

The result cancels out the partial time derivative of the vector potential **A** and is the same as the simple Newtonian equations (17.1.1-3). The Lagrangian and Hamiltonian forms have no obvious advantage if you just need Cartesian equations of motion. But, the Hamiltonian form wins for curved coordinates and for deducing symmetry and conservation laws. Also, both *L* and *H* lead to theoretical insight for relativity, quantum theory, and other areas where Newtonian theory seems quite clueless. (Recall Sec. 5.3.)

(c) Classical plane wave perturbations

Understanding the electromagnetic perturbation terms **A•P** or **A•A** in (17.1.10b) is helped by first considering an electron or other charge *e* in a radiation field of a monochromatic plane standing wave.

$$\mathbf{A} = \mathbf{e}_x 2|a|\sin(kz - \omega t) \qquad (17.1.12a)$$

The electric **E** and magnetic **B**-fields are given by Maxwell's definitions (17.1.2).

$$\mathbf{E}^{rad} = -\frac{\partial \mathbf{A}}{\partial t} = \mathbf{e}_x E_0 \cos(kz - \omega t), \quad \text{where: } E_0 = 2|a|\omega \qquad (17.1.12b)$$

$$\mathbf{B}^{rad} = \nabla \times \mathbf{A} = \mathbf{k} \times \mathbf{e}_x B_0 \cos(kz - \omega t), \quad \text{where: } B_0 = 2|a|k \qquad (17.1.12c)$$

Let us assume for a moment the scalar potential Φ associated with the radiation field is zero. This is a well-known *transversality*, *Coulomb*, or *transverse gauge* convention. It comes at a price: lack of relativistic covariance associated with arbitrarily zeroing the time-like component Φ of the 4-vector potential $(A_\mu)=(\Phi, c\mathbf{A})$. This means zeroing all field divergence where no charge density $\rho=\nabla\bullet\mathbf{E}\varepsilon_0$ exists.

$$\nabla \bullet \mathbf{E}^{rad} = 0 \ , \qquad \nabla \bullet \mathbf{A} = 0 \qquad (17.1.13a)$$

For an arbitrary plane wave $\mathbf{A}(\mathbf{R},t)=|a|e^{i(\mathbf{k}\bullet\mathbf{R}-\omega t)}$ this means fields **A** and **E** are transverse to wavevector **k**.

$$\mathbf{k} \bullet \mathbf{E}^{rad} = 0 \ , \qquad \mathbf{k} \bullet \mathbf{A} = 0 \qquad (17.1.13b)$$

Transversality (17.1.13.a) conveniently makes the quantum operator $\boldsymbol{P}=(\hbar/i)\partial/\partial\mathbf{R}=(\hbar/i)\nabla$ on **A** give zero.

$$\boldsymbol{P}\bullet\mathbf{A}=0 \qquad (17.1.14a)$$

So, the perturbation terms $\boldsymbol{P}\bullet\mathbf{A}$ and $\mathbf{A}\bullet\boldsymbol{P}$ both have the same effect even if **A** is a function of position **R**.

$$\boldsymbol{P}\bullet\mathbf{A}\psi=\mathbf{A}\bullet\boldsymbol{P}\psi \qquad (17.1.14b)$$

Transversality sets $\Phi^{rad}=0$ in a Schrodinger equation for a mass-*M*-charge-*q* particle.

$$i\hbar\frac{\partial\psi}{\partial t} = H\psi = \left[\frac{(P - q\mathbf{A})^2}{2M} + V(\mathbf{R})\right]\psi = \left[\frac{(\hbar\nabla/i - q\mathbf{A})^2}{2M} + V(\mathbf{R})\right]\psi. \qquad (17.1.15a)$$

As noted in Ch.2-3, Schrodinger's equation is non-relativistic. It expands as follows, using (17.1.14).

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{-\hbar^2\nabla^2}{2M}+i\frac{q\hbar}{M}\mathbf{A}\bullet\nabla+\frac{q^2}{2M}\mathbf{A}\bullet\mathbf{A}+V(\mathbf{R})\right]\psi. \qquad (17.1.15b)$$

The residual scalar potential $V(\mathbf{R})$ is meant to account for forces other than the radiation field arising from a nucleus, atom, molecule, or solid. Its presence further spoils relativistic symmetry.

(d) Change of picture: Boosts and gauge change

The **A•P** and **A•A** perturbations in Schrodinger equation (17.1.15b) are regarded as unnecessarily complicated for non-relativistic atomic physics. Therefore, a change-of-basis transformation is done to relate momentum **P** to a **p** which is Newtonian particle momentum $M\mathbf{v}$ by (17.1.6) or (17.1.10c). A transformation **B** is found which adds $q\mathbf{A}$ to momentum $\mathbf{p}=\mathbf{P}-q\mathbf{A}$ to give **P** and *vice-versa* for $\mathbf{B}^\dagger$.

$\mathbf{B}\mathbf{p}\mathbf{B}^\dagger=\mathbf{B}(\mathbf{P}-q\mathbf{A}\mathbf{1})\mathbf{B}^\dagger=\mathbf{P}=\mathbf{p}+q\mathbf{A}\mathbf{1}$ (17.1.16a) $\qquad \mathbf{B}^\dagger\mathbf{P}\mathbf{B}=\mathbf{B}^\dagger(\mathbf{p}+q\mathbf{A}\mathbf{1})\mathbf{B}=\mathbf{p}=\mathbf{P}-q\mathbf{A}\mathbf{1}$ (17.1.16b)

The **B** transformation was found by Synder and Richards (1948). We now consider their definition.

$$\mathbf{B}=e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar} \qquad (17.1.16b)$$

(A classical transformation was given earlier by Marie Geopert-Mayer (1931). $e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ was generalized by Power, *et. al*. (1976). Later in Sec. (g), **B** is related to a *(**A**,Φ)-gauge transformation* of Maxwell's equations.) Here we explain **B** in simpler terms: **B** is a *uniform boost* by $(-q\mathbf{A})$ of momentum if **A** is **R**-independent, otherwise, it is a *non-uniform boost* or "squeezing" operator. An up-boost $\mathbf{B}^\dagger=e^{+iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ by $(+q\mathbf{A})$ of coordinate basis $\{|\mathbf{R}\rangle..\}$ to $\{\mathbf{B}^\dagger|\mathbf{R}\rangle=|\mathbf{r}\rangle..\}$ is defined and discussed below.

Quantum translation operators

To understand quantum translation in space, let's make an analogy with translation in time that by Chapter 8 is done by a time evolution operator $\mathbf{U}(T)$. Equation (9.2.5c) in Chapter 9 gives **U** as $\mathbf{U}(T)=e^{-iT\mathbf{H}/\hbar}$ where **H** is the Hamiltonian generator of time translation. By Planck's axiom $E=\hbar\omega$, the energy operator **H** relates to frequency (per-second) operator $\mathbf{H}/\hbar$ through Planck's $\hbar$-constant, and by definition (9.1.1), **U** advances time: $\mathbf{U}(T)\psi(x,t)=\psi(x,t+T)$. Now consider space translation.

By analogy space translation operator $\mathbf{T}(R)=e^{-iR\mathbf{P}/\hbar}$ should use momentum **P** to generate coordinate translation. Momentum operator **P** relates to wavevector (per-meter) operator $\mathbf{K}=\mathbf{P}/\hbar$ by DeBroglie's relation $p=\hbar k$. So, does **T** translate? Is $\mathbf{T}(R)\psi(x,t)=\psi(x-R,t)$?

The quickest test of a translation operator is on a plane wave $\psi(x,t)=e^{i(kx-\omega t)}$ where you see a sign difference between space ($\psi(x-R,t)$ is *shifted* by positive R.) and time. ($\psi(x,t+T)$ is *ahead* by positive T.) The

effect of $\mathbf{T}(R) = e^{-iR\mathbf{P}/\hbar}$ on $e^{i(kx-\omega t)}$ is to apply the $\mathbf{P}/\hbar=\mathbf{K}=k$ representation e^{-iRk} which shifts by R.

$\mathbf{P}$'s coordinate representation $\mathbf{P}/\hbar=-i\partial_x$ does the same thing, but requires writing out a Taylor series.

$$\mathsf{T}(R)\psi(x) = e^{-iRP/\hbar}\psi(x) = 1 - R\frac{\partial\psi}{\partial x} + \frac{R^2}{2!}\frac{\partial^2\psi}{\partial x^2} - ... = \psi(x-R)$$

A rule emerges: Add R to quantum variable Q by exponential $e^{-iR\mathbf{P}/\hbar}$ of its *per*-Q-operator $\mathbf{P}$ times $-iR/\hbar$. For example, exponentiated angular momentum $\mathbf{S}$ in $e^{-i\boldsymbol{\Theta}\bullet\mathbf{S}/\hbar}$ rotates by angle Θ as in (10.5.25).

Quantum boost operators

A similar rule gives a momentum shift of $P=\hbar K$ by a boost operator $\mathsf{B}(P) = e^{+iP\mathsf{X}/\hbar} = e^{+ik\mathsf{X}}$ whose effect on a plane wave $\psi_k(x,t)=e^{i(kx-\omega t)}$ is simply $\mathbf{B}(P)\psi_k(x,t)=e^{iKx}e^{i(kx-\omega t)}=\psi_{k+K}(x,t)$. Now we denote by $\mathbf{B}$ the boost $\mathbf{B}(-qA)=e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ by momentum $-q\mathbf{A}$. New position ket $|\mathbf{r}\rangle$ relates to old $|\mathbf{R}\rangle=\mathbf{B}|\mathbf{r}\rangle$ as follows.

$$|\mathbf{r}\rangle = \mathbf{B}^\dagger|\mathbf{R}\rangle \ , \quad |\mathbf{R}\rangle = \mathbf{B}|\mathbf{r}\rangle \ , \quad \langle\mathbf{r}| = \langle\mathbf{R}|\,\mathbf{B} \ , \quad \langle\mathbf{R}| = \langle\mathbf{r}|\,\mathbf{B}^\dagger \ . \tag{17.1.17a}$$

A wavefunction $\psi(\mathbf{R}) = \langle\mathbf{R}|\psi\rangle$ of any state $|\psi\rangle$ times $B = e^{-iq\mathbf{A}\bullet\boldsymbol{R}/\hbar}$ gives wave $\psi(\mathbf{r}) = \langle\mathbf{r}|\psi\rangle$ in $\mathbf{r}$-basis.

$$\psi(\mathbf{r})=\langle\mathbf{r}|\psi\rangle=\langle\mathbf{R}|\,\mathbf{B}|\psi\rangle=\langle\mathbf{R}|\,e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}|\psi\rangle=e^{-iq\mathbf{A}\bullet\boldsymbol{R}/\hbar}\psi(\mathbf{R})=\psi^B(\mathbf{R}) \ . \tag{17.1.17b}$$

Position operator-$\mathbf{r}$ values are not affected since $\mathbf{B}$ is a momentum boost only and not an x-translation.

$$\mathbf{B}\,\mathbf{R}\,\mathbf{B}^\dagger = \mathbf{r} = \mathbf{R} \tag{17.1.18a}$$

The upper case$\{\mathbf{P},\mathbf{R}\}$ and lower case$\{\mathbf{p},\mathbf{r}\}$ notation is used for the original basis and the "reduced-momentum" basis, respectively. However, spatial coordinate labels $\mathbf{R}$ and $\mathbf{r}$ may be used interchangeably.

$$\mathbf{r}|\mathbf{r}\rangle = \mathbf{r}|\mathbf{r}\rangle \quad , \mathbf{A}(\mathbf{r},t)\bullet\,\mathbf{r}|\mathbf{r}\rangle \ = \ \mathbf{A}(\mathbf{r},t)\bullet\mathbf{r}|\mathbf{r}\rangle \tag{17.1.18b}$$

$$\mathbf{r}|\mathbf{R}\rangle = \mathbf{R}|\mathbf{R}\rangle \quad , \mathbf{A}(\mathbf{r},t)\bullet\,\mathbf{r}|\mathbf{R}\rangle = \mathbf{A}(\mathbf{R},t)\bullet\mathbf{R}|\mathbf{R}\rangle \tag{17.1.18c}$$

Representation of $\mathbf{p}$ in new $|\mathbf{r}\rangle$-basis is the same as $\mathbf{P}$ in the old $|\mathbf{R}\rangle$-basis: an $(\hbar/i)$-gradient $\boldsymbol{(P=(\hbar/i)\partial/\partial\mathbf{R})}$.

Inserting $\mathbf{1}=\mathbf{B}^\dagger\mathbf{B}$ and using $\mathbf{BpB}^\dagger=\mathbf{P}$ (17.1.16a) and $\langle\mathbf{R}| = \langle\mathbf{r}|\,\mathbf{B}^\dagger$ (17.1.17a) gives the following.

$$\boldsymbol{p}\,\psi(\mathbf{r}) = \langle\mathbf{r}|\,\mathbf{p}|\psi\rangle = \langle\mathbf{r}|\mathbf{B}^\dagger\mathbf{B}\,\mathbf{p}\,\mathbf{B}^\dagger\mathbf{B}|\psi\rangle = \langle\mathbf{R}|\,\mathbf{PB}|\psi\rangle = \boldsymbol{PB}\,\psi(\mathbf{R})$$

$$\boldsymbol{p}\,\psi(\mathbf{r}) = \boldsymbol{P}\psi^B(\mathbf{R}) = \boldsymbol{P}\psi(\mathbf{r}) = (\hbar/i)\partial/\partial\mathbf{R}\,\psi^B(\mathbf{R}) = (\hbar/i)\partial/\partial\mathbf{r}\,\psi(\mathbf{r}) \tag{17.1.18d}$$

Here, the notation (17.1.17b) for the boosted wavefunction $\psi^B(\mathbf{R})=\boldsymbol{B}\psi(\mathbf{R})=\psi(\mathbf{r})$ is used again.

Bookkeeping for Boosts: Operators vs. States

There arise questions about ±signs in B operations. It is important to clarify these for both operators and states, particularly since they differ. First, our mnemonic labeling of operators is

$$\mathsf{B} \ \textit{means} \begin{pmatrix} \text{"}\textit{make}\ \mathsf{B}\textit{igger}\text{"} \\ (\text{add } qA \text{ to } \mathsf{p} \text{ to make } \mathsf{P}) \\ \mathsf{BpB}^\dagger = \mathsf{p} + qA = \mathsf{P} \end{pmatrix} \qquad \mathsf{B}^\dagger \ \textit{means} \begin{pmatrix} \text{"}\textit{chop}(\dagger)\ \textit{down}\text{"} \\ (\text{cut } qA \text{ from } \mathsf{P} \text{ to make } \mathsf{p}) \\ \mathsf{B}^\dagger\mathsf{PB} = \mathsf{P} - qA = \mathsf{p} \end{pmatrix}$$

We may expand the exponential form of $\mathbf{B} = e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ to check its effect.

$$\begin{aligned}\mathsf{BpB}^\dagger &= e^{-iqA\cdot\mathsf{x}/\hbar}\mathsf{p}e^{+iqA\cdot\mathsf{x}/\hbar} = (1-iqA\cdot\mathsf{x}/\hbar\ldots)\mathsf{p}(1+iqA\cdot\mathsf{x}/\hbar\ldots)\\ &= \mathsf{p}-iqA\cdot\mathsf{xp}/\hbar+iqA\cdot\mathsf{px}/\hbar\ldots\\ &= \mathsf{p}-iqA\cdot[\mathsf{x},\mathsf{p}]/\hbar\ldots \quad \text{where: } [\mathsf{x},\mathsf{p}]=\hbar i\\ &= \mathsf{p}+qA\end{aligned}$$

Applying B (or $\mathsf{B}^\dagger$) again just adds (or subtracts) another qA, since here $\mathsf{B}qA\mathsf{B}^\dagger = qA = \mathsf{B}^\dagger qA\mathsf{B}$

$$\mathsf{BPB}^\dagger = \mathsf{P}+qA = \mathsf{p}+2qA \qquad \mathsf{B}^\dagger\mathsf{pB} = \mathsf{p}-qA = \mathsf{P}-2qA$$

$$\mathsf{B}(\mathsf{P}+qA)\mathsf{B}^\dagger = \mathsf{P}+2qA = \mathsf{p}+3qA \qquad \mathsf{B}^\dagger(\mathsf{p}-qA)\mathsf{B} = \mathsf{p}-2qA = \mathsf{P}-3qA$$

$$\vdots \qquad\qquad \vdots$$

B has the opposite effect on states or wavefunctions. Look at its effect on a plane wave.

$$\mathsf{B}\psi_k(x) = e^{-iqA\cdot x/\hbar}e^{ik\cdot x} = e^{i(k-qA/\hbar)\cdot x} = \psi_{k-qA/\hbar}(x)$$

B makes state momentum expectation *smaller* by the term qA, not bigger. This has to be since a basis change *cannot change matrix elements*. What the operator gains the states must lose and *vice-versa*.

$$\begin{aligned}\langle\psi_k|\mathsf{p}|\psi_k\rangle = \hbar k &= \langle\psi_k|\mathsf{B}^\dagger\mathsf{BpB}^\dagger\mathsf{B}|\psi_k\rangle\\ &= \langle\psi_{k-qA/\hbar}|\mathsf{BpB}^\dagger|\psi_{k-qA/\hbar}\rangle\\ &= \langle\psi_{k-qA/\hbar}|(\mathsf{p}+qA)|\psi_{k-qA/\hbar}\rangle\\ &= \langle\psi_{k-qA/\hbar}|\mathsf{p}|\psi_{k-qA/\hbar}\rangle + qA\\ &= \hbar(k-qA/\hbar)+qA = \hbar k\end{aligned}$$

How one might visualize the various boosting effects is discussed in connection with Fig. 17.1.1. But, these questions usually boil down to the relativity between states and operators that "analyze" the states. The fact that what we observe is an *interference* between the two has been emphasized repeatedly in Chapter 1 through 15. Newtonian absolutes have no place in modern theory. The relativity of boosts and momentum seem very confusing from a Newtonian point of view, and the Schrodinger wavefunction $\psi(x)$ notation, unlike Dirac's $\langle x|\psi\rangle$ notation, does little to clarify.

However, as shown in Unit 2, the quantum theory and relativity are inseparably mixed in a universe of waves. To treat either separately, as a Newtonian or Schrodinger paradigm might prefer, is to invite paradox and confusion. The simplistic Galilean B boosts used here should be replaced by Lorentz transformations derived in Unit 4 using the σ-operator forms developed in Unit 3. However, for now, we persevere to finish the Schrodinger approach.

Schrodinger E•r wave equation

Now $\psi(\mathbf{R})$-representation (17.1.15) of the electromagnetic Schrodinger equation is transformed to a $\psi(\mathbf{r})$-representation where: $\psi(\mathbf{r})=\psi^B(\mathbf{R})=B\,\psi(\mathbf{R})=e^{-iq\mathbf{A}\bullet\mathbf{R}/\hbar}\psi(\mathbf{R})$. We start by acting on (17.1.15) by B .

$$i\hbar B\frac{\partial\psi(\mathbf{R},t)}{\partial t}=B\left[\frac{(P-q\mathbf{A})^2}{2M}+V(\mathbf{R})\right]B^\dagger B\psi(\mathbf{R},t)=B\left[\frac{1}{2M}\left(\frac{\hbar}{i}\frac{\partial}{\partial R}-q\mathbf{A}\right)^2+V(\mathbf{R})\right]B^\dagger B\psi(\mathbf{R},t),$$

Also $1=B^\dagger B$ is inserted so as to use $B\,(P-q\mathbf{A}1)\,B^\dagger=P$, and $P\psi^B(\mathbf{R})=(\hbar/i)\partial/\partial\mathbf{r}\,\psi(\mathbf{r})$. (17.1.19a)

$$i\hbar B\frac{\partial\psi(R,t)}{\partial t}=\left[\frac{P^2}{2M}+V(\mathbf{r})\right]\psi(\mathbf{r},t)=\left[\frac{-\hbar^2\partial^2}{2M\partial r^2}+V(\mathbf{r})\right]\psi(\mathbf{r},t) \qquad (17.1.19b)$$

If vector potential **A** is constant in space and time (a trivial case with zero **E**-and **B**-fields) then the B factor can pass $\partial/\partial t$ to make $B\,\partial\psi(R)/\partial t$ into $\partial\psi(r)/\partial t$. Note that $(\mathbf{A}=0)$ just gives $\mathbf{B}=e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}=\mathbf{1}$.

Consider the simplest non-trivial case: a time dependent $\mathbf{A}(t)$ that is constant in space or nearly so.

$$\mathbf{A}=\mathbf{e}_x 2|a|\sin(kz-\omega t)\cong\mathbf{e}_x 2|a|\sin(-\omega t) \qquad (17.1.20a)$$

This is called the *long wavelength* or *dipole approximation* in which kz is negligible compared to ωt. (Imagine atomic sized $z\sim 0.5\,10^{-10}m$ and optical wavelengths $\lambda\sim 0.5\,10^{-6}m$ so $kz=2\pi\cdot 10^{-4}$ is *10,000* times smaller than $\omega t\sim 2\pi$ after one cycle.) Even so, the boost operator B does *not* commute with $\partial/\partial t$.

$$\begin{aligned}i\hbar B\frac{\partial\psi(R,t)}{\partial t}&=i\hbar\frac{\partial B\psi(R,t)}{\partial t}-i\hbar\frac{\partial B}{\partial t}\psi(R,t)=i\hbar\frac{\partial\psi(r,t)}{\partial t}-i\hbar\frac{\partial e^{-iq\mathbf{A}(t)\bullet\mathbf{r}/\hbar}}{\partial t}\psi(R,t)\\&=i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}-q\left(\frac{\partial\mathbf{A}(t)}{\partial t}\bullet\mathbf{r}\right)\psi(\mathbf{r},t)\quad\text{where: } B\psi(R,t)=\psi(\mathbf{r},t)\end{aligned} \qquad (17.1.20b)$$

An electric dipole potential $-q\mathbf{E}\bullet\mathbf{r}$ arises from $B\,\partial\psi(R)/\partial t$ and Maxwell equation $\mathbf{E}=-\partial\mathbf{A}/\partial t$.(17.1.2)

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{-\hbar^2\nabla_{\mathbf{r}}{}^2}{2M}+V(\mathbf{r})-q\mathbf{E}(t)\bullet\mathbf{r}\right]\psi(\mathbf{r},t) \qquad (17.1.20c)$$

Here we assume zero radiation scalar potential $(\Phi=0)$ in Maxwell equation (17.1.2). Nevertheless the radiation interaction appears as part of a "total" scalar potential $U(r)=V(r)-q\mathbf{E}\bullet\mathbf{r}$. This rather special situation owes its existence to the transversality condition and dipole approximations. This and other issues concerning **A•p** versus **E•r** interactions are discussed next.

(e) Comparing |R⟩ and |r⟩ = B|R⟩ pictures: A·P vs. E·r

Transformation $|\mathbf{r}\rangle=\mathbf{B}^\dagger|\mathbf{R}\rangle$ is more than just a change-of-basis. Since $\mathbf{B}=e^{-iq\mathbf{A}(t)\bullet\mathbf{r}/\hbar}$ is explicitly time-dependent, this is called a *change-of-picture*, as in "*motion* picture." Let us compare the Hamiltonian in the two pictures. The original $|\mathbf{R}\rangle$-picture has a Hamiltonian like the right hand side of (17.1.15).

$$H(\mathbf{R},\mathbf{P},t)=H_0(\mathbf{R},\mathbf{P})+H_I(\mathbf{R},\mathbf{P},t)=\left(\frac{\mathbf{P}^2}{2M}+V(\mathbf{R})\right)+\left[\frac{-q}{M}\mathbf{A}\bullet\mathbf{P}+\frac{q^2}{2M}\mathbf{A}\bullet\mathbf{A}\right]. \qquad (17.1.21a)$$

The new $|\mathbf{r}\rangle = \mathbf{B}^\dagger|\mathbf{R}\rangle$-picture has a Hamiltonian like the right hand side of (17.1.20).

$$H(\mathbf{r},\mathbf{p},t)=H_0(\mathbf{r},\mathbf{p})+H_I(\mathbf{r},t) \quad =\left(\frac{\mathbf{p}^2}{2M}+V(\mathbf{r})\right)+\left[-q\mathbf{E}(t)\bullet\mathbf{r}\right]. \qquad (17.1.21b)$$

The time independent $H_0=T+V$-parts look the same except for altering notation (**P**,**R**) to (**p**, **r**). Both **P** and **p** are represented by a gradient $(\hbar/i)\nabla$ and **R** equals **r**, so one might think the H_0 in (17.1.21a-b) are equal.

This is one of the worst traps in theoretical physics and leads to the mistake of equating a dipole potential $-q\mathbf{E}\bullet\mathbf{r}$ to the interaction $-(q/M)\mathbf{A}\bullet\mathbf{P}+(q^2/2M)\mathbf{A}\bullet\mathbf{A}$. *Not!* Transforming $H(\mathbf{p},\mathbf{r})$ to $H(\mathbf{P},\mathbf{R})$ is done by $\mathbf{B}^\dagger=e^{iq\mathbf{A}\bullet\mathbf{r}/\hbar}$. $\mathbf{B}^\dagger$ is a $q\mathbf{A}$-boost of **r**-space relative to **R**-space (assuming **A** is **r**-independent).

$$H(\mathbf{p},\mathbf{r},t)=\mathbf{B}^\dagger H(\mathbf{P},\mathbf{R},t)\mathbf{B} \qquad (17.1.21c)$$

The $(-q\mathbf{A})$-boost $\mathbf{B}=e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ was defined by (17.1.16) and (17.1.18). $\mathbf{B}^\dagger$ is **B**'s inverse.

$$\mathbf{p}=\mathbf{B}^\dagger\mathbf{P}\mathbf{B}=\mathbf{P}-\mathbf{1}q\mathbf{A}(t), \qquad (17.1.21d)\ , \qquad \mathbf{r}=\mathbf{B}^\dagger\mathbf{R}\mathbf{B}=\mathbf{R}. \qquad (17.1.21e)$$

Hence, part of $H_0(\mathbf{p},\mathbf{r},t)$ winds up in $H_I(\mathbf{P},\mathbf{R},t)$, and *vice-versa*; equating $H_0(\mathbf{p},\mathbf{r})$ to $H_0(\mathbf{P},\mathbf{R})$ is wrong but so is equating $H_0(\mathbf{p},\mathbf{r},t)$ to $\mathbf{B}^\dagger H_0(\mathbf{P},\mathbf{R},t)\mathbf{B}$. The transformation relation (17.1.21c) only applies to the total atom-plus-radiation Hamiltonian $H=H_0+H_I$. An attempt to visualize this is shown in Fig. 17.1.1.

