Fourier transformations by numerical grid summations

$$F_{hkl} \underset{\mathcal{F}^{-1}}{\overset{\mathcal{F}}{\rightleftarrows}} \rho(x,y,z) \qquad \begin{cases} \rho(x,y,z) = \mathcal{F}\left[F_{hkl}\right] & \textbf{Fourier synthesis} \\ F_{hkl} = \mathcal{F}^{-1}\left[\rho(x,y,z)\right] & \textbf{Fourier analysis} \end{cases}$$

Fourier Synthesis

$$\rho(x_p,y_q,z_r) = \frac{1}{V_{\text{cell}}} \sum_{h_{\min}}^{h_{\max}} \sum_{k_{\min}}^{k_{\max}} \sum_{l_{\min}}^{l_{\max}} |F_{hkl}| \cos\left[\varphi_{hkl} - 2\pi\left(hx_p + ky_q + lz_r\right)\right]$$

$$0 \le x_p, y_q, z_r < 1 \quad \begin{cases} x_p = p/N_{\text{x}}, & y_q = q/N_{\text{y}}, & z_r = r/N_{\text{z}} \\ p = 0,1,2,\ldots,N_{\text{x}}-1, & q = 0,1,2,\ldots,N_{\text{y}}-1, & r = 0,1,2,\ldots,N_{\text{z}}-1 \\ \Delta x = a/N_{\text{x}}, & \Delta y = b/N_{\text{y}} & \Delta z = c/N_{\text{z}} \end{cases}$$

Shannon sampling: $d_{hkl} \ge d_{\min} = \dfrac{\lambda}{2\sin\theta_{\max}}$ and $\max(\Delta x, \Delta y, \Delta z) \lesssim \dfrac{1}{2} d_{\min}$

Fourier Analysis

$$F_{hkl} = \frac{V_{\text{cell}}}{N_{\text{x}} N_{\text{y}} N_{\text{z}}} \sum_{p=0}^{N_{\text{x}}-1} \sum_{q=0}^{N_{\text{y}}-1} \sum_{r=0}^{N_{\text{z}}-1} \rho(x_p,y_q,z_r) \exp\left[+2\pi i\left(hx_p + ky_q + lz_r\right)\right]$$

Shannon sampling: $d_{hkl} \ge d_{\min} \gtrsim 2\max(\Delta x, \Delta y, \Delta z) = 2\max\left(a/N_{\text{x}}, b/N_{\text{y}}, c/N_{\text{z}}\right)$

Structure factor amplitudes and phases by numerical Fourier inversion of a grid density

Fourier Analysis

$$F_{hkl} = \frac{V_{\text{cell}}}{N_{\text{x}} N_{\text{y}} N_{\text{z}}} \sum_{p=0}^{N_{\text{x}}-1} \sum_{q=0}^{N_{\text{y}}-1} \sum_{r=0}^{N_{\text{z}}-1} \rho\left(x_p, y_q, z_r\right) \exp\left[+2\pi i \left(h x_p + k y_q + l z_r\right)\right]$$

$$F_{hkl} = \left|F_{hkl}\right| \mathrm{e}^{i\varphi_{hkl}} = \left|F_{hkl}\right| \left(\cos\varphi_{hkl} + i \sin\varphi_{hkl}\right) = A_{hkl} + i B_{hkl}$$

$$\begin{cases} A_{hkl} = \dfrac{V_{\text{cell}}}{N_{\text{x}} N_{\text{y}} N_{\text{z}}} \displaystyle\sum_{p=0}^{N_{\text{x}}-1} \sum_{q=0}^{N_{\text{y}}-1} \sum_{r=0}^{N_{\text{z}}-1} \rho\left(x_p, y_q, z_r\right) \cos\left[+2\pi \left(h x_p + k y_q + l z_r\right)\right] \\ B_{hkl} = \dfrac{V_{\text{cell}}}{N_{\text{x}} N_{\text{y}} N_{\text{z}}} \displaystyle\sum_{p=0}^{N_{\text{x}}-1} \sum_{q=0}^{N_{\text{y}}-1} \sum_{r=0}^{N_{\text{z}}-1} \rho\left(x_p, y_q, z_r\right) \sin\left[+2\pi \left(h x_p + k y_q + l z_r\right)\right] \end{cases}$$

$$\begin{cases} \left|F_{hkl}\right| = \sqrt{A_{hkl}^2 + B_{hkl}^2} \\ \varphi_{hkl} = \tan^{-1}\left(\dfrac{B_{hkl}}{A_{hkl}}\right) \end{cases}$$

Shannon sampling : $d_{hkl} \geq d_{\min} \gtrsim 2 \max\left(\Delta x, \Delta y, \Delta z\right) = 2 \max\left(a/N_{\text{x}}, b/N_{\text{y}}, c/N_{\text{z}}\right)$

Shannon sampling

$$\begin{cases} \textbf{Reciprocal lattice}: & \max\left|\mathbf{h}_j\right| = \dfrac{1}{d_{\min}} = 2\left(\dfrac{\sin\theta_{\max}}{\lambda}\right), \qquad j = 1,2,...,n \\ \textbf{Density grid}: & \min\left|\mathbf{r}_{j+1} - \mathbf{r}_j\right| = \dfrac{d_{\min}}{2} = \dfrac{\lambda}{4\sin\theta_{\max}}, \qquad j = 0,1,...,2n-1 \end{cases}$$

n points in **h**-space $\Leftrightarrow$ 2*n* points in **r**-space

Claude E. Shannon, "Communication in the presence of noise", *Proc. Institute of Radio Engineers*, vol. **37**, no. 1, pp. 10–21, (Jan. 1949). Reprint as classic paper in: *Proc. IEEE*, vol. **86**, no. 2, (Feb. 1998)

http://en.wikipedia.org/wiki/Nyquist–Shannon_sampling_theorem

$F_{hkl} \overset{\mathcal{F}}{\underset{\mathcal{F}^{-1}}{\rightleftarrows}} \rho(x,y,z)$

Basic principle of the FFT

A sum of N terms can be decomposed into two sums of $N/2$ terms.

$F_{hkl} \overset{\text{FFT}}{\underset{\text{FFT}^{-1}}{\rightleftarrows}} \rho(x,y,z)$

The projection of a unit-cell scattering density distribution onto the *a* axis is given by Fourier transformation of the axial structure factors,

$$\begin{aligned}
\rho(x) &= \mathcal{F}\left[F_{h\,0\,0}\right] \\
&= \frac{1}{a}\sum_{h=0}^{N_h-1} F_{h\,0\,0}\exp(-2\pi i h x) \\
&= \frac{1}{a}\sum_{h=0}^{(N_h/2)-1} F_{2h\;0\;0}\exp\left[-2\pi i(2h)x\right] + \frac{1}{a}\sum_{h=0}^{(N_h/2)-1} F_{(2h+1)\;0\;0}\exp\left[-2\pi i(2h+1)x\right] \\
&= \frac{1}{a}\sum_{h=0}^{(N_h/2)-1} F_{2h\;0\;0}\exp\left[-2\pi i(2h)x\right] + \frac{1}{a}\exp(-2\pi i x)\sum_{h=0}^{(N_h/2)-1} F_{(2h+1)\;0\;0}\exp\left[-2\pi i(2h)x\right].
\end{aligned}$$

Thus $\exp\left[-2\pi i(2h)x\right]$ needs be evaluated only $N_h/2$ times but can be used N_h times.

Similarly, the axial structure factors are given by Fourier inversion of the one-dimensional projected density,

$$\begin{aligned}
F_{h00} &= \mathcal{F}^{-1}\left[\rho(x)\right] \\
&= a\sum_{n=0}^{N_x-1} \rho(x_n)\exp(+2\pi i h x_n) \\
&= a\sum_{n=0}^{N_x-1} \rho(n/N_x)\exp(2\pi i h n/N_x) \\
&= a\sum_{n=0}^{(N_x/2)-1} \rho\left(\frac{2n}{N_x}\right)\exp\left[2\pi i h(2n)/N_x\right] + a\sum_{n=0}^{(N_x/2)-1} \rho\left(\frac{2n+1}{N_x}\right)\exp\left[2\pi i h(2n+1)/N_x\right] \\
&= a\sum_{n=0}^{(N_x/2)-1} \rho\left(\frac{2n}{N_x}\right)\exp\left[2\pi i h(2n)/N_x\right] + a\exp(+2\pi i h)\sum_{n=0}^{(N_x/2)-1} \rho\left(\frac{2n+1}{N_x}\right)\exp\left[2\pi i h(2n)/N_x\right],
\end{aligned}$$

and $\exp\left[2\pi i h(2n)/N_x\right]$ needs be evaluated only $N_x/2$ times but can be used N_x times.

Basic principle of the FFT (cont'd)

• Subdivision of a sum of N terms into separate even-index and odd-index sums of $N/2$ terms can be repeated recursively.

• Each of the sums of $N/2$ terms can be subdivided into sums of $N/4$ terms over even-index and odd-index terms, and the process of subdivision can be continued until finally only two-term sums remain to be summed.

• The net effect of economies in evaluations of $e^{i\theta}$ by subdivision in FFT algorithms is a reduction of the size of a calculation for N data points from order N^2 to order $N \log_2 N$. As shown in the table below, this represents for large N an enormous reduction.

• Depending on the factorability of N, subdivisions into other than two sums of $N/2$ terms indexed by $2n$ and $2n+1$, such as three sums of $N/3$ terms indexed by $3n$, $3n+1$, and $3n+2$, are also possible.

• After the advent of high-speed digital electronic computing, the invention of the Cooley-Tukey FFT algorithm (Cooley and Tukey, 1965) made large-scale Fourier transform calculations important and commonplace in many, many areas of science and engineering.

• The *N*-factorization/divide-and-conquer principle for series evaluation had in fact been discovered by Gauss (1777-1855), but its practical exploitation had to await the appearance of fast computers.

Basic principle of the FFT (cont'd)

The net effect of the computational economies in FFT algorithms is a reduction of the size of the calculation from order N^2 to order $N \log_2 N$.

