Hans Bethe, Quantum Mechanics, and the Lamb Shift

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An elementary derivation of the Lamb Shift, as originally given by Hans Bethe, is attempted, with a short historical background on the evolution of QED since the beginning of the last century. The treatment is for a non-relativistic electron, in keeping with Bethe's proverbial insight into the problem, which renders irrelevant the effect of the electron spin on the problem. The Kramer idea of renormalization is implemented through a simple subtraction of the self-energy of a free electron from that of the electron bound in a hydrogen atom.

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1. Introduction: Bethe's Impact on Physics

Hans Albrecht Bethe, the last link among the founding fathers of physics of the last century, passed away on March 6, 2005 at the age of 98. In the world of physics, it is difficult to describe Bethe's impact in adequate terms, since it extended over a whole spectrum, from atomic processes responsible for the properties of matter, to the nuclear forces governing the structure of atomic nuclei, within a 75 year time span ranging from the mid-thirties to the last decade of the twentieth century. No less was his concern for the social responsibility of science, a subject on which he had written numerous articles in influential journals. Whichever sector of physics he had set his eyes on, Bethe invariably left an indelible mark of his masterly grasp with deep insight born out of his twin characteristics of *simplicity* and *thoroughness*, be it in solid state physics (Bethe Ansatz), or nuclear physics (Bethe Second Principle Theory), or even quantum field theory (Bethe–Salpeter Equation). His fantastic powers

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of fast yet accurate calculation (in the days long before the computer revolution) had made him a legend of his time, thanks to his single-handed success in determining the energy production in the Sun and the stars by a *correct* choice of a sequence of nuclear reactions resulting in the fusion of four hydrogen atoms into one helium atom, through four steps of the 'carbon cycle', leaving the original carbon to come out unscathed in the end. (The story of how Bethe achieved this feat while travelling in a train is vividly described by George Gamow in his book *Birth and Death of the Sun*). His Nobel Prize (in 1967), three decades after this great discovery, was a rather belated recognition of his genius.

Some of Bethe's early works have become household words in physics textbooks. The Bethe–Weiszacker mass formula is a classic example of physical insight, inasmuch as each term in the formula represents a distinct physical effect. Another household word is the Bethe–Heitler formula for Bremsstrahlung whose agreement with data then available provided one of the earliest experimental supports for the then nascent structure of QED. Bethe was equally dexterous in applying *classical* mathematical methods to i) the calculation of electron densities in crystals; ii) the order-disorder transition in alloys (the Bethe–Peierls Approximation); iii) the ionization processes in shock waves, to name only a few. No wonder he headed the group of theoreticians for the Manhattan Project in Los Alamos, since his deep and versatile knowledge of physics had few equals.

At the next higher level of sophistication, there has been rich evidence of Bethe's transparent approach, all bearing the unmistakable marks of a "yin-yang" Tao of simplicity with thoroughness. Some examples are his famous papers on (i) Lamb Shift in QED; (ii) Bethe–Salpeter Equation in the strong interaction sector of quantum field theory (QFT); and (iii) effective range theory, and Bethe–Brueckner theory of nuclear matter.

1.1 *Lamb Shift: The Bethe Connection*

The Lamb Shift, which is the subject of the present paper, first needs a little historical background which has both theoretical and experimental aspects, of which the latter was a by-product of World War II in connection with the radar development which was concerned with a region of the order of 1 cm, termed the *microwave* region, lying between the far infrared and short radio waves.