Fig. 17.1.1 compares $H(\boldsymbol{p},\boldsymbol{r},t)$ to $H(\boldsymbol{P},\boldsymbol{R},t)$ with a 1D-HO potential $V(x)=(k/2)x^2$ and constant $E=-Å$.

$$H(\boldsymbol{p},\boldsymbol{r},t) = p^2/2M+(k/2)r^2 - qEr \qquad (17.1.22a)$$

$$H(\boldsymbol{P},\boldsymbol{R},t)=(P-qÅt)^2/2M+(k/2)R^2 \qquad (17.1.22)$$

A constant (DC) E-field adds a linear potential $-qEr=qÅ\,r$ to $V(r)$ if **A** increases at a constant rate $Å$.

$$E=-\partial A/\partial t=-Å \ \text{ where: } \ A=Åt \qquad (17.1.23b)$$

A positive rate $\partial A/\partial t = Å$ means a negative E but a positive slope $-qE$ of the interaction potential line $-qEr$. This causes the minimum of total potential $U(r)$ to shift left from $r=0$ to $r_o=-qÅ/k$ as seen in Fig. 17.1.1a.

$$MIN\ U(r) = (k/2)\,r_o^2-qEr_o=-q^2E^2/2k=-q^2Å^2/2k \quad \text{at: } r_o=qE/k=-qÅ/k \qquad (17.1.24)$$

The momentum derivative $\dot{p}$ for a particle at $r=0$ shifts from $\dot{p}=0$ to $\dot{p}=qE=-qÅ$ when E is turned on.

$$\dot{r}=\frac{\partial H}{\partial p}=\frac{p}{M}=\begin{cases}0\\ \pm qÅ/\sqrt{kM}\\ 0\end{cases} \qquad \dot{p}=-\frac{\partial H}{\partial r}=-kr+qE=\begin{cases}-qÅ & \text{at: } r=0\\ 0 & \text{at: } r=-qÅ/k\\ qÅ & \text{at: } r=-2qÅ/k\end{cases}$$

(17.1.25a) (17.1.25b)

The *H(**p**,**r**,t)* phase space origin also shifts from *r=0* to r_o=*-qÅ/k* as shown in Fig. 17.1.1b. Phase points rotate clockwise as in an Australian "typhoon" around a fixed-point or "eye" at origin *(r,p)=(r_o,0)*.

The *H(**P**,**R**,t)* phase space has a similar "typhoon" of clockwise phase *(**P**,**R**)*-point flow.

$$\dot{R} = \frac{\partial H}{\partial P} = \frac{p}{M} = \begin{cases} 0 \\ \pm qÅ/\sqrt{kM} \\ 0 \end{cases} \quad , \quad \dot{P} = -\frac{\partial H}{\partial R} = -kR = \begin{cases} -qÅ & \text{at: } R = qÅ/k \\ 0 & \text{at: } R = 0 \\ qÅ & \text{at: } R = -qÅ/k \end{cases}$$

(17.1.25c) (17.1.25d)

In contrast to *H(**p**,**r**,t)*, the *H(**P**,**R**,t)* "typhoon" is not shifted horizontally but simply drifts upward along with the *r*-axis at rate *qÅ=-qE* relative to *R*-axis in Fig. 17.1.1c. Momentum-*p* flow rate $\dot{p} = \dot{P} - qÅ$ is less than $\dot{P}$ by the rate *qÅ* of up-boost *qA=qÅt* since *p* is measured relative to the *r*-axis, but *P* is relative to *R*.

$$\dot{p} = \dot{P} - qÅ = \begin{cases} -2qÅ & \text{at: } R = qÅ/k \\ -qÅ & \text{at: } R = 0 \\ 0 & \text{at: } R = -qÅ/k \end{cases} \qquad (17.1.25e)$$

Note that boost *qA=qÅt* shifts the "eye" or ($\dot{p} = 0$)-point from *R=0* to *R=-qÅ/k* on the negative *r*-axis in Fig. 17.1.1c consistent with the shifted but stationary "eye" on the *r*-axis in Fig. 17.1.1b. This shows the subtle nature of the boost transformations (17.1.16), (17.1.18a), and (17.1.21) that relate electromagnetic Hamiltonian pictures of *H(**p**,**r**,t)* to *H(**P**,**R**,t)*. Even for a constant *E*-field this is not a trivial relation.

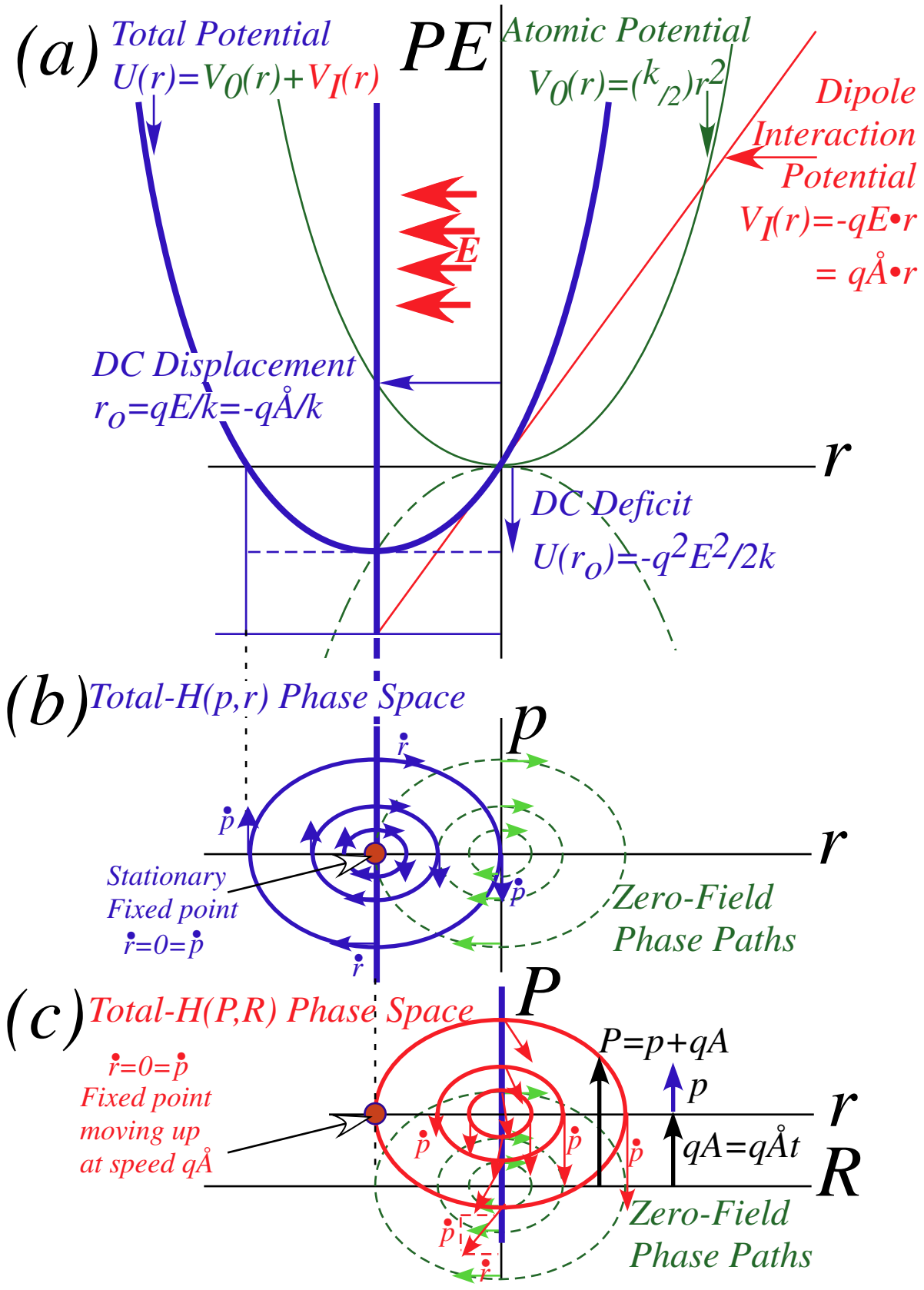

Fig. 17.1.1 (a) H(p,r) with E•r coupling. (b) Phase space. (c) H(P,R)=H(p+qA,R) boosted phase space.

Linear-plus-constant field geometry: Adding potential parabolas and lines

Perhaps, no other physical process is more important than optical excitation of atoms, molecules, and solids. All the color you see around you, indeed *everything* you can see, is due to this process. Whether this process is described by classical or quantum theory, it is often modeled by a parabolic atomic potential $V^A=kx^2/2$ (linear force $F^A=-kx$) in a linear electric potential field $\Phi=-qE\,x$ (uniform electric force field $F^E=qE$). This ideal atom model is *Lorentz's linear or harmonic atomic binding model* and the ideal model of a stimulating electric radiation field is the *long wave or dipole field approximation*. In Fig. 17.1.2 the geometry of fields is introduced beginning with two *force-vs.-x* lines in Fig. 17.1.2(a).

To plot total force, we only have to add two lines, the constant ($F^E=qE$)-line of the electric field and the sloping ($F^A=-kx$)-line of the atomic restoring force. This is done in Fig. 17.1.2(b) for a negative qE-field ($qE=-0.6$) and a positive atomic "spring" constant ($k=0.8$) to yield a total force ($F^{Total}=-kx+qE$)-line.

$$F^{Total}= F^A+ F^E =-kx+qE=-0.8x-0.6 \qquad \text{(A.1)}$$

The equilibrium "resting" point ($x=0,\ F^A=0$) of the atomic ($F^A=-kx$)-line moves to a new zero point of the total force ($F^{Total}=-kx+qE$)-line at the electric-atom equilibrium point ($x=x_E,\ F^{Total}=0$).

$$0=F^{Total}=0 =-kx+qE=-0.8x-0.6 \qquad \text{at: } x=x_E,=qE/k=-0.6/0.8=-0.75 \qquad \text{(A.2)}$$

To plot potential $V^{Total}(x)$ we use parabolic geometry beginning with finding the V^{Total}-parabola focus in Fig. 17.1.2(c). The new V^{Total}-parabola axis is at the x_E value indicated by the little circle on the x-axis at the equilibrium point $x_E=-3/4$ in Fig. 17.1.2(b-c) where the total force goes to zero.

Now imagine a light ray going down the old axis. Angle-ϕ of incidence equals angle+ϕ of OF-line for the ray reflecting off the parabolic tangent to hit the focus. (Atom force F^A and potential $V^A=kx^2/2$ are zero at $x=0$ where qE-field potential Φ and slope equal those of V^{Total}.)

The total atom-plus-field potential $V^{Total}=V^A+\Phi$ is a parabola of the same shape as $V^A=kx^2/2$ for the undisturbed atom, but its axis is over the new x_E–point where total force (potential slope) are now zero. Also, its minimum (zero-slope) point falls to a negative value $V^{Total}(x_E)$ that is zero only for $qE=0$.

$$V^{Total}(x_E) =V(x_E)+\Phi(x_E) = k\,x_E^2/2-qE\,x_E = -(qE)^2/(2k) =-(0.6)^2/1.6=-0.225 \qquad \text{(A.3)}$$

This new minimum $V^{Total}(x_E)$ and the new potential $V^{Total}(x)$ are constructed in Fig. 17.1.2(d-f). While it is perhaps difficult to explain, it is quite easy to do. First the directrix line is found in Fig. 17.1.2(d). It uses the fact that each point on the directrix lies below the contact point of the tangent normal to a line connecting that point to the focus as shown in Fig. 17.1.2(e). The normal points or "elbows" of the tangents all lie on the horizontal tangent to the $V^{Total}(x)$ parabola's minimum. This gives an easy tangent-contact construction of the $V^{Total}(x)$ parabola seen in Fig. 17.1.2(f).

Alternatively, one may start with the original field-free atomic parabola $V^A=kx^2/2$ shown in Fig. 17.1.2(g). Its tangents at $x=\pm1$ are parallel to the force plot lines $\pm F^A=-kx$ for any value of external qE-field as shown by lines for $qE=\pm k$ and $qE=\pm k/2$. The latter are tangent at $x=\pm1$ and provide a contact construction of $V^A(x)$ like the one for $V^{Total}(x)$ in Fig. 17.1.2(d-f). Then any $V^{Total}(x)$ parabola is found by translating the origin of $V^A(x)$ along an inverted copy $[-V^A(x)]$ of itself as shown in Fig. 17.1.2(h).

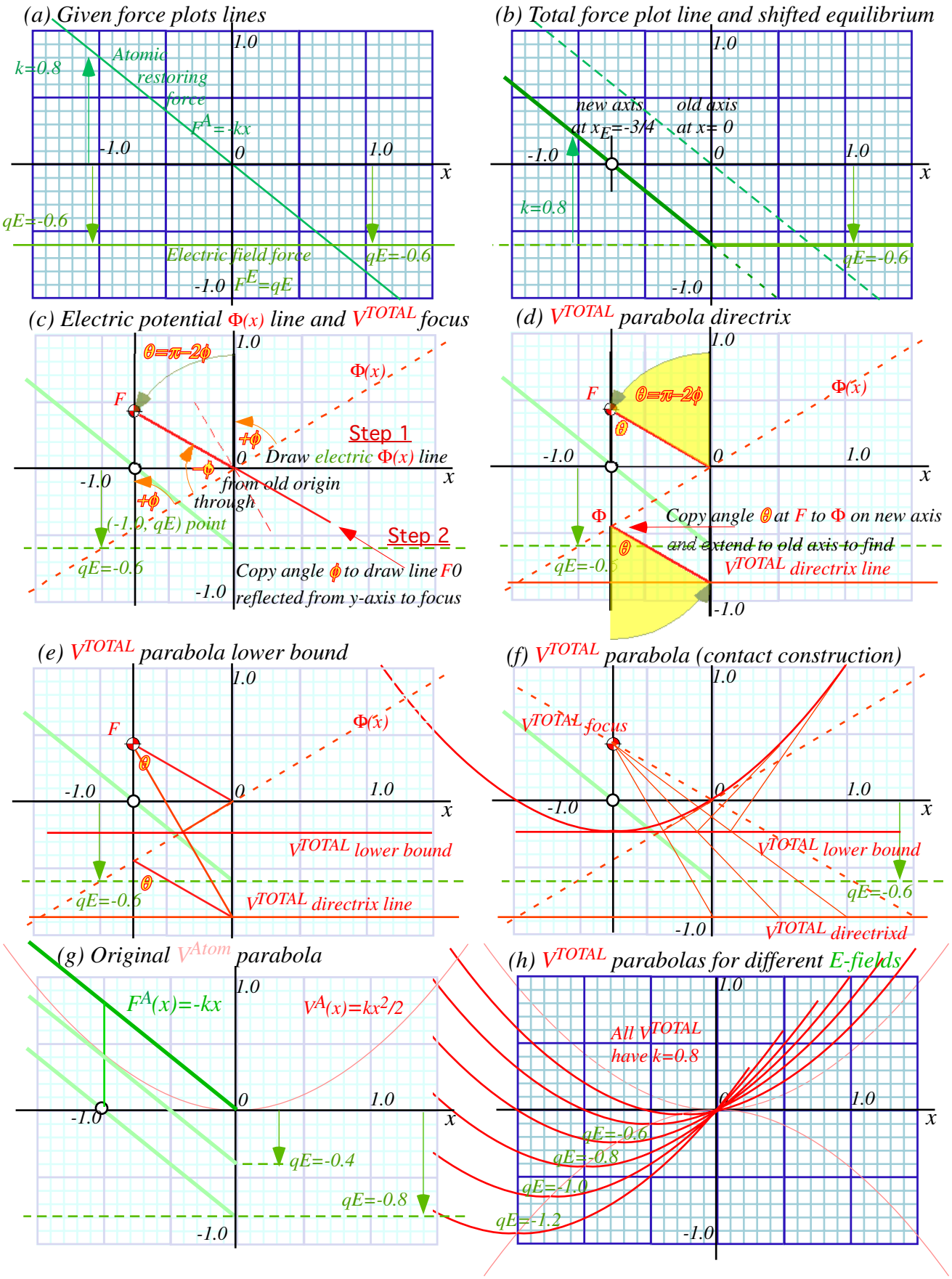
(a) Given force plots lines
k=0.8
Atomic restoring force
$F^A=-kx$
1.0
-1.0
0
1.0
x
qE=-0.6
Electric field force $F^E=qE$
qE=-0.6
(b) Total force plot line and shifted equilibrium
new axis at x_E=-3/4
old axis at x= 0
k=0.8
qE=-0.6
(c) Electric potential Φ(x) line and V^{TOTAL} focus
θ=π−2ϕ
F
Φ(x)
Step 1
Draw electric Φ(x) line from old origin through (-1.0, qE) point
Step 2
Copy angle ϕ to draw line F0 reflected from y-axis to focus
qE=-0.6
(d) V^{TOTAL} parabola directrix
Copy angle θ at F to Φ on new axis and extend to old axis to find V^{TOTAL} directrix line
(e) V^{TOTAL} parabola lower bound
V^{TOTAL} lower bound
V^{TOTAL} directrix line
(f) V^{TOTAL} parabola (contact construction)
V^{TOTAL} focus
V^{TOTAL} directrixd
(g) Original V^{Atom} parabola
$F^A(x)=-kx$
$V^A(x)=kx^2/2$
qE=-0.4
qE=-0.8
(h) V^{TOTAL} parabolas for different E-fields
All V^{TOTAL} have k=0.8
qE=-0.6
qE=-0.8
qE=-1.0
qE=-1.2

Fig. 17.1.2 Geometry of atomic oscillator potential $V^{Total}(x)=V(x)+\Phi(x) = kx^2/2-qE\,x$ with uniform E-field.

(f) Comparing diabatic with adiabatic: "Catcher-In-the-Eye"

For variable *E*-fields the preceding pictures can be insightful. Suppose a particle is sitting at $r=0$ near the bottom of the atomic potential $V(r)=(k/2)r^2$ with the *E*-field turned off. Now imagine turning on the *E*-field in very tiny steps so that the $\dot{p}=qE=-q\dot{A}$ excursions in (17.1.25a-b) are tiny for each step and so the shift $r_o=qE/k$ is made arbitrarily high but the particle stays around r_o with near-zero $\dot{p}$. If you are clever at catching the particle in the "eye" just when its momentum is turning around, you can make $\dot{p}$ *exactly* zero. Such a "catcher-in-the eye" game can produce large r_o with zero $\dot{p}$ in just a couple of steps.

Suppose now that a high r_o with low $\dot{p}$ has been obtained. What happens if suddenly the applied field goes to zero? Forgetting, for the moment, the resulting transient radiation field, it is clear that the particle will find itself high up on the zero-*E* potential, that is, at energy $V(r_o)=(k/2)r_o^2$ with a low initial velocity. In about a quarter cycle, all that potential will be converted entirely to kinetic energy! Such an extreme diabatic transition is quite a contrast to an adiabatic one that would leave the particle back at $r_o=0$ and $\dot{p}=0$ after the field was turned off slowly or reduced cleverly by "catcher-in-the-eye" maneuvers.

Oscillating particles may also undergo adiabatic transitions by conserving classical action $S=\int p dx$. Adiabatic conservation of classical action implies quantum number conservation or *adiabatic following* . A system starting in the *n*-th state remains in the *n*-th state even if the states are changing like mad.

In contrast to adiabatic following, *resonant excitation* changes action and quantum numbers. If a potential $U(r)$ in Fig. 17.1.1(a) shakes at the natural oscillator frequency, the system will be excited rapidly to a combination of two or more states. Chapter 18 discusses of this sort of resonant excitation.

(g) Gauge transformation

Consider a non-relativistic electromagnetic Hamiltonian and Schrodinger equation with both a scalar potential $\Phi(\mathbf{R},t)$ and vector potential $\mathbf{A}(\mathbf{R},t)$ operative.

$$i\hbar\frac{\partial\psi}{\partial t}=\frac{1}{2M}\left(P-q\mathbf{A}\right)^2\psi+q\Phi(\mathbf{R})\psi+V(\mathbf{R})\psi \qquad (17.1.26a)$$

Isolating time-like parts from space-like parts more closely respects the equation's relativistic origins.

$$\left(i\hbar\frac{\partial}{\partial t}-q\Phi(\mathbf{R})\right)\psi=\frac{1}{2M}\left(-i\hbar\frac{\partial}{\partial\mathbf{R}}-q\mathbf{A}\right)^2\psi+V(\mathbf{R})\psi \qquad (17.1.26b)$$

Now consider the corresponding equation for a *Γ-gauge-transformed* wavefunction

$$\psi^G(\mathbf{R}) = e^{iq\Gamma(\mathbf{R},t)/\hbar}\,\psi(\mathbf{R}) = G\psi(\mathbf{R}), \qquad (17.1.27)$$

that is, a wavefunction whose phase has been messed up by an arbitrary *gauge function* $\Gamma(\mathbf{R},t)$.

$$e^{iq\Gamma(\mathbf{R},t)/\hbar}\left(i\hbar\frac{\partial}{\partial t}-q\Phi(\mathbf{R})\right)e^{-iq\Gamma(\mathbf{R},t)/\hbar}\psi^G=e^{iq\Gamma(\mathbf{R},t)/\hbar}\frac{1}{2M}\left(-i\hbar\frac{\partial}{\partial\mathbf{R}}-q\mathbf{A}\right)^2e^{-iq\Gamma(\mathbf{R},t)/\hbar}\psi^G+V(\mathbf{R})\psi^G \tag{17.1.26b}$$

Here an inverted version $\psi=G^\dagger\psi^G$ of (17.1.27) is put in for ψ and $G=e^{iq\Gamma(\mathbf{R},t)/\hbar}$ is applied to the left.

$$\begin{aligned}e^{iq\Gamma(\mathbf{R},t)/\hbar}\left(i\hbar\frac{\partial}{\partial t}-q\Phi\right)e^{-iq\Gamma(\mathbf{R},t)/\hbar}&=\left(i\hbar\frac{\partial}{\partial t}-q\Phi^G\right)\\ e^{iq\Gamma(\mathbf{R},t)/\hbar}\left(-i\hbar\frac{\partial}{\partial\mathbf{R}}-q\mathbf{A}\right)^2e^{-iq\Gamma(\mathbf{R},t)/\hbar}&=\left(-i\hbar\frac{\partial}{\partial\mathbf{R}}-q\mathbf{A}^G\right)^2\end{aligned} \tag{17.1.27a}$$

Gauge transformed wave ψ^G obeys wave equation (17.1.6) with *gauge transformed potentials* Φ^G and $\mathbf{A}^G$.

$$\Phi^G=\Phi-\frac{\partial\Gamma(\mathbf{R},t)}{\partial t}\ ,\qquad\qquad \mathbf{A}^G=\mathbf{A}+\frac{\partial\Gamma(\mathbf{R},t)}{\partial\mathbf{R}} \tag{17.1.27b}$$

The electric and magnetic fields **E** and **B** are not affected by a gauge transformation.

$$\begin{aligned}\mathbf{E}^G&=-\frac{\partial\Phi^G}{\partial\mathbf{R}}-\frac{\partial\mathbf{A}^G}{\partial t}=-\frac{\partial\Phi}{\partial\mathbf{R}}+\frac{\partial^2\Gamma(\mathbf{R},t)}{\partial\mathbf{R}\partial t}-\frac{\partial^2\Gamma(\mathbf{R},t)}{\partial t\partial\mathbf{R}}-\frac{\partial\mathbf{A}}{\partial t}=\mathbf{E}\\ \mathbf{B}^G&=\nabla\times\mathbf{A}^G=\nabla\times\mathbf{A}+\nabla\times\nabla\Gamma(\mathbf{R},t)=\nabla\times\mathbf{A}=\mathbf{B}\end{aligned} \tag{17.1.27c}$$

The boost transformation $\mathbf{B}=e^{-iq\mathbf{A}(t)\bullet\mathbf{r}/\hbar}$ in (17.1.16) uses a gauge function $\Gamma(\mathbf{R},t)=-\mathbf{A}(t)\bullet\mathbf{R}$ to cancel the vector potential with $-\mathbf{A}=\partial\Gamma/\partial\mathbf{R}$ and add a dipole term $-\partial\Gamma/\partial t=\partial\mathbf{A}/\partial t\bullet\mathbf{R}=-\mathbf{E}\bullet\mathbf{R}$ to the scalar potential Φ.

Such a simple algebraic result covers up the transformation physics and phase space geometry described earlier. A gauge transformation is a change-of-basis that is as severe as any can be and should be treated as such even though, as it is often described, it does not seem to affect fundamental fields **E** and **B**, coordinates **R**, or momenta **P**. In fact it does! It is a non-uniform boost in space and time that changes origin and scale in frequency-wavevector space. The **B**-transformation is as close to a relativistic Lorentz boost as is possible in a non-relativistic theory. Changing the space and time wrinkles of waves (their **k** and ω) is the same as a change of their momentum and energy.

A serious problem here is our abandonment of relativistic symmetry, which occurred in Chapter 7 as we entered the Schrodinger world. The elegant relation between relativity and quantum theory in Chapters 4 through 6 is, in my mind, so compelling. Dirac once commented, "Nature is a stickler for good form." Dirac's theory of relativistic electron spin (to be explored later) is still as much a monument to good form as the gauge confusion alluded to above is to the lack thereof.

Mechanical analogy for cyclotron motion in magnetic field

A smooth sphere or ball rolling on a horizontal rotating table, as shown in Fig. 17.1.2 obeys the same equations as a charged particle in a uniform magnetic **B** field.