N	N	N^2	$N \log_2 N$
1	2^0	1	1
2	2^1	4	2
4	2^2	16	8
8	2^3	64	24
⋮			
1,024	2^{10}	$104{,}856 \approx 10^5$	$10{,}240 \approx 10^4$
2,048	2^{11}		
4,096	2^{12}		
8,192	2^{13}		
16,383	2^{14}		
32,768	2^{15}	$1{,}073{,}741{,}824 \approx 10^9$	$491{,}520 \approx 0.5\times10^6$
⋮	⋮	⋮	⋮

The unit cell scattering density distribution $\rho(\mathbf{r}) = \rho(x,y,z)$ and the crystal structure factors $F_{\mathbf{h}} = F_{hkl}$ as atomic summations

$$\rho(\mathbf{r}) = \sum_{a=1}^{N} \rho_a(\mathbf{r} - \mathbf{r}_a) = \sum_{a=1}^{N} \rho_a(\mathbf{r}) * \delta(\mathbf{r} - \mathbf{r}_a)$$

$$\begin{aligned}
F_{\mathbf{h}} &= \mathcal{F}^{-1}\left[\rho(\mathbf{r})\right] \\
&= \mathcal{F}^{-1}\left[\sum_{a=1}^{N} \rho_a(\mathbf{r} - \mathbf{r}_a)\right] \\
&= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r} - \mathbf{r}_a)\right] \\
&= \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r}) * \delta(\mathbf{r} - \mathbf{r}_a)\right]
\end{aligned}$$

$$F_{\mathbf{h}} = \sum_{a=1}^{N} \mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] \mathcal{F}^{-1}\left[\delta(\mathbf{r} - \mathbf{r}_a)\right]$$

$$\mathcal{F}^{-1}\left[\rho_a(\mathbf{r})\right] = f_a(\mathbf{h})$$

$$\mathcal{F}^{-1}\left[\delta(\mathbf{r} - \mathbf{r}_a)\right] = \exp(2\pi i \mathbf{h} \bullet \mathbf{r}_a)$$

$$F_{\mathbf{h}} = \sum_{a=1}^{N} f_a(\mathbf{h}) \exp(2\pi i \mathbf{h} \bullet \mathbf{r}_a)$$

The Kronecker Delta

$$\delta_{ij} = \begin{cases} 0\,, & i \neq j \\ 1\,, & i = j \end{cases}$$

The Dirac Delta Function

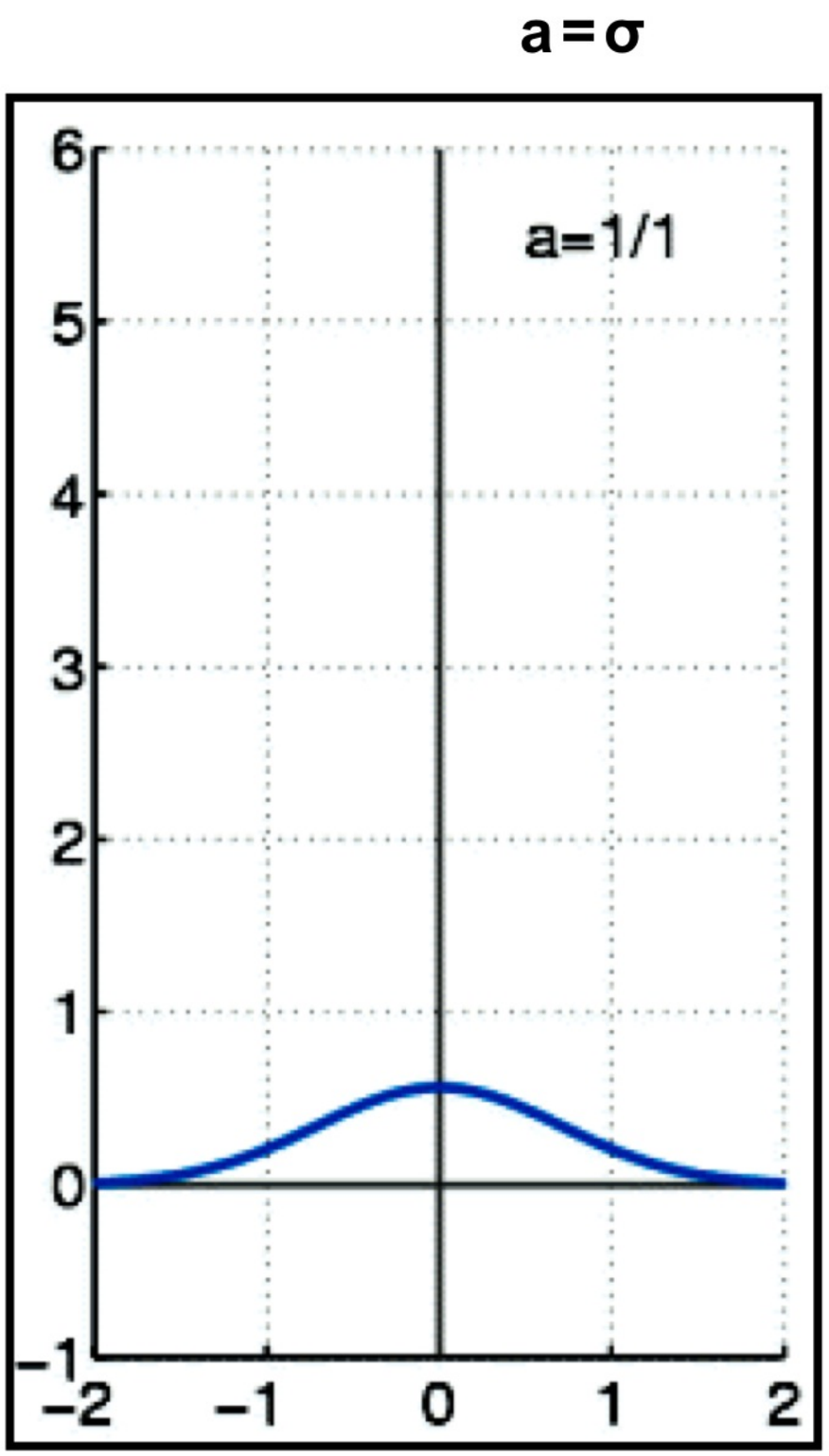
$$\delta\left(x - x_0\right) = 0\,, \quad \forall x \neq x_0$$

$$\int_{-\infty}^{+\infty} \delta\left(x - x_0\right) \mathrm{d}x = 1$$

$$\int_{-\infty}^{+\infty} f\left(x\right) \delta\left(x - x_0\right) \mathrm{d}x = f\left(x_0\right)$$

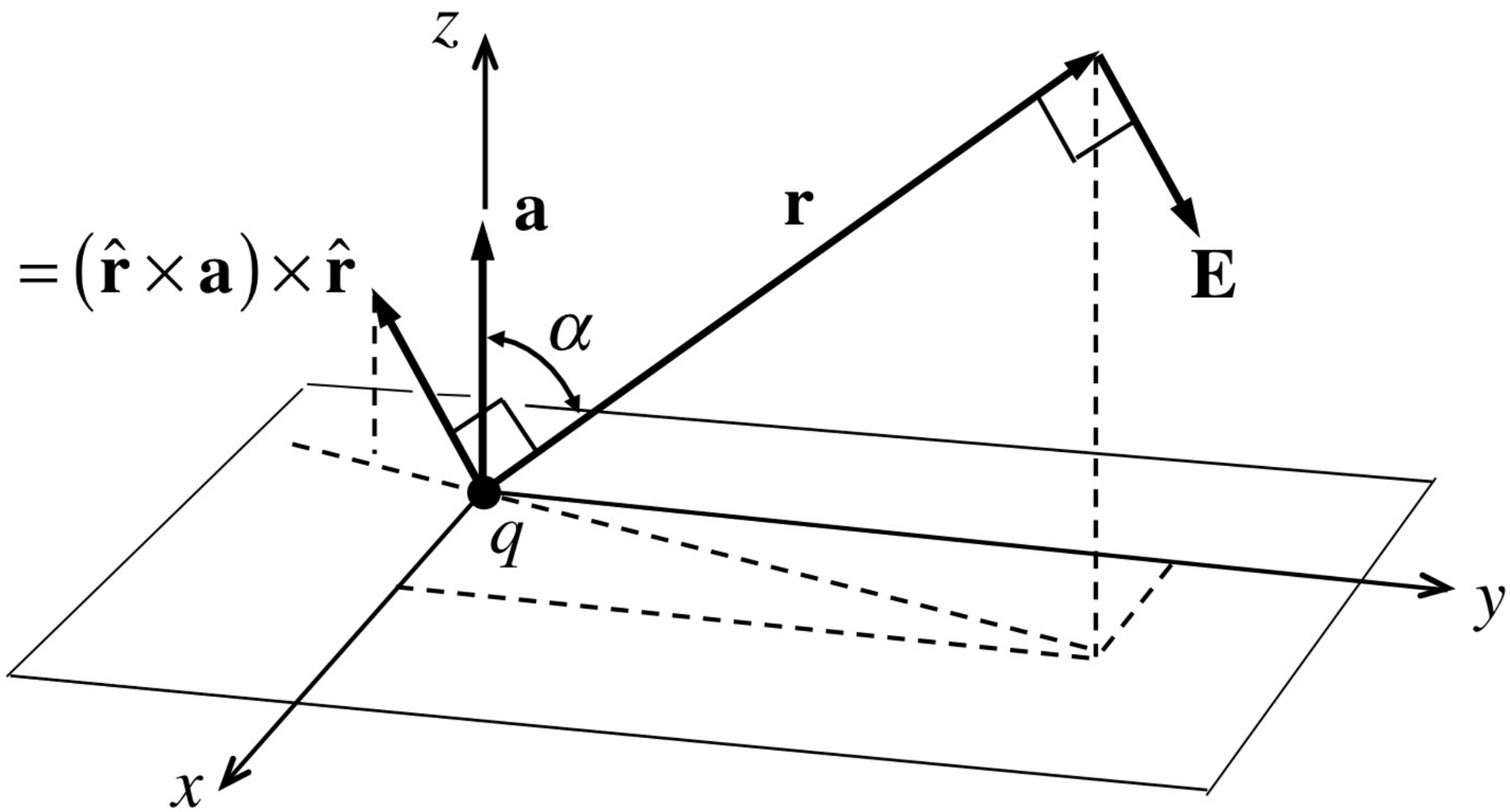
$$\int_{x_0 - \varepsilon}^{x_0 + \varepsilon} \delta\left(x - x_0\right) \mathrm{d}x = 1\,, \qquad \varepsilon > 0$$

$$\int_{x_0 - \varepsilon}^{x_0 + \varepsilon} f\left(x\right) \delta\left(x - x_0\right) \mathrm{d}x = f\left(x_0\right)\,, \quad \varepsilon > 0$$



$$\delta\left(x\right) = \lim_{\sigma \to 0} \left\{ \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{x}{\sigma} \right)^2 \right] \right\}$$