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The techniques of the microwave region came in very handy at the hands of W E Lamb and his colleague R C Retherford [1], in making fine structure measurements of the atomic spectra. The 'Lamb Shift' was the frequency of a microwave field that induced transitions from one excited state of a hydrogen atom to another. In particular, they found that the $2s_{1/2}$ levels of hydrogen were slightly above the $2p_{1/2}$ level, by about 1050 MHz, contrary to what was predicted by Dirac's theory, and obeyed by experiment till then! This 'Lamb Shift' was addressed by Bethe in his own inimitable style: He was returning to Cornell after attending a select workshop in the summer of 1947 in Shelter Island (NY), where the anomaly posed by the Lamb–Retherford discovery was the subject of several brain-storming sessions, with top experts in the field participating in threadbare discussions on various aspects of the 'problem' vis-a-vis the existing knowledge on QED [2]. One of the participants was H Kramers of Holland, who unfolded his idea of *renormalization* in this context (see Section 2 for a logical exposition of the concept). Apparently he found the solution in the train itself (!), on his return journey – a repetition of a similar feat a decade earlier on the mechanism of energy production in the Sun, which was to fetch him his Nobel Prize. It was a two-page paper with a few crisp symbols and equations [3], that said it all.

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The story of *how* [2] Bethe obtained the desired solution is the subject of this article. Since the intricacies of QED were not involved in his derivation, it is of considerable physical interest to a wider readership, to reproduce the derivation without going into the avoidable sophistications of QED (including the Dirac theory). To keep the article reasonably self-contained, however, some historical perspective on the status of quantum theory (QT), preceding the growth of QED is offered for completeness. To that end, the article is organized as follows. Section 2 attempts an overview of the principal developments in QT, leading to the status of QED up to the early forties of the last century, with special reference to Bethe's involvement in early QED applications. Section 3 provides the actual derivation of the Lamb Shift as given originally by Bethe, wherein the electron is treated as a non-relativistic particle, and the photon as a field which can be Fourier analysed in terms of wave numbers and frequencies. Section 4 concludes with a short discussion.

2. Quantum Theory to QED: A Panoramic View

The last century started with a bang, with Max Planck's (1901) revolutionary quantum proposal on the one hand, and Einstein's single year (1905) of 3 earth-shaking papers which changed the face of physics, on the other. The Special Theory of Relativity, which was inspired by the invariance of Maxwell's equations under Lorentz transformations, as well as by the null result of the Michelson–Morley experiment, unified space and time (hitherto regarded as two separate entities) into a *single* space-time invariant $(x^2 - c^2t^2)$ under Lorentz transformations, albeit at the cost of a new universal constant c representing the velocity of light in vacuum. (Einstein later generalized the Special Theory into the General Theory of Relativity, but such generalization is not relevant in the present context). As a logical consequence of the Special Theory, Einstein deduced the dynamical result $E = mc^2$ whose importance in the world of

physics hardly needs telling. The International Year of Physics (2005) incidentally marks the centenary of this great discovery.

2.1 *Old Quantum Theory*

The ramifications of the quantum concept took much longer to sink in, although Einstein quickly upheld Planck's hypothesis with his celebrated photoelectric effect which gave the photon a particle property over and above its already known wave character. What was now needed was a viable atomic model to account for some crucial empirical data like Ritz's classification of spectral lines, the Franck–Hertz experiment on the discrete energy losses of electrons on collision with atoms, etc. The necessary boost was provided by Rutherford's discovery (1911) of atomic structure which led Niels Bohr (1913) to propose his atomic model in terms of two postulates: i) an atomic system can stay in particular quantized states each of which corresponds to a definite energy of the system; ii) a radiation quantum has a frequency equal to the difference of two atomic energy levels divided by h. These postulates, fortified by Wilson–Sommerfeld (WS) quantization conditions, sufficed to give a quantitative description of large number of spectroscopic data for atoms and diatomic molecules. The WS conditions in turn were based on the Hamilton–Jacobi formulation of classical mechanics wherein the energy of the system was expressible entirely in terms of the so-called 'action' integrals (after elimination of the cyclic 'angle' variables). In this representation, the WS conditions consisted simply in demanding that the action integrals be 'quantized', i.e., represented as integral multiples of h. This was the so-called '*old* Quantum Theory' which was to rule the world of atomic physics for about a decade at the end of which it gave way to the *new* Quantum Mechanics (QM) of Heisenberg, Schrödinger and Dirac.