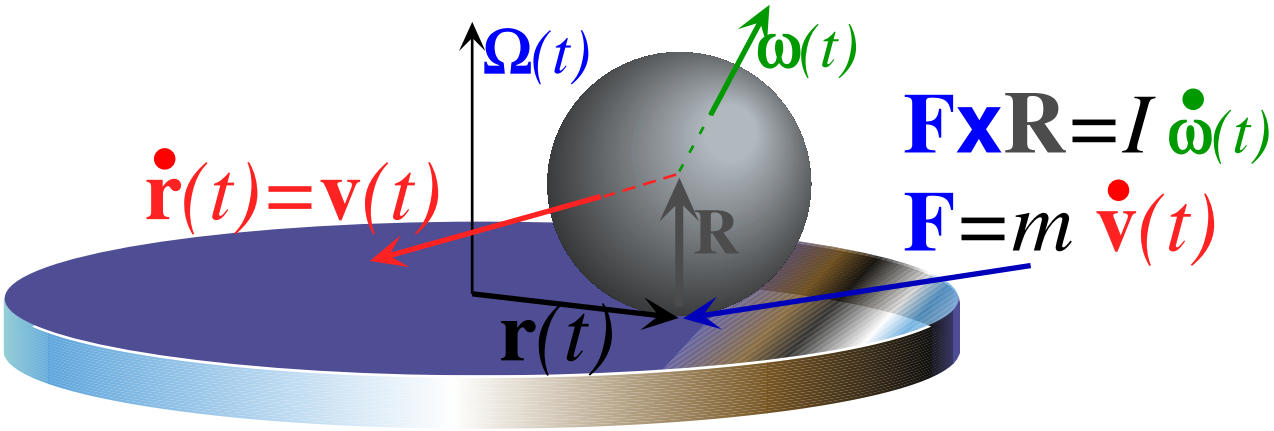

Fig. 17.1.2 Mechanical analog of magnetic **vxB** *cyclotron mechanics.*

The key to making this device work is to have rolling "stiction" with as little rolling friction as possible. A plexiglas pool ball on a plexiglas disc attached to a record turntable will suffice. The constraint relation which demands no slippage of the ball on the table is as follows.

$$\mathbf{v} = \boldsymbol{\Omega}\times\mathbf{r} + \boldsymbol{\omega}\times\mathbf{R} = \boldsymbol{\Omega}\times\mathbf{r} + \boldsymbol{\omega}\times\hat{\mathbf{z}}R \qquad (17.1.28)$$

Combining with Newton equations for translation and rotation in the Fig. 17.1.2 gives

$$I\dot{\boldsymbol{\omega}} = \mathbf{F}\times\mathbf{R} = m\dot{\mathbf{v}}\times\mathbf{R} = m\dot{\mathbf{v}}\times\hat{\mathbf{z}}R \qquad (17.1.29)$$

The acceleration $\mathbf{a} = \dot{\mathbf{v}}$ is given by the time derivative of the velocity constraint (17.1.28).

$$\dot{\mathbf{v}} = \boldsymbol{\Omega}\times\dot{\mathbf{r}} + \dot{\boldsymbol{\omega}}\times\hat{\mathbf{z}}R = \boldsymbol{\Omega}\times\mathbf{v} + \dot{\boldsymbol{\omega}}\times\hat{\mathbf{z}}R \qquad (17.1.30a)$$

Putting in (17.1.29) gives the velocity equation of translational motion on the table.

$$\dot{\mathbf{v}} = \boldsymbol{\Omega}\times\mathbf{v} + \frac{1}{I}(m\dot{\mathbf{v}}\times\hat{\mathbf{z}}R)\times\hat{\mathbf{z}}R = \boldsymbol{\Omega}\times\mathbf{v} - \frac{mR^2}{I}\dot{\mathbf{v}} \qquad (17.1.30b)$$

This has the form of the cyclotorn orbit equation $m\dot{\mathbf{v}} = e\mathbf{v}\times\mathbf{B}$.

$$\left(1+\frac{mR^2}{I}\right)\dot{\mathbf{v}} = \boldsymbol{\Omega}\times\mathbf{v} \quad \text{or:} \quad \dot{\mathbf{v}} = \frac{e}{m}\mathbf{v}\times\mathbf{B} \quad \text{where:} \quad \mathbf{B} = -\frac{\boldsymbol{\Omega}}{\left(1+\frac{mR^2}{I}\right)} \qquad (17.1.30c)$$

A solid ball with inertia $I={}^2/_5mR^2$ leads to an effective cycloton frequency of $2\Omega/7$, that is, the ball will orbit exactly twice for each *seven* rotations of the table. The actual surface velocity $\mathbf{V}=\boldsymbol{\Omega}\mathbf{x}\mathbf{r}$ of the table is analogous to a vector potential $\mathbf{A}={}^1/_2\mathbf{B}\mathbf{x}\mathbf{r}$ of a uniform magnetic field.

17.2 Introduction to Autonomy of Time Dependence

Quantum theory contrasts two kinds of time dependence based on whether the Hamiltonian **H** has explicit time dependence or not. An *autonomous* system with constant **H** is the ideal case, but many applications use a time-dependent **H***(t)* to describe non-autonomous systems. We compare the two cases.

(a) Autonomy: The ideal "hands-off" view

In the preceding chapters, time dependence of a quantum system has been autonomous, that is, it occurs without any help from the outside world. Time evolution introduced in Chapter 8 involved a Hamiltonian time evolution generator **H** which was constant **H***(t)*=**H***(0)*. This means the observed time dependence of a state could be written using an evolution operator **U***(t)* formed by an exponential of **H**.

$$|\Psi(t)\rangle = \mathbf{U}(t)\,|\Psi(0)\rangle = e^{-i\mathbf{H}\,t/\hbar}\,|\Psi(0)\rangle \qquad (17.2.1a)$$

This is displayed in equation (9.2.5c) and is equivalent to Schrodinger's equation (9.2.6a) repeated here.

$$i\hbar\frac{\partial}{\partial t}\big|\Psi(t)\big\rangle = \mathbf{H}\big|\Psi(t)\big\rangle \qquad (17.2.1b)$$

The physics behind this is as simple as it is beautiful, and it is based upon Planck's energy-frequency equivalence $E = \hbar\omega$. Each stationary "own-state" or eigenstate $|\varepsilon_k\rangle$ of the Hamiltonian **H** has a definite "own-energy-frequency" or eigen-energy-frequency $\varepsilon_k = \hbar\omega_k$.

$$\mathbf{H}|\varepsilon_k\rangle = \varepsilon_k|\varepsilon_k\rangle = \hbar\omega_k\,|\varepsilon_k\rangle \qquad (17.2.2)$$

An eigenstate of constant Hamiltonian is constant. Only its internal clock will secretly "tick" by (17.2.1).

$$|\varepsilon_k(t)\rangle = e^{-i\varepsilon_k\,t/\hbar}\,|\varepsilon_k(0)\rangle = e^{-i\omega_k\,t}\,|\varepsilon_k\rangle \qquad (17.2.3)$$

Also constant is the probability $P(x,t) = |\langle x|\varepsilon_k(t)\rangle|^2$ for an eigenstate $|\varepsilon_k\rangle$ to end up in any given state $|x\rangle$. Squaring $\Psi^*\Psi=|\Psi|^2$ cancels the single "ticking" phase factor $e^{-i\omega_k\,t}$ with its conjugate $(e^{-i\omega_k\,t})^*=e^{+i\omega_k\,t}$.

$$P_{\varepsilon_k}(x,t) = \langle x|\varepsilon_k(t)\rangle^*\,\langle x|\varepsilon_k(t)\rangle = \langle x|\varepsilon_k\rangle^*\,\langle x|\varepsilon_k\rangle = P_{\varepsilon_k}(x,0) \qquad (17.2.4)$$

But, general states $|\Psi(0)\rangle$ must be some combination $c_1|\varepsilon_1\rangle+c_2|\varepsilon_2\rangle+...$of $|\varepsilon_k\rangle$.(The $|\varepsilon_k\rangle$ are a complete set.)

$$\big|\Psi(0)\big\rangle = \sum_k \big|\varepsilon_k\big\rangle\big\langle\varepsilon_k\big|\Psi(0)\big\rangle = \sum_k \big|\varepsilon_k\big\rangle\, c_k \qquad (17.2.5a)$$

Coefficients $c_k = \langle\varepsilon_k|\Psi(0)\rangle$ are constant as time passes, but eigenstates "tick" their phases by (17.2.3).

$$\big|\Psi(t)\big\rangle = \sum_k e^{-i\omega_k t}\big|\varepsilon_k\big\rangle\, c_k \qquad (17.2.5b)$$

So if state $|\Psi(0)\rangle$ initially combines two or more eigenstates $c_j|\varepsilon_j\rangle+c_k|\varepsilon_k\rangle+...$, the time dependence of its *x*-probability will contain "beats" of amplitude $|c_j\,c_k\,|$,... at each of the difference frequencies $(\omega_j-\omega_k)$,....

$$P_\Psi(x,t) = \langle \Psi(t)|x\rangle\langle x|\Psi(t)\rangle = \sum_{j,k,\cdots} \langle x|\varepsilon_j(t)\rangle^* \langle x|\varepsilon_k(t)\rangle = \sum_k e^{-i(\omega_j-\omega_k)t}\, c_j{}^* c_k \qquad (17.2.5c)$$

It is such a combination of beats that determines the time behavior of an autonomous quantum world as a Fourier sum (or integral) over the system's spectrum. If you really knew all the spectral amplitude coefficients c_j, c_k,... then you can predict the state of an autonomous system forever.

(b) Non-Autonomy: The practical "quantum control" view

There are a couple of real-world problems with the ideal quantum deterministic view of the world. First of all, the observable "reality" of a state $|\Psi(t)\rangle$ are given by probability values $P_\Psi(x,t)$ or expectation values $\langle\Psi(t)|\mathbf{x}|\Psi(t)\rangle$. So, however well you know a state $|\Psi(t)\rangle$, it only gives you some raffle-lottery tickets. A probability $P_\Psi(x,t) = |\langle x|\Psi(t)\rangle|^2$ is just that, odds for an outcome of some more or less clumsy "measurement" process involving eigenstates $\{\langle x|, \langle x'|,..\}$ of another "counter" system different and outside of the one with eigenstates $\{|\varepsilon_1\rangle, |\varepsilon_2\rangle,..\}$ being considered. Remember Axioms 1-4 are based on relative transformation matrix elements $\{\langle x|\varepsilon_1\rangle, \langle x'|\varepsilon_1\rangle,..\langle x|\varepsilon_2\rangle, \langle x'|\varepsilon_2\rangle,..\}$ between two systems.

This then brings up the second problem: A truly autonomous system would be totally isolated and therefore unavailable for "measurement" or any kind of observation. A total measurement ends autonomy just as the act of cashing in all of one's chips ends a game of chance.

One way out of this conundrum is to find ways to "tweak" or perturb a system by time-varying some part of its Hamiltonian in a way that affects outcome probabilities. A general outcome scenario starts a system in some initial state $|\Psi(0)\rangle$ and perturbs $\mathbf{H}$ to stimulate probability in some final state-$|x\rangle$.

$$P_\Psi(x,t) = |\langle x|\Psi(t)\rangle|^2 = |\langle x|\mathbf{U}(t,0)|\Psi(0)\rangle|^2\,, \qquad (17.2.6a)$$

A more usual outcome scenario starts a system in some initial eigenstate-$|\varepsilon_k(0)\rangle = |\varepsilon_k\rangle$ and perturbs $\mathbf{H}$ to stimulate *transition probability* $P_{\varepsilon_k}(\varepsilon_j,t)$ to wind up in some other final eigenstate $|\varepsilon_j\rangle$.

$$P_{\varepsilon_k}(\varepsilon_j,t) = |\langle\varepsilon_j|\varepsilon_k(t)\rangle|^2 = |\langle\varepsilon_j|\mathbf{U}(t,0)|\varepsilon_k(0)\rangle|^2 \qquad (17.2.6b)$$

For the latter case we turn on the perturbation at time $t=0$ and then turn it off sometime later so that the eigenstates of the unperturbed Hamiltonian are meaningful bases for describing the initial and final states.

(c) Diabatic versus adiabatic quantum control

How rapidly we turn on or turn off a perturbation is an important consideration. Sudden or *diabatic* changes in $\mathbf{H}(t)$ cause wave systems to exhibit complicated "ringing" behavior because oscillators respond excitedly when spectral bandwidth of a stimulus overlaps their resonant frequencies. In contrast, gradual or *adiabatic* variation of $\mathbf{H}(t)$ may allow an old eigenstate $|e_k(0)\rangle = |\varepsilon_k\rangle$ of $\mathbf{H}(0)$ to gradually morph into a new eigenstate $|\varepsilon_k(t)\rangle$ of $\mathbf{H}(t)$ without producing combinations of any other $\mathbf{H}(t)$ eigenstates (Such a transition is

known as *adiabatic following*.) But, sudden changes (*Diabatic* means *non-adiabatic* in modern double-negative jargon) are so fast the initial state $|\varepsilon_k(0)\rangle$ cannot follow. The "surprised" state $|\varepsilon_k\rangle$ may be a combination of two or more new eigenstates $|\varepsilon_k(t)\rangle$, $|\varepsilon_{k'}(t)\rangle$, $|\varepsilon_{k''}(t)\rangle$, .. of $\mathbf{H}(t)$ so these "beat" against each other at frequencies $\omega_k(t)-\omega_{k'}(t)$, $\omega_k(t)-\omega_{k''}t)$, .. as in (17.2.5c) while the $\omega_k(t)$ also vary with $\mathbf{H}(t)$.

The distinction between adiabatic and diabatic applies equally to the space-time or wavevector-frequency domain. For example, recall how a sharp barrier causes a wiggling transmission spectrum in Fig. 13.1.6 but softening boundaries even a little quenches the wiggles as in Fig. 13.1.7. For another example, compare Fig. 12.2.7 and 12.2.8. To (over) accommodate long adiabatic turn-on and turn-off times it is often the formal convention that outcome probabilities like (17.2.6) have the initial time $t=0$ replaced by $t=-\infty$, and the final time t replaced by $t=+\infty$. This is a theorist's way of taking the sublime to the ridiculous.

Consider an example of a perturbation operator $\mathbf{V}$ added to $\mathbf{H}$ with a turn-on-turn-off time T.

$$\mathbf{H}(t)=\begin{cases}\mathbf{H}(0) & \text{for } t<0\\ \mathbf{H}(0)+\mathbf{V}\left(1-\cos\left(2\pi t/T\right)\right) & \text{for } 0\le t\le T\\ \mathbf{H}(0) & \text{for } t>T\end{cases} \qquad (17.2.7)$$

If operator $\mathbf{V}$ were, itself, a constant operator, then a system starting in an $\mathbf{H}(0)$-eigenstate $|\varepsilon_k\rangle$ at $t=0$, might, if T was long, always be in a state $|\varepsilon_k(t)\rangle$ which was at all times an eigenstate of the current $\mathbf{H}(t)$ and return to the same original eigenstate $|\varepsilon_k(T)\rangle=|\varepsilon_k\rangle$ after time $t=T$. For some systems this is possible even if $\mathbf{V}$ is large enough to conduct $|\varepsilon_k(t)\rangle$ through a "grand tour" which visits a wide range of the state space.

(d) Which is better? Autonomy or Not

There is something about quantum autonomy that rankles the classicist in all of us. Most of us are, deep down, control freaks worrying over details as picayune as whether to hyphenate the expression anal-retentive! So a driverless quantum system seems to demand..., well,... a driver.

Nevertheless, driving a quantum system *exactly* is not an option. One must question the wisdom of applying a "hard" and precise classical field $\mathbf{E}(t)$ to "soft" and uncertain quantum wavefunctions. After all, the stuff in a classical field involves, deep down, quantized waves, too. All perturbing fields like $\mathbf{E}(t)$ have underlying quantum uncertainty. The same goes for those "hard" classical potentials $V(\mathbf{r})$ or $U(\mathbf{r},t)$. Pure quantum theory cannot tolerate absolute certainty and still be consistent. The smallest indivisible unit of any phase space area is Planck's coefficient $\hbar\sim10^{-35}$*Joule seconds*. The unit is tiny, but it is not zero.

However, practicality of non-autonomous $\mathbf{E}(t)$ wins out if 10^{-35}*Joule seconds* means much more to the system in a perturbing field $\mathbf{E}(t)$ or potential $U(\mathbf{r},t)$ than it does to the field or potential itself. In other

words, if a field or potential has gobs of quanta, then it can say, "What are a few quanta to help a friend?" Such non-autonomy is called *semi-classical* quantum mechanics: a non-autonomous system uses $\Psi(x,t)$ amplitudes to predict each quantum state according to uncertainty relations but demands absolute certainty of phase and amplitude for classical driving perturbation $\mathbf{E}(t)$ or potential $U(\mathbf{r},t)$ in which quanta are negligible. Semi-classical quantum theory and electrodynamics constitutes much of modern theory.

Nevertheless, the parts of modern theory that are most prized are the autonomous ones in which the details of quantum theory are most completely accounted. Quantum electrodynamics (QED) that uses Dirac's electron model is one of the most famous examples. Here both the electronic matter and the electromagnetic field are described in terms of quantum states and operators. No explicit time dependence is attached to any part. Furthermore, QED is fully relativistic, and so Schrodinger's equation, which isolates time as a parameter rather a space-time dimension, must fall by the wayside, as must purely scalar $V(\mathbf{r})$ potentials. The intimate relation between quantum theory and relativity (shown in Ch. 5) indicates that a timeless autonomous quantum theory is ultimately what we want.

But, a perennial question remains, "How can a "measurer" be part of its own system?" This question will bother us for quite some time!

Problems for Chapter 17.

Newton recovers

17.1.1 Verify that Hamilton's equations (17.1.10e) yield the Newtonian pondermotive relation (17.1.1).

Euclid recovers

17.2.1 With a ruler and compass construct on graph paper the *qE*-dipole-shifted atomic *k*-parabolic potential for cases with *k=2.0* and (a) *qE=0* , (a) *qE=1.0* , (a) *qE=2.0* , (a) *qE=4.0* . You might show in each how the phase *(x,v)*-space elliptical paths are located for a mass of *M=1.0* and for *M= 4.0*.

Jailhouse Rock'n Roll

17.2.2 Prisoner-*M* is in the infinite-well maximum-security prison of Chapter 12 suffering from an Earthquake (caused perhaps by a heavy-metal rock band) that seems to go on forever. Now the prison floor tilt angle varies: $\phi=\phi^{limit}\sin(\omega_{rock}t)$ giving gravity PE function $V_{rock'n\ roll}(x)=Mgh$. (Let floor height be defined $h=0$ at $x=0$.)

(a) Give the lowest order term in $V_{rock'n\ roll}(x)$. Discuss how or when that might be a valid approximation.

(b) If prisoner-*M* has a charge *Q* derive his potential in an em-wave $E_x = e_0 \cos(kz-\omega_{rock}t)$ whose polarization is along the cell *x*-axis. Discuss the conditions for it to have the form desired in part (a).

"Zoom" versus "Catcher in the eye"

17.2.3 Conventional wisdom about potential fields claims that a classical or quantum oscillator will "follow" a field that takes a long time to "turn on." Indeed, the phenomena is called "adiabatic following." Suppose it takes *1000* oscillator periods to turn on a uniform field that moves an oscillator's equilibrium position form $r_0=0$ to $r_0=1$. (See Fig. 17.1.1(a)) Then an oscillator sitting at $r_0=0$ (or oscillating around $r_0=0$) is expected, after that field is fully turned on, to have "followed" the varying r_0 all the way from $r_0=0$ to end up sitting at $r_0=1$ (or oscillating around $r_0=1$) with the same action $S=\oint p dx$ it had before. Consider two extreme cases: (a) "Zoom" and (b) "Catcher-in-the eye."

(a) However, suppose that the field increase occurs so that equilibrium starts at $r_0=0$ and makes tiny jumps by $\Delta r_0=1/1000$ each period. Such a field appears to rise slowly but may excite a stationary oscillator to high action. Discuss this case for an initially stationary oscillator and one that is moving. Draw a space-time plot of the force, equilibrium $r_0(t)$ and the oscillator $x(t)$ for several jumps.

(b) Suppose that the field increase occurs so that equilibrium starts at $r_0=0$ and makes tiny jumps by $\Delta r_0=1/2000$ each *1/2*-period.. Discuss this case for an initially stationary oscillator and one that is moving. Draw a space-time plot of the force, equilibrium $r_0(t)$ and the oscillator $x(t)$ for several jumps.

"Ping-pong" versus "pong-pong"

17.2.4 One way to visualize adiabatic-versus-diabatic action variation is to examine a mass bouncing back and forth between two perfectly elastic ping-pong paddles. In each case we imagine that the left "ping" paddle is slowly closing in on a fixed right "pong" paddle so that after 1000 or so bounces it reduces the spacing by one-half. Consider two extreme cases: (a) "Ping-pong" and (b) "Pong-pong."

(a) Suppose the "ping" paddle moves in at velocity v_0 that is slow compared with the initial bounce velocity $V(0)$ of the ball. Each collision increases the speed $V(t)$ and momentum $p(t)=MV(t)$ of the ball. How much? Meanwhile, distance $x(t)$ that the ball travels between each "ping" and "pong" is slowly being reduced. Show that the action $S=\oint p dx$ is nearly constant.

(b) Suppose the "ping" paddle moves at velocity v_0 except that when it hits the ball it stops briefly so each collision leaves the speed $V(t)$ and momentum $p(t)=MV(t)$ of the ball unchanged in magnitude. Show how the action $S=\oint p dx$ varies under these conditions.

Time-Variable Perturbation

W. G. Harter

Chapter 18 treats the case of weak or off-resonant fields for which a perturbation approach to field-stimulated transitions gives an accurate picture of their dynamics. Perturbation may be regarded as an iterative process and is simple when only the first iteration is needed. Several famous results come from such an approximation. These include Fermi's Golden Rule, the TRK-oscillator strength-sum rule, and virial identities. Relations between E•r and A•p approaches are seen, too.

CHAPTER 18 INTRODUCTION TO TIME-VARIABLE PERTURBATION 1

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Chapter 18 Introduction to Time-Variable Perturbation

18.1 Time Dependent Potential

The following is an analysis of time dependent perturbations like E•r in (17.1.20) and more general perturbations $\mathbf{V}(t)$ that are arbitrary functions of time. Perturbation theory attempts to give solutions to the time Schrodinger equation (17.2.1b) with an explicitly time-dependent (non-autonomous) Hamiltonian.

$$\mathbf{H}(t) = \mathbf{H}_0 + \mathbf{V}(t) = \mathbf{H}_0 + \mathbf{H}_I \tag{18.1.1a}$$

A non-autonomous Schrodinger equation is generated by the total Hamiltonian $\mathbf{H}(t)$.

$$i\hbar\frac{\partial}{\partial t}\big|\Psi(t)\big\rangle = \mathbf{H}(t)\big|\Psi(t)\big\rangle = \big(\mathbf{H}_0 + \mathbf{V}(t)\big)\big|\Psi(t)\big\rangle \tag{18.1.1b}$$

We represent it using a basis $\{|\varepsilon_1\rangle, |\varepsilon_2\rangle,..\}$ of eigenstates of the unperturbed part $\mathbf{H}_0$ of the Hamiltonian.

$$\mathbf{H}_0|\varepsilon_k\rangle = \varepsilon_k|\varepsilon_k\rangle = \hbar\omega_k\,|\varepsilon_k\rangle \tag{18.1.3}$$

This is the same as (17.2.2) as is the expansion (17.2.5a) repeated here of the initial state in this basis.

$$\big|\Psi(0)\big\rangle = \sum_k \big|\varepsilon_k\big\rangle\big\langle\varepsilon_k\big|\Psi(0)\big\rangle = \sum_k \big|\varepsilon_k\big\rangle\, c_k \tag{18.1.4}$$

(a) Perturbation approximations

The next steps involve the art of a particular approximation and differ from the time-independent formulation of (17.2.5). First, definition (17.2.5b) has variable $c_k(t)$ replacing constant c_k .

$$\big|\Psi(t)\big\rangle = \sum_k e^{-i\omega_k t}\big|\varepsilon_k\big\rangle\, c_k(t) \tag{18.1.5}$$

The idea is that a small varying $\mathbf{V}(t)$ will cause a slow variation of the otherwise constant $|\varepsilon_k\rangle$-expansion coefficients $c_k(t)$ of the initial state. The comparatively rapid phase oscillation frequencies ω_k of the unperturbed ε-states are assumed constant; the comparatively slow variation of the state is to be entirely accounted for by $c_k(t)$.

While the $|\varepsilon_k\rangle$ and ε_k are rarely eigenkets or eigenvalues of the total Hamiltonian $\mathbf{H}_0 + \mathbf{H}_I$, they do constitute a complete set of eigensolutions of the unperturbed Hamiltonian $\mathbf{H}_0$ and therefore able to make an arbitrary state $|\Psi(t)\rangle$ at any time. This approximation does not try to adjust either the eigenvectors or the eigenvalues to be instantaneous eigensolutions of the total Hamiltonian $\mathbf{H}(t)$. That adjustment is entirely made up by the coefficients $c_k(t)$ for which an approximate solution will now be derived.

Assumed state $|\Psi(t)\rangle$ obeys Schrodinger equation (18.1.1b). The left hand side is a time derivative.

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = i\hbar\frac{\partial}{\partial t}\sum_k e^{-i\omega_k t}|\varepsilon_k\rangle\, c_k(t)$$

$$= i\hbar\sum_k \frac{\partial e^{-i\omega_k t}}{\partial t}|\varepsilon_k\rangle\, c_k(t) + i\hbar\sum_k e^{-i\omega_k t}|\varepsilon_k\rangle\frac{\partial c_k(t)}{\partial t} \qquad (18.1.6)$$

$$= \sum_k \hbar\omega_k e^{-i\omega_k t}|\varepsilon_k\rangle\, c_k(t) + i\hbar\sum_k e^{-i\omega_k t}|\varepsilon_k\rangle\frac{\partial c_k(t)}{\partial t}$$

Schrodinger equation (18.1.1) is rewritten in (18.1.7) below. It may be subtracted from (18.1.6) to cancel the left hand time derivatives and first sum on the right hand side since $\mathbf{H}_0|\varepsilon_k\rangle$ equals $\hbar\omega_k\,|\varepsilon_k\rangle$ by (18.1.3).

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = \sum_{k'} e^{-i\omega_{k'}t}\mathbf{H}_0|\varepsilon_{k'}\rangle\, c_{k'}(t) + \sum_{k'} e^{-i\omega_{k'}t}\mathbf{V}(t)|\varepsilon_{k'}\rangle c_{k'}(t) \qquad (18.1.7)$$

So, the second sum with the $c_k(t)$ derivative in (18.1.6) equals the second sum in (18.1.7).

$$i\hbar\sum_k e^{-i\omega_k t}|\varepsilon_k\rangle\frac{\partial c_k(t)}{\partial t} = \sum_{k'} e^{-i\omega_{k'}t}\mathbf{V}(t)|\varepsilon_{k'}\rangle c_{k'}(t) \qquad (18.1.8)$$

Using eigenstate orthonormality ($\langle\varepsilon_j|\varepsilon_k\rangle=\delta_{jk}$) gives a Schrodinger-like equation for coefficients $c_k(t)$.

$$i\hbar\frac{\partial c_k(t)}{\partial t} = \sum_{k'} e^{i\omega_k t}e^{-i\omega_{k'}t}\langle\varepsilon_k|\mathbf{V}(t)|\varepsilon_{k'}\rangle c_{k'}(t) \qquad (18.1.9)$$

The equation has oscillatory coupling involving perturbation matrix elements $\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle$ and $e^{i(\omega_j-\omega_k)t}$.

$$i\hbar\frac{\partial c_j(t)}{\partial t} = \sum_k e^{i(\omega_j-\omega_k)t}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle c_k(t) = \sum_k V_{jk}(t)c_k(t) \qquad (18.1.10a)$$

Each coupling component has a phase factor oscillating at a beat or transition frequency $\Omega_{jk}=\omega_j-\omega_k$..

$$i\hbar\frac{\partial c_j(t)}{\partial t} = \sum_k e^{i(\omega_j-\omega_k)t}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle c_k(t) = \sum_k V_{jk}(t)c_k(t) \qquad (18.1.10b)$$

The (j,k)-coupling time dependence is a modulation by $\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle$ of the transition beat phasor $e^{i\Omega_{jk}}$.

$$V_{jk}(t) = e^{i\Omega_{jk}}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle = e^{i(\omega_j-\omega_k)t}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle \qquad (18.1.10c)$$

The time variation of the state amplitude of general state $|\Psi(t)\rangle$ in (18.1.5) is

$$\langle\varepsilon_k|\Psi(t)\rangle = e^{-i\omega_k t}\, c_k(t)\ . \qquad (18.1.10d)$$

Apart from its phase factor, $\langle\varepsilon_k|\Psi(t)\rangle$ varies only if the coefficient $c_k(t)$ varies and that happens only if the perturbation $\mathbf{V}(t)$ is non-zero. But, no matter what $\mathbf{V}(t)$ does, the $\mathbf{H}_0$ eigenstates $|\varepsilon_k\rangle$ and their eigenvalues $\varepsilon_k=\hbar\omega_k$ are assumed constant. Only $c_k(t)$ is influenced by $\mathbf{V}(t)$.