Electric field **E** at a point at **r** from a charge **q** that experiences an acceleration **a**



$$\mathbf{E} = -\frac{q}{c^2 r}(\hat{\mathbf{r}} \times \mathbf{a}) \times \hat{\mathbf{r}}\,, \qquad \hat{\mathbf{r}} = \frac{\mathbf{r}}{|\mathbf{r}|}\,, \qquad |\mathbf{r}| = r$$

$$E = -\frac{q}{c^2 r} a \sin\alpha\,, \qquad E = |\mathbf{E}|\,, \qquad a = |\mathbf{a}|$$

X-ray scattering by a free electron at rest (Gaussian cgs units)

driven harmonic oscillator

Coulombic em driving force

$$\mathbf{F} = q\mathbf{E} = q_{\mathrm{e}}\mathbf{E} = -e\underbrace{\mathbf{E}_0\,\mathrm{e}^{i\omega t}}_{\substack{\text{incident}\\ \text{X-ray}\\ \text{plane wave}}} = -e\,\mathbf{E}_0\left[\cos(\omega t) + i\sin(\omega t)\right]$$

Newton's second law of motion

$$\mathbf{F} = m\mathbf{a} = m_{\mathrm{e}}\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2}$$

$$m\,\mathbf{a} = q\mathbf{E}$$

$$m_{\mathrm{e}}\mathbf{a} = -e\mathbf{E}_0\,\mathrm{e}^{i\omega t}$$

$$\mathbf{a} = \frac{-e\mathbf{E}_0}{m_{\mathrm{e}}}\mathrm{e}^{i\omega t} = \mathbf{a}_0\,\mathrm{e}^{i\omega t}, \qquad \mathbf{a}_0 = \frac{-e\mathbf{E}_0}{m_{\mathrm{e}}}$$

em radiation from an accelerated charge

$$\begin{cases} \boldsymbol{\mathcal{E}} = -\dfrac{q}{c^2 r}\mathbf{a}_{\perp}, \qquad |\boldsymbol{\mathcal{E}}| = -\dfrac{q}{c^2 r}|\mathbf{a}|\sin\alpha, \qquad \alpha = \measuredangle\,\mathbf{a},\mathbf{r} \\ \boldsymbol{\mathcal{E}} = -\dfrac{q}{c^2 r}(\hat{\mathbf{r}}\times\mathbf{a})\times\hat{\mathbf{r}} = -\dfrac{q}{c^2 r}\left(\dfrac{\mathbf{r}}{r}\times\mathbf{a}\right)\times\dfrac{\mathbf{r}}{r} \end{cases}$$

$$\boldsymbol{\mathcal{E}}_0 = -\frac{q_{\mathrm{e}}}{c^2 r}\mathbf{a}_0 = -\frac{-e}{c^2 r}\left(\frac{-e\mathbf{E}_0}{m_{\mathrm{e}}}\right) = \underbrace{-\left(\frac{e^2}{m_{\mathrm{e}}c^2}\right)\frac{\mathbf{E}_0}{r}}_{\substack{\text{scattered X-ray}\\ \text{spherical wave}\\ \text{Amplitude at r in the equatorial plane}\\ \text{perpendicular to the polarization direction}}} = -r_{\mathrm{e}}\frac{\mathbf{E}_0}{r}$$

X-ray scattering by a free electron, at rest or moving uniformly at a nonrelativistic velocity

(Gaussian cgs units)

$$\begin{cases} \mathbf{F}_{\text{Coulomb}} = q\mathbf{E} \\ \mathbf{F}_{\text{Newton}} = m\mathbf{a} \end{cases}$$

$$m\mathbf{a} = -e\mathbf{E}_0 \mathrm{e}^{i\omega t}$$

Newton's second law force $\mathbf{F}=m\mathbf{a}$

em Coulombic driving force $\mathbf{F}=q\mathbf{E}$

$$\mathbf{a} = -\frac{e}{m}\mathbf{E}_0 \mathrm{e}^{i\omega t}$$

$$\boldsymbol{\mathcal{E}} = -\frac{q\,\mathbf{a}_\perp}{c^2 r} = -\frac{q}{c^2 r}(\hat{\mathbf{r}}\times\mathbf{a})\times\hat{\mathbf{r}}\,, \qquad \hat{\mathbf{r}} = \frac{\mathbf{r}}{|\mathbf{r}|}\,, \qquad |\boldsymbol{\mathcal{E}}| = -\frac{q}{c^2 r}|\mathbf{a}|\sin\alpha\,, \qquad \alpha = \measuredangle\,\mathbf{a},\mathbf{r}$$

$$\boldsymbol{\mathcal{E}} = -\frac{q\,\mathbf{a}}{c^2 r} = -\left(\frac{-e}{c^2 r}\right)\left(\frac{-e\mathbf{E}_0}{m}\right)\mathrm{e}^{i\omega t} = \underbrace{-\underbrace{\left(\frac{e^2}{mc^2}\right)}_{\text{Thomson scattering length}}\frac{\mathbf{E}_0}{r}\,\mathrm{e}^{i\omega t}}_{\boldsymbol{\mathcal{E}}_0} = \boldsymbol{\mathcal{E}}_0 \mathrm{e}^{i\omega t}$$

X-ray scattering by a free electron (Gaussian cgs units)

$$\underbrace{\boldsymbol{\mathcal{E}}_0 \mathrm{e}^{i\omega t}}_{\substack{\text{scattered}\\ \text{X-ray}\\ \text{wave}}} = -\underbrace{\left(\frac{e^2}{mc^2}\right)}_{\substack{r_\mathrm{e}\\ \text{Thomson}\\ \text{scattering}\\ \text{length}}} \frac{\mathbf{E}_0}{r}\mathrm{e}^{i\omega t} = -r_\mathrm{e}\,\frac{\mathbf{E}_0}{r}\mathrm{e}^{i\omega t} = -\frac{r_\mathrm{e}}{r}\mathbf{E}_0\mathrm{e}^{i\omega t}$$

$$r_\mathrm{e} = \underbrace{\left(\frac{e^2}{mc^2}\right)}_{\substack{\text{classical}\\ \text{electron}\\ \text{radius}}}$$

$$\frac{\text{charge}^2}{\text{mass}\bullet\text{velocity}^2} = \frac{\text{charge}^2}{\text{mass}\bullet\text{distance}^2\bullet\text{time}^{-2}} = \frac{\text{force}}{\text{mass}\bullet\text{time}^{-2}} = \frac{\text{acceleration}}{\text{time}^{-2}} = \text{distance}$$

Classical electron radius

Electrostatic potential energy

$$E = q\phi(r) = q(q/r) = e^2/r_\mathrm{e}$$

Relativistic mass - energy

$$E = m_\mathrm{e}c^2$$

$$\Bigg\} \quad r_\mathrm{e} = \frac{e^2}{m_\mathrm{e}c^2}$$

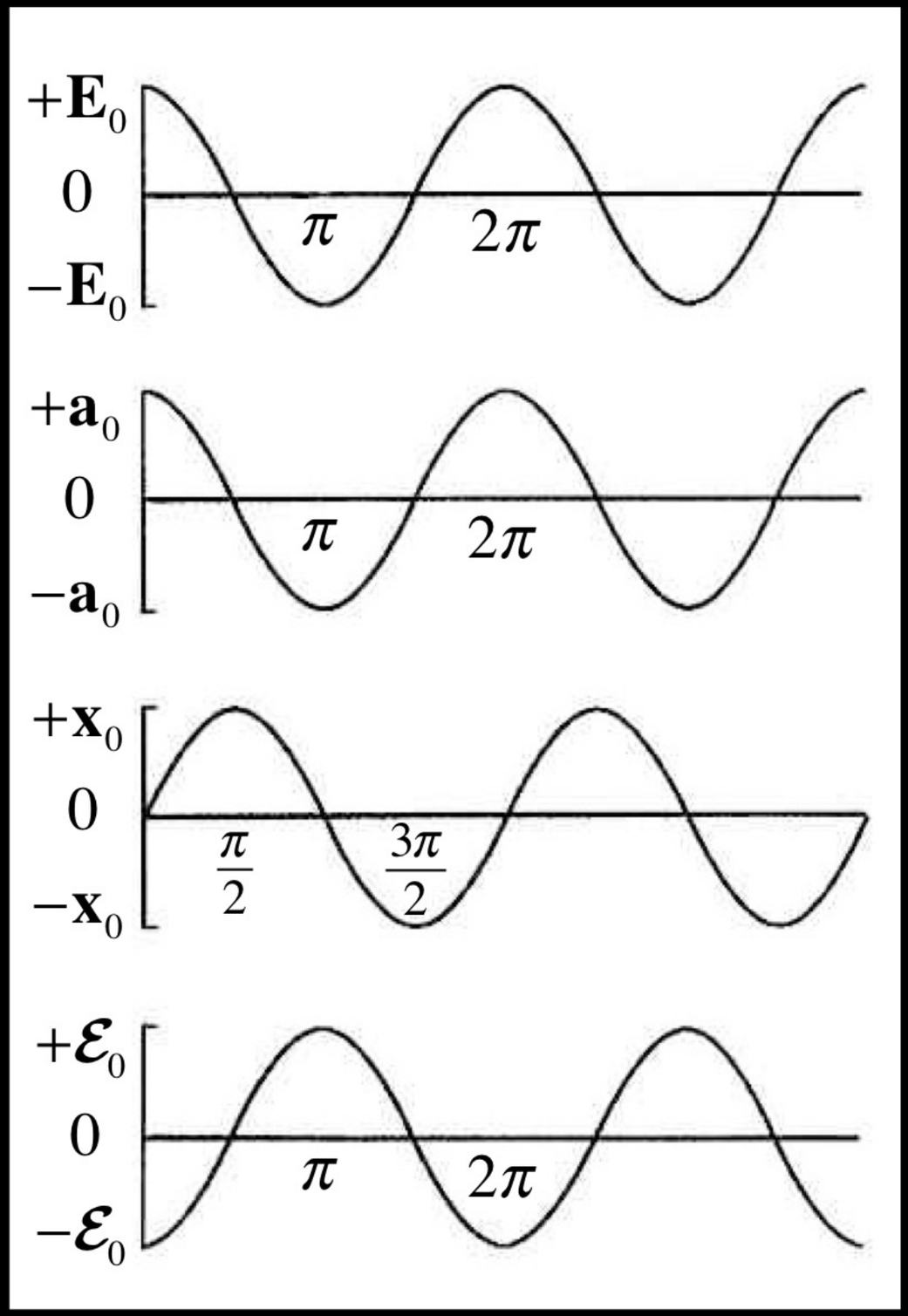
Phase reversal upon scattering of an electromagnetic wave by a point charge