The need for change was occasioned by some major inadequacies in the *old* QT, such as its inapplicability to aperiodic systems, and incomplete treatment of the intensities of spectral lines, as well as some inner contradictions resulting in its failure to give a conceptually satisfactory account of fundamental phenomena. For example, it was difficult to understand why the Coulomb interaction between the electron and the proton was so effective for the spectra, while the ability of an electron to emit em radiation from a *stationary* state was zero! And the assumption of a dual character of light appeared self-contradictory [4].

2.2 *New Quantum Mechanics*

The advent of the *new* QM was preceded by two conceptual discoveries. The first was the proposal by de Broglie about the wave nature of material particles with wave length given by $\lambda = h/p$, which suggested that wave-particle duality was a *universal* phenomenon, not confined to the electromagnetic field alone, a result which found overwhelming support from the Davisson–Germer (1927) and G P Thompson (1928) experiments. The second was S N Bose's (1924) proposal for a new mode of counting based on true *indistinguishability* which emphasized the classification of *states* according to the number of photons in their kitty, instead of the 'classical' Maxwell–Boltzmann mode of counting in which the individual 'names' of the photons could not be fully erased, (despite division by $n!$!). Bose's proposal found a natural echo in Heisenberg's Matrix Mechanics in which a dynamical variable (like position or momentum) was no longer considered associated with individual particle motions, but was regarded as an operator (matrix), operating on states that were supposed to be labelled by the number of particles with specified characteristics. In this formulation, the correspondence with the classical picture was established by reinterpreting the Hamiltonian equation $H(q,p) = E$ as an operator (ma-

trix) equation which made sense only after specifying the state (vector) on which it was supposed to operate!

Heisenberg's matrix formulation succeeded in removing the conceptual obstacles associated with the *old* Quantum Theory, while improving if anything the agreement with the data. An alternative formulation by Schrödinger, which proved more effective in practice, consisted in using a *local* 'differential' representation for the operators in q space:

$$p = -i\hbar\partial_q; \quad E = +i\hbar\partial_t; \quad H = H(q, -i\hbar\partial_q); \qquad (1)$$

and writing the equation of motion as

$$H\psi(q,t) = i\hbar\partial_t\psi(q,t), \qquad (2)$$

where the wave-function ψ stands for the state under study. In this description, the wave function is the repository for the full dynamical information of the quantum state under study. The Hamiltonian is adapted from the corresponding 'classical' structure, with due regard to its operator character in the quantum context. (For its precise form under the electromagnetic interaction, see below).

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2.3 *Relativistic QM: Quantum Field*

The next stage of the development, viz., relativistic formulation of the quantum equations, proved crucial not only in concrete mathematical terms, but *conceptually* in terms of mathematical self-consistency of the generalization envisaged. Now the generalization from the (non-relativistic) Newtonian equations of motion to those in conformity with the special theory of relativity had presented no problem. Indeed for a free particle, it only means the replacement

$$p^2/2m = E; \quad \Rightarrow E^2 = p^2c^2 + m^2c^4. \qquad (3)$$

For a particle interacting with the electromagnetic field

$(\mathbf{A}, \phi)$, the form given above stays relativistically invariant, since it means the replacements

$$E \Rightarrow E - e\phi; \quad \mathbf{p} \Rightarrow \mathbf{p} - e\mathbf{A}/c. \tag{4}$$

Thus the classical relativistic equation in the presence of an em field reads as

$$(E - e\phi)^2 = (c\mathbf{p} - e\mathbf{A})^2 + m^2c^4, \tag{5}$$

which also happens to be consistent with *gauge* invariance! The non-relativistic form of the last equation now follows in the limit of small p/mc as

$$E - e\phi = (\mathbf{p} - e\mathbf{A}/c)^2/2m, \tag{6}$$

where the energy E on the left-hand-side excludes the rest energy mc^2.

