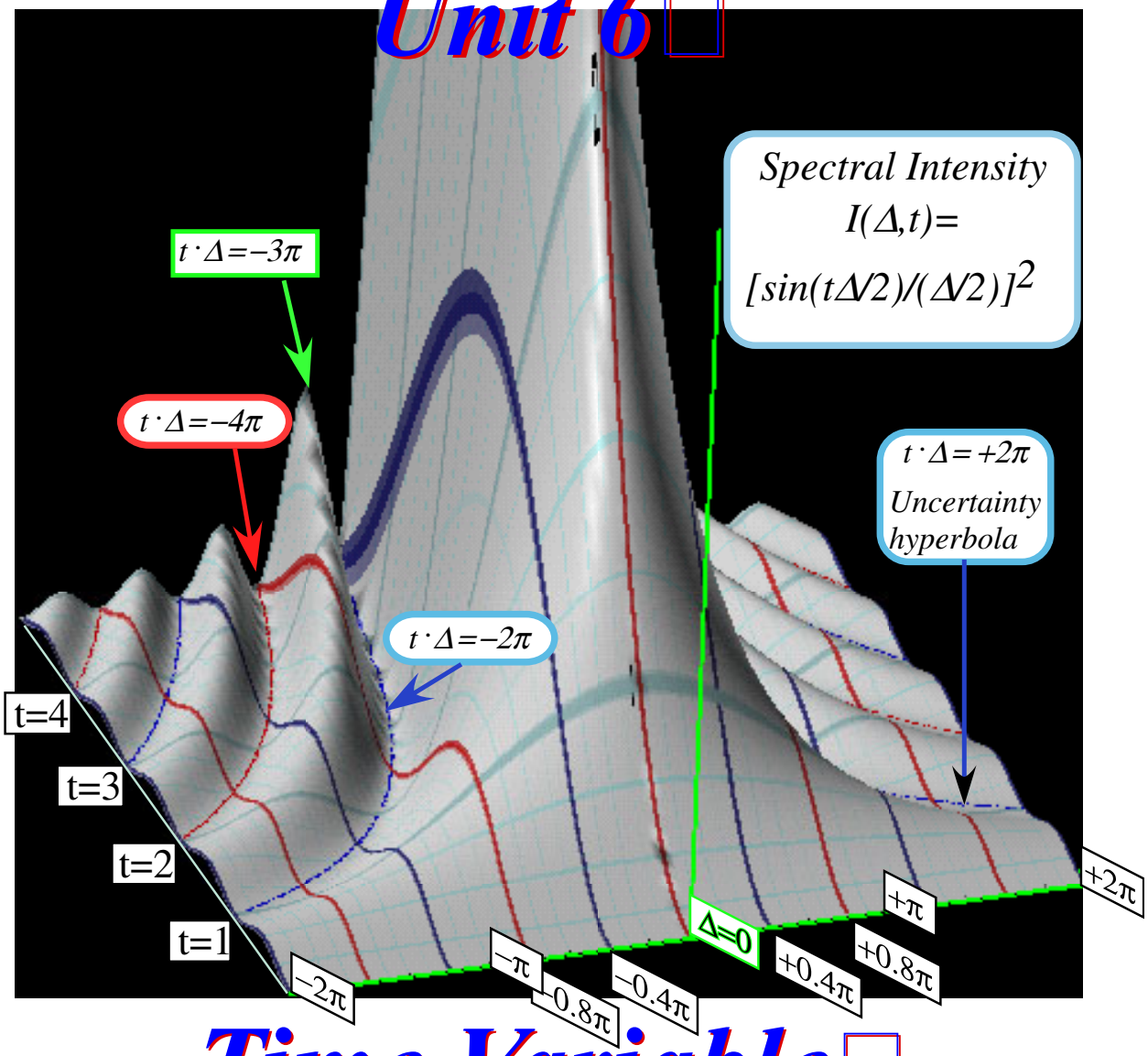
# Quantum Theory for the Computer Age

# 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.

**W. G. Harter**

**Department of Physics**

**University of Arkansas**

**Fayetteville**

*Hardware and Software by*

**HARTER**-*Soft*

*Elegant Educational Tools Since 2001*

## *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.

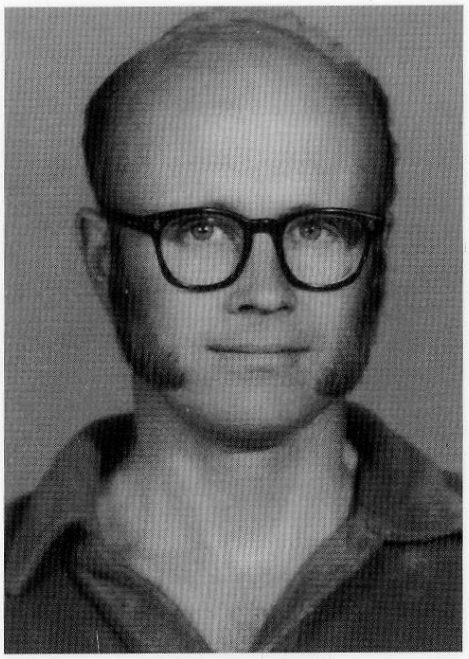
Let me introduce an "Indiana Jones" of modern physics. While he may never have been called "Montana Ken," such a name would describe a real life hero from Bozeman, Montana, whose accomplishments in many ways surpass the fictional character in *Raiders of the Lost Arc* and other cinematic thrillers.

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.

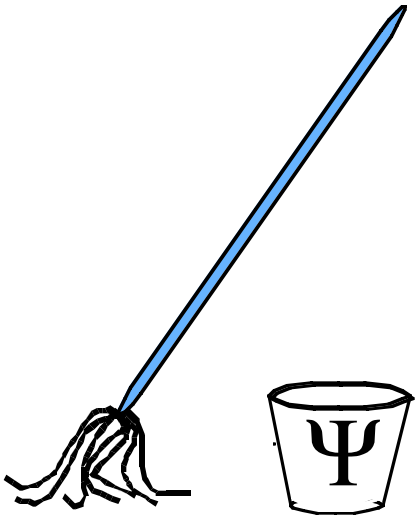
Those who knew him will always miss Ken. But, his indelible legacy of persistence lives on as ultra-precision atomic and molecular wave and pulse quantum optics continue to advance and provide mankind with heretofore-unimaginable capability.



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.

.

# 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 $\nabla$ 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 *($\mu$=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 $\Phi$ 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 $\Phi$ 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 $\Phi$ 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 $\Theta$ 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 $\mathsf{B}$ (or $\mathsf{B}^\dagger$) again just adds (or subtracts) another $qA$, since here $\mathsf{B}qA\mathsf{B}^\dagger = qA = \mathsf{B}^\dagger qA\mathsf{B}$

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

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

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

$\mathsf{B}$ has the opposite effect on states or wavefunctions. Look at its effect on a plane wave.

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

$\mathsf{B}$ 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 $\mathsf{B}$ boosts used here should be replaced by Lorentz transformations derived in Unit 4 using the $\sigma$-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 $\omega t$. (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.