incident em wave

charge acceleration

charge displacement

scattered em wave



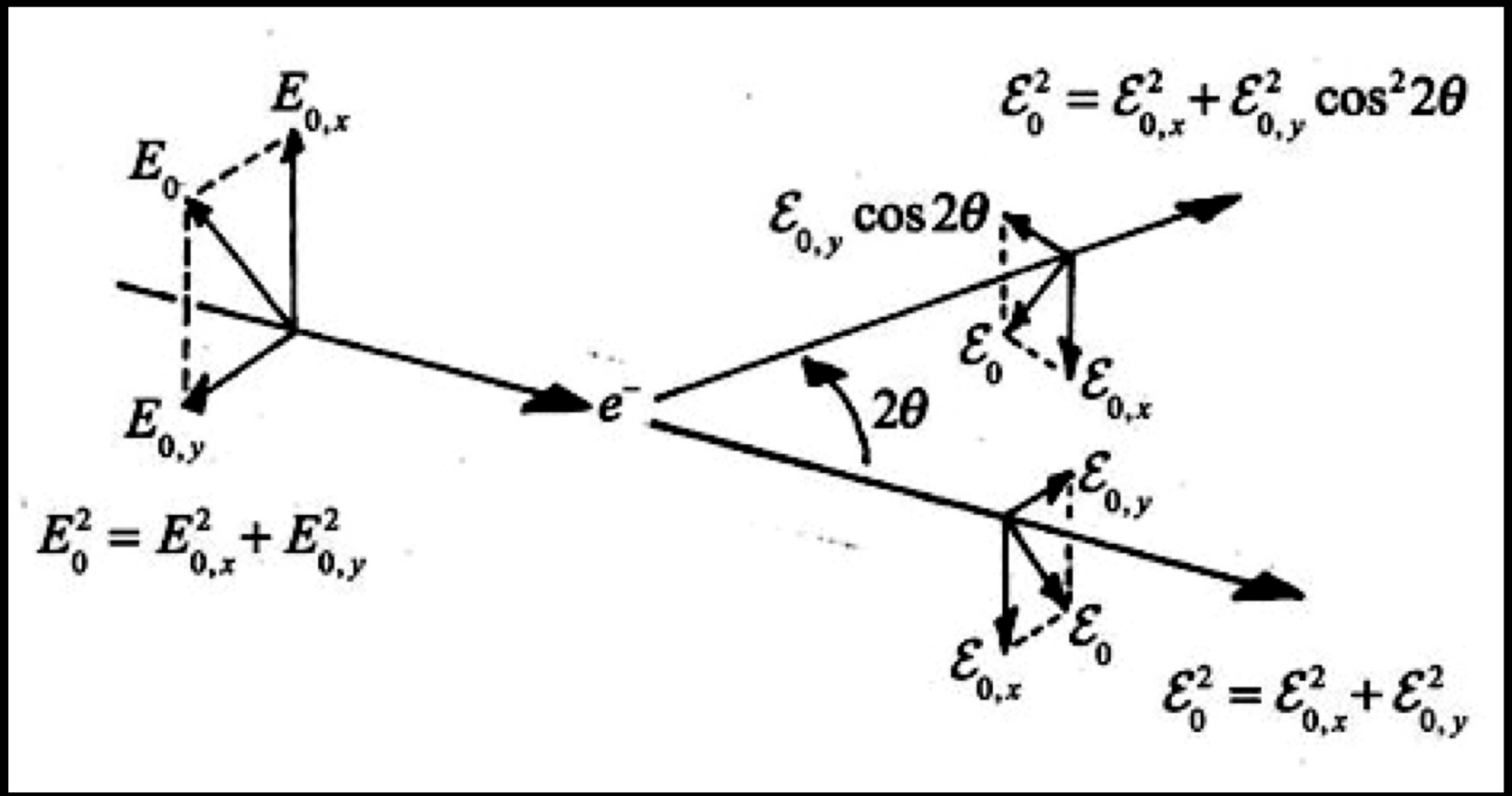
$$\begin{cases} \varphi_{\mathbf{E}} \\ \mathbf{E} = \mathbf{E}_0 e^{i\omega t} \end{cases}$$

$$\begin{cases} \varphi_{\mathbf{a}} = \varphi_{\mathbf{E}} \\ \mathbf{a} = \mathbf{a}_0 e^{i\omega t} \end{cases}$$

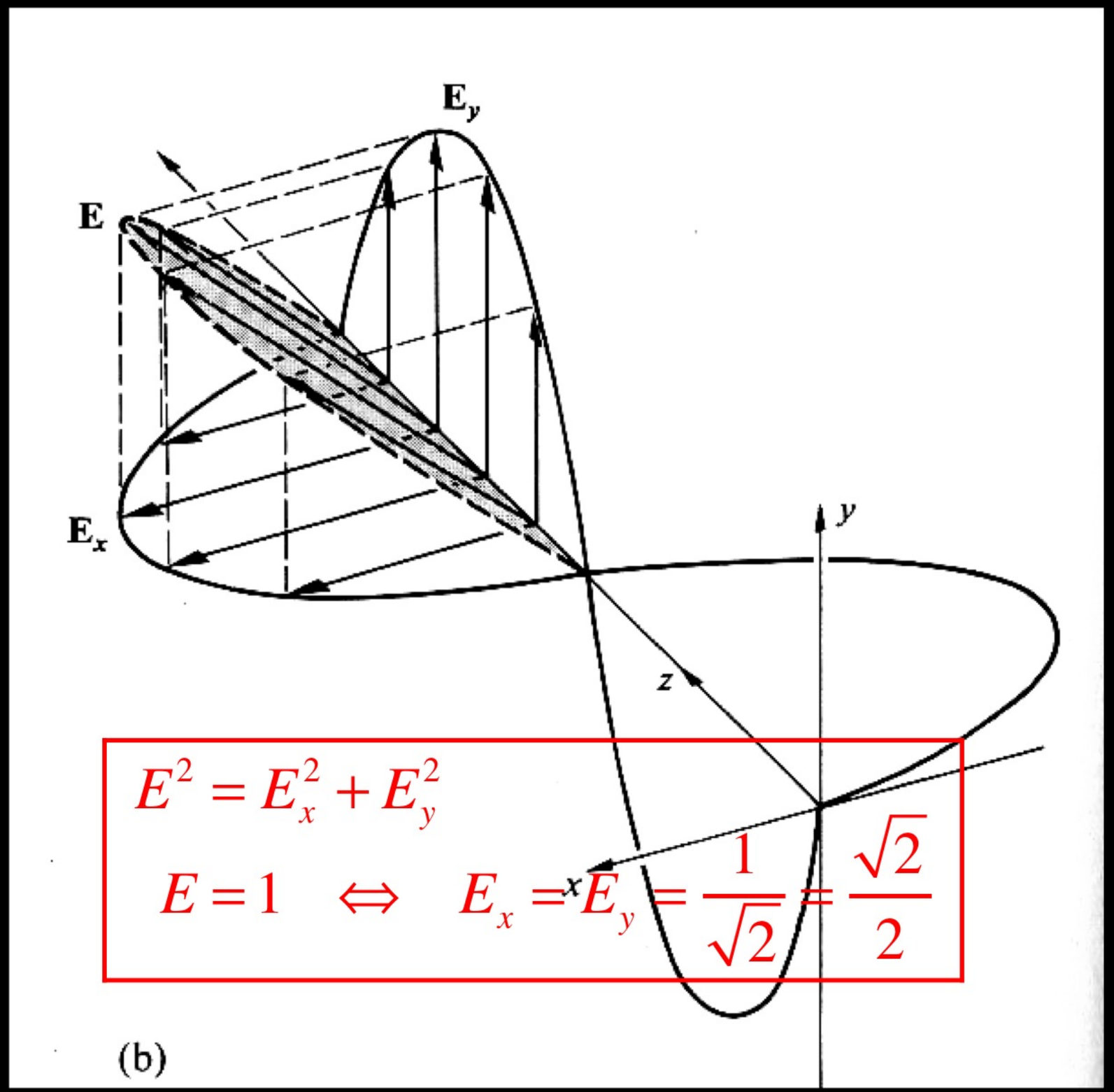
$$\begin{cases} \varphi_{\mathbf{x}} = \left(\varphi_{\mathbf{a}} - \dfrac{\pi}{2}\right) = \left(\varphi_{\mathbf{E}} - \dfrac{\pi}{2}\right) \\ \mathbf{x} = \mathbf{x}_0 \exp\left[i\left(\omega t - \dfrac{\pi}{2} \right) \right] \end{cases}$$

$$\begin{cases} \varphi_{\mathcal{E}} = \left(\varphi_{\mathbf{x}} - \dfrac{\pi}{2}\right) = \left(\varphi_{\mathbf{E}} - \pi\right) \\ \mathcal{E} = \mathcal{E}_0 \exp\left[i(\omega t - \pi) \right] \end{cases}$$