(b) Iterative perturbation expansion

To begin solving (18.1.10a) assume the initial state is a pure $\mathbf{H}_0$ eigenstate $|\varepsilon_k\rangle=|\varepsilon_1\rangle$, that is,

$$c_k(0)=\delta_{k1}=c_k^{(0)}. \tag{18.1.11}$$

Then coupled equations (18.1.10a) simplify for a short time *(t~0)*. The first approximation is

$$i\hbar\frac{\partial c_j^{(1)}(t)}{\partial t}=\sum_k V_{jk}(t)c_k^{(0)}(t)=\sum_k V_{jk}(t)\delta_{k1}=V_{j1}(t). \tag{18.1.12}$$

The first approximation for each coefficient is given by a single integral of the perturbation component.

$$c_j^{(1)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}(t_1) \tag{18.1.13}$$

The second approximation to (18.1.10a) uses the first approximation as a starting point.

$$\begin{aligned} i\hbar\frac{\partial c_j^{(2)}(t)}{\partial t}&=\sum_k V_{jk}(t)c_k^{(1)}(t)=\sum_k V_{jk}(t)\left[\delta_{k1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{k1}(t_1)\right] \\ &=V_{j1}(t)+\frac{1}{i\hbar}\sum_k V_{jk}(t)\int_0^t dt_1 V_{k1}(t_1) \end{aligned} \tag{18.1.14a}$$

Integrating with initial value (18.1.11) gives the second iterate of each coefficient.

$$c_j^{(2)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}(t_1)+\frac{1}{(i\hbar)^2}\sum_k\int_0^t dt_2 V_{jk}(t_2)\int_0^{t_2} dt_1 V_{k1}(t_1) \tag{18.1.14b}$$

The third approximate iteration is done similarly and so on for each higher one.

$$c_j^{(3)}(t)=c_j^{(2)}(t)+\frac{1}{(i\hbar)^3}\sum_{k,k'}\int_0^t dt_3 V_{jk'}(t_3)\int_0^{t_3} dt_2 V_{k'k}(t_2)\int_0^{t_2} dt_1 V_{k1}(t_1) \tag{18.1.15}$$

The complexity of each iterative contribution increases rapidly. The situation is reminiscent of the matrix perturbation expansion outlined in Ch. 3 by equation (3.2.5) . Carrying (18.1.15) out means summing all possible sequences between two state-1 and state-j while (3.2.5) sums all path sequences between state-1 and itself. For a constant perturbation operator $\mathbf{V}(t)=\mathbf{V}$ the integrals in (18.1.15) produce energy denominators which are similar to those in (3.2.5).

18.2 First-Order Perturbation Theory and Fermi-Golden-Rule

Much of quantum transition theory is based on first order approximations. These are described in this section in a way that can be compared and improved with better approximations in later Chapters.

(a) First order iteration of dipole approximation

As is the case for matrix perturbation, time dependent perturbation gets the most mileage from its simplest approximation, the first iteration (18.1.13). Consider a perturbation with a single time Fourier component: a charge q sitting at point $\mathbf{r}$ in an x-polarized plane wave electric field $\mathbf{E}(t) = \mathbf{e}_x E_o e^{i(\mathbf{k}\bullet\mathbf{r}-\omega t+\phi)}$.

$$\mathbf{V}^-(t) = -q\,\mathbf{E}(t)\bullet\mathbf{r} = -q\,\mathbf{r}\bullet\mathbf{e}_x E_o e^{i(\mathbf{k}\bullet\mathbf{r}-\omega t+\phi))} \sim -qE_o\, e^{-i(\omega t-\phi)}\mathbf{r}\bullet\mathbf{e}_x \qquad (18.2.1)$$

If the charge is an electron $(q=-|e|=1.6E\text{-}19\ C)$ in an atom whose radius $(\sim 0.5\ A=0.5E\text{-}10m)$ is ten thousand times smaller than optical wavelength $(0.5\mu m=0.5E\text{-}6m)$ then it is convenient to invoke the *dipole approximation* (mentioned after (17.1.20a)) ignoring the small k-dependency of the plane wave.

$$e^{i(\mathbf{k}\bullet\mathbf{r}-\omega t)} \sim e^{-i\omega t} \quad \text{(for negligible } \mathbf{k}\bullet\mathbf{r}\text{)}$$

The dipole approximation reduces the perturbation to an $\mathbf{x}$-operator with an oscillating phase factor.

$$\mathbf{V}^-(t) \sim -qE_o\ e^{-i(\omega t-\phi)}\,\mathbf{r}\bullet\mathbf{e}_x = -qE_o\ e^{-i(\omega t-\phi)}\,\mathbf{x} \qquad (18.2.2a)$$

Let us define a positive frequency $\mathbf{V}^+(t)$ that is the complex conjugate of $\mathbf{V}^-(t)$. (E_o is real here.)

$$\mathbf{V}^+(t) \sim -qE_o\ e^{+i(\omega t-\phi)}\,\mathbf{r}\bullet\mathbf{e}_x = -qE_o\ e^{+i(\omega t-\phi)}\,\mathbf{x} \qquad (18.2.2b)$$

A real standing cosine potential $\mathbf{V}^c(t)$ is a sum of $\mathbf{V}^-(t)$ and $\mathbf{V}^-(t)$.

$$\mathbf{V}^c(t)= [\mathbf{V}^+(t)+\mathbf{V}^-(t)]/2 \sim -qE_o\ \mathbf{r}\bullet\mathbf{e}_x\cos(\omega t-\phi) = -qE_o\ \mathbf{x}\cos(\omega t-\phi) \qquad (18.2.2c)$$

A vector potential which would give the same field $\mathbf{E}=-\partial\mathbf{A}/\partial t$ is the following. (Recall (17.1.12).)

$$\mathbf{A}=\mathbf{e}_x\, 2|a|\sin(kx-\omega t-\phi)\sim\mathbf{e}_x\ 2|a|\ \sin(\omega t-\phi)= \mathbf{e}_x\,|a|(-ie^{-i(\omega t-\phi)}+ie^{+i(\omega t-\phi)})$$

$$= \mathbf{e}_x\,(ae^{-i\omega t}+ a^*e^{+i\omega t})$$

$\mathbf{E}$-field magnitude E_o is given in terms of a complex $\mathbf{A}$ amplitude a and ϕ is initial cosine phase of $\mathbf{E}$.

$$E_o=2|a|\omega \qquad \text{where: } a = -i|a|\,e^{i\phi}, \qquad (18.2.3a)$$

This is for later comparison with quantum fields. The corresponding $\mathbf{A}\bullet\mathbf{P}$ interaction term would be

$$-(q/M)\mathbf{A}\bullet\mathbf{P}\sim\ 2(q/M)|a|\sin(\omega t-\phi)\ \mathbf{P}\bullet\mathbf{e}_x = \mathbf{P}_x\,(-q/M)(ae^{-i\omega t}+a^*e^{+i\omega t}). \qquad (18.2.3b)$$

Let the $\mathbf{E}\bullet\mathbf{r}$ interaction $\mathbf{V}^c(t)$ be given in terms of $a = -i|a|\,e^{i\phi}$.

$$\mathbf{V}^c(t) \sim\ -2q\omega|a|\cos(\omega t-\phi)\ \mathbf{r}\bullet\mathbf{e}_x = -\mathbf{x}\,q\,(\,i\omega\,ae^{-i\omega t}- i\omega\,a^*e^{+i\omega t}). \qquad (18.2.4)$$

Consider now, first-order amplitudes $c_j^{(1)}(t)$ from (18.1.13) of eigenstate $|\varepsilon_j\rangle$ for a system starting out in state $|\varepsilon_1\rangle$ at $t=0$ and perturbed by a cosine potential $\mathbf{V}^c(t)$ in (18.2.4) above.

$$c_j^{(1)}(t) = \delta_{j1} + \frac{1}{i\hbar}\int_0^t dt_I V_{j1}^c(t_I) = \delta_{j1} + \frac{1}{i\hbar}\int_0^t dt_I e^{i\Omega_{j1}} \langle \varepsilon_j \,|\, \mathbf{V}^c(t_I) \,|\, \varepsilon_1 \rangle \qquad (18.2.5a)$$

The key quantities are the beats or *(j←1)-transition frequencies* Ω_{j1} and *(j←1)-dipole matrix elements* r_{j1}.

$$\Omega_{j1} = \omega_j - \omega_1. \qquad r_{j1} = \mathbf{e}\bullet\langle j|\,\mathbf{r}\,|1\rangle \qquad (18.2.5b)$$

The three components of a dipole are labeled *(x,y,z)*. Each are treated equivalently.

$$x_{j1} = \mathbf{e_x}\bullet\langle j|\,\mathbf{r}\,|1\rangle = \langle j|\,\mathbf{x}\,|1\rangle, \qquad y_{j1} = \mathbf{e_y}\bullet\langle j|\,\mathbf{r}\,|1\rangle = \langle j|\,\mathbf{y}\,|1\rangle, \qquad z_{j1} = \mathbf{e_z}\bullet\langle j|\,\mathbf{r}\,|1\rangle = \langle j|\,\mathbf{z}\,|1\rangle$$

Using $\mathbf{V}^c(t)$ from (18.2.3) gives the amplitude integral expressions.

$$c_j^{(1)}(t) = \delta_{j1} + q\frac{r_{j1}}{\hbar}\int_0^t dt_1 \left(-\omega a e^{i(\Omega_{j1}-\omega)t_1} + \omega a^* e^{i(\Omega_{j1}+\omega)t_1} \right) \qquad (18.2.5c)$$

Carrying out the integrals and inserting the amplitude $a = -i|a|\, e^{i\phi}$ gives the following.

$$\begin{aligned} c_j^{(1)}(t) &= \delta_{j1} + q\frac{r_{j1}}{\hbar}\left(i\omega a \frac{e^{i(\Omega_{j1}-\omega)t} - 1}{\Omega_{j1}-\omega} - i\omega a^* \frac{e^{i(\Omega_{j1}+\omega)t} - 1}{\Omega_{j1}+\omega} \right) \\ &= \delta_{j1} + q\frac{r_{j1}\omega|a|}{\hbar}\left(e^{i\phi}\frac{e^{i(\Omega_{j1}-\omega)t} - 1}{\Omega_{j1}-\omega} + e^{-i\phi}\frac{e^{i(\Omega_{j1}+\omega)t} - 1}{\Omega_{j1}+\omega} \right) \end{aligned} \qquad (18.2.5d)$$

It is helpful to rewrite the amplitudes $c_j^{(1)}(t)$ as follows (Here: $E_o = 2|a|\omega$ appears again.)

$$c_j^{(1)}(t) = \delta_{j1} + \frac{q\, r_{j1} E_0}{2\hbar}\left[e^{i\phi} S\left(\Delta^{\uparrow}, t\right) + e^{-i\phi} S\left(\Delta^{\downarrow}, t\right) \right], \qquad (18.2.5e)$$

using an important *spectral amplitude function S(Δ,t)* of an angular frequency *detuning parameter Δ*

$$S(\Delta, t) = \int_0^t d\tau\, e^{i\tau\Delta} = \frac{e^{it\Delta/2}\sin(t\Delta/2)}{\Delta/2}. \qquad (18.2.5f)$$

S maximizes for $\Delta = \Delta^{\uparrow} = 0$ if ω excites an energy increase $(\omega_j > \omega_1)$ or for $\Delta^{\downarrow} = 0$ if energy drops $(\omega_j < \omega_1)$.

$$\Delta^{\uparrow} = \Omega_{j1} - \omega : \text{(excitation: } \varepsilon_1 \to \varepsilon_j > \varepsilon_1) \qquad \Delta^{\downarrow} = \Omega_{j1} + \omega : \text{(de-excitation: } \varepsilon_1 \to \varepsilon_j < \varepsilon_1) \qquad (18.2.5g)$$

(b) The spectral intensity function and energy-time uncertainty

It is important to visualize the spectral function $S(\Delta,t)$ since it appears repeatedly in quantum theory, spectroscopy, acoustics, optics, and practically any subject with oscillation. $S(\Delta,t)$ first appears in this book in connection with pulse trains in Fig. 5.3.2 and wavepacket revivals in Fig. 12.2.5 to Fig. 12.2.7.

One may view $S(\Delta,t)$ as a function $S_t(\Delta)$ of frequency Δ for a fixed time parameter t or *vice-versa* as a time function $S_\Delta(t)$ for a fixed frequency Δ. $S(\Delta,t)=S_t(\Delta)$ is the Fourier Δ-spectrum of a "box-car" function $x(t)$ that is constant $x(\tau)=1$ between time $\tau=0$ and time $\tau=t$ but zero $(x=0)$ before or after. $S(\Delta,t)=S_\Delta(t)$ is the zero-frequency spectral component at time t of a pure single frequency Δ turned on at time $t=0$.

Amplitude-square $|c_j^{(1)}(t)|^2$ is a probability which includes *spectral intensity functions* $I(\Delta,t)$

$$I(\Delta,t)=\left|S(\Delta,t)\right|^2=\frac{\sin^2\left(t\Delta/2\right)}{\left(\Delta/2\right)^2}. \qquad (18.2.6a)$$

The spectral intensity function $I(\Delta,t)$ is plotted versus detuning Δ and time t in Fig. 18.2.1. Its most notable feature is a peak at zero detuning $(\Delta=0)$ soaring up as the square $(I=t^2)$ of time.

$$\lim_{\Delta\to 0} I(\Delta,t) = \lim_{\Delta\to 0}\frac{\sin^2\left(t\Delta/2\right)}{\left(\Delta/2\right)^2}=t^2. \qquad (18.2.6b)$$

Off the main peak, at non-zero-Δ, are lesser $4/\Delta^2$-high peaks whose $2/\Delta$-amplitudes oscillate or "beat" at frequency $\Delta/2$. (Note $t\cdot\Delta=\pm 3\pi, \pm 5\pi,\ldots$ peaks of diminishing heights $4/\Delta^2=4t^2/9\pi^2$, $4t^2/25\pi^2$,… in Fig. 18.2.1) The central t^2-peak is the biggest of these beats, but unlike its companion "beatlets", the $(\Delta=0)$-peak has *zero* beat frequency and *infinite* amplitude. It just keeps on climbing and *never* comes back down!

The $\Delta/2$ frequency of each "beatlet" might be a source of worry since we have noted generally that a system with two states $|\varepsilon_1\rangle$ and $|\varepsilon_j\rangle$ with frequency ω_1 and ω_j, respectively, would beat at frequency $\Omega_{j1}=\omega_j-\omega_1=\Delta$, not at $\Delta/2$. But, as should be the case, $\Omega_{j1}=\Delta$ is the frequency of the *probability*

$$|c_j(t)|^2\sim \sin^2(t\Delta/2)=(1-\cos(t\Delta))/2. \qquad (18.2.7)$$

Meanwhile the *amplitude* $c_j(t)\sim\sin(t\Delta/2)$ has the half-frequency $\Delta/2$. Recall (2.3.14) for similar situations.

Infinite or near infinite amplitudes are a bigger source of worry here. No probability value $|c_j(t)|^2$ should exceed 100% or unity $(c_j(t)\le 1)$ let alone approach infinity! Indeed, the $|c_j^{(1)}(t)|^2$ values are only the first order approximate iteration (18.2.5). Low-Δ-high-t amplitudes $c_j^{(1)}(t)$ need to be fixed by (at least) higher order approximations $c_j^{(2)}(t)$, $c_j^{(3)}(t)$,... in order to make accurate predictions for longer time or finer detuning frequency Δ. However, as we've noted before, perturbation theory often becomes a doomed enterprise of dark arts and crafts. An alternative quasi-exact solution will be discussed in Chapter 19. (Compare Fig. 18.2.1 with a deceptively similar Fig. 19.1.4)

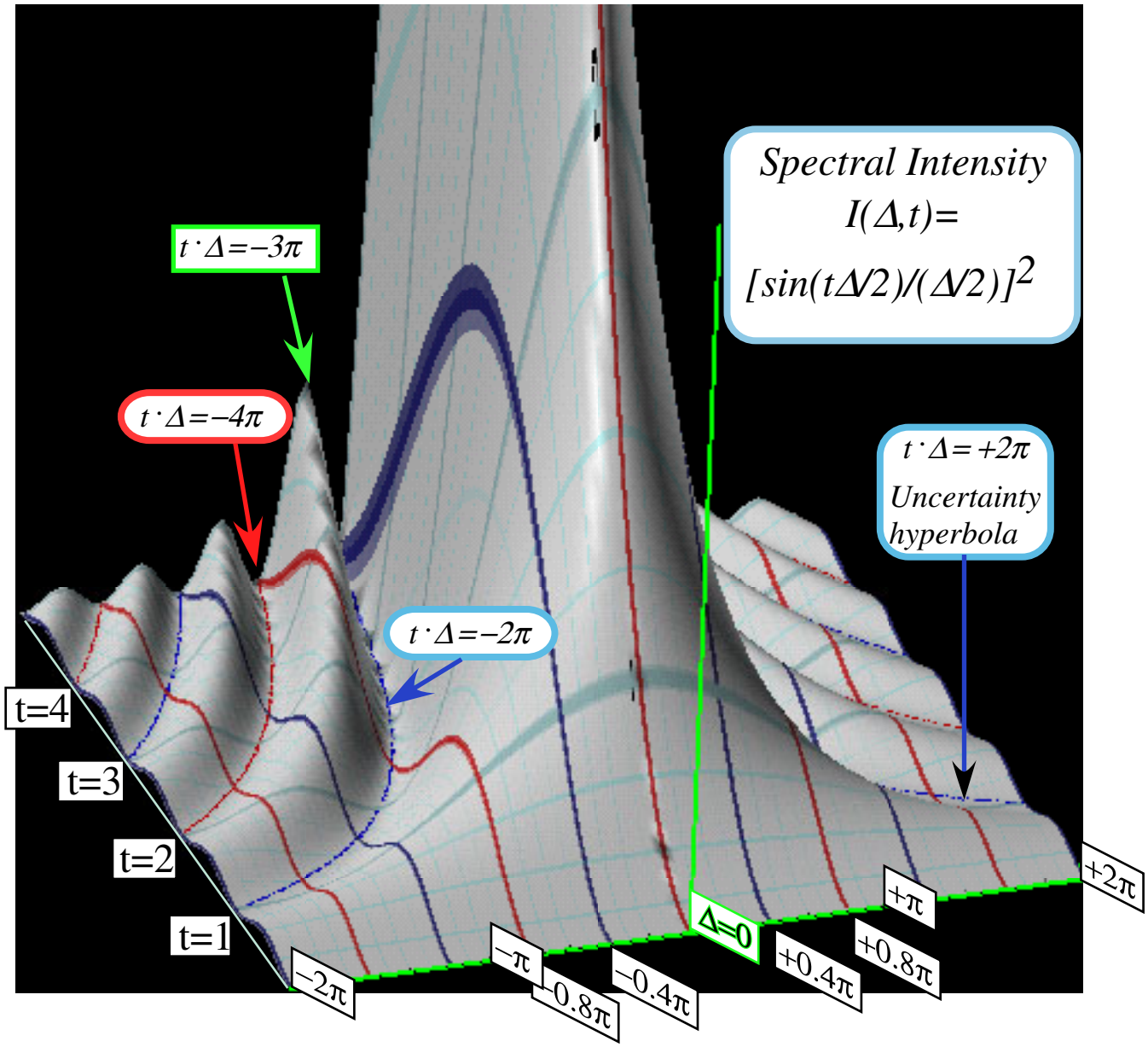


Fig. 18.2.1 Spectral intensity function I(Δ,t) for first order iterate.

The zeros of $I(\Delta,t)$ nearest to $\Delta=0$ are at $t\Delta/2=\pm\pi$ and define a *time-frequency uncertainty relation*

$$t\cdot\Delta = (\Delta\tau)\cdot(\Delta\omega) = \pm 2\pi\ . \qquad (18.2.8)$$

The longer time $t=\Delta\tau$ that the perturbation acts, the less the width $\Delta=\Delta\omega$ of the main peak. From Planck's energy-frequency axiom $E=\hbar\omega$ arises the *Heisenberg time-energy uncertainty relation*

$$\Delta\tau\cdot\Delta E = \pm 2\pi\hbar = \pm h. \qquad (18.2.9)$$

The longer the time $t=\Delta\tau$ allowed for a transition, the smaller the tolerance ΔE for ω-deviation or "non-conservation" of energy. Extremely short times yield a broad energy spectral peak whose bounding zeros at

$\Delta = \pm 2\pi/t$ will, as time t advances, converge as they follow a pair of hyperbolas asymptotic to the t-axis and $\Delta=0$ line in Fig. 18.2.1. The hyperbolas appear to "squeeze" or focus the peak.

The fringe "beatlet" peaks on either side of the main one are left out of this uncertainty relation. They are a small but non-zero part of the total probability spectrum. However, the fringes are an artifact of the "sharp-turn-on" of the perturbation $V(t)$ at initial time $t=0$. They are analogous to the ringing fringes of the $\sin(K_{cut}x)/x$ wave in Fig. 12.2.2 associated with a sharp cut-off of the energy spectrum. Fringes go away for more realistic cut-off that are more gradual as was seen by comparing the ringing fringes of a "box-car" spectrum in Fig. 12.2.7 with a smooth Gaussian spectrum in Fig. 12.2.8 which has no fringes.

(c) Fermi's "Golden Rule"

It is interesting to note that, for short time $(t\sim 0)$ intensity rises as $I=t^2$ for a range of Δ inside a pair of uncertainty hyperbolas $(-2\pi/t < \Delta < \pm 2\pi/t)$. All energy states get an initial "t^2-jolt" no matter how far they are detuned from resonance, another artifact of a diabatic or "sudden" turn-on. As shown in Fig. 18.2.2, the t^2-rise continues for a decreasing range around $\Delta=0$ since greater-$|\Delta|$ amplitudes succumb more quickly to their assigned Δ-beating. This leaves a decreasing number $2\pi/t$ of peak Δ-values still on a t^2-rise. So I-peak area in Fig. 18.2.2 varies as the product of its squeezing base $\Delta=2\pi/t$ and soaring height t^2 *increasing linearly* something like $2\pi t$. So does *total transition probability* $\Sigma(t)$ according to famous "golden-rules" of atomic transitions. Such rules are quantified by investigating the frequency Δ-integral $\Sigma(t)$ of $I(\Delta,t)$.

$$\Sigma(t) = \int_{-\infty}^{\infty} d\Delta \left|S(\Delta,t)\right|^2 = \int_{-\infty}^{\infty} d\Delta \frac{\sin^2\left(t\Delta/2\right)}{\left(\Delta/2\right)^2}. \qquad (18.2.10a)$$

The time derivative of the frequency integral $\Sigma(t)$ is more calculus-friendly.

$$\frac{d\Sigma(\Delta,t)}{dt} = \int_{-\infty}^{\infty} d\Delta \frac{2\sin\left(t\Delta/2\right)\cos\left(t\Delta/2\right)}{\left(\Delta/2\right)^2}\Delta/2 = \int_{-\infty}^{\infty} d\Delta \frac{2\sin\left(t\Delta\right)}{\Delta}. \qquad (18.2.10b)$$

This is reduced to contour integrals and evaluated using Cauchy's theorem $f(a) = \frac{1}{2\pi i}\oint \frac{f(z)}{z-a}dz$. (See exercise.)

$$\frac{d\Sigma(\Delta,t)}{dt} = \frac{1}{i}\oint_{C_1} dz \frac{e^{itz}}{z} - \frac{1}{i}\oint_{C_2} dz \frac{e^{-itz}}{z} = 2\pi. \qquad (18.2.\ 10c)$$

This gives the mathematical basis for *Fermi's golden rule for constant transition rates*.

$$\Sigma(t) = \int_{-\infty}^{\infty} d\Delta \left|S(\Delta,t)\right|^2 = 2\pi\cdot t \qquad (18.2.10d)$$

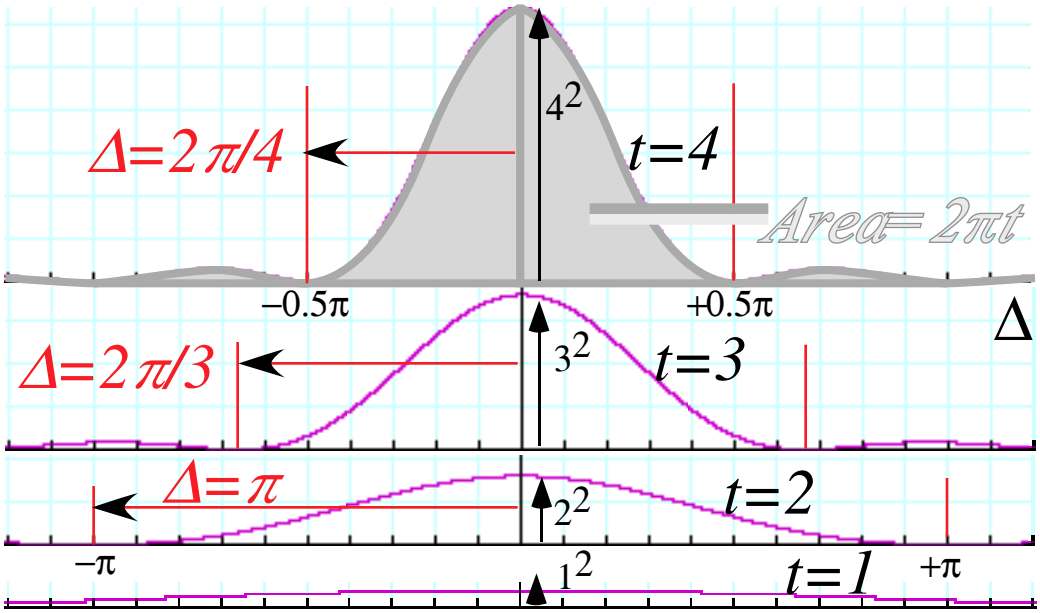


Fig. 18.2.2 Time dependence of spectral intensity function and area.