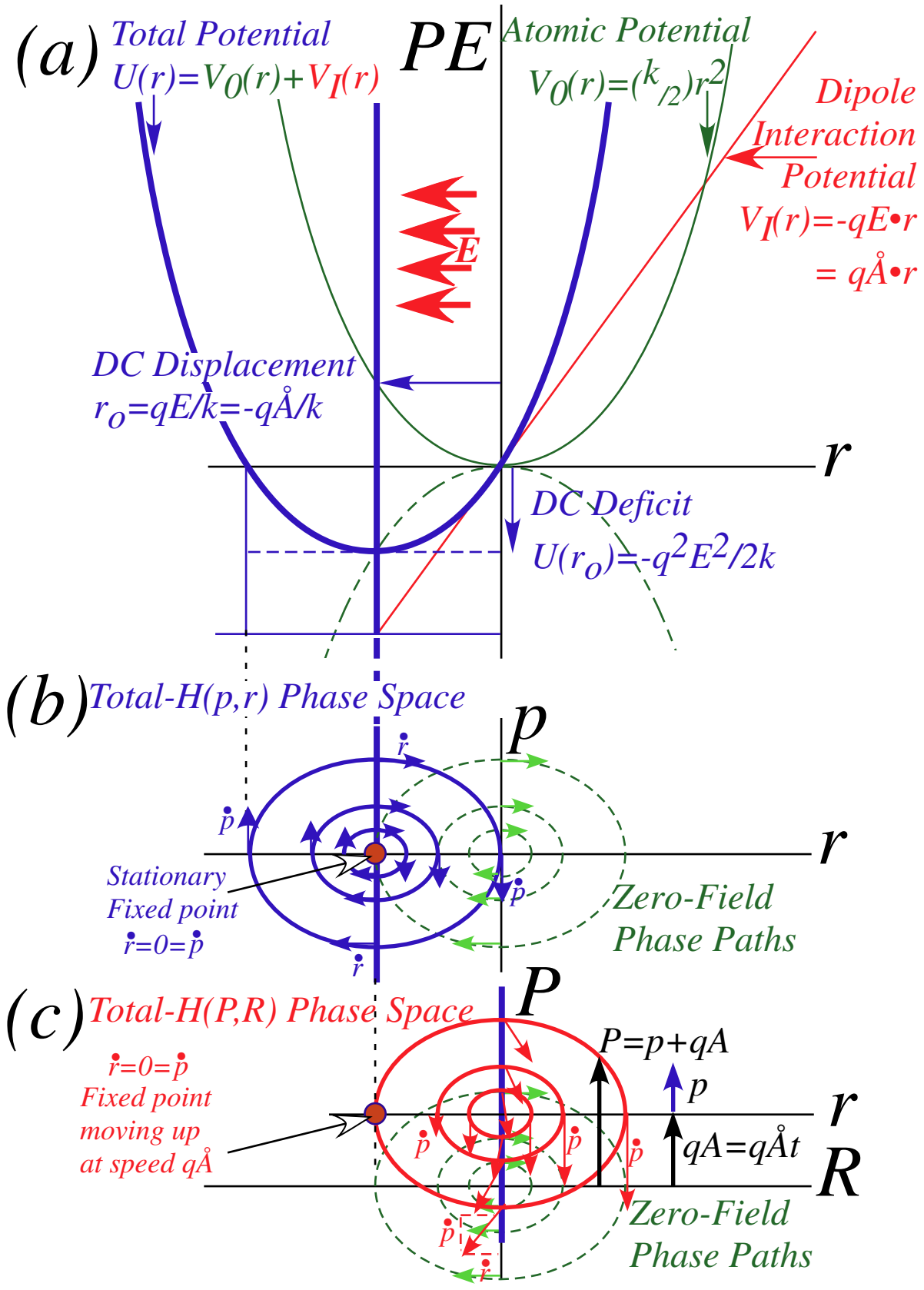



*Fig. 17.1.1 (a) H(p,r) with E•r coupling. (b) Phase space. (c) H(P,R)=H(p+qA,R) boosted phase space.*

## *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-$\phi$ of incidence equals angle+$\phi$ 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 $\Phi$ 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).