Scattering of a linearly polarized beam with an arbitrary direction of polarization



Resolved perpendicular components of polarization



$$E^2 = E_x^2 + E_y^2$$

$$E = 1 \quad \Leftrightarrow \quad E_x = E_y = \frac{1}{\sqrt{2}} = \frac{\sqrt{2}}{2}$$

http://www.star.le.ac.uk/~rw/courses/lect4313_fig5.jpg

Scattering of polarized em radiation

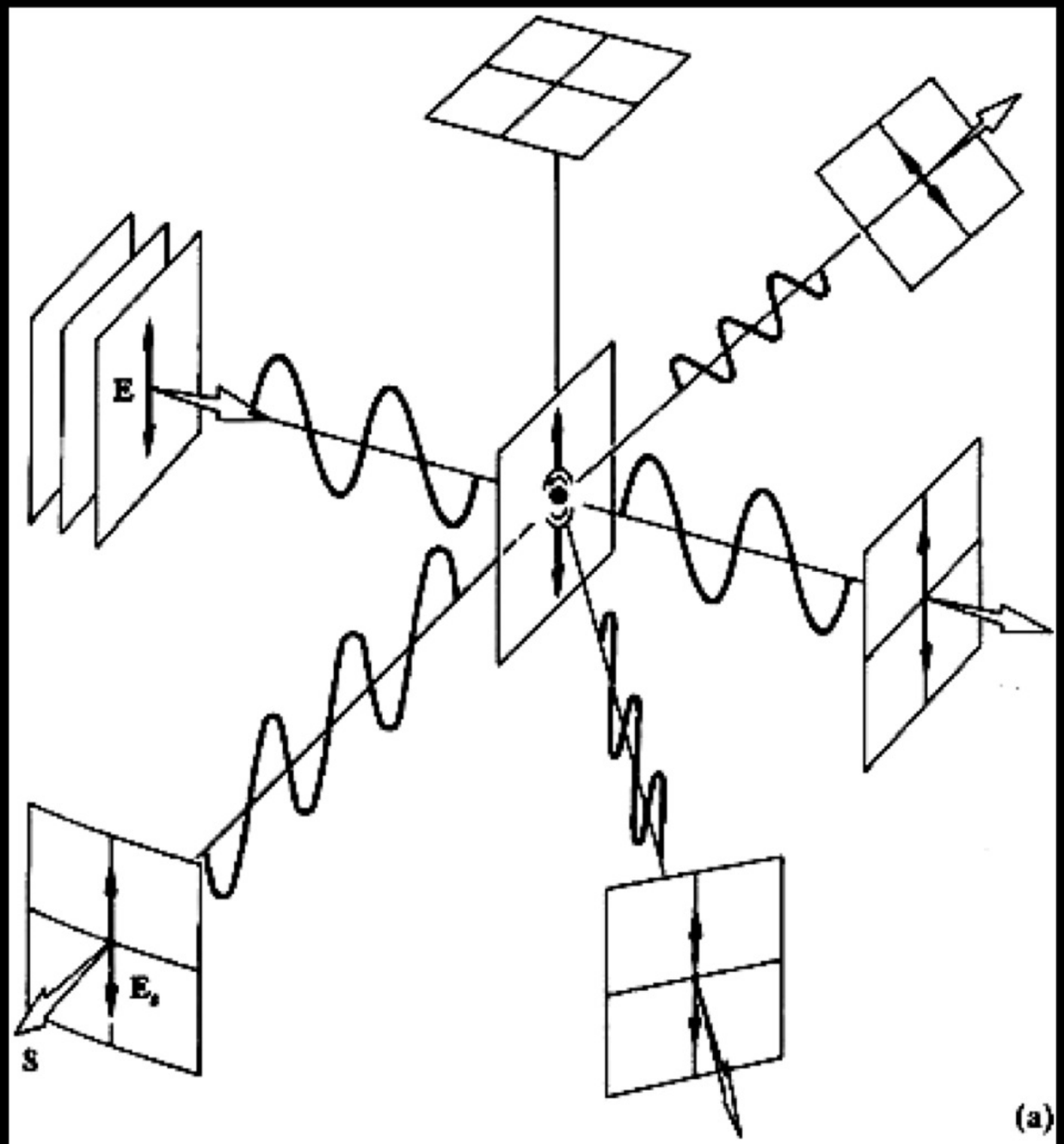


FIGURE 8.35a Scattering of polarized light by a molecule.

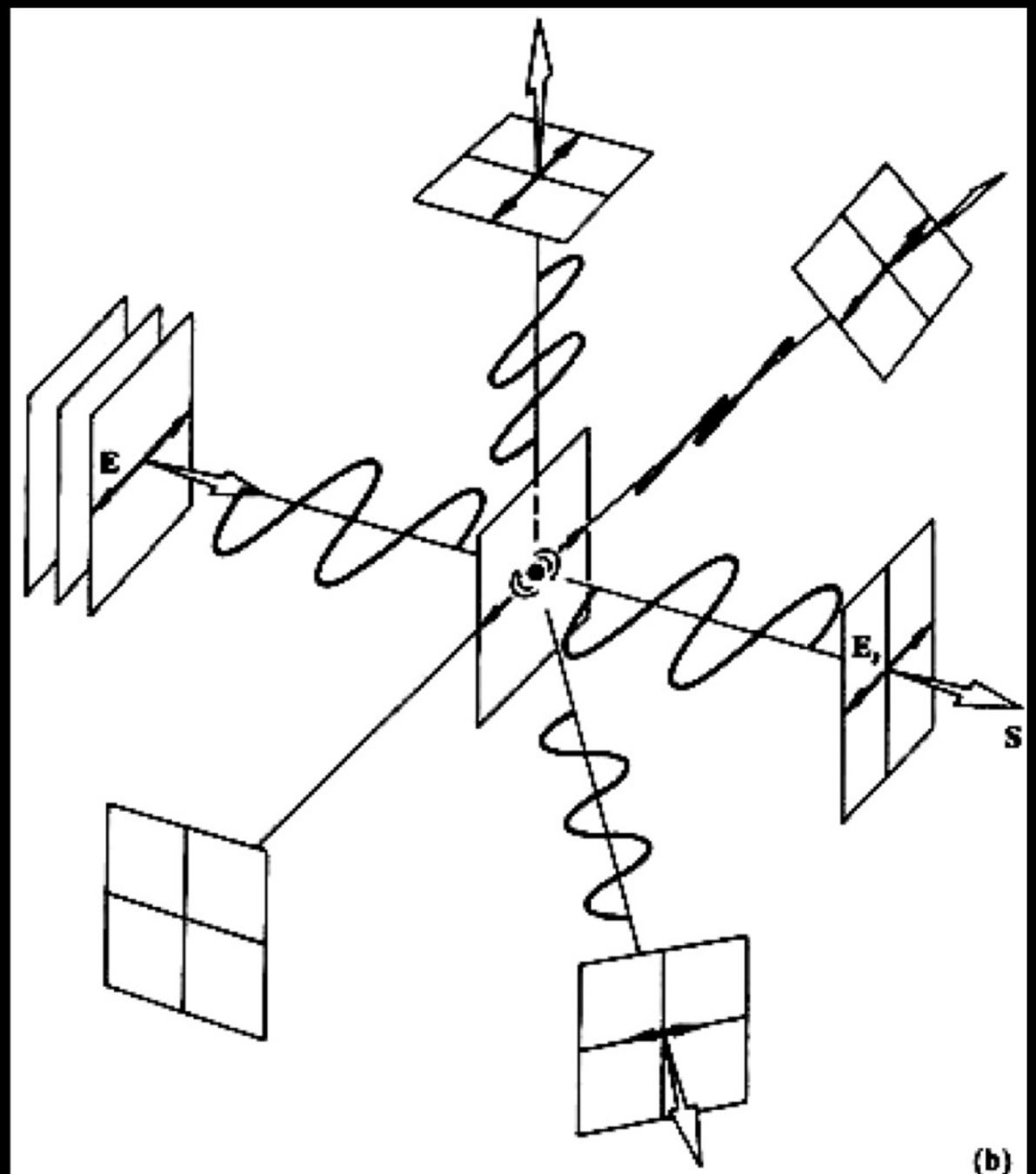
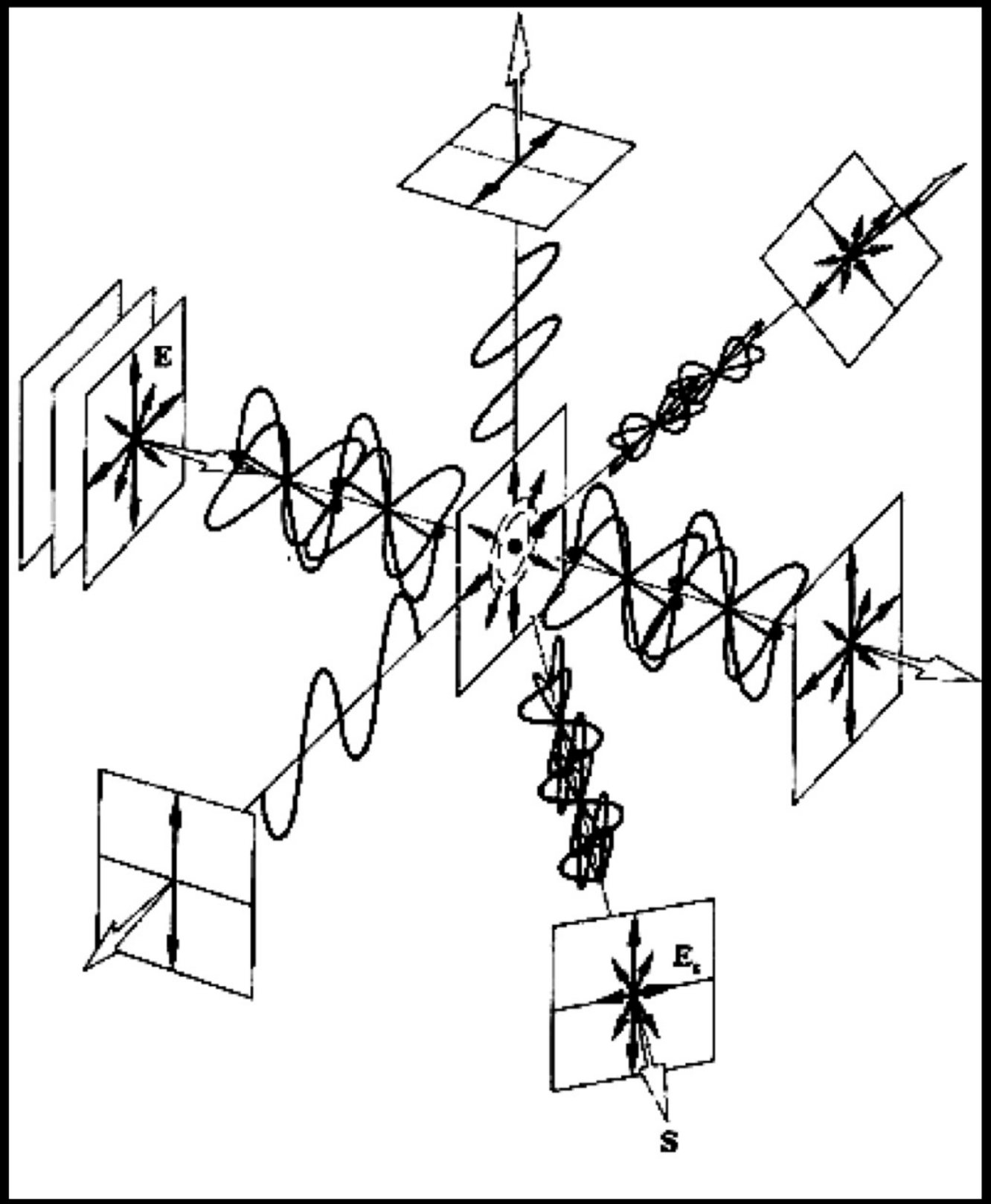