Only one *S*-term of (18.2.5e) can resonate. The $S(\Delta^{\uparrow},t)$-term peaks at $\omega=\omega_j-\omega_1$ when $\Delta^{\uparrow}=\omega_j-\omega_1-\omega$ is zero as it must be for upward ($\omega_j>\omega_1$) transitions. For downward ($\omega_j>\omega_1$) transitions, the $S(\Delta^{\downarrow},t)$-term peaks at $\Delta^{\downarrow}=\omega_j-\omega_1+\omega=0$ or $\omega=\omega_1-\omega_j$. The latter follows a golden rule if sum $\Sigma j=\Sigma j\Delta n_j$ over final states-*j* finds uniform energy state density $dn_j/d\Delta$ near $\Delta\sim 0$. Then total transition rate *R* is $d\Sigma(t)/dt=2\pi$ times a constant which is a product of r_{j1} and $dn_j/d\Delta$ evaluated near the resonant $S(0,t)$ peak at $\omega=\Omega_{1j}=\omega_1-\omega_j$.

$$R=\frac{d}{dt}\sum_j\left|c_j^{(1)}(t)\right|^2=\frac{d}{dt}\int_{-\infty}^{\infty}d\Delta\left|c_j^{(1)}(t)\right|^2\frac{dn_j}{d\Delta}=\left|\frac{q\,r_{j1}E_0}{2\hbar}\right|^2\frac{dn_j}{d\Delta}\frac{d\Sigma(t)}{dt}=(const.)\qquad(18.2.11a)$$

Upward rates are golden if perturbation $E_0(\omega)$ has a uniform spectrum near a resonance $\omega=\Omega_{j1}=\omega_j-\omega_1$.

$$R_{j\leftarrow 1}=\frac{d}{dt}\int_{-\infty}^{\infty}d\Delta\left|c_j^{(1)}(t)\right|^2=\left|\frac{q\,r_{j1}E_0(\Omega_{j1})}{2\hbar}\right|^2\frac{d\Sigma(t)}{dt}=(const.)\qquad(18.2.11b)$$

Rate constancy needs some sort of quasi-continuous spectrum so the many beats will cancel each other and not contribute spurious coherent oscillation.

Constant rate *R* means constant drainage out an initial state $|\varepsilon_1\rangle$ through matrix element r_{j1} to a final state $|\varepsilon_j\rangle$ as long as the perturbation is in effect. So if, for example, the rate *R* is one transition per 10^6 seconds for each atom, a bottle of $N(0)=10^6$ atoms would make a quantum counter go "click.click...click. click ...click.." at the average rate of one click per second whenever the perturbation is turned on. That is an

average rate. Don't try to set a clock using quantum clicks unless you are willing to average over an enormous number of them. Each click only comes when it's good and ready to come!

But if the perturbation is left on the click rate must go down as the population 'dies off." Only if one somehow replaces the "live" states will the observed rate remain constant. More precisely, $N(0)$ atoms in state $|\varepsilon_1\rangle$ at $t=0$ leaves $N(t)=N(0)e^{-Rt}$ atoms in state $|\varepsilon_1\rangle$ at time t with an instantaneous "click" rate of $N(t)R=N(0)Re^{-Rt}$. A constant *relative* rate R gives pure e^{-Rt} exponential decay rate in a decay experiment.

18.3 Classical Lorentz vs. Quantum Oscillator response

It is instructive to compare classical and quantum-semi-classical oscillator response to harmonic perturbation. This tests **E•r** versus **A•p** interactions and shows what are the classical correspondences of amplitude $c_j^{(1)}(t)$ and the beat frequency $\Omega_{j1}=\omega_j-\omega_1$. We also see how the multiplicative or parametric resonance of quantum theory yields the additive or linear (Lorentz) resonance of classical oscillation.

(a) Classical Lorentz response

The following is a classical equation for a charge-q and mass-M harmonic oscillator of natural frequency ω_0 stimulated by an E-field of frequency ω_S.

$$\ddot{x}+\omega_0{}^2 x=\frac{qE_0}{M}\cos(\omega_S t) \tag{18.3.1a}$$

The solution to this equation for zero initial position or velocity *(x(0) =0= v(0))* is as follows.

$$x_{classical}(t)=\frac{qE_0}{M}\frac{\cos\omega_S t-\cos\omega_0 t}{\omega_0{}^2-\omega_S{}^2} \tag{18.3.1b}$$

Now this is compared with the corresponding quantum physics of harmonic resonance due to a field

$$\mathbf{V}^{\mathbf{c}}(t)=-qE_o\ \cos(\omega t-\phi)\ \mathbf{x}\ . \qquad (18.2.2b)_{repeated}$$

(b) First-order semi-classical response

The general perturbed state (18.1.5) is repeated below and expanded to first order for $c_1^{(1)}(t)=1$.

$$|\Psi(t)\rangle=\sum_j e^{-i\omega_j t}|\varepsilon_j\rangle\, c_j(t) \qquad (18.1.5)_{repeated}$$

$$\cong e^{-i\omega_1 t}\left(|\varepsilon_1\rangle+\sum_{j\neq 1} e^{-i\Omega_{j1}t}c_j(t)|\varepsilon_j\rangle\right),\ \text{where:}\ \ \Omega_{j1}=\omega_j-\omega_1 \tag{18.3.2}$$

The first order iterate for a harmonic perturbation of frequency ω is given by (18.2.5d) repeated here.

$$c_j^{(1)}(t)=\delta_{j1}+q\frac{r_{j1}\omega|a|}{\hbar}\left(e^{i\phi}\frac{e^{i(\Omega_{j1}-\omega)t}-1}{\Omega_{j1}-\omega}+e^{-i\phi}\frac{e^{i(\Omega_{j1}+\omega)t}-1}{\Omega_{j1}+\omega}\right) \qquad (18.2.5d)_{repeated}$$

$$=\delta_{j1}+q\frac{r_{j1}E_0}{2\hbar}\left(\frac{e^{i(\Omega_{j1}-\omega)t}-1}{\Omega_{j1}-\omega}+\frac{e^{i(\Omega_{j1}+\omega)t}-1}{\Omega_{j1}+\omega}\right) \tag{18.3.2}$$

Then $E_o=2|a|\omega$ from (18.2.3b) is used with $\phi=0$ to match the E-field of (18.2.2b) to (18.3.1a) above. The preceding two approximations are now used to estimate the coordinate expectation value $\langle\Psi|\mathbf{x}|\Psi\rangle$.

$$\langle x\rangle=\langle\Psi|\mathbf{x}|\Psi\rangle = \sum_{j\neq 1} e^{-i\Omega_{j1}t}\, c_j(t)\, r_{1j} + \sum_{j'\neq 1} e^{+i\Omega_{j'1}t}\, c^*_{j'}(t)\, r^*_{1j'} = 2\mathrm{Re}\sum_{j\neq 1} e^{-i\Omega_{j1}t}\, c_j(t)\, r_{1j}$$

where: $\langle j|\mathbf{x}|1\rangle = r_{j1} = r^*_{1j}$ and: $\Omega_{j1}=\omega_j-\omega_1$ (18.3.3)

We assume a zero initial (ground state-$|1\rangle$) position value. ($\langle 1|\mathbf{x}|1\rangle=0$) Also, we neglect second order terms $c_j(t)c^*_{j'}(t)\, r_{j'j}$ in a first order calculation. Putting $c_1^{(1)}(t)$ from (18.3.2) in the $\langle x\rangle$ expression gives

$$\begin{aligned}\langle x\rangle &= 2\,\mathrm{Re}\sum_{j\neq 1} e^{-i\Omega_{j1}t}\; c_j^{(1)}(t) r_{1j} \\ &= 2\,\mathrm{Re}\frac{q r_{j1} r_{1j} E_0}{2\hbar}\left(\frac{e^{-i\omega t}-e^{-i\Omega_{j1}t}}{\Omega_{j1}-\omega}+\frac{e^{i\omega t}-e^{-i\Omega_{j1}t}}{\Omega_{j1}+\omega}\right)\end{aligned} \qquad (18.3.4a)$$

This resembles the classical response equation (18.3.1b). Sum restriction $j\neq 1$ is automatic since $\Omega_{11}=0$.

$$\langle x\rangle = \sum_{j\neq 1}\frac{q|r_{j1}|^2 E_0}{\hbar}\mathrm{Re}\left(\frac{\left(\Omega_{j1}+\omega\right)\left(e^{-i\omega t}-e^{-i\Omega_{j1}t}\right)+\left(\Omega_{j1}-\omega\right)\left(e^{i\omega t}-e^{-i\Omega_{j1}t}\right)}{{\Omega_{j1}}^2-\omega^2}\right)$$

$$= \sum_{j=1}\frac{2\Omega_{j1} q|r_{j1}|^2 E_0}{\hbar}\left(\frac{\cos\omega t-\cos\Omega_{j1}t}{{\Omega_{j1}}^2-\omega^2}\right) \qquad (18.3.4b)$$

(c) Oscillator strength

Factors of the corresponding $x_{classical}$ in (18.3.1b) and quantum $\langle x\rangle$ above are isolated.

$$\begin{aligned}\langle x\rangle &= \sum_{j=1}\frac{2\Omega_{j1}|r_{j1}|^2 M}{\hbar}\left(\frac{qE_0}{M}\frac{\cos\omega t-\cos\Omega_{j1}t}{{\Omega_{j1}}^2-\omega^2}\right) \\ &= \sum_{j=1} f_{j1}\cdot x_{classical}\end{aligned} \qquad (18.3.5a)$$

Each classical response term has a natural frequency ω_0 that is the *Lorentz-atomic-oscillator* frequency

$$\omega_0=\Omega_{j1}=\omega_j-\omega_1. \qquad (18.3.5b)$$

This is the *(j←1)-transition frequency* Ω_{j1} or quantum beat. Each is driven by stimulus frequency ω_S.

$$\omega_S=\omega. \qquad (18.3.5c)$$

Each Lorentz oscillator responds with a certain *(j←1)-oscillator strength* f_{j1} defined here.

$$f_{j1}=\frac{2\Omega_{j1}|r_{j1}|^2 M}{\hbar} \qquad (18.3.5d)$$

(1) Harmonic oscillator

The following uses some facts about the quantum 1D-harmonic oscillator which are derived in Chapter 20.For a harmonic oscillator potential $(V(r)=\frac{1}{2}\omega^2 r^2)$ the only f_{j1} arising from the $(j=1)$-state $|\upsilon=0\rangle$ is from $(j=2)$-state, that is, the first excited state $|\upsilon=1\rangle$. The oscillator dipole matrix is derived in (20.3.8).

$$r_{\upsilon 0} = \langle \upsilon|x|0\rangle = \langle \upsilon|a+a^\dagger|0\rangle\sqrt{\frac{\hbar}{2M\omega}} = \delta_{\upsilon 1}\sqrt{\frac{\hbar}{2M\Omega_{0,1}}} \quad , \qquad \text{So: } f_{\upsilon,0}=\delta_{\upsilon,1} \qquad (18.3.6)$$

Therefore (18.3.5a) for ground state excitation reduces to a single $(f_{1,0}=1)$-term ($j=1$ means $\upsilon=0$ and $j=2$ means $\upsilon=1$.) equal to the classical response, that is, $\langle x\rangle=x_{classical}$ is true exactly.

The quantum result is exactly the classical one despite the fact that it is based on a first order $c_j^{(1)}(t)$ approximation! We know that the $c_j^{(1)}(t)$ approximation is wrong near its central peak since it blows up. How can such an untrustworthy quantum result come up with an exact classical one?

The classical result blows up at resonance $(\omega_S=\omega)$ but legitimately so. To approximate near-resonance behavior of any quantum system one needs higher-than-first-order approximations. This is particularly the case for a harmonic oscillator whose quantum $(\upsilon+1\leftarrow\upsilon)$ transitions all have the same frequency $(\omega=\Omega_{\upsilon+1\leftarrow\upsilon})$ and therefore are all in resonance at once. After the first excited state $|\upsilon=1\rangle$ acquires an amplitude from the ground state $|\upsilon=0\rangle$ there will begin a transition to $|\upsilon=2\rangle$, then $|\upsilon=3\rangle$, and so on, as each $(\upsilon+1\leftarrow\upsilon)$ pair contributes oscillator strength to the $\langle x\rangle$-value near resonance $(\omega_S=\omega)$.

No such problem arises if the stimulus is far enough from resonance. The first order theory accounts for the beats, which for a cold oscillator, consist solely of the $(1\leftarrow 0)$ beats plotted in Fig. 18.2.1.

While an oscillator potential $\frac{1}{2}\omega^2 r^2$ restricts oscillator strength to $(\upsilon+1\leftarrow\upsilon)$-transitions between neighboring pairs of levels, other potentials $V(r)$ may have strength in general $(k\leftarrow j)$-transitions. If so, the first order response (18.3.5a) has multiple interfering terms contributing to $\langle x\rangle$. Even so, if the stimulus ω is close to a particular resonance Ω_{j1} with a non-zero oscillator strength f_{j1} (but not close enough to ruin the first-order approximation) then the f_{j1}-term in the sum will dominate as $1/(\Omega_{j1}^2-\omega_1^2)$ blows up.

(d) Thomas-Reiche-Kuhn sum and virial identities

It turns out that a sum of oscillator strengths is invariant to choice of potential. The sum is $\Sigma_j f_{j1}=1$ for an oscillator by (18.3.6). The general sum in question is like the one in (18.3.5a) sans $x_{classical}$.

$$\sum_{j=1} f_{j1} = \sum_{j=1} 2\Omega_{j1} r^*_{1j} r_{j1} M/\hbar = \sum_{j=1} 2\Omega_{j1} \langle 1|x|j\rangle\langle j|x|1\rangle M/\hbar \qquad (18.3.7)$$

An x-matrix element is related to a p-matrix element using commutation $[p,x]=\hbar/i$ with $H_0=p^2/2M+V(x)$.

$$[H_0\,,\,x] = [\,p^2,\,x\,]/2M = \hbar\, p/Mi \qquad (18.3.8)$$

Now the definitions $H_0|j\rangle=\hbar\omega_j H_0|j\rangle$ and $\Omega_{j1}=\omega_j-\omega_1$ are used with this commutation.

$$\langle j|\,p|\,1\rangle = Mi\,\langle j|\,[H_0\,,\,x]|\,1\rangle/\hbar = Mi\,(\omega_j-\omega_1)\langle j|\,x|\,1\rangle = Mi\Omega_{j1}\,r_{j1}$$

The resulting replacements

$$\langle j|\,x|\,1\rangle = \langle j|\,p|\,1\rangle/(Mi\Omega_{j1}) \quad \text{or:} \quad \langle 1|\,x|j\rangle = \langle 1|\,p|j\rangle/(Mi\Omega_{1j}) = -\langle 1|\,p|j\rangle/(Mi\Omega_{j1}) \qquad (18.3.9)$$

then yield the *Thomas-Reiche-Kuhn sum rule for oscillator strength*. This holds for any H_0 eigenstate $|1\rangle$.

$$\sum_{j=1} f_{j1} = \sum_{j=1} 2\langle 1|x|j\rangle\langle j|p|1\rangle/\hbar i = 2\langle 1|xp|1\rangle/\hbar i = -2\langle 1|px|1\rangle/\hbar i = 1 \qquad (18.3.10a)$$

A corollary of the TRK rule is the *virial identity* that also holds for any H_0 eigenstate $|m\rangle$.

$$\langle m|\,xp|m\rangle = \hbar i/2 = -\langle m|\,px|m\rangle \qquad (18.3.10b)$$

The time derivative of the virial matrix element is zero. Schrodinger's equation $|\dot m\rangle = -i/\hbar H|m\rangle$ gives

$$0 = \frac{\partial}{\partial t}\langle m|xp|m\rangle = \langle \dot m|xp|m\rangle + \langle m|xp|\dot m\rangle = \frac{i}{\hbar}\langle m|Hxp|m\rangle - \frac{i}{\hbar}\langle m|xpH|m\rangle = \frac{i}{\hbar}\langle m|[H,xp]|m\rangle$$

For a power-law-potential Hamiltonian $H=p^2/2M+V\cdot x^P$ the commutation reduces as follows.

$$0 = \frac{i}{\hbar}\langle m|\left[\frac{p^2}{2M},xp\right]|m\rangle - \frac{i}{\hbar}\langle m|\left[V\cdot x^P,xp\right]|m\rangle = \langle m|\frac{p^2}{M}|m\rangle - P\langle m|V\cdot x^P|m\rangle$$

From this follows a *quantum eigenstate virial theorem* which is similar to the classical viral theorem.

$$\langle KE\rangle = \langle m|\frac{p^2}{2M}|m\rangle = \frac{P}{2}\langle m|V\cdot x^P|m\rangle = \frac{P}{2}\langle PE\rangle \qquad (18.3.10c)$$

Interference terms $a_m^* a_n\,\langle m|H|n\rangle$ in $\langle\Psi|H|\Psi\rangle$ matrices for mixed state $|\Psi\rangle=\Sigma a_m|m\rangle$ give beating $\langle KE(t)\rangle$ and $\langle PE(t)\rangle$ which disobey the virial theorem. However, if averages of $a_m^* a_n$ may be assumed to be zero for $m\neq n$ this leaves only the diagonal probabilities $P(n)=a_n^* a_n=|a_n|^2$. Then an *averaged virial theorem* still holds for a randomized ensemble of mixed states, and the classical result is recovered.

$$\overline{\langle KE\rangle} = \overline{\langle\Psi|\frac{p^2}{2M}|\Psi\rangle} = \frac{P}{2}\overline{\langle\Psi|V\cdot x^P|\Psi\rangle} = \frac{P}{2}\overline{\langle PE\rangle} \qquad (18.3.10d)$$

For the harmonic oscillator *(P=2)*, average kinetic energy $\langle KE\rangle$ average potential energy $\langle PE\rangle$ are equal.

(e) A·P interaction again

One might inquire what the oscillator response $\langle x\rangle$ would be if the $-q\mathbf{A}\bullet\mathbf{P}/M$ perturbation from (17.1.21a) is substituted for the $-q\mathbf{E}\bullet\mathbf{r}$ interaction of (17.1.21b) used in the preceding equation (18.2.5). We have been using (18.2.4) which is repeated below. (Recall amplitude definition: $\omega a = -i\omega |a| e^{i\phi}$)

$$-q\mathbf{E}\bullet\mathbf{r}\sim \quad -2q\omega|a|\mathbf{r}\bullet \mathbf{e}_x\cos(\omega t-\phi) \quad = \mathsf{x}\, q\,(i\omega\, ae^{-i\omega t}- i\omega\, a^*e^{+i\omega t}). \qquad (18.2.4)_{repeated}$$

to derive the following dipole interaction matrix element which then was used to calculate response.

$$-\langle j|q\mathbf{E}\bullet\mathbf{r}|1\rangle \quad = \langle j|\mathsf{x}|1\rangle\, q\,(-i\omega\, ae^{-i\omega t}+ i\omega\, a^*e^{+i\omega t}). \qquad (18.3.11)$$

Instead, for the same electromagnetic field $\mathbf{E}=-\partial\mathbf{A}/\partial t$, consider using the following interaction

$$-(q/M)\mathbf{A}\bullet\mathbf{P}\sim\ 2(q/M)|a|\mathbf{P}\bullet\ \mathbf{e}_x\ \sin(\omega t-\phi)=\mathsf{P}_x\,(-q/M)(ae^{-i\omega t}+a^*e^{+i\omega t}), \qquad (18.2.3b)_{repeated}$$

which gives the following dipole interaction matrix element.

$$-\langle j|(q/M)\mathbf{A}\bullet\mathbf{P}|1\rangle = \langle j|\mathsf{P}_x|1\rangle\,(q/M)(-ae^{-i\omega t}- a^*e^{+i\omega t}) \qquad (18.3.12a)$$

The momentum matrix can be related to the position dipole using $\langle j|\,\mathsf{p}|1\rangle = Mi\Omega_{j1}\langle j|\,\mathsf{x}|1\rangle$ from (18.3.9).

$$-\langle j|(q/M)\mathbf{A}\bullet\mathbf{P}|1\rangle = \langle j|\mathbf{X}|1\rangle\,(qi\Omega_{j1})(-ae^{-i\omega t}- a^*e^{+i\omega t}) \qquad (18.3.12b)$$

$$= \langle j|\mathbf{X}|1\rangle\, q(-i\Omega_{j1}ae^{-i\omega t}-i\Omega_{j1}a^*e^{+i\omega t}) \qquad (18.3.12c)$$

Comparison of (18.3.11) to (18.3.12c) reveals a discrepancy in factors of the form $\pm\omega/\Omega_{j1}$ and dispels any notion that $-q\mathbf{E}\bullet\mathbf{r}$ and $-q\mathbf{A}\bullet\mathbf{P}/M$ are equal. However, for an excitation resonance $(\omega=\Omega_{j1})$ the first terms will match and for a de-excitation resonance $(\omega=\Omega_{1j}=-\Omega_{j1})$ the second terms will match. So golden rule rates, which are insensitive to coherence between the terms, might incorrectly suggest equality of $-q\mathbf{E}\bullet\mathbf{r}$ and $-q\mathbf{A}\bullet\mathbf{P}/M$. Such a coincidence sets a trap into which many have fallen, but attempts to use $-q\mathbf{A}\bullet\mathbf{P}/M$ to derive coherent response fails if the $(\mathbf{X},\mathbf{P})$-$(\mathbf{x},\mathbf{p})$ transformation (6.2.21) is ignored.

For convenience we collect here a summary of classical dipole fields $\mathbf{E}=-\partial\mathbf{A}/\partial t$:

$$\mathbf{E}= \ 2\omega|a|\mathbf{e}_x\ \cos(\omega t-\phi) = \ (i\omega\, ae^{-i\omega t}- i\omega\, a^*e^{+i\omega t})\mathbf{e}_x \quad \text{where: } \omega\, a = -i\omega|a|\ e^{i\phi} = -iE_o/2\ e^{i\phi}$$

$$\mathbf{A}=-2|a|\ \ \mathbf{e}_x\ \sin(\omega t-\phi) = (\quad ae^{-i\omega t} + \quad a^*e^{+i\omega t})\mathbf{e}_x \qquad (18.3.13)$$

This will be compared to very similar looking expressions for quantum fields in which the amplitudes $\mathbf{E}$, $\mathbf{A}$, and a are replaced by operators. Sometimes such a replacement is given an oxymoronic label of *second quantization*. This is a result of the long history of semi-classical treatments of particles (quantized nuclei, atoms, molecules, solids, etc.) in fields (classical electromagnetic fields) which has been so useful. The idea is that a "second coming" is needed to "fix up" the field, too. This is ironic in

light of the fact that quantum theory owes its very existence to Planck's hypothesis of *electromagnetic* quanta.

As we will see, one needs to regard the particles and field as a single spacetime quantum system. Classical reductionism goes only so far before it becomes misleading and paradoxical. A first step toward such a re-en"light"enment is a non-perturbative treatment of a radiation field interacting with just two levels of an atom, molecule, or a single spin-1/2 of an electron, nucleon, atom, molecule, solid, etc.

In the next section we revisit the *ABCD* formulation from Chapters 9 and 10 of two-level *U(2)* quantum states. The difference now will be that one or more of those *A, B, C*, or *D* parameters can wiggle in time and even be controlled from the outside. Indeed, it's more semi-classical theory but one with a twist!

Problems for Chapter 18.

Golden Cauchy Potato

18.2.1 Use Cauchy's theorem to verify the Fermi Golden Rule (18.2.10) for constant transition rates. Show relevant integration contours and explain your steps.

Beat to death

(a) Compare the relative heights of 0^{th} , 1^{st}, 2^{nd}, ...N^{th} beat probability peaks in Fig. 18.2.1.

(b) Use whatever means to deduce the probability versus time to be under the 0^{th} beat peak in Fig. 18.2.1. (Only numbers and time t are allowed in your answer!)

(a) Compare the relative probabilities under 0^{th}, 1^{st}, 2^{nd},3^{rd} beat peaks in Fig. 18.2.1. How does that relative distribution vary with time?

Jailhouse Rock'round the Clock

18.3.1 In Problem 18.1.1 (*Jailhouse Rock'n Roll*) prisoner-M is in the infinite-well maximum security prison of Chapter 12 suffering from an Earthquake (caused perhaps by a heavy-metal rock band) that seems to go on forever. M remains in any of its eigenstates only in the absence of perturbations. But now the prison floor tilt angle varies: $\phi=\phi^{limit} sin(\omega_{rock}t)$ giving $V_{rock'n\ roll}(x)$ of Proplem 18.1.1. Use that here.

Discuss transition from the ground state $|\varepsilon_1\rangle$ to $|\varepsilon_m\rangle$ stimulated by frequency ω_{rock} of amplitude $\phi^{limit}=\pi/10$. Consider cases: $\omega_{rock} = \varepsilon_1$ ($=1$ in theorist $\hbar=1$ units) , $2\ \varepsilon_1$, $3\ \varepsilon_1$, $4\ \varepsilon_1$.

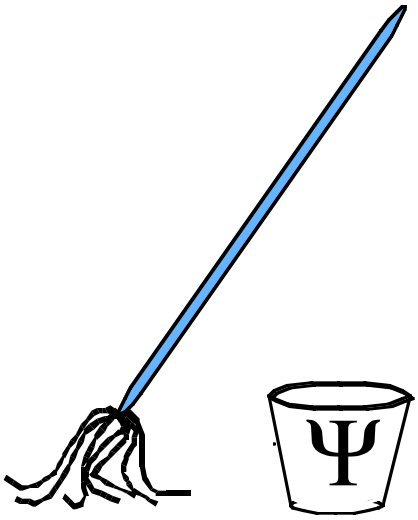
(a) Using only the first term in $V_{rock'n\ roll}(x)$, derive first order transition amplitudes $c^{(1)}_m$.

(b) Derive the resulting expectation value $\langle x\rangle$ of position if M is "waked up" from its ground state.

(c) Derive the resulting expectation value $\langle p\rangle$ of momentum if M is "waked up" from its ground state.

(d) Discuss the Thomas-Reiche-Kuhn sum rule and the Virial Theorem for the prison.