Next, the quantum formulation, *á la* Schrödinger, from the non-relativistic form of classical mechanics goes through by regarding (2) or (6) as operator equations and applying them to ψ on the right. But the same prescription does *not* work with the relativistic form (5), without sacrificing mathematical self-consistency! To see the nature of the self-consistency that is involved, consider the quantum form of the second part of (3):

$$-\hbar^2\partial_t^2\psi = [-\hbar^2\nabla^2c^2 + m^2c^4]\psi, \tag{7}$$

where the differential forms of E and p, *á la* (1), have been inserted. Now the presence of the second derivative w.r.t. time implies that the particle density

$$\rho = i(\psi^*\partial_t\psi - \partial_t\psi^*\psi),$$

that is needed to conserve the current, is no longer positive definite, which is the source of the inconsistency. This problem was resolved by Pauli–Weisskopf [5] by reinterpreting the quantity ρ as the average charge density of the ψ *field*, (which can have either sign locally),

instead of as a *single* particle density! This is the price of quantization in the relativistic regime: the minimum d.o.f. is that of a *field* (infinite number of particles), and *not* of a single particle, as stipulated by Dyson [6].

The same story goes for the Dirac formulation for an electron with spin [5], despite the appearance of E in a linear form, since the inconsistency now shows up in the form of *negative* energy states! Here again, the solution lies in demanding that the negative energy states be normally full, thus preventing (*à la* exclusion principle) the electron from entering them, unless enough energy ($> 2mc^2$) is pumped in from outside to 'lift' one of such electrons to a positive energy state, so as to accommodate the outside electron in the 'hole' so created. Thus the message is the same again, viz., one must deal with an infinite number of electrons – a quantum (fermion) *field*! The 'hole' is a signature for an anti-electron (positron) with exactly opposite properties to the electron's. In the case of the boson field ψ of (7) too, the corresponding anti-particle is a boson of opposite charge. Thus the message is the same for both [5]: The marriage of Relativity with Quantum theory resulted in the prediction of anti-matter.

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In the non-relativistic domain on the other hand, the field concept is optional for quantization, since the corresponding Schrödinger equation is now

$$i\hbar\partial_t\psi = -\frac{\hbar^2\nabla^2}{2m}\psi,$$

for which $\rho = \hbar\psi^*\psi$ is positive definite even for a single particle. The same logic goes through in the presence of an em field too, for which the quantum equation can be read off from the corresponding classical equation (6):

$$[E - e\phi]\psi = [(\mathbf{p} - e\mathbf{A}/c)^2/2m]\psi \qquad (8)$$

involving a single time derivative when the differential forms are inserted from (1). On the other hand, for the

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em field, which is always relativistic, the quantization is necessarily for the entire field, and not for a single photon.

2.4 *QFT Methods for QED: Perturbation Theory*

The quantum field (QFT) concept is essentially one of extending the methods of quantum mechanics to an infinite number of harmonic oscillators. Here's how. The quantization for a free field is achieved by first Fourier analyzing the field variable say A_μ in terms of a discrete but infinite set of q_k, p_k variables (under box normalization). In a (q, p) representation, the free field Hamiltonian behaves like an infinite set of harmonic oscillators, so that the problem of quantization gets reduced to solving for an infinite set of non-interacting harmonic oscillators, in the standard manner. The treatment gets greatly simplified by an alternative complex representation:

$$(a, a^\dagger) = (q \pm ip)/\sqrt{2}$$

wherein the a and $a^\dagger$ behave like step-down (annihilation) and step-up (creation) operators respectively in a number (N) representation for the quanta of the free field under study.

The same procedure is applicable for the interaction of two fields, say the electron and em fields, with separate tracks of their respective N representations. And since in practice, only one or two quanta of the respective fields are involved, the N-degrees of freedom usually get eliminated in a trivial manner, leaving the remaining (non-trivial) parts of the matrix elements to the rules of ordinary quantum mechanics.