FIGURE 8.35b

http://www.physics.gatech.edu/MOPED/Theory/PbS_files/image002.jpg

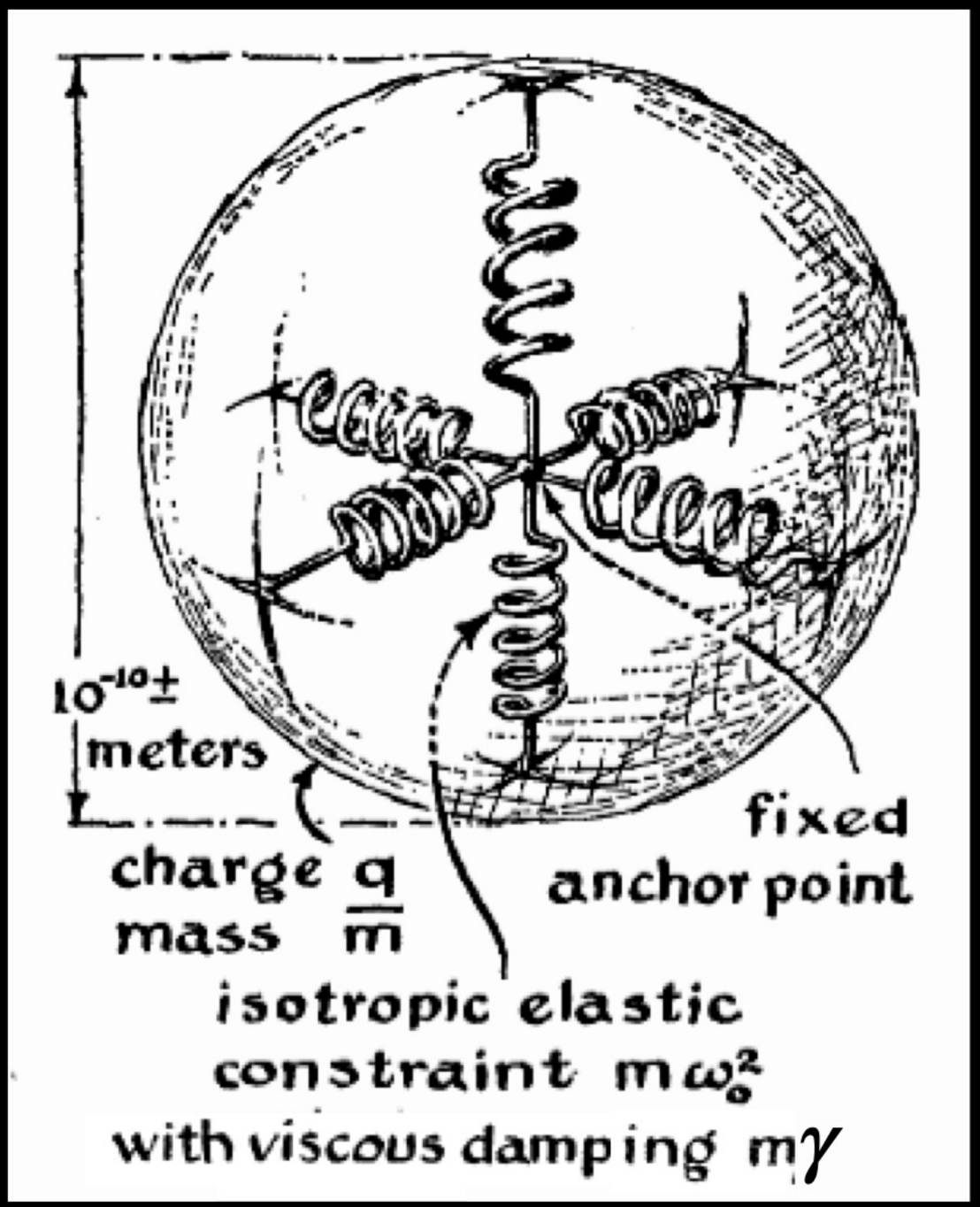
Scattering of unpolarized em radiation

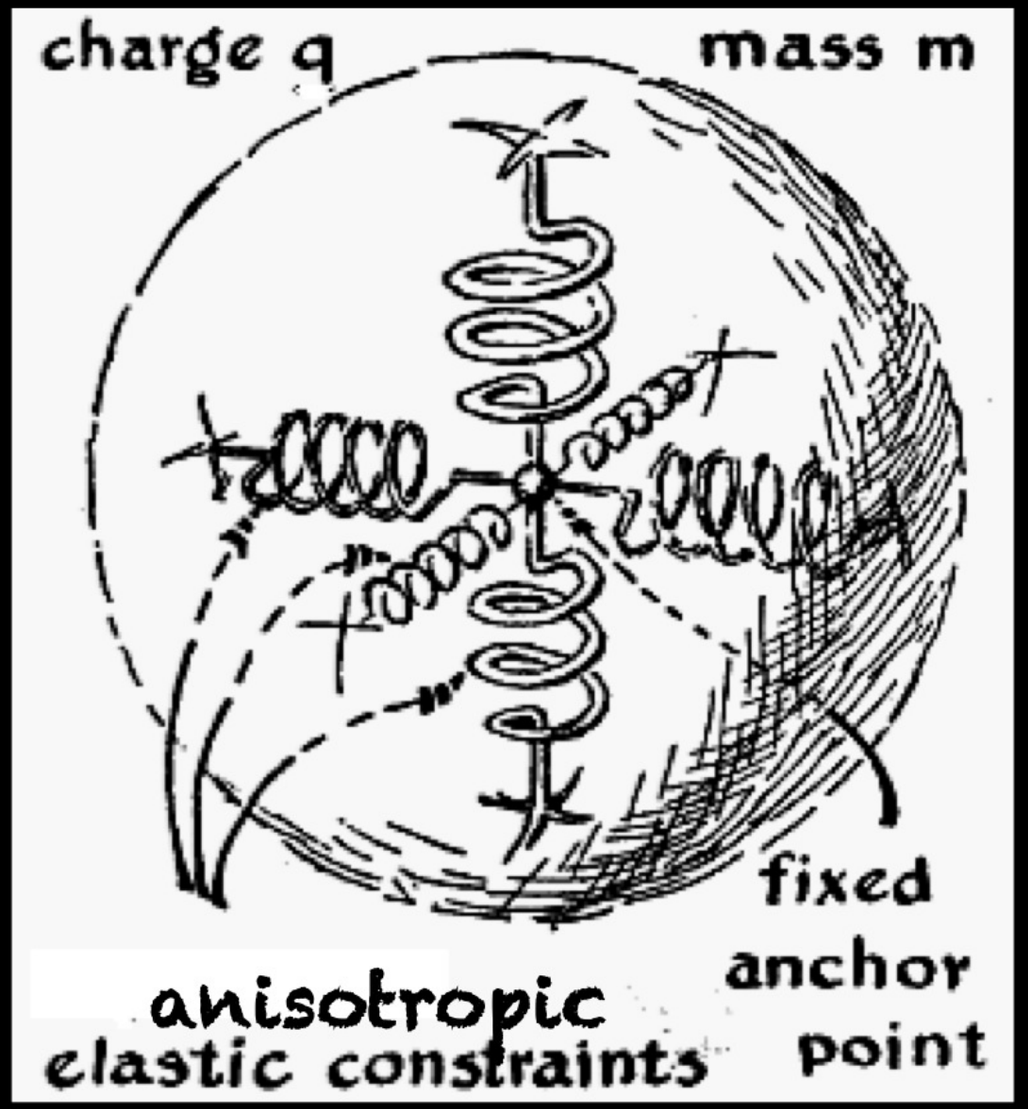


http://www.physics.gatech.edu/MOPED/Theory/PbS_files/image006.jpg

Mechanical models for electron oscillators

Spheres of uniform charge density with total charge *q* and mass *m*





Classical electron radius

Electrostatic potential energy

$$E = q\phi(r) = q(q/r) = e^2/r_e$$