Unit 6



QM for AMOP

Chapter 19

Time-Variable Perturbation Of Two-State Systems

W. G. Harter

CHAPTER 19 TIME-VARIABLE PERTURBATION OF TWO-STATE SYSTEMS..... 1

For two-state systems the perturbation effects due to oscillating components A, B, C, and D of its Hamiltonian may be described analytically and geometrically. We comparison of these results with the first-order approximation given in the preceding Chapter 18. One type of the effects, as applied to transitions of NH_3 states introduced in Chapter 10, are called the AC-Stark shifts. Related effects were studied much earlier in nuclear magnetic resonance (NMR) and electronic spin resonance (ESR) systems. The effects in this Chapter are known mostly by the names Rabi-Ramsey-Schwinger and Feynman-Vernon-Helwarth after two famous papers by these triplets of authors. Rotation operator and spin vector visualization tools developed in Chapter 10 help to clarify spin resonance and time-dependent “dressed” eigenstates.

Chapter 19 Time-Variable Perturbation of Two-State Systems

19.1 "Exact" Time Dependent Perturbation

Low order approximations of time-dependent perturbation (TDP) theory is successful beyond what one has a right to expect. Using the first-order iterate (18.2.5) one may derive much of the basic theory that is used in modern physics. The constant transition rate is such a well-established result that it is called the "golden rule." Roughly speaking, TDP gives time behavior as a power series in time and the "golden rule" is based on the first term. (But, a quasi-continuum of beats has to average to zero!)

The problem with power series is that eventually they blow up. The spectral intensity function described around Fig. 18.2.1 is such an example in which $c_j^{(1)}(t)$ diverges with time t and probability $|c_j^{(1)}(t)|^2$ blows up as t^2. One should note some similarity in error growth for $c_j^{(n)}(t)$ iteration and a related failure of matrix perturbation depicted in Fig. 3.2.2 of Chapter 3.

It seems that polynomials are bad descriptors of quantum phenomena which, being fundamentally wave-like, are better described by sine, cosine, and exponential, that is, by circular and hyperbolic functions. Polynomial approximation of the two-level hyperbola in Fig. 3.2.2 eventually fails badly.

Here we consider time-dependent perturbation of a two-level system that, like the matrix perturbation example in Fig. 3.2.2, has an "exact" hyperbolic description. A hyperbolic "avoided crossing" was described again in Chapter 10 around Fig. 10.3.1 in connection with E-field splitting of ammonia (NH_3) inversion levels. This is known as a *DC Stark effect*.

This section will be devoted to basically the same problem, but with an oscillatory or AC electric field. This is known as an *AC Stark effect*. Here, as in the DC case, it will be seen how an "exact" theory can be constructed to replace a failing perturbation sequence. Such a replacement is absolutely necessary in the presence of strong coherent radiation fields of high spectral purity. Then strong quantum beats dominate and the "golden rule" goes out the window.

Among the first work to describe and demonstrate oscillatory perturbation of two-state systems was a paper by Rabi, Ramsey, and Schwinger in connection with nuclear magnetic resonance (NMR). The analogy between spin resonance and resonance of other two-state systems including NH_3-inversion was pointed out in a paper shortly thereafter by Feynman, Vernon, and Helwarth.

The NH_3-inversion experiments by Townes' group was labeled by the acronym MASER (Microwave Amplification by Stimulated Emission of Radiation). Soon thereafter, the optical transitions were found to give light amplification by stimulated emission and the LASER was born. The AC Stark effect and NMR is closely related to much of laser physics and deserves special attention not only for its historic significance but also for its fundamental quantum theoretical implications.

These implications include resonance effects in other much older 2-state systems such as optical polarization and galloping wave dynamics introduced in Chapter 4. It is ironic that earliest physical realizations of *U(2)* phenomena are the latest to receive modern attention. So-called *photonics* is both an ancient and an ultra-modern field!

(a) Perturbed 2-state systems

The most general 2-state Hamiltonian $H=H^\dagger$ has four real parameters A, B, C, and D.

$$H=\begin{pmatrix} A & B-iC \\ B+iC & D \end{pmatrix} \tag{19.1.1}$$

Chapter 10 discusses three main symmetry types of $ABCD$-Hamiltonians. First, the *AD-type* is *asymmetric-diagonal*, the *B-type* has *balanced-bilateral* symmetry, and the *C-type* is *complex-chiral* and associated with *circular* polarization, *cyclotron* resonance, or *coriolis* forces.

$$H^A=\begin{pmatrix} A & 0 \\ 0 & -A \end{pmatrix} \tag{19.1.2a}$$
$$=A\sigma_A=A\sigma_Z$$

$$H^B=\begin{pmatrix} 0 & B \\ B & 0 \end{pmatrix} \tag{19.1.2b}$$
$$=B\sigma_B=B\sigma_X$$

$$H^C=\begin{pmatrix} 0 & -iC \\ iC & 0 \end{pmatrix} \tag{19.1.2c}$$
$$=C\sigma_C=C\sigma_Y$$

(Standard XYZ labels of Pauli operators are included, too.) The general Hamiltonian (19.1.1) combines the A, B, and C symmetry operators with the $U(2)$-symmetric unit matrix operator $\sigma_0=\mathbf{1}$.

$$\mathbf{H}=\frac{A+D}{2}\mathbf{1}+\frac{A-D}{2}\sigma_A+B\sigma_B+C\sigma_C \tag{19.1.3a}$$
$$=(A+D)\mathbf{S}_0+(A-D)\mathbf{S}_A+(2B)\mathbf{S}_B+(2C)\mathbf{S}_C=\Omega_0 S_0+\Omega\bullet\mathbf{S}$$

Here the spin-$^1/_2$ angular momentum operators $\mathbf{S}_N=\sigma_N/2$ are preferred bases because their coefficients

$$\Omega_0=(A+D),\quad \Omega_A=(A-D),\quad \Omega_B=2B,\quad \Omega_C=2C. \tag{19.1.3b}$$

are angular velocities. The "crank-vector" $\mathbf{\Omega}=(\Omega_A,\Omega_B,\Omega_C)$ determines where and how fast the spin expectation value $\langle\mathbf{S}\rangle$ precesses (or if it precesses) in (S_A, S_B, S_C)-space due to an $ABCD$-Hamiltonian H.

The time Schrodinger equation, in units with $\hbar=1$, is as follows.

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix}=i\frac{\partial}{\partial t}|\Psi(t)\rangle=\mathbf{H}|\Psi(t)\rangle=\begin{pmatrix} A & B-iC \\ B+iC & D\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} \tag{19.1.4a}$$

The solution for constant A, B, C, and D is by (2.10.20) a t-exponential Ω_0-phase-plus-$\mathbf{\Omega}$-rotation.

$$|\Psi(t)\rangle=e^{-i\mathbf{H}t}|\Psi(0)\rangle=e^{-i\left(\frac{\Omega_0}{2}\mathbf{1}+\mathbf{\Omega}\bullet\mathbf{S}\right)t}|\Psi(0)\rangle=e^{-i\left(\frac{\Omega_0}{2}\mathbf{1}+\frac{\mathbf{\Omega}\bullet\mathbf{\sigma}}{2}\right)t}|\Psi(0)\rangle \tag{19.1.4b}$$
$$=e^{-i\frac{\Omega_0}{2}t}e^{-i(\Omega_A\mathbf{S_A}+\Omega_B\mathbf{S_B}+\Omega_C\mathbf{S_C})t}|\Psi(0)\rangle=e^{-i\frac{\Omega_0}{2}t}e^{-\frac{i}{2}(\Omega_A\sigma_\mathbf{A}+\Omega_B\sigma_\mathbf{B}+\Omega_C\sigma_\mathbf{C})t}|\Psi(0)\rangle$$

A similar NMR Hamiltonian for a spin moment $\mathbf{m}=g\,\mathbf{S}$ in a $\mathbf{B}$-field (but without an overall phase Ω_0) is

$$\mathbf{H}=\begin{pmatrix}\langle\uparrow|\mathbf{H}|\uparrow\rangle & \langle\uparrow|\mathbf{H}|\downarrow\rangle\\ \langle\downarrow|\mathbf{H}|\uparrow\rangle & \langle\downarrow|\mathbf{H}|\downarrow\rangle\end{pmatrix}=-\mathbf{m}\bullet\mathbf{B}=-g\mathbf{B}\bullet\mathbf{S}=\frac{g}{2}\begin{pmatrix}B_Z & B_X-iB_Y\\ B_X+iB_Y & -B_Z\end{pmatrix} \tag{19.1.5a}$$

(Again, let $\hbar=1$.) The constant-$\mathbf{B}$ solution is just an $(\mathbf{S}=\mathbf{\sigma}/2)$-vector rotation at a beat frequency Ω.

$$|\Psi(t)\rangle=e^{-ig\mathbf{B}\bullet\mathbf{S}t}|\Psi(0)\rangle=e^{-i\frac{g\mathbf{B}\bullet\mathbf{\sigma}}{2}t}|\Psi(0)\rangle=\left(\mathbf{1}\cos\frac{g|\mathbf{B}|}{2}\mathrm{t}-i\frac{\mathbf{B}\bullet\mathbf{\sigma}}{|\mathbf{B}|}\sin\frac{g|\mathbf{B}|}{2}\mathrm{t}\right), \tag{19.1.5b}$$

The *NMR beat frequency* $\Omega=g|\mathbf{B}|\hbar$ is the length of "crank vector" $\mathbf{\Omega}=g(B_X, B_Y, B_Z)$.

$$\Omega = g|\mathbf{B}| = g\sqrt{B_X^2 + B_Y^2 + B_Z^2} \qquad (19.1.5c)$$

This NMR example is essentially the same as the general *ABCD*-case except it zeros overall phase Ω_0.

Solution $|\Psi(t)\rangle$ needs to be upgraded if the parameters $\{A, B, C, D\}$ or fields (B_X,B_Y,B_Z) are time dependent. An NMR device fixes a large B_Z field to get a microwave level splitting $\Omega=gB_Z$, and oscillates low-amplitude transverse "tickler" components $B_X(t)$ or $B_Y(t)$ close to the resonance frequency Ω.

Analogous resonant transitions are stimulated in NH_3 by an E_z-field oscillating near the resonance frequency $\Omega=2S\sim24\ GHz$ of an ammonia inversion as described in Chapter 10. The Hamiltonian matrix

$$\begin{pmatrix} \langle N_{up}|\mathbf{H}|N_{up}\rangle & \langle N_{up}|\mathbf{H}|N_{dn}\rangle \\ \langle N_{dn}|\mathbf{H}|N_{up}\rangle & \langle N_{dn}|\mathbf{H}|N_{dn}\rangle \end{pmatrix} = \begin{pmatrix} H - pE_z & -S \\ -S & H + pE_z \end{pmatrix} \qquad (19.1.6a)$$

from (10.3.3) contains on its diagonal the field potential energy $-pE_z$ of an "up" Nitrogen atom state $|N_{up}\rangle$ versus $+pE_z$ of a "down" Nitrogen atom state $|N_{dn}\rangle$. Inversion tunneling amplitude $-S$ is off-diagonal. The matrix has the form of an *AB*-type Hamiltonian. Transforming to a $\{|+\rangle,|-\rangle\}$ basis interchanges S and pE_z.

$$\begin{pmatrix} \langle(+)|\mathbf{H}|(+)\rangle & \langle(+)|\mathbf{H}|(-)\rangle \\ \langle(-)|\mathbf{H}|(+)\rangle & \langle(-)|\mathbf{H}|(-)\rangle \end{pmatrix} = \begin{pmatrix} H - S & -pE_z \\ -pE_z & H + S \end{pmatrix} \text{ where: } \begin{matrix} |(+)\rangle = \left(|N_{up}\rangle + |N_{dn}\rangle\right)/\sqrt{2} \\ |(-)\rangle = \left(|N_{up}\rangle - |N_{dn}\rangle\right)/\sqrt{2} \end{matrix} \qquad (19.1.6b)$$

In an NH_3 resonance experiment, the dipole perturbation $pE_z(t)$ will be a time-dependent and is precisely analogous to the $B_X(t)$-component of the NMR "tickler" field, while NH_3 eigenstates $\{|(+)\rangle,|(-)\rangle\}$ are precisely analogous to NMR *spin-up-z* and *spin-dn-z* eigenstates $\{|\uparrow\rangle,|\downarrow\rangle\}$ in the fixed polarizing B_Z-field.

(b) Visualizing quasi-spin space: NH_3 *vs.* NMR

Generally, the *A*-axis *a.k.a. Z*-axis is the quantization axis of choice. For the NMR problem a favored-*Z* convention is forced by a big fixed B_Z-field. (A small $B_X(t)$ will be wiggled.) For the NH_3 problem we plan to wiggle $B=-pE_z(t)$ in (19.1.6b) and not S. (Nature fixes tunneling amplitude S.) *NH_3* eigenstates $\{|(+)\rangle,|(-)\rangle\}$ will now be associated with *spin-up-A* and *spin-down-A*, with field-free eigenvalues $A=H-S$ and $D=H+S$, respectively. In going between (19.1.6a and b), A and B are switched.

Do not confuse the *z*-axis of the NH_3 molecule with the *A* or *Z*-axis in its quasi-spin (S_A, S_B, S_C)-space. Nor is the *x*-axis of the NH_3 molecule to be confused with the *B* or *X*-axis. But, all three **B**-field components $(B_X(t),B_Y(t),B_Z)$ are meaningful real parameters $\{A=B_Z, B=B_X(t), C=B_Y(t), D=-B_Z,\}$ of the NMR Hamiltonian (19.1.5a), while the NH_3 inversion Hamiltonian (19.1.6b) has only the *z*-dipole energy $pE_z(t)$ as a meaningful real field parameter in the set $\{A=H-S, B=-pE_z(t), C=0, D=H+S\}$.

The dipole *balance parameter B* quantifies a $(-q\mathbf{E}\bullet\mathbf{r})$ coupling between two states $|(+)\rangle$ and $|(-)\rangle$.

$$B=-pE_z(t)=-\langle(+)|q\mathsf{z}E_z(t)|(-)\rangle = r\cos(\omega t)=(r/2)(e^{i\omega t}+e^{-i\omega t}) \qquad (19.1.7a)$$

B is $gB_x(t)/2$ for the NMR example. For NH_3 it is the *interaction strength* or *Rabi rate parameter r*.

$$B= r = -pE_z(0) \qquad (19.1.7b)$$

B contains the oscillator strength or *electric dipole matrix element*

$$p=q\langle(+)|\mathsf{z}|(-)\rangle, \qquad (19.1.7c)$$

in product with the field magnitude $E_z(0)$ for which a real monochromatic radiation field is assumed.

$$E_z(t) = \cos(\omega t)=(1/2)(e^{i\omega t}+e^{-i\omega t}) \ . \qquad (19.1.7d)$$

Below is the exact NH_3 inversion-resonance Hamiltonian (19.1.6b) in its Schrodinger equation.

$$i\frac{\partial}{\partial t}\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix}=\begin{pmatrix}H+\frac{\varepsilon}{2} & \frac{r}{2}\cos\omega t\\ \frac{r}{2}\cos\omega t & H-\frac{\varepsilon}{2}\end{pmatrix}\begin{pmatrix}\psi_+\\ \psi_-\end{pmatrix}, \quad \text{where: } \varepsilon=-2S \qquad (19.1.8a)$$

The **H**-crank **Ω**-components (19.1.3b) are below. The unperturbed *(r=0)* case is shown in Fig. 19.1.1b.

$$\Omega_0 = H\ , \qquad \Omega_A = \varepsilon, \quad \Omega_B = r\cos\omega t, \quad \Omega_C = 0. \qquad (19.1.8b)$$

The **H**-crank vector **Ω** swings to-and-fro in the AB-plane at constant $\Omega_A=\varepsilon$ as shown later. (Fig. 19.1.2b)

The NH_3-electric dipole moment of any state is related to the transverse $\langle\mathbf{S}_\perp\rangle$–component of the quasi-spin vector $\langle\mathbf{S}\rangle$ expectation. In NMR, $\langle\mathbf{m}_\perp\rangle=g\langle\mathbf{S}_\perp\rangle$ is the magnetic moment transverse to the main B_Z-field. The NH_3 dipole $\langle p_z\rangle=q\langle z\rangle$ is a product of p and $2S_B=2\mathrm{Re}\psi_+^*\psi_-$ using (2.10.8b) and (19.1.7).

$$\begin{aligned}\langle p_z\rangle &= \langle\Psi|\rho_z|\Psi\rangle = \left(\psi_+^*\langle+|+\psi_-^*\langle-|\right)\rho_z\left(\psi_+|+\rangle+\psi_-|-\rangle\right)\\ &= 2\mathrm{Re}\psi_+^*\psi_-\langle+|\rho_z|-\rangle \quad (\text{using } \langle+|\rho_z|-\rangle=\langle-|\rho_z|+\rangle) \qquad (19.1.9a)\\ &= 2S_B p = p\cos\alpha\sin\beta \quad (\text{using (2.10.8b) and } \langle+|\rho_z|-\rangle = p)\end{aligned}$$

Symmetry rules out diagonal z-matrix elements $\langle+|z|+\rangle=0=\langle-|z|-\rangle$. Here is the time derivative of $\langle p_z\rangle$.

$$\begin{aligned}\langle\dot\rho_z\rangle &= \langle\dot\Psi|\rho_z|\Psi\rangle+\langle\Psi|\rho_z|\dot\Psi\rangle = \left(\dot\psi_+^*\psi_-+\dot\psi_-^*\psi_++\psi_+^*\dot\psi_-+\psi_-^*\dot\psi_+\right)\langle+|\rho_z|-\rangle\\ &= -2\varepsilon\,\mathrm{Im}\psi_+^*\psi_-\langle+|\rho_z|-\rangle \qquad (\text{using: } i\dot\psi_\pm=\pm\frac{\varepsilon}{2}\psi_\pm\ ) \qquad (19.1.9b)\\ &= -2\varepsilon S_C p = -\varepsilon p\sin\alpha\sin\beta \qquad (\text{using (2.10.8b) and } \langle+|\rho_z|-\rangle = p)\end{aligned}$$

Fig. 19.1.1a shows a "real" NMR spin moment $\mathbf{m}=g\mathbf{S}$ precessing around its Ω-cranking gB_Z-field. Fig. 19.1.1b shows an analogous NH_3 quasi-spin **S** similarly precessing around its A-axis at rate $\varepsilon=2S$. The transverse NMR moment $\mathbf{m}_\perp$ lies in the projection or "shadow" of **m** in the XY-plane. An analogous NH_3 *Lorentz phasor* vector $\mathbf{p}_\perp=q(\langle z\rangle,-\langle\dot z\rangle/\varepsilon)$ rotates in the BC-plane according to (19.1.9) at rate $\Omega=2S=\varepsilon$. This relates the first Euler angle α to an *atomic oscillator phase angle* $\phi=-\alpha$, as shown in Fig. 19.1.1b.

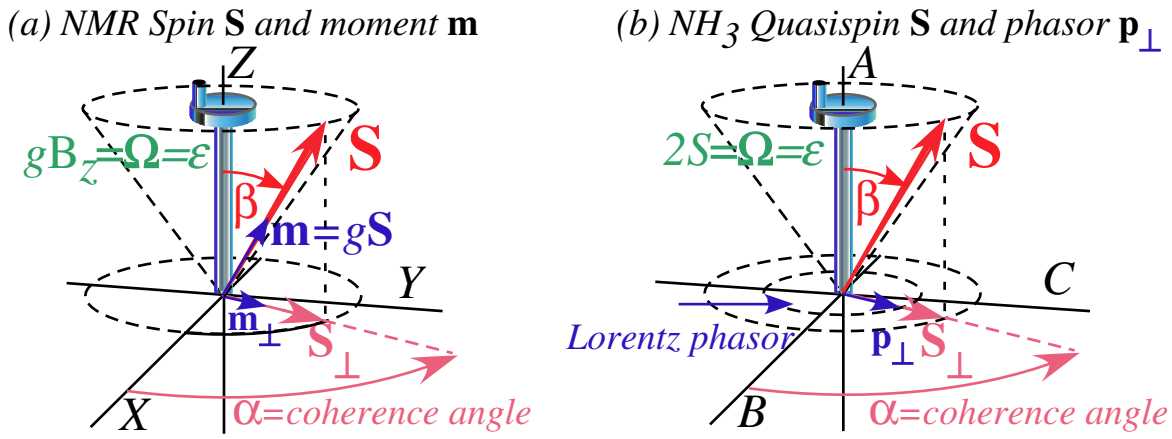


Fig. 19.1.1 Ω-Cranked polarization and spin vectors for (a) NMR and (b) NH_3 inversion resonance.

$\mathbf{p}_\perp$ is a quantum version of the classical Lorentz atomic oscillator phasor $p(t)=p(0)e^{-i\varepsilon t}$ which has a real value $p(0)\cos\varepsilon t$ and an imaginary value $-p(0)\sin\varepsilon t$ corresponding to dipole time derivative $(dp/dt)/\varepsilon$.

Lorentz oscillators are classical harmonic oscillators and grow to infinity if the driving frequency ω approaches the natural frequency $\Omega=\varepsilon$. Not so for the quantum model of a two level atom pictured in Fig. 19.1.1b. The dipole expectation value $\langle p_z\rangle=q\langle z\rangle$ starts at zero for the ground $|(+)\rangle$-eigenstate $(\beta=0)$ then grows toward its *saturation* value of p for a (50-50) state such as a *spin-up-B* wave $(\psi_+,\psi_-)=(1/\sqrt{2},\ 1/\sqrt{2})$ with spin at $\beta=\pi/2$. The value p is as large as $\langle p_z\rangle$ can be for the 2-level system.

Saturated (50-50)-states have **S**-vector normal $(\beta=\pi/2)$ to the crank **Ω**-vector. This includes the Nitrogen-up state $|N_{up}\rangle=(|(+)\rangle+|(-)\rangle)/\sqrt{2}$ the Nitrogen-down state $|N_{dn}\rangle=(|(+)\rangle-|(-)\rangle)/\sqrt{2}$ whose **S**-vector is along the $\pm B$-axes, or transition states $|\pm C\rangle=(|(+)\rangle\pm i|(-)\rangle)/\sqrt{2}$ whose **S**-vector is along the $\pm C$-axes. An increase in amount of excited state $|(-)\rangle$ above 50-50 *decreases* the dipole moment in the BC-plane; it is zero for a pure excited state $|(-)\rangle$ or a pure ground state $|(+)\rangle$. Lorentz "phasor space" unbounded and flat, but a 2-state $(|(+)\rangle,|(-)\rangle)$ phasor or *coherence* space is a bounded spherical projection and periodic. The quantum quasi-spin world, unlike Lorentz's "flat" classical phasor world, is "round."

(c) Rotating wave solutions

We first solve a *rotating wave approximation* to (19.1.8) obtained by dropping $e^{i\omega t}$ from $E_z(t)$.

$$i\frac{\partial}{\partial t}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix}=\begin{pmatrix}\frac{\varepsilon}{2} & \frac{r}{2}e^{-i\omega t}\\ \frac{r}{2}e^{+i\omega t} & \frac{-\varepsilon}{2}\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},\ \text{where: } \varepsilon=-2S\ ,\ \text{and: } \begin{matrix}\psi_1=\psi_+=\psi_\uparrow\\ \psi_2=\psi_-=\psi_\downarrow\end{matrix} \qquad (19.1.10a)$$

The **H**-crank vector **Ω** rotates around the Z-axis tracing an inverted cone of altitude ε as in Fig. 19.1.2a.

$$\Omega_0=H=0,\quad \Omega_Z=\Omega_A=\varepsilon,\ \Omega_X=\Omega_B=r\cos\omega t,\ \Omega_Y=\Omega_C=r\sin\omega t. \qquad (19.1.10b)$$

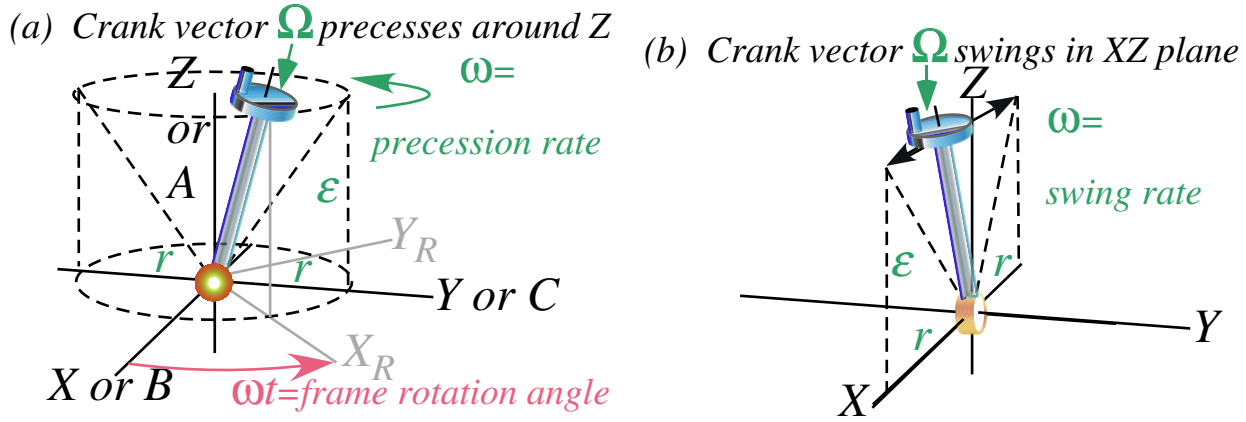


Fig. 19.1.2 Ω-Crank time dependence for (a) Rotating crank approximation (b) Exact planar swing.

This **H** is like that of an NMR resonance with a fixed B_z field added to a rotating $B_x(t)$ and $B_y(t)$ field.

$$B_z = 2\varepsilon, \quad B_x(t) = 2r\cos\omega t, \quad B_y(t) = 2r\sin\omega t. \tag{19.1.10c}$$

For such a **B**-field (19.1.10a) is an exact equation. In the analogous NH_3 equation (19.1.8) only the *X*-or-*B*-component oscillates as shown in Fig. 19.1.2b. But, it turns out that the circular polarized **B** or **Ω** motion (19.1.10b-c) like Fig. 19.1.2a has much the same effect as a *ZX*-plane swinging **Ω** (19.1.8b) in Fig. 19.1.2b provided the amplitude B_x (or Rabi radius *r*) is much less than the splitting frequency ε ($r<<\varepsilon$).