The first application of the QFT methods was to the problem of interaction of the em field with the Dirac electron, termed quantum-electrodynamics, QED for short. To that end, the unperturbed part H_0 of the

Hamiltonian includes the resultant of the longitudinal and temporal parts of the em field, together with an external field if any (e.g., the field of a proton in a hydrogen atom), as an effective Coulomb interaction, while the *transverse* part of the em field, termed the radiation field, is treated by standard perturbation theory with the interaction term :

$$e\bar{\psi}A_\mu\gamma_\mu\psi; \quad e = \sqrt{4\pi/137}.$$

(The smallness of the electron's charge, a measure of its coupling with the em field, justifies the perturbation approach).

Bethe realized from intuition that it was most practicable to treat the electron as a particle, and the photon as a field.

2.5 *Bethe's Involvement in Early QED*

Some of the earliest applications of QED were to several second order processes like Compton scattering (Klein–Nishina formula [7]), and the related process known as Bremsstrahlung which was given by Bethe in collaboration with Heitler [8], both of which turned out to give excellent agreement with experiment. Thus Bethe was from the beginning of QED closely associated with its applications to atomic phenomena. He seemed to have realized from intuition that it was most practicable to treat the electron as a particle, and the photon as a field. So he went on to collaborate with Fermi, who had developed the QED on these lines [2], to calculate the retarded interaction of two electrons via the exchange of a photon [9]. After the Fermi collaboration, he wrote a big review article [10] on the quantum theory of one-electron and two-electron systems, which is a standing testimony to the thoroughness of his approach to atomic problems with the tools of QED.

2.6 *Infinities in QED: Renormalization?*

The QED applications in the thirties, were not only successful in the second order, but also for higher order processes, provided the calculation was made in the

Kramers idea of renormalization helped remove the infinities in the calculation of electron mass.

lowest 'e-order' for the process under study, i.e., no *virtual* sub-process (with emission and re-absorption of radiation) was involved. On the other hand it was found that if the e-order of a given process involved some *virtual* sub-process, then invariably some divergences were encountered. A primary virtual process is one in which an electron emits and reabsorbs a radiation quantum, thus contributing to its 'self-energy'. If this is an entire process, it corresponds to the 'self-energy' of a *free* electron. Or it could be part of a bigger process, e.g., an electron inside a hydrogen atom, in which case it is termed the self-energy of a *bound* electron. For all such processes, the rules of perturbative QED invariably give infinities. Why? In a second order process involving the emission of a photon, followed by reabsorption of the *same* photon, the photon momentum $\mathbf{k}$ can have any value, so that all such amplitudes must be summed over all possible values of $\mathbf{k}$, which produces a divergent expression! Unfortunately, the theory as developed up to the 1940s, was not equipped to deal with such hazards. On the other hand, any physical quantity to be observable, must have a finite value, and there seemed to be no obvious way to get rid of such infinities before confronting the corresponding amplitudes with observation.

2.6.1 ***Kramers' Idea***: It was a brilliant idea of H Kramers that led him to propose that the bulk of the infinity in such calculations was *not* significant, but only a small (hopefully finite!) part that remains after the amount corresponding to a free or *bare* electron was isolated and subtracted out, since the self-energy contribution for the latter would never be observable ! Therefore the 'true' self-energy of an electron bound in a hydrogen atom is the result of subtraction of the value accruing from the free or *bare* electron, and should hopefully be finite. This was the idea of *Renormalization* which amounted to redefining the observed mass of the elec-

tron as a sum of its bare mass m_0 and the 'self-mass' δm (obtained as above, after dividing by c^2). It was however left to Bethe to show how to calculate the net effect with his great insight [2] that led him to consider equation (8) instead of its full-fledged relativistic counterpart, thus avoiding the field concept for the electron. This derivation is sketched below.