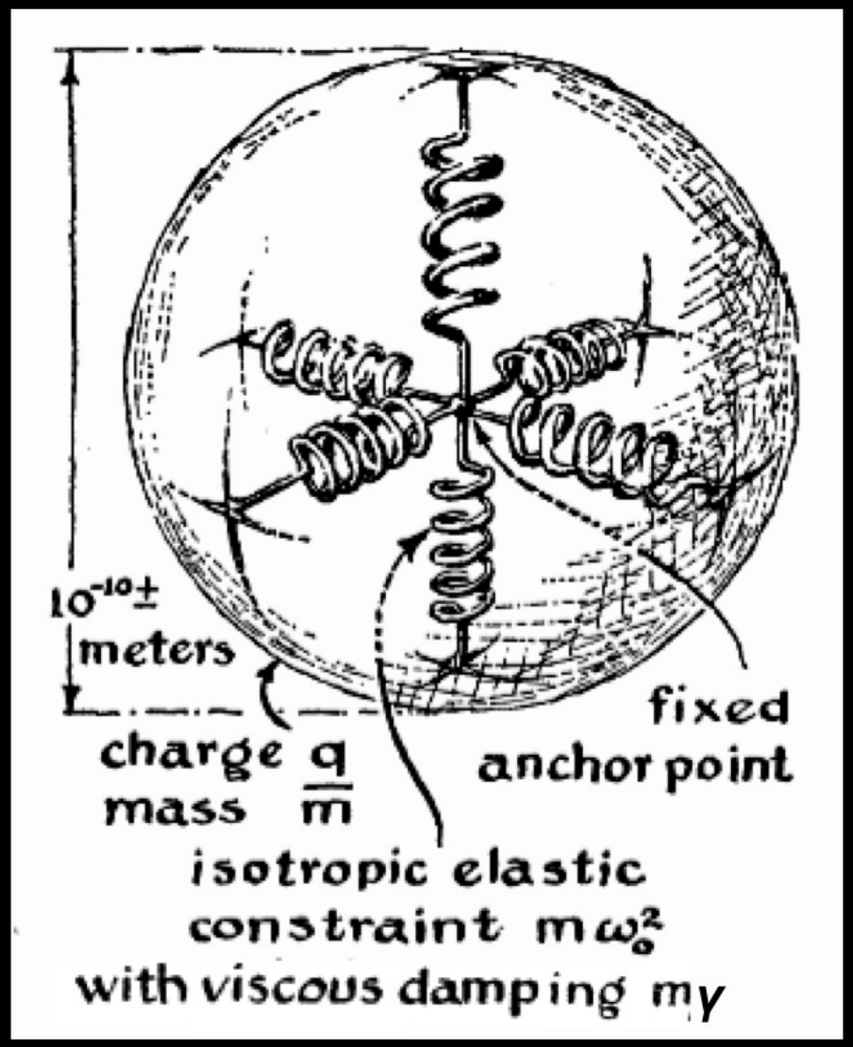
Relativistic mass - energy

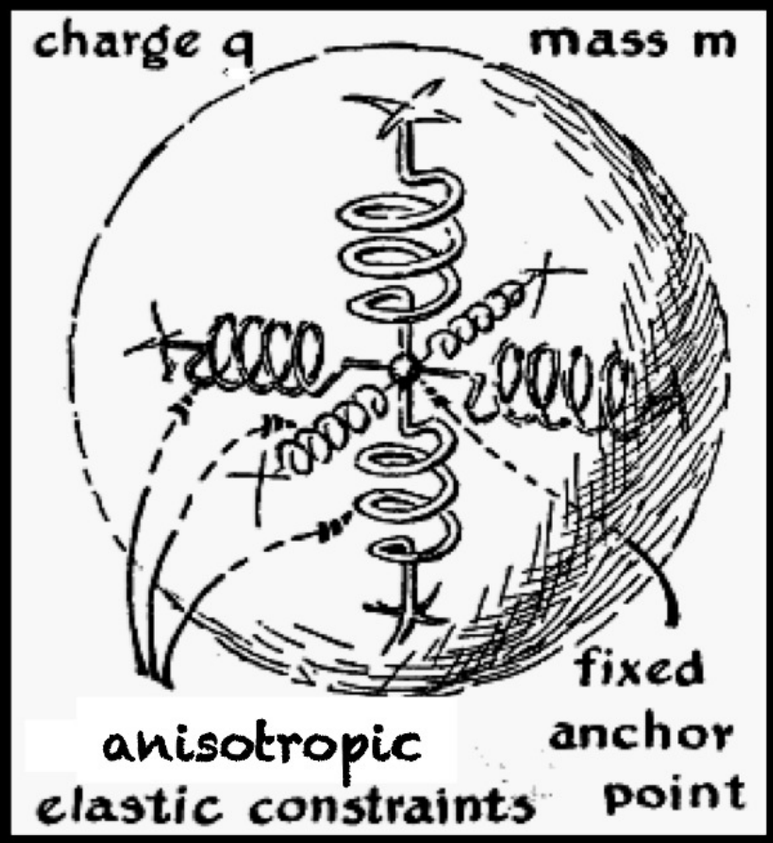
$$E = m_e c^2$$

$$r_e = \frac{e^2}{m_e c^2}$$

John Strong (1958). *Concepts of Classical Optics*. San Francisco: W.H. Freeman & Co.

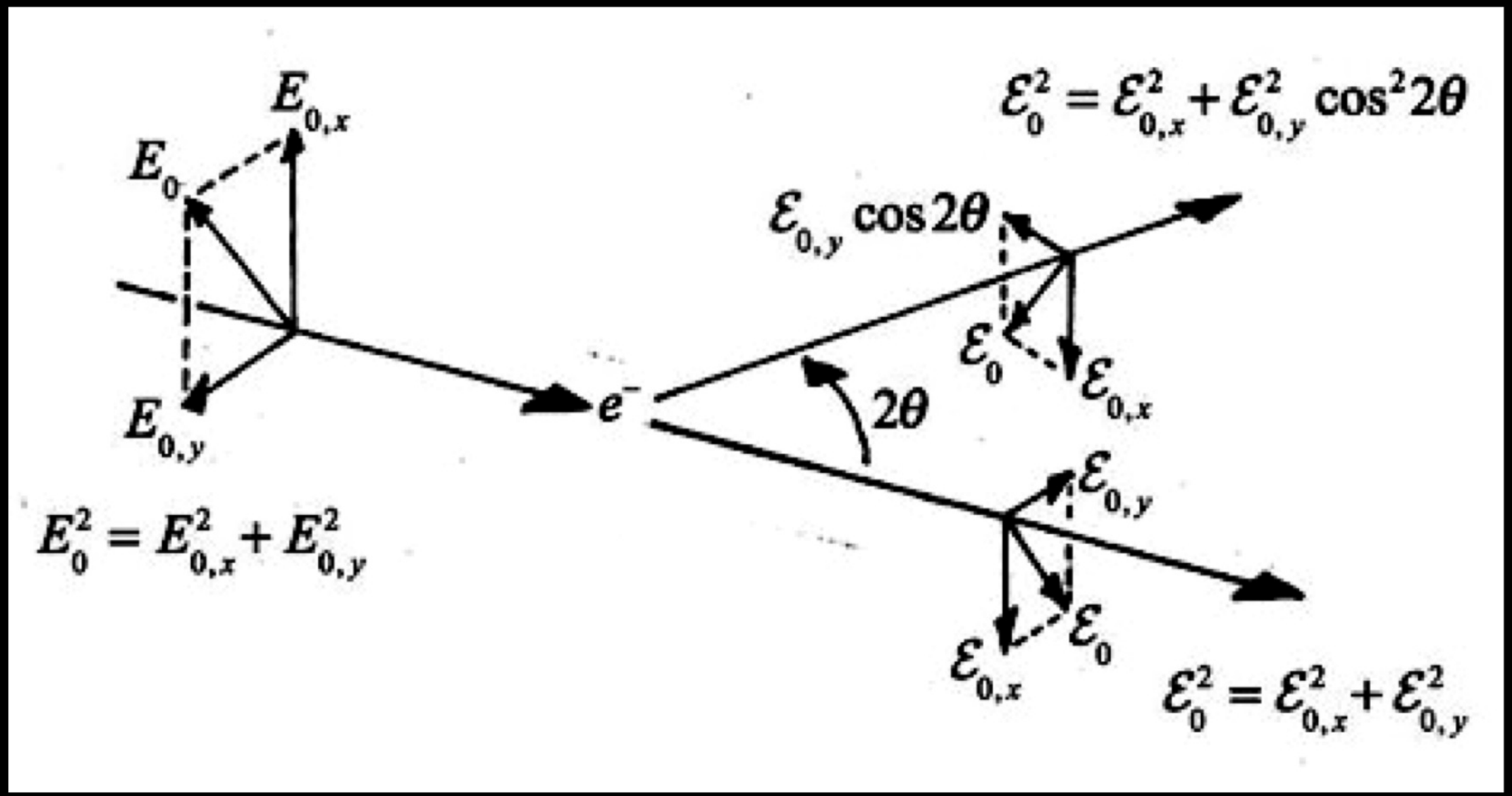
Mechanical models for 3-D oscillators





If a electron is driven to oscillate by an ***unpolarized em wave***, the electron oscillations will be ***three dimensional***.