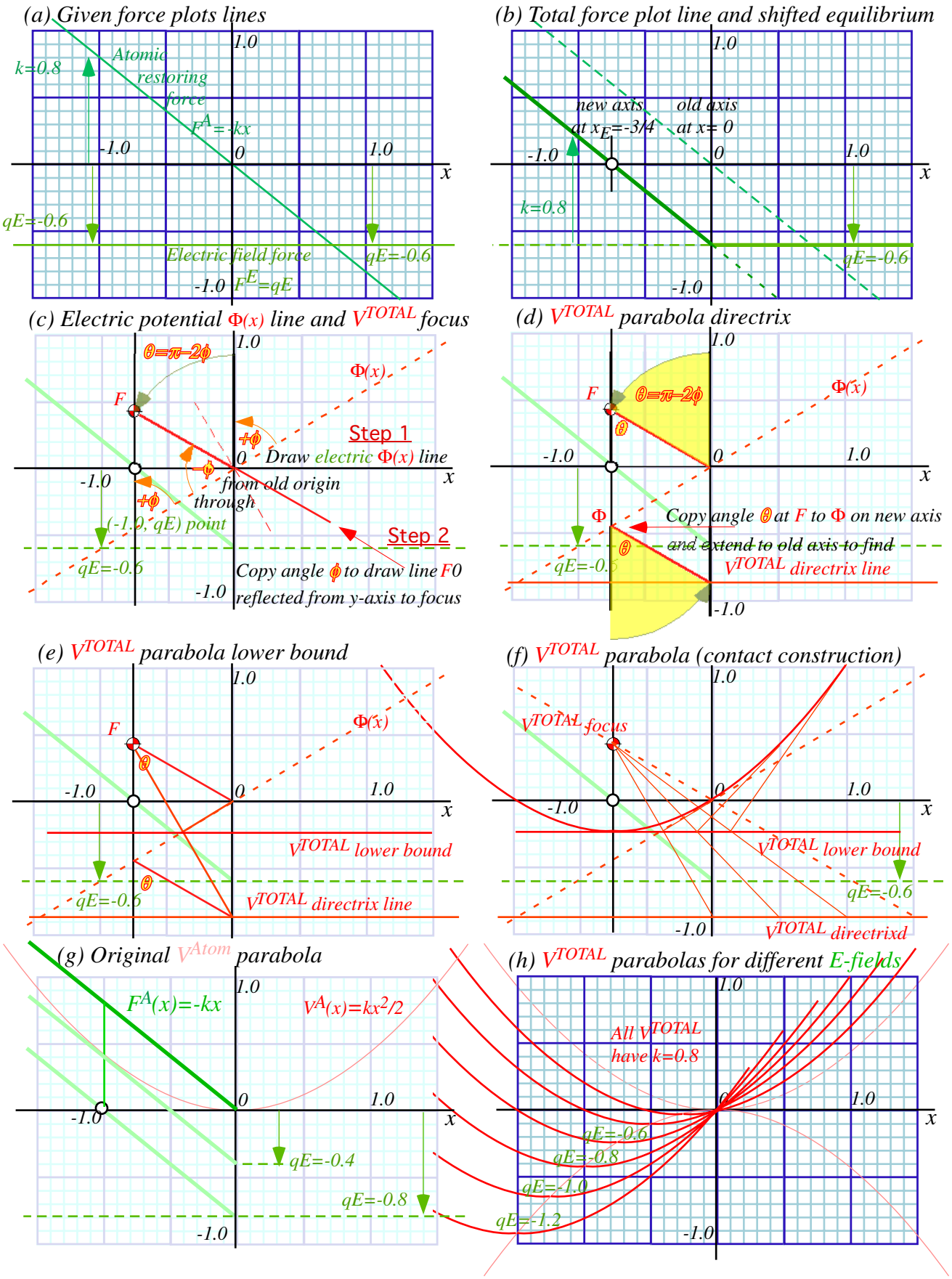

(a) Given force plots lines
k=0.8
Atomic restoring force
$F^A=-kx$
1.0
-1.0
0
1.0
x
qE=-0.6
Electric field force $F^E=qE$
qE=-0.6
(b) Total force plot line and shifted equilibrium
new axis at $x_E$=-3/4
old axis at x= 0
k=0.8
qE=-0.6
(c) Electric potential Φ(x) line and $V^{TOTAL}$ focus
θ=π−2ϕ
F
Φ(x)
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 $\psi$ 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 $\psi^G$ obeys wave equation (17.1.6) with *gauge transformed potentials* $\Phi^G$ 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 $\Phi$.

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 $\omega$) 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.

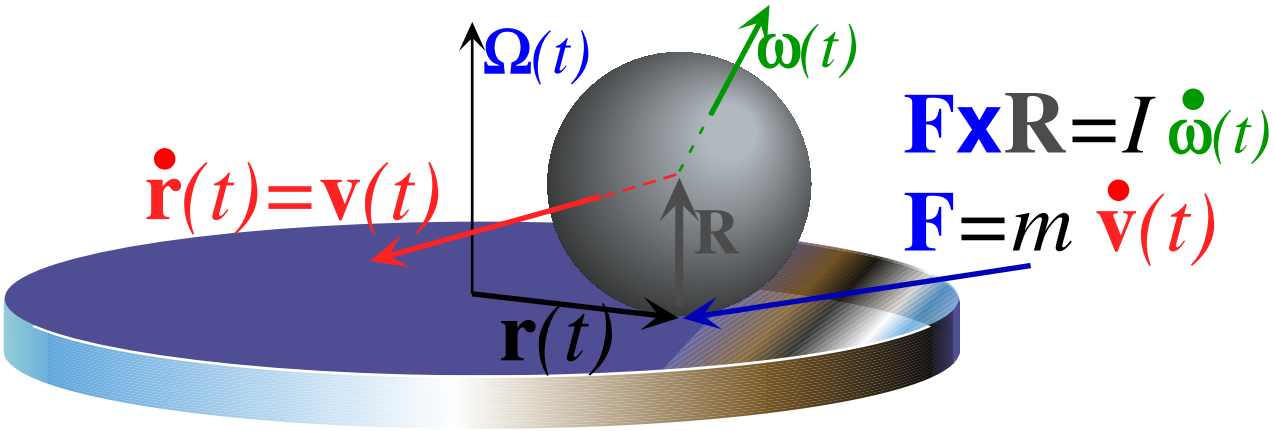



*Fig. 17.1.2 Mechanical analog of magnetic* **vxB** *cyclotron mechanics.*

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.