To solve (19.1.10a) we boost by rotation $R_Z[\omega t]$ to a rotating frame $\{X_R, Y_R, Z_R, =Z\}$ shown in Fig. 19.1.2a, where the crank vector **Ω** would appear to be standing still. This is something like the change-of-picture boost which zeros the vector potential **A** in (17.1.16). New *R*-base states $|k\rangle^R$ are defined first.

$$|\uparrow\rangle^R = \mathsf{R}_Z[\omega t]|\uparrow\rangle = e^{-i\omega t\,J_Z}|\uparrow\rangle = e^{-i\omega t/2}|\uparrow\rangle, \quad {}^R\langle\uparrow| = \langle\uparrow|\mathsf{R}^\dagger[\omega t] = \langle\uparrow|e^{+i\omega t/2} \tag{19.1.11a}$$

$$|\downarrow\rangle^R = \mathsf{R}_Z[\omega t]|\downarrow\rangle = e^{-i\omega t\,J_Z}|\downarrow\rangle = e^{+i\omega t/2}|\downarrow\rangle, \quad {}^R\langle\downarrow| = \langle\downarrow|\mathsf{R}^\dagger[\omega t] = \langle\downarrow|e^{-i\omega t/2} \tag{19.1.11b}$$

This gives the needed transformation matrix and inverse.

$$\begin{pmatrix} \langle\uparrow|\uparrow\rangle^R & \langle\uparrow|\downarrow\rangle^R \\ \langle\downarrow|\uparrow\rangle^R & \langle\downarrow|\downarrow\rangle^R \end{pmatrix} = \begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{+i\omega t/2} \end{pmatrix} \qquad \begin{pmatrix} {}^R\langle\uparrow|\uparrow\rangle & {}^R\langle\uparrow|\downarrow\rangle \\ {}^R\langle\downarrow|\uparrow\rangle & {}^R\langle\downarrow|\downarrow\rangle \end{pmatrix} = \begin{pmatrix} e^{+i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix} \tag{19.1.11c}$$

Then transformed wave amplitudes $\psi^R = \mathsf{R}^\dagger\psi$ and a new Hamiltonian $\mathsf{H}^R = \mathsf{R}^\dagger\mathsf{H}\cdot\mathsf{R}$ follow.

$$\begin{pmatrix} \psi^R_\uparrow \\ \psi^R_\uparrow \end{pmatrix} = \begin{pmatrix} {}^R\langle\uparrow|\psi\rangle \\ {}^R\langle\downarrow|\psi\rangle \end{pmatrix} = \begin{pmatrix} {}^R\langle\uparrow|\uparrow\rangle & {}^R\langle\uparrow|\downarrow\rangle \\ {}^R\langle\downarrow|\uparrow\rangle & {}^R\langle\downarrow|\downarrow\rangle \end{pmatrix}\begin{pmatrix} \langle\uparrow|\psi\rangle \\ \langle\downarrow|\psi\rangle \end{pmatrix} = \begin{pmatrix} e^{+i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}\begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} \tag{19.1.11d}$$

The new Hamiltonian H^R does indeed have a constant **Ω**-vector and no explicit time dependence.

$$\begin{pmatrix} {}^R\langle\uparrow|H|\uparrow\rangle^R & {}^R\langle\uparrow|H|\downarrow\rangle^R \\ {}^R\langle\downarrow|H|\uparrow\rangle^R & {}^R\langle\downarrow|H|\downarrow\rangle^R \end{pmatrix} = \begin{pmatrix} {}^R\langle\uparrow|\uparrow\rangle & {}^R\langle\uparrow|\downarrow\rangle \\ {}^R\langle\downarrow|\uparrow\rangle & {}^R\langle\downarrow|\downarrow\rangle \end{pmatrix}\begin{pmatrix} \langle\uparrow|H|\uparrow\rangle & \langle\uparrow|H|\downarrow\rangle \\ \langle\downarrow|H|\uparrow\rangle & \langle\downarrow|H|\downarrow\rangle \end{pmatrix}\begin{pmatrix} \langle\uparrow|\uparrow\rangle^R & \langle\uparrow|\downarrow\rangle^R \\ \langle\downarrow|\uparrow\rangle^R & \langle\downarrow|\downarrow\rangle^R \end{pmatrix} \tag{19.1.12}$$

$$= \begin{pmatrix} e^{+i\omega t/2} & 0 \\ 0 & e^{-i\omega t/2} \end{pmatrix}\begin{pmatrix} \varepsilon/2 & re^{-i\omega t}/2 \\ re^{-i\omega t}/2 & -\varepsilon/2 \end{pmatrix}\begin{pmatrix} e^{-i\omega t/2} & 0 \\ 0 & e^{+i\omega t/2} \end{pmatrix} = \begin{pmatrix} \varepsilon/2 & r/2 \\ r/2 & -\varepsilon/2 \end{pmatrix}$$

But, change-of-picture (19.1.11d) has time dependence so time derivative $i\partial/\partial t\ \psi^R$ yields extra terms.

$$i\frac{\partial}{\partial t}\begin{pmatrix}\psi^R_\uparrow\\ \psi^R_\downarrow\end{pmatrix}= \quad i\frac{\partial}{\partial t}\begin{pmatrix}e^{+i\omega t/2} & 0\\ 0 & e^{-i\omega t/2}\end{pmatrix}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix}+\begin{pmatrix}e^{+i\omega t/2} & 0\\ 0 & e^{-i\omega t/2}\end{pmatrix}i\frac{\partial}{\partial t}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix} \tag{19.1.13a}$$

$$=\begin{pmatrix}\frac{-\omega}{2} & 0\\ 0 & \frac{\omega}{2}\end{pmatrix}\begin{pmatrix}e^{+i\omega t/2} & 0\\ 0 & e^{-i\omega t/2}\end{pmatrix}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix}+\begin{pmatrix}e^{+i\omega t/2} & 0\\ 0 & e^{-i\omega t/2}\end{pmatrix}\mathsf{H}\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix} \tag{19.1.13b}$$

The original Schrodinger equation $i\partial/\partial t|\psi\rangle=\mathsf{H}|\psi\rangle$ becomes one for $|\psi^R\rangle=\mathsf{R}^\dagger[\omega t]|\psi^R\rangle$ by inserting $\mathsf{R}^\dagger\mathsf{R}=1$.

$$i\frac{\partial}{\partial t}\begin{pmatrix}\psi^R_\uparrow\\ \psi^R_\downarrow\end{pmatrix}=\begin{pmatrix}\frac{-\omega}{2} & 0\\ 0 & \frac{\omega}{2}\end{pmatrix}\cdot\mathsf{R}^\dagger[\omega t]\cdot\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix}+\mathsf{R}^\dagger[\omega t]\cdot\mathsf{H}\cdot\mathsf{R}[\omega t]\mathsf{R}^\dagger[\omega t]\begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix} \tag{19.1.14}$$

The new H^R has extra diagonal terms $\pm\omega/2$ but off-diagonal time dependence $e^{\pm i\omega t}$ of (19.1.10) is gone.

$$i\frac{\partial}{\partial t}\left|\psi^R\right\rangle=\mathsf{R}^\dagger\mathsf{H}\mathsf{R}\left|\psi^R\right\rangle=\mathsf{H}^R\left|\psi^R\right\rangle \quad \text{or:} \quad i\frac{\partial}{\partial t}\begin{pmatrix}\psi^R_\uparrow\\ \psi^R_\downarrow\end{pmatrix}=\begin{pmatrix}\frac{\varepsilon-\omega}{2} & \frac{r}{2}\\ \frac{r}{2} & \frac{-\varepsilon+\omega}{2}\end{pmatrix}\begin{pmatrix}\psi^R_\uparrow\\ \psi^R_\downarrow\end{pmatrix} \tag{19.1.15a}$$

The crank vector $\mathbf{\Omega}^R$ in the rotating frame is indeed motionless but has $(-\omega)$ added to its Z-component.

$$\Omega^R{}_0 = H^R{}_{11}+H^R{}_{22}, \quad \Omega_Z = H^R{}_{11}-H^R{}_{22}, \quad \Omega_X = 2\mathrm{Re}H^R{}_{12}, \quad \Omega_Y = 2\mathrm{Im}H^R{}_{12}.$$
$$= 0, \qquad = \varepsilon-\omega=\Delta, \qquad = r, \qquad = 0. \tag{19.1.15b}$$

The resulting crank $\mathbf{\Omega}^R$ depends on the *detuning* parameter $\Delta=\varepsilon-\omega$ as shown in Fig. 19.1.3. Δ is zero at resonance. A zero detuning makes the beat frequency or crank length become a minimum value r.

$$\Omega^R=\pm\sqrt{\Delta^2+r^2}\cong\begin{cases}\pm\Delta & \text{for: } r<<|\Delta| \text{ (far from resonance)}\\ \pm r & \text{for: } |\Delta|<<r \text{ (close to resonance)}\end{cases} \tag{19.1.15c}$$

The minimum beat frequency r is called the *Rabi frequency* and was given (for $\hbar=1$) by (19.1.7).

$$r = -q\langle(+)|\mathsf{z}|(-)\rangle E_z(0) \tag{19.1.16}$$

Two-state quantum resonant beat frequency Ω^R, unlike a classical resonance, approaches r but not zero as detuning Δ goes through zero. But, when detuning exceeds r, we recover the classical relation $\Omega^R=\Delta$ between beat rate and natural-minus-stimulus frequency difference $\Delta=\varepsilon-\omega$, as shown in (19.1.15c).

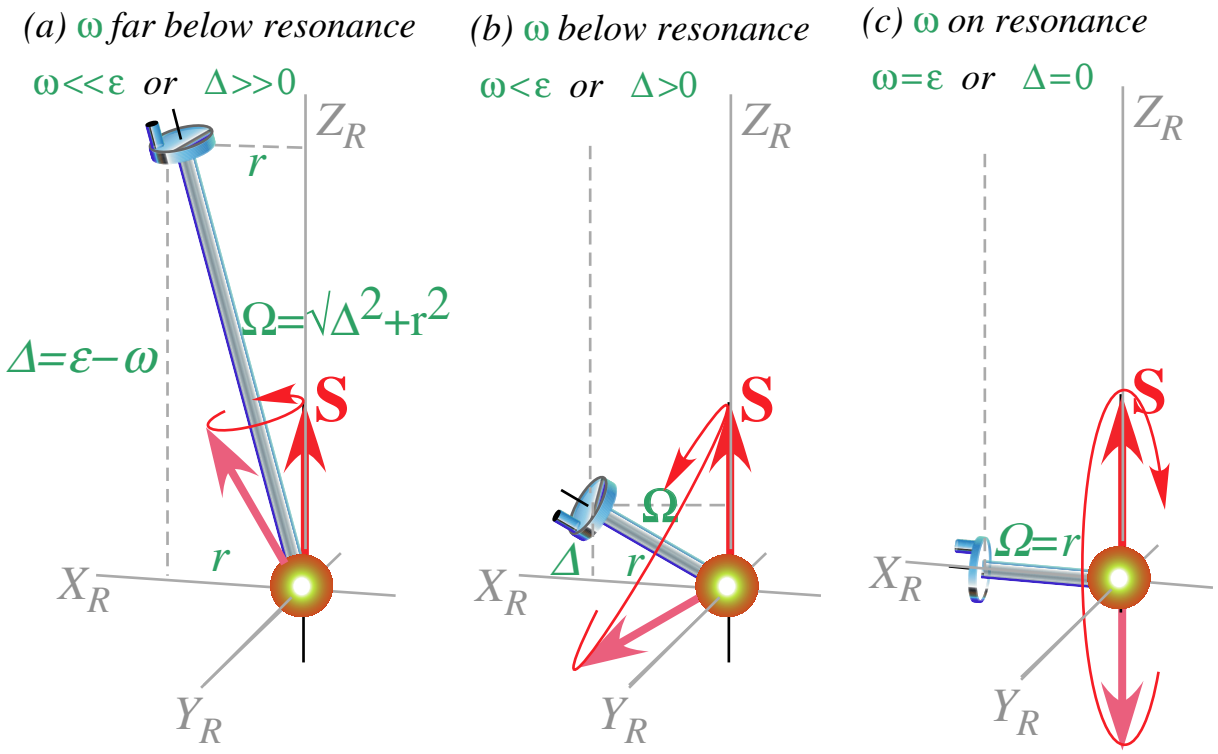


Fig. 19.1.3 $\mathbf{\Omega}^R$*-crank turns spin S-up state in rotating frame (a)* $\omega<<\varepsilon$ *(b)*$\omega<\varepsilon$ *(c) Resonance* $\omega=\varepsilon$.

Two-state quantum response does not blow up at $\Delta=0$ like the classical Lorentz oscillator (18.3.1) or like the first order approximation (18.2.6). As noted after Fig. 19.1.1, maximum dipole response has its spin **S** normal to the *Z*-axis *(*$\beta=\pi/2$*)*. This happens to an initial ground state (*spin-up* $|\uparrow\rangle^R$) if Δ lies inside $\pm r$ as in Fig. 19.1.3b-c. Time evolution operator $U^R(t)=e^{-iH^Rt}$ is a rotation around crank $\mathbf{\Omega}^R$ of polar angle ϑ^R for $\cos\vartheta^R=\Delta/\Omega^R$ and $\sin\vartheta^R=r/\Omega^R$. Rotation matrix $e^{-i\mathbf{\Omega}t\bullet\mathbf{J}}$ comes from (10.5.25c) in Ch. 10.

$$U^R(t)|\uparrow\rangle^R = e^{-i\mathbf{\Omega}^R t\bullet\mathbf{J}}|\uparrow\rangle^R = \begin{pmatrix} \cos\frac{\Omega^R t}{2} - i\cos\vartheta^R \sin\frac{\Omega^R t}{2} & \cdot \\ -i\sin\vartheta^R \sin\frac{\Omega^R t}{2} & \cdot \end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \begin{pmatrix} \cos\frac{\Omega^R t}{2} - i\frac{\Delta}{\Omega^R}\sin\frac{\Omega^R t}{2} & \cdot \\ -i\frac{r}{\Omega^R}\sin\frac{\Omega^R t}{2} & \cdot \end{pmatrix} \tag{19.1.17}$$

The excited $|\downarrow\rangle^R$-state component gives the transition probability from ground $|\uparrow\rangle^R$-state as a function of time *t*, Rabi amplitude *r*, and detuning Δ. For large Δ it reduces to the spectral intensity value (18.2.6).

$$\begin{aligned} \left|{}^R\langle\downarrow|\psi(t)\rangle\right|^2 &= \left(\frac{r}{\Omega^R}\sin\frac{\Omega^R t}{2}\right)^2 = \frac{r^2}{\Delta^2+r^2}\sin\frac{\sqrt{\Delta^2+r^2}\,t}{2} \\ &\cong \frac{r^2\sin^2 t\Delta/2}{\Delta^2} = \frac{r^2}{4}|S(\Delta,t)|^2 \quad \text{for: } |\Delta|>>r \end{aligned} \tag{19.1.18}$$

A plot of 2-state transition is given in Fig. 19.1.4 to compare with a first order approximation in Fig. 18.2.1. The Rabi surface in Fig. 19.1.4 below has the same markings as the first-order approximation in Fig. 18.2.1. Notice the uncertainty hyperbolas that are at the bottom of valleys in Fig. 18.2.1 have been lifted up in Fig.

19.1.4 by encroaching beatlet peaks that used to surround them. This lifting effect becomes most pronounced near the resonance origin (Δ=0) but diminishes in regions far from resonance.

As mentioned before, the first-order approximation is most happy to stay away from resonance where it unhappily blows up. Fig. 18.2.1 and Fig. 19.1.4 are practically the same everywhere except in the tiny region blown up in the two figures.

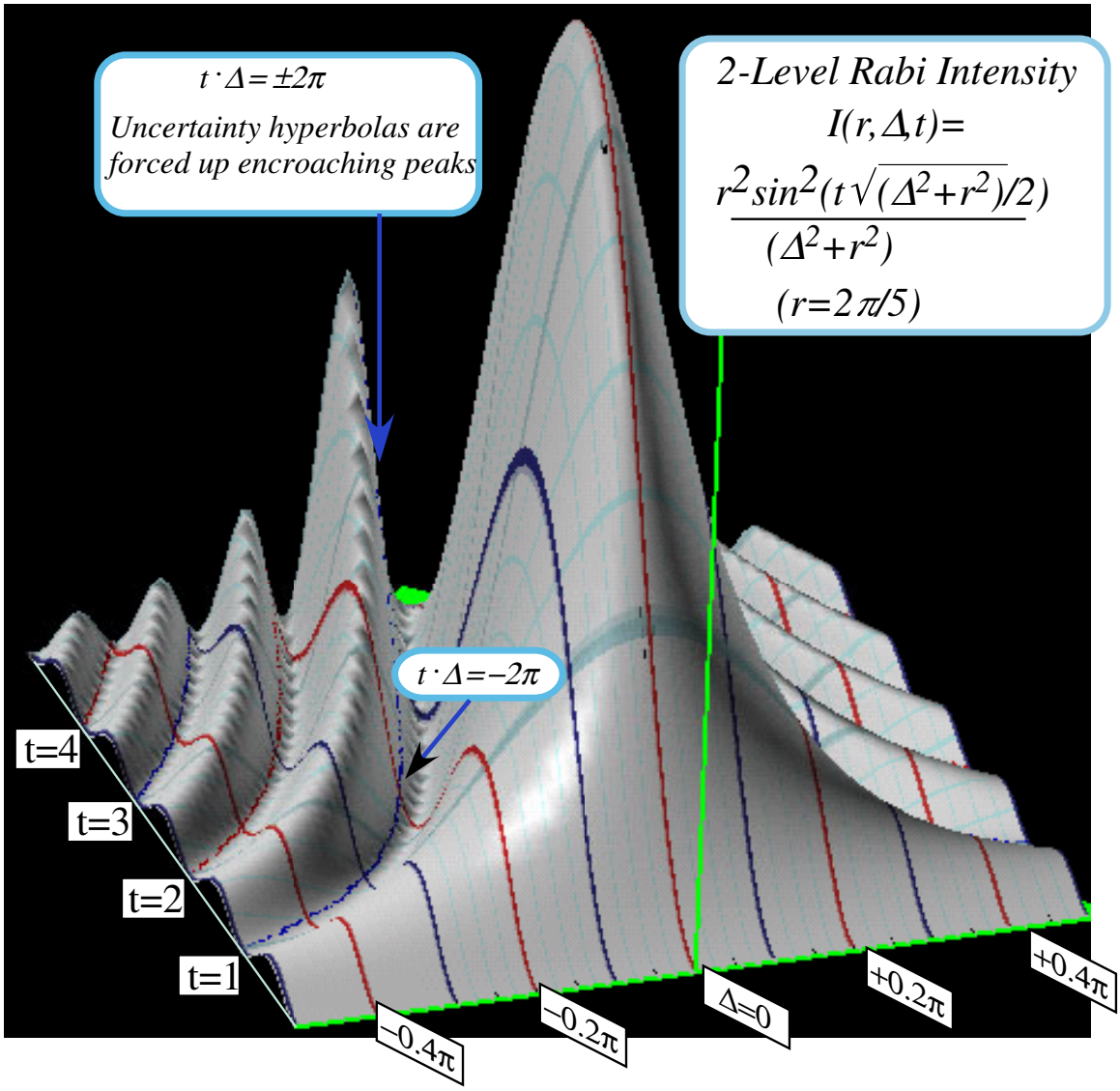


Fig. 19.1.4 Rabi spectral intensity function I(r,Δ,t) for 2-level rotating wave for r=2π/5.

The most striking contrast between Rabi 2-level *I(r,Δ,t)* and the approximate *I(Δ,t)* is that the Rabi *(Δ=0)*-peak goes to a maximum value: *I(r, Δ=0, t=π/r)=1* then back to zero at *t=2π/r. Meanwhile*, the approximate $I(\Delta=0,t)=t^2$ just goes up! In other words, after one Rabi period, the transition probability is back to zero since the spin vector in Fig. 19.1.3c has completed one full revolution. No such return to initial state is possible in a first (or even 2nd or 3rd) order polynomial perturbation approximation.

Rabi 2-level response $I(r,\Delta,t)$ beats faster than $I(\Delta,t)$ near $\Delta=0$. Beat rate Ω^R (19.1.15c) depends on stimulus amplitude through Rabi rate r as well as on stimulus frequency ω through $\Delta=\varepsilon-\omega$. If r increases, beats get faster and bigger near $\Delta=0$ since Rabi-r is both a *rate* and a *radius* of $\mathbf{\Omega}^R$-cranking. A top view of $I(r,\Delta,t)$ with twice the rate r $(r=4\pi/5)$ is shown below in Fig. 19.1.5. Note how the zeros of $I(r,\Delta,t)$ veer away from uncertainty hyperbolas of $I(r,t)$ and toward a $(\Delta=0)$-rendezvous at each Rabi period.

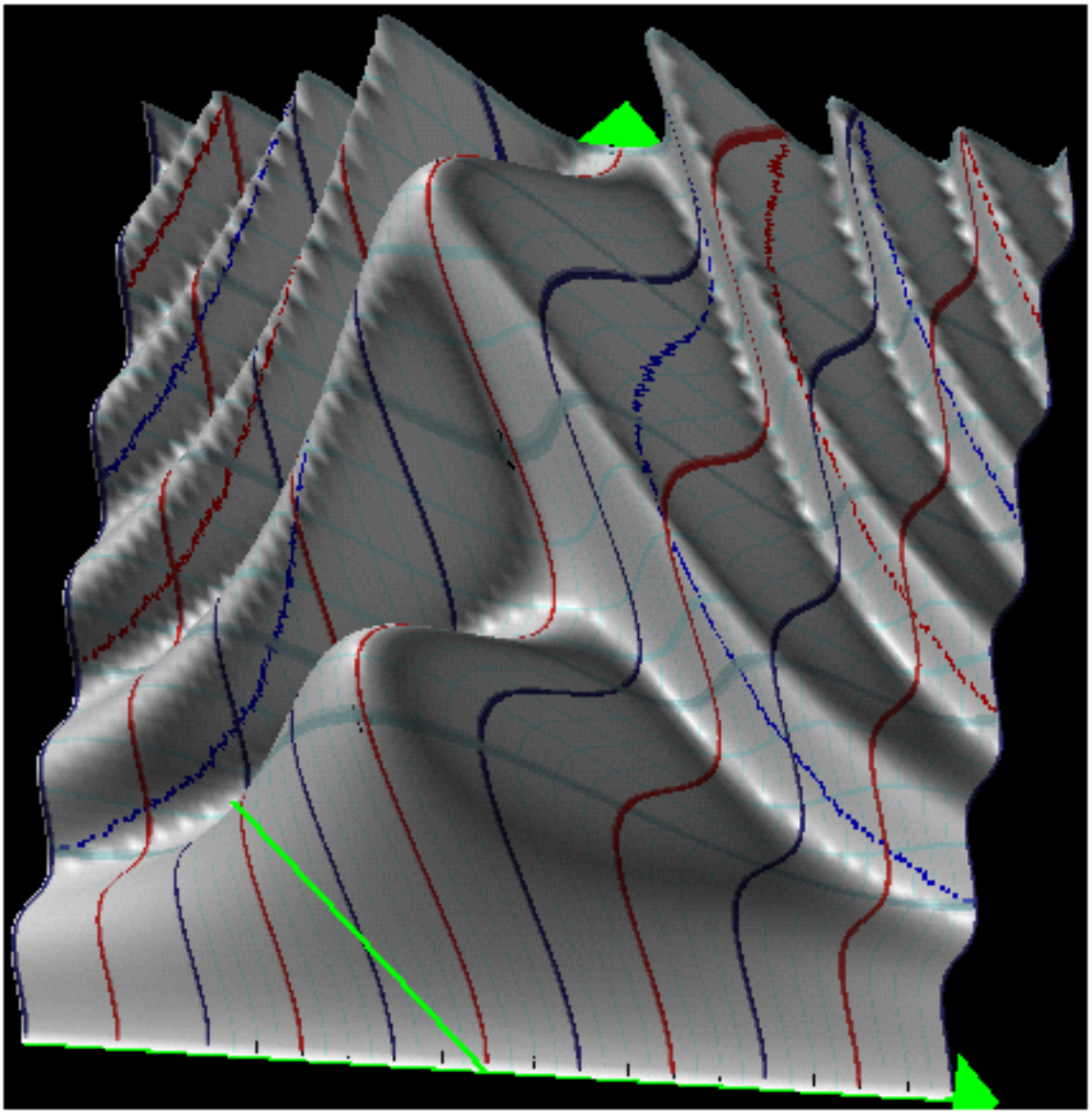


Fig. 19.1.5 Top-down view of Rabi spectral intensity function $I(r,\Delta,t)$ for $r=4\pi/5$.

As zeros move toward low-Δ, the probability moves away. Larger and faster beats also appear in the $\pm\Delta$ wings of the spectrum as r is increased. This effect, known as *power broadening*, changes the spectral profile (19.1.17) from a narrow inverse-Δ-square (r^2/Δ^2) to a fatter Lorentzian $(r^2/[\Delta^2+r^2])$.

The frame $\{X_R, Y_R, Z_R,\}$ of Fig. 19.1.3 rotates at the stimulus frequency ω about the $(Z=Z_R)$-axis as shown in Fig. 19.1.2. So, an X_R, spin component or related polarization $\mathbf{p}_\perp$ or $\mathbf{m}_\perp$in Fig. 19.1.2 also has a ω-field-driven rotation. Oscillation or rotation of electric or magnetic moments radiates electromagnetic waves at the frequency ω of the oscillation. ω-Radiation from 2-state system rises when the slower $\mathbf{\Omega}^R$-rotation drives the spin vector **S** away from the Z_R-axis in Fig. 19.1.3, but it falls as the same $\mathbf{\Omega}^R$ brings **S** back to the Z_R-axis. Neither a pure ground state $|(+)\rangle$ or $|\uparrow\rangle$ nor a pure excited state $|(-)\rangle$ or $|\downarrow\rangle$ can radiate. Radiating moments require state mixture, preferably a saturated 50-50 mixture.

(d) AC Stark levels: Dressed eigenstates

To better understand an increasingly intimate relation between atomic and nuclear moments for two levels $(E\uparrow=0,\ E\downarrow=\hbar\varepsilon)$ and its stimulating radiation field $E_R=\hbar\omega$, let us plot the important frequencies as a function of *detuning* Δ=ε−ω by the *stimulus frequency* ω off the *zero-field transition frequency* ε. The simplest of these plots is the zero-coupling case of Fig. 19.1.6a for which the Rabi-rate is zero. $(r=0)$ It is a 45° line representing the laser stimulus crossing horizontal lines representing the two levels 0 and ε.