Scattering of a linearly polarized beam with an arbitrary direction of polarization



Diffracted X-ray beam polarization

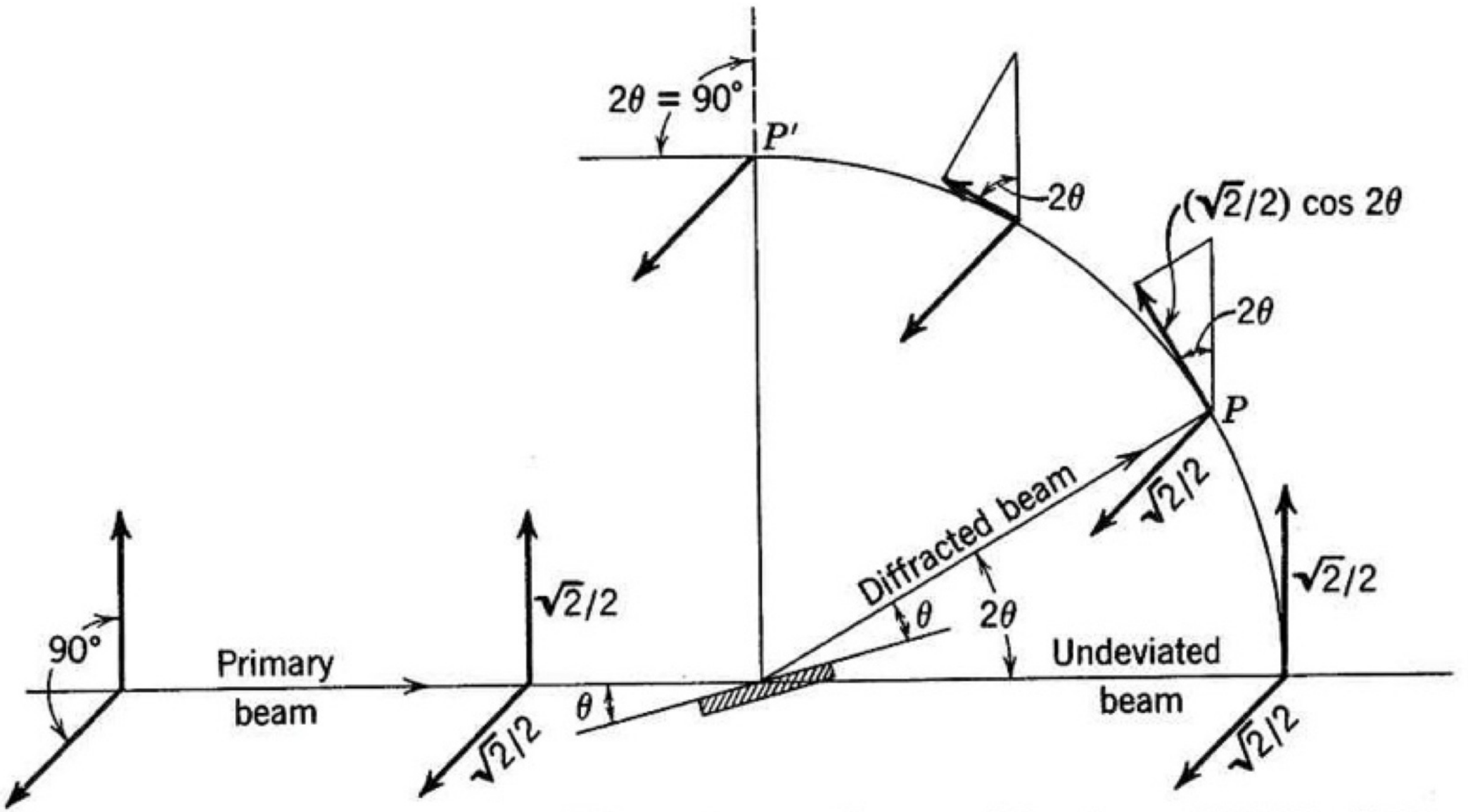


Fig. 3–11. Polarization of a diffracted x-ray beam. (Courtesy of Blake, *Revs. Mod. Phys.*, 5, 169.)

Any vector of unit length can be resolved into a pair of perpendicular components each of length $\sqrt{2}/2$. The component perpendicular to the equatorial plane of the incident and diffracted beams remains constant; the in-plane component varies as cos $\left(\sqrt{2}/2\right)$

Harold P. Klug and Leroy E. Alexander (1954). *X-Ray Diffraction Procedures for Polycrystalline and Amorphous Materials*. New York: John Wiley.

X-ray scattering by a bound electron in a free atom

(Gaussian cgs units)

$$m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -e\mathbf{E}_0\mathrm{e}^{i\omega t} \quad -k\mathbf{x} \quad , \qquad k = m\omega_0^2 \quad \text{elastic force constant}$$

Newton's second law force $\mathbf{F}=m\mathbf{a}$

em Coulombic driving force $\mathbf{F}=q\mathbf{E}$

Hooke's law elastic restoring force $\mathbf{F}=-k\mathbf{x}$

$$\begin{cases} \mathbf{x} = \mathbf{x}_0\mathrm{e}^{i\omega t} \, , \qquad \mathbf{v} = \dfrac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = i\,\omega\mathbf{x}_0\mathrm{e}^{i\omega t} \, , \qquad \mathbf{a} = \dfrac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = \dfrac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\omega^2\mathbf{x}_0\mathrm{e}^{i\omega t} \\ -m\,\omega^2\mathbf{x}_0\mathrm{e}^{i\omega t} = -e\mathbf{E}_0\mathrm{e}^{i\omega t} - k\mathbf{x}_0\mathrm{e}^{i\omega t} \\ m\omega^2\mathbf{x} = e\mathbf{E} + k\mathbf{x} \end{cases}$$

$$\mathbf{x} = \frac{e\mathbf{E}}{m\omega^2 - k} = \frac{e\mathbf{E}}{m\left(\omega^2 - \dfrac{k}{m}\right)} = \frac{e\mathbf{E}_0}{m}\left(\frac{1}{\omega^2 - \omega_0^2}\right)\mathrm{e}^{i\omega t} \, , \qquad \omega_0 = \sqrt{k/m}$$

$$\mathbf{a} = -\omega^2\mathbf{x} = -\frac{e\mathbf{E}}{m}\left(\frac{\omega^2}{\omega^2 - \omega_0^2}\right)$$

$$\boldsymbol{\mathcal{E}} = -\frac{q\,\mathbf{a}}{c^2 r} = -\left(\frac{-e}{c^2 r}\right)\frac{e\mathbf{E}}{m}\left(\frac{\omega^2}{\omega^2 - \omega_0^2}\right)\mathrm{e}^{i\omega t} = \underbrace{\underbrace{\left(\frac{e^2}{mc^2}\right)}_{r_\mathrm{e}}\frac{\mathbf{E}_0}{r}}_{\boldsymbol{\mathcal{E}}_0}\left(\frac{\omega^2}{\omega^2 - \omega_0^2}\right)\mathrm{e}^{i\omega t} = \boldsymbol{\mathcal{E}}_0\mathrm{e}^{i\omega t}$$

Resonant X-ray scattering by a bound atomic electron

(Gaussian cgs units)

damped driven harmonic oscillator

$$m\frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\kappa\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} \quad -k\,\mathbf{x} \quad -e\mathbf{E}_0\,\mathrm{e}^{i\omega t}\ ,$$

Newton's second law force $\mathbf{F}=m\mathbf{a}$

radiation loss damping force $\mathbf{F}=-\kappa\mathbf{v}$

Hooke's law restoring force $\mathbf{F}=-k\mathbf{x}$

Coulombic em driving force $\mathbf{F}=q\mathbf{E}$

$$\begin{cases} k = m\omega_0^2 & \text{nucleus-electron elastic force constant} \\ \kappa = m\gamma & \text{radiation loss damping force constant} \end{cases}$$

$$\mathbf{x} = \mathbf{x}_0\,\mathrm{e}^{i\omega t}\ , \qquad \mathbf{x}_0 = \frac{e\mathbf{E}_0}{m}\left(\frac{1}{\omega^2-\omega_0^2-i\gamma\omega}\right)$$

$$\mathbf{a} = \frac{\mathrm{d}^2\mathbf{x}}{\mathrm{d}t^2} = -\omega^2\mathbf{x}_0\,\mathrm{e}^{i\omega t} = \mathbf{a}_0\,\mathrm{e}^{i\omega t}\ , \qquad \mathbf{a}_0 = -\omega^2\mathbf{x}_0 = -\frac{e\mathbf{E}_0}{m}\left(\frac{\omega^2}{\omega^2-\omega_0^2-i\gamma\omega}\right)$$

$$\mathcal{E}_0 = -\frac{q\,\mathbf{a}_0}{c^2 r} = \underbrace{-\left(\frac{e^2}{m_\mathrm{e}c^2}\right)\frac{\mathbf{E}_0}{r}}_{\text{free } e^- \text{ scattered X-ray wave amplitude at r}}\underbrace{\left(\frac{\omega^2}{\omega^2-\omega_0^2-i\gamma\omega}\right)}_{\text{bound } e^- \text{ scattered X-ray wave amplitude at r}}$$

$$f_\mathrm{e} = \frac{\mathcal{E}_0(\text{bound})}{\mathcal{E}_0(\text{free})} = \frac{\omega^2}{\omega^2-\omega_0^2-i\gamma\omega} = \frac{1}{1-\left(\frac{\omega_0}{\omega}\right)^2-\frac{i\gamma}{\omega}}$$

X-ray scattering by a bound atomic electron is approximately the same as scattering by a free electron at rest (Gaussian cgs units)

$$\mathcal{E}_0 = -\frac{q\,\mathbf{a}_0}{c^2 r} = \underbrace{-\left(\frac{e^2}{m_e c^2}\right)\frac{\mathbf{E}_0}{r}}_{\substack{\text{free } e^- \text{ scattered} \\ \text{X-ray wave} \\ \text{amplitude at r}}}\underbrace{\left(\frac{\omega^2}{\omega^2 - \omega_0^2 - i\gamma\omega}\right)}_{\substack{\text{bound } e^- \text{ scattered} \\ \text{X-ray wave} \\ \text{amplitude at r}}}$$

$$f_e = \frac{\mathcal{E}_0(\text{bound})}{\mathcal{E}_0(\text{free})} = \frac{\omega^2}{\omega^2 - \omega_0^2 - i\gamma\omega} = \frac{1}{1 - \left(\frac{\omega_0}{\omega}\right)^2 - \frac{i\gamma}{\omega}}$$

$\gamma \ll \omega \quad \Rightarrow \quad f_e \approx \dfrac{1}{1 - \left(\dfrac{\omega_0}{\omega}\right)^2}$ undamped oscillation

$\omega_0 \ll \omega \quad \Rightarrow \quad f_e \approx 1$ high frequency limit

} free electron at rest $f_e = 1$