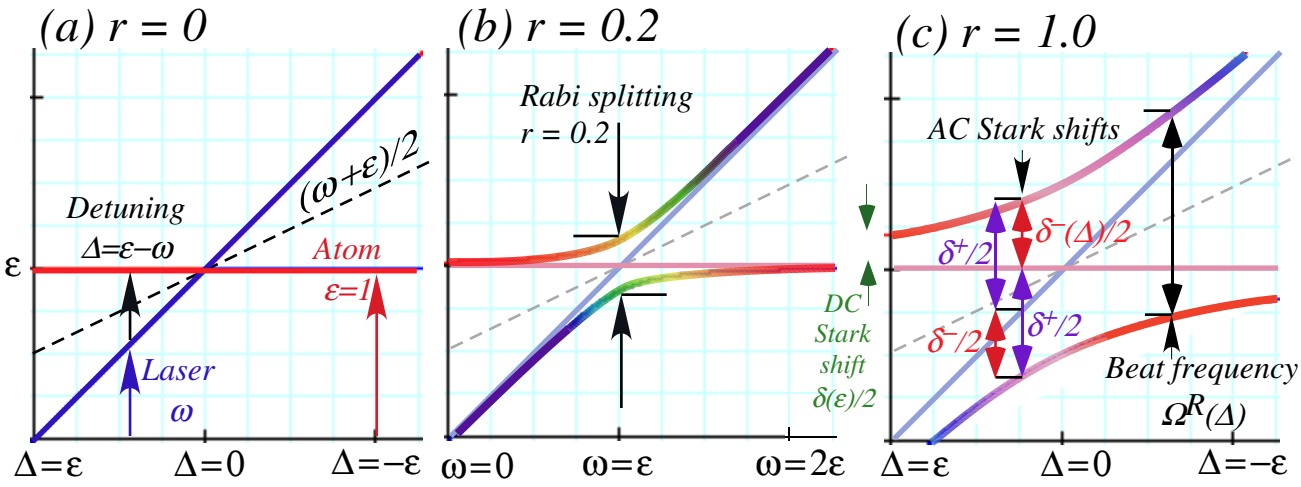


Fig. 19.1.6 Rotating wave eigenfrequencies versus detuning frequency. Rabi rate r=(a) 0, (b) 0.2, (c) 1.0.

Plotted are eigenvalues of the rotating wave Hamiltonian (19.1.15) plus an overall frequency $\Omega_0=(\varepsilon+\omega)/2$.

$$\mathsf{H}^R+\Omega_0\mathsf{1}=\begin{pmatrix}\frac{\Delta}{2} & \frac{r}{2}\\ \frac{r}{2} & \frac{-\Delta}{2}\end{pmatrix}+\Omega_0\mathsf{1}=\begin{pmatrix}\frac{\varepsilon-\omega}{2} & \frac{r}{2}\\ \frac{r}{2} & \frac{-\varepsilon+\omega}{2}\end{pmatrix}+\frac{\varepsilon+\omega}{2}\mathsf{1}=\begin{pmatrix}\varepsilon & \frac{r}{2}\\ \frac{r}{2} & \omega\end{pmatrix} \qquad (19.1.19)$$

Eigenvalues of $\mathsf{H}^R+\Omega_0\,\mathsf{1}$ are called *dressed eigenfrequencies* $\Omega_0\pm\Omega^R/2$. Ω^R is the crank rate (19.1.15c).

$$\Omega^{hi}=\Omega_0+\Omega^R/2=\varepsilon+(\Omega^R-\varepsilon+\omega)/2=\varepsilon+(\Omega^R-\Delta)/2=\varepsilon+\delta^-/2 \qquad (19.1.20a)$$

$$\Omega^{lo}=\Omega_0-\Omega^R/2=\omega-(\Omega^R-\varepsilon+\omega)/2=\omega-(\Omega^R-\Delta)/2=\omega-\delta^-/2 \qquad (19.1.20b)$$

Eigenstate $|\Omega^{hi}\rangle$ or $|\Omega^{lo}\rangle$ has spin **S** aligned or anti-aligned to crank vector $\mathbf{\Omega}^R$. ($\beta=\vartheta^R$ or $\beta=\pi+\vartheta^R$)

The polar angle ϑ^R of the rotating crank $\mathbf{\Omega}^R$ is shown in Fig. 19.1.3 with $\cos\vartheta^R=\Delta/\Omega^R$ and $\sin\vartheta^R=r/\Omega^R$.

The eigenstate components use $\cos^2\vartheta^R/2=(1+\Delta/\Omega^R]/2$ and $\sin^2\vartheta^R/2=(1-\Delta/\Omega^R]/2$ to give *AC-Stark states*

$$\left|\Omega^{lo}\right\rangle^D=\begin{pmatrix}\cos\frac{\vartheta^R}{2}\\ \sin\frac{\vartheta^R}{2}\end{pmatrix}=\begin{pmatrix}\frac{r}{\sqrt{2\Omega^R\delta^-}}\\ \frac{\delta^-}{\sqrt{2\Omega^R\delta^-}}\end{pmatrix},\quad(19.1.20c)\qquad \left|\Omega^{hi}\right\rangle^D=\begin{pmatrix}-\sin\frac{\vartheta^R}{2}\\ \cos\frac{\vartheta^R}{2}\end{pmatrix}=\begin{pmatrix}\frac{-\delta^-}{\sqrt{2\Omega^R\delta^-}}\\ \frac{r}{\sqrt{2\Omega^R\delta^-}}\end{pmatrix},\quad(19.1.20d)$$

where we define the *AC-Stark shifts* $\delta^\pm$ as follows. (See also: Fig. 19.1.6.)

$$\delta^-=\delta(\Delta)\ =\Omega^R-\Delta=\sqrt{[\Delta^2+r^2]}-\Delta \qquad (19.1.20e)$$

$$\delta^+=\delta(-\Delta)=\Omega^R+\Delta=\sqrt{[\Delta^2+r^2]}+\Delta \qquad (19.1.20e)$$

Half shifts $\delta^-/2$ and $\delta^+/2$ give the deviation of each eigenfrequency from the zero-field frequencies ω or ε as seen in (19.1.20a-b) and Fig. 19.1.6c. The sum of $\delta^-/2$ and $\delta^+/2$ is the total splitting Ω^R , their difference is the detuning Δ, and the shift product $\delta^-\delta^+$ is the Rabi rate squared.

$$\delta^-/2+\delta^+/2=\Omega^R\quad(19.1.20f)\qquad \delta^-/2-\delta^+/2=\Delta\quad(19.1.20g)\qquad .\delta^-\delta^+=r^2\quad(19.1.20h)$$

Finally, note the AC Stark state norm.

$$\delta^\pm+r^2=(\Omega^R\pm\Delta)^2+r^2=2\Omega^R(\Omega^R\pm\Delta)=2\Omega^R\delta^\pm \qquad (19.1.20i)$$

The AC Stark states are also called *adiabatic dressed eigenstates* because the dipole moment $\mathbf{p}_\perp$ or $\mathbf{m}_\perp$ oscillation is correlated or "clothed" with that of the stimulating radiation particularly near resonance. They are the states that arise from a zero-field eigenstate if r or Δ are turned on slowly (adiabatic).

Consider two AC dressed eigenstate amplitudes in a 50-50 duet at frequencies Ω^{hi} and Ω^{lo}.

$$e^{-i\Omega^{hi}t}+e^{-i\Omega^{lo}t}=e^{-i(\varepsilon+\delta/2)t}+e^{-i(\omega-\delta/2)t}=e^{-i(\varepsilon+\omega)t/2}\cos(\varepsilon-\omega+\delta)t/2$$

$$=e^{-i\Omega 0t}\cos\Omega^R t/2$$

It is an *amplitude modulation (AM)* of a carrier frequency $\Omega_0=(\varepsilon+\omega)t/2$ by a modulation frequency $\Omega^R t/2$ giving two *side bands* belonging to the two Ω^{hi} and Ω^{lo} curves in Fig. 19.1.6 above and below Ω_0 .

$$\omega_{high\ sideband}=\Omega_0+\Omega^R/2=\Omega^{hi}=\varepsilon+\delta^-/2 \qquad (19.1.18a)$$

$$\omega_{low\ sideband}=\Omega_0-\Omega^R/2=\Omega^{lo}=\omega-\delta^-/2 \qquad (19.1.18b)$$

The modulation arises because the radiating dipole $\mathbf{p}_\perp=p\sin\vartheta^R$ varies with polar angle ϑ^R of spin vector **S** as the crank vector $\mathbf{\Omega}^R$ turns in Fig. 19.1.3. As the **S** vector rotates from the spin-up ground state ($\vartheta^R=0$) the radiation moment beats up and down. For $\Delta=r$, a maximum $\mathbf{p}_\perp=p$ occurs at $\vartheta^R=\pi/2$ as in Fig. 19.1.3b. For $\Delta\sim 0$, angle ϑ^R rotates at uniform rate $\Omega^R\sim r$ from 0 to 2π as in Fig. 19.1.3c. Dipole $\mathbf{p}_\perp$ has beat maxima

at $\pi/2$ and $3\pi/2$ and a zero in between at angle $\vartheta^R=\pi$ of the excited (spin-down) state. As in the discussion of (18.210), amplitude beat frequency is $\Omega^R/2$ while intensity (square-amplitude) beats at Ω^R.

A geometric sketch of the spin-crank angle ϑ^R and related frequencies Ω^R, $\delta^{\pm}$ and Δ is given in Fig. 19.1.7. Concentric circles of radii δ^- and δ^+ define the $\mathbf{\Omega}^R$ vector by (19.1.20f) and Δ by (19.1.20g). The figure relates angles ϑ^R , $\vartheta^R/2$, and components $(\cos\vartheta^R/2, \sin\vartheta^R/2)$ of AC states (19.1.20c-d).

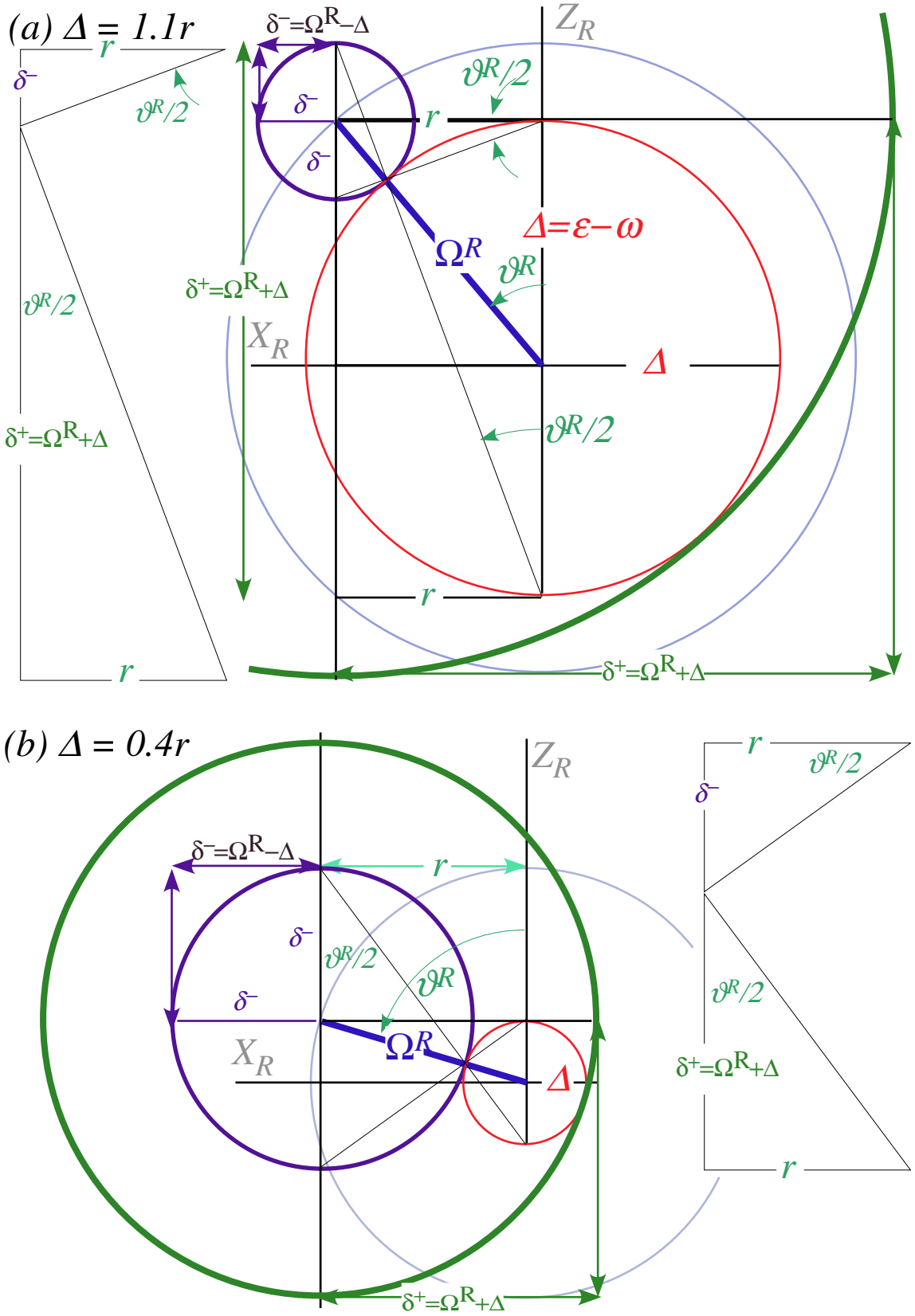


Fig. 19.1.6 AC Stark eigensolution geometry. Rabi rate r=(a) 1.2, (b) 0.4.

Problems for Chapter 19.

Jailhouse Rock'round the Clock(again)

19.1.1 In Problem 18.3.1 (*Jailhouse Rock'n Roll*) prisoner-*M* is in the infinite-well maximum-security prison of Chapter 12 suffering from an Earthquake (caused perhaps by a heavy-metal rock band) that seems to go on forever. *M* remains in any of its eigenstates only in the absence of perturbations. But now the prison floor tilt angle varies: $\phi=\phi^{limit} sin(\omega_{rock}t)$ giving $V_{rock'n\ roll}(x)$ of Problem 18.1.1. Using only the first term in $V_{rock'n\ roll}(x)$, discuss transition from the ground state $|\varepsilon_1\rangle$ to $|\varepsilon_2\rangle$ stimulated by frequency ω_{rock} of amplitude $\phi^{limit}=\pi/10$. At first assume no other levels participate, then estimate possible "leakage.".

(a) $\omega_{rock} = \varepsilon_1$ (*=1* in theorist $\hbar=1$ units)

(b) $\omega_{rock} = 2\varepsilon_1$.

(c) $\omega_{rock} = 3\varepsilon_1$..

(d) $\omega_{rock} = 4\varepsilon_1$...

In each case plot the resulting Rabi-Spin **S**-vector and its driving crank **Ω**-vector. Indicate on a plot like Fig. 19.1.6 the dressed eigenstates and the maximum transition amplitude.

Review Topics & Formulas for Unit 6

Lorentz *pondermotive* form for Newton's $\mathbf{F}=M\mathbf{a}=M\dot{\mathbf{v}}=M\ddot{\mathbf{R}}$ equation for a mass M of charge e.

$$M\frac{d\mathbf{v}}{dt}=\mathbf{F}=e(\mathbf{E}+\mathbf{v}\times\mathbf{B}) \tag{17.1.1}$$

Velocity is $\mathbf{v}=\dot{\mathbf{R}}$. *Scalar potential field* $\Phi=\Phi(\mathbf{R},t)$ and a *vector potential field* $\mathbf{A}=\mathbf{A}(\mathbf{R},t)$ use Maxwell's.

$$\mathbf{E}=-\nabla\Phi-\frac{\partial\mathbf{A}}{\partial t},\qquad \mathbf{B}=\nabla\times\mathbf{A} \tag{17.1.2}$$

Canonical electromagnetic Lagrange equations.

$$\frac{d}{dt}\frac{\partial L}{\partial\mathbf{v}}=\frac{d}{dt}\frac{\partial}{\partial\mathbf{v}}\left(\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-(e\Phi-\mathbf{v}\bullet e\mathbf{A})\right)=\nabla(e\Phi-\mathbf{v}\bullet e\mathbf{A})=\frac{\partial L}{\partial\mathbf{R}} \tag{17.1.5c}$$

Here the *electromagnetic Lagrangian* is

$$L=L(\mathbf{R},\mathbf{v},t)=\frac{1}{2}M\mathbf{v}\bullet\mathbf{v}-\big(e\Phi(\mathbf{R},t)-\mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\big) \tag{17.1.5d}$$

The *canonical electromagnetic momentum* is

$$\mathbf{P}=\frac{\partial L}{\partial\mathbf{v}}=\frac{\partial}{\partial\mathbf{v}}\left(\frac{1}{2}m\mathbf{v}\bullet\mathbf{v}-\big(e\Phi(\mathbf{R},t)-\mathbf{v}\bullet e\mathbf{A}(\mathbf{R},t)\big)\right)=m\mathbf{v}+e\mathbf{A}(\mathbf{R},t) \tag{17.1.5e}$$

Electromagnetic Hamiltonian function.

$$H=\frac{1}{2M}\big(\mathbf{P}-e\mathbf{A}(\mathbf{R},t)\big)\bullet\big(\mathbf{P}-e\mathbf{A}(\mathbf{R},t)\big)+e\Phi(\mathbf{R},t)\qquad\begin{pmatrix}\text{Formally}\\ \text{correct}\end{pmatrix} \tag{17.1.10a}$$

$$H=\frac{\mathbf{P}\bullet\mathbf{P}}{2M}-\frac{e}{2M}(\mathbf{P}\bullet\mathbf{A}+\mathbf{A}\bullet\mathbf{P})+\frac{e^2}{2M}\mathbf{A}\bullet\mathbf{A}+e\Phi(\mathbf{R},t) \tag{17.1.10b}$$

Schrodinger's equation is non-relativistic.

$$i\hbar\frac{\partial\psi}{\partial t}=H\psi=\left[\frac{(P-q\mathbf{A})^2}{2M}+V(\mathbf{R})\right]\psi=\left[\frac{(\hbar\nabla/i-q\mathbf{A})^2}{2M}+V(\mathbf{R})\right]\psi. \tag{17.1.15a}$$

$$i\hbar\frac{\partial\psi}{\partial t}=\left[\frac{-\hbar^2\nabla^2}{2M}+i\frac{q\hbar}{M}\mathbf{A}\bullet\nabla+\frac{q^2}{2M}\mathbf{A}\bullet\mathbf{A}+V(\mathbf{R})\right]\psi. \tag{17.1.15b}$$

Boost $\mathbf{B}(-q\mathbf{A})=e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}$ by momentum $-q\mathbf{A}$.

$\mathbf{BpB}^\dagger=\mathbf{B}(\mathbf{P}-q\mathbf{A}\mathbf{1})\mathbf{B}^\dagger=\mathbf{P}=\mathbf{p}+q\mathbf{A}\mathbf{1}$ (17.1.16a) $\qquad$ $\mathbf{B}^\dagger\mathbf{PB}=\mathbf{B}^\dagger(\mathbf{p}+q\mathbf{A}\mathbf{1})\mathbf{B}=\mathbf{p}=\mathbf{P}-q\mathbf{A}\mathbf{1}$ (17.1.16b)

New position ket $|\mathbf{r}\rangle$ relates to old $|\mathbf{R}\rangle=\mathbf{B}|\mathbf{r}\rangle$ as follows.

$$|\mathbf{r}\rangle=\mathbf{B}^\dagger|\mathbf{R}\rangle\ ,\quad |\mathbf{R}\rangle=\mathbf{B}|\mathbf{r}\rangle\ ,\quad \langle\mathbf{r}|=\langle\mathbf{R}|\,\mathbf{B}\ ,\quad \langle\mathbf{R}|=\langle\mathbf{r}|\,\mathbf{B}^\dagger. \tag{17.1.17a}$$

A wavefunction $\psi(\mathbf{R})=\langle\mathbf{R}|\psi\rangle$ of any state $|\psi\rangle$ times $B=e^{-iq\mathbf{A}\bullet\boldsymbol{R}/\hbar}$ gives wave $\psi(\mathbf{r})=\langle\mathbf{r}|\psi\rangle$ in $\mathbf{r}$-basis.

$$\psi(\mathbf{r})=\langle\mathbf{r}|\psi\rangle=\langle\mathbf{R}|\,\mathbf{B}|\psi\rangle=\langle\mathbf{R}|\,e^{-iq\mathbf{A}\bullet\mathbf{r}/\hbar}|\psi\rangle=e^{-iq\mathbf{A}\bullet\boldsymbol{R}/\hbar}\psi(\mathbf{R})=\psi^B(\mathbf{R})\ . \tag{17.1.17b}$$

An electric dipole potential $-q\mathbf{E}\bullet\mathbf{r}$ arises from $B\ \partial\psi(R)/\partial t$ and Maxwell equation $\mathbf{E}=-\partial\mathbf{A}/\partial t$.

$$i\hbar\frac{\partial\psi(\mathbf{r},t)}{\partial t}=\left[\frac{-\hbar^2\nabla_{\mathbf{r}}{}^2}{2M}+V(\mathbf{r})-q\mathbf{E}(t)\bullet\mathbf{r}\right]\psi(\mathbf{r},t) \tag{17.1.20c}$$

Time-dependent (non-autonomous) Hamiltonian.

$$\mathbf{H}(t)=\mathbf{H}_0+\mathbf{V}(t)=\mathbf{H}_0+\mathbf{H}_I \tag{18.1.1a}$$

$$i\hbar\frac{\partial}{\partial t}\left|\Psi(t)\right\rangle=\mathbf{H}(t)\left|\Psi(t)\right\rangle=\left(\mathbf{H}_0+\mathbf{V}(t)\right)\left|\Psi(t)\right\rangle \tag{18.1.1b}$$

Eigenstates of the unperturbed part $\mathbf{H}_0$ of the Hamiltonian.

$$\mathbf{H}_0|\varepsilon_k\rangle=\varepsilon_k|\varepsilon_k\rangle=\hbar\omega_k\,|\varepsilon_k\rangle \tag{18.1.3}$$

$$\left|\Psi(t)\right\rangle=\sum_k e^{-i\omega_k t}\left|\varepsilon_k\right\rangle c_k(t) \tag{18.1.5}$$

$$i\hbar\frac{\partial c_j(t)}{\partial t}=\sum_k e^{i(\omega_j-\omega_k)t}\left\langle\varepsilon_j\left|\mathbf{V}(t)\right|\varepsilon_k\right\rangle c_k(t)=\sum_k V_{jk}(t)c_k(t) \tag{18.1.10b}$$

The *(j,k)*-coupling time dependence is a modulation by $\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle$ of the transition beat phasor $e^{i\Omega_{jk}}$.

$$V_{jk}(t)=e^{i\Omega_{jk}}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle=e^{i(\omega_j-\omega_k)t}\langle\varepsilon_j|\mathbf{V}(t)|\varepsilon_k\rangle \tag{18.1.10c}$$

The time variation of the state amplitude of general state $|\Psi(t)\rangle$ in (18.1.5) is

$$\langle\varepsilon_k|\Psi(t)\rangle=e^{-i\omega_k t}\,c_k(t)\ . \tag{18.1.10d}$$

Iterative solution:

$$c_k(0)=\delta_{k1}=c_k^{(0)}. \tag{18.1.11}$$

$$c_j^{(1)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}(t_1) \tag{18.1.13}$$

$$c_j^{(2)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}(t_1)+\frac{1}{(i\hbar)^2}\sum_k\int_0^t dt_2 V_{jk}(t_2)\int_0^{t_2} dt_1 V_{k1}(t_1) \tag{18.1.14b}$$

$$c_j^{(3)}(t)=c_j^{(2)}(t)+\frac{1}{(i\hbar)^3}\sum_{k,k'}\int_0^t dt_3 V_{jk'}(t_3)\int_0^{t_3} dt_2 V_{k'k}(t_2)\int_0^{t_2} dt_1 V_{k1}(t_1) \tag{18.1.15}$$

$$c_j^{(1)}(t)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 V_{j1}^c(t_1)=\delta_{j1}+\frac{1}{i\hbar}\int_0^t dt_1 e^{i\Omega_{j1}}\,\langle\varepsilon_j\,|\,\mathbf{V}^c(t_1)\,|\,\varepsilon_1\rangle \tag{18.2.5a}$$

The key quantities are the beats or *(j←1)-transition frequencies* Ω_{j1} and *(j←1)-dipole matrix elements* r_{j1}.

$$\Omega_{j1}=\omega_j-\omega_1. \qquad r_{j1}=\mathbf{e}\bullet\langle j|\,\mathbf{r}\,|1\rangle \tag{18.2.5b}$$

It is helpful to rewrite the amplitudes $c_j^{(1)}(t)$ as follows (Here: $E_o=2|a|\omega$ appears again.)

$$c_j^{(1)}(t) = \delta_{j1} + \frac{q\, r_{j1} E_0}{2\hbar}\left[e^{i\phi} S\left(\Delta^{\uparrow}, t\right) + e^{-i\phi} S\left(\Delta^{\downarrow}, t\right)\right], \qquad (18.2.5e)$$

using an important *spectral amplitude function S(Δ,t)* of an angular frequency *detuning parameter Δ*

$$S(\Delta, t) = \int_0^t d\tau\, e^{i\tau\Delta} = \frac{e^{it\Delta/2}\sin(t\Delta/2)}{\Delta/2}. \qquad (18.2.5f)$$

Total transition probability $\Sigma(t) = \int_{-\infty}^{\infty} d\Delta \left|S(\Delta,t)\right|^2 = \int_{-\infty}^{\infty} d\Delta \frac{\sin^2(t\Delta/2)}{(\Delta/2)^2}.$ (18.2.10a)

Fermi's golden rule for constant transition rates. $\Sigma(t) = \int_{-\infty}^{\infty} d\Delta \left|S(\Delta,t)\right|^2 = 2\pi \cdot t$ (18.2.10d)

Oscillator strength and dipole response

$$\langle x\rangle = \sum_{j=1} \frac{2\Omega_{j1}\left|r_{j1}\right|^2 M}{\hbar}\left(\frac{qE_0}{M}\frac{\cos\omega t - \cos\Omega_{j1} t}{{\Omega_{j1}}^2 - \omega^2}\right) \qquad (18.3.5a)$$

$$= \sum_{j=1} \quad f_{j1} \quad \cdot \quad x_{classical}$$

Lorentz-atomic-oscillator frequency $\omega_0 = \Omega_{j1} = \omega_j - \omega_1$. (18.3.5b)

This is the *(j←1)-transition frequency* Ω_{j1} or quantum beat driven by stimulus frequency $\omega_S = \omega$.

(j←1)-oscillator strength f_{j1} $f_{j1} = \frac{2\Omega_{j1}\left|r_{j1}\right|^2 M}{\hbar}$ (18.3.5d)

Thomas-Reiche-Kuhn sum rule for oscillator strength. This holds for any H_0 eigenstate $|1\rangle$.

$$\sum_{j=1} f_{j1} = \sum_{j=1} 2\langle 1|x|j\rangle\langle j|p|1\rangle/\hbar i = 2\langle 1|xp|1\rangle/\hbar i = -2\langle 1|px|1\rangle/\hbar i = 1 \qquad (18.3.10a)$$

Quantum eigenstate virial theorem that is similar to the classical viral theorem.

$$\langle KE\rangle = \langle m|\frac{p^2}{2M}|m\rangle = \frac{P}{2}\langle m|V\cdot x^P|m\rangle = \frac{P}{2}\langle PE\rangle \qquad (18.3.10c)$$