3. Bethe's Derivation of the Lamb Shift

We now give a brief sketch of Bethe's original derivation [3,8] of the Lamb Shift, one in which the spirit of renormalization was implemented in a pragmatic fashion, merely by subtracting the 'free' electron self energy from the full (bound electron) amount. To that end we write the full Hamiltonian from an inspection of (8), and specializing to a Coulomb potential, as

$$H = p^2/2m - Ze^2/r + H_1;\ H_1 = -e\mathbf{p}.\mathbf{A}/mc;\ \nabla.\mathbf{A} = 0, \tag{9}$$

where the interaction H_1 with the (transverse) radiation field is explicitly shown. The radiation field $\mathbf{A}$ is Fourier analyzed as

$$\mathbf{A}(\vec{x}) = \sqrt{\frac{\hbar c}{(2\pi)^3}} \int \frac{d^3k}{\sqrt{2\omega_k}} \sum_1^2 \vec{\epsilon}_{ki}(a_{ki} + a_{ki}^\dagger), \tag{10}$$

where the two transverse polarizations of the photon are indicated by the index i. Now the second order self-energy of a bound electron in a quantum state of energy E_m, due to emission and reabsorption of radiation of energy kc, is given by the standard formula:

$$\Delta E = \sum_{nk} \frac{< H_1 >_{mk;nk} < H_1 >_{nk;mk}}{E_m - E_n - ck},$$

where the sum is over all possible intermediate states n of the atom, as well as over all possible states k of the emitted and reabsorbed photon. Substituting from (9) and (10), and skipping a couple of steps of the trivial

d.o.f.'s of the N-representation, the simplified form of the self-energy becomes [11]

$$\Delta E = -\frac{2\alpha}{3\pi m^2 c^2}\int_0^L kdk \sum_n \frac{p_{mn}p_{nm}}{E_n + k - E_m}. \qquad (11)$$

Here p is the momentum operator for the electron; the sum over the two polarization directions as well as the angular integration over the photon directions have been carried out; and k inside the integral has been normalized to the dimension of energy. The upper limit L of k-integration is supposed to be infinite. The crucial step is now to *subtract* the 'free' electron contribution, which may be read off from (11) by replacing the denominator on the r.h.s. with k only, so that the subtracted denominator reads as:

$$\frac{1}{E_n + k - E_m} \Rightarrow \frac{1}{E_n + k - E_m} - \frac{1}{k} = \frac{E_m - E_n}{k(E_n + k - E_m)}.$$

Then the 'renormalized' form of ΔE becomes

$$\Delta E = \frac{2\alpha}{3\pi m^2 c^2}\int_0^L dk \sum_n \frac{p_{mn}p_{nm}(E_n - E_m)}{E_n + k - E_m}. \qquad (12)$$

Note that the degree of divergence in k now reduces to logarithmic from linear, so that the sensitivity to the upper limit L is greatly reduced. This is as far as could be achieved with Bethe's non-relativistic treatment. However, Bethe correctly surmised that with a proper relativistic treatment, the divergence would be further reduced from logarithmic to a convergent integral [11].

To treat (12) further, the k-integration gives a factor $\ln L/[E_n - E_m]$, where L may be taken as of order mc^2, as befits a non-relativistic treatment. Further, the relative insensitivity of the logarithm to its argument warrants an approximation which eliminates its (m, n) dependence, by replacing $E_n - E_m$ with an average value

$< E - E_m >$ which can then be taken out of the n-summation! The result of all these manipulations is

$$\Delta E = \frac{2\alpha}{3\pi m^2 c^2} \sum_n p_{mn} p_{nm} (E_n - E_m)$$

$$[\ln mc^2 / < E - E_m >]. \qquad (13)$$

Now using the rules of quantum mechanics, one finds [11]

$$\sum_n (E_n - E_m) p_{nm} p_{mn} = \frac{1}{2} < [p, [-Ze^2/r, p]] >_{mm} =$$

$$2\pi \hbar^2 e^2 Z [\psi_m(0)]^2.$$

To see how the last form comes about, the double commutator reduces to a $\nabla^2(1/r)$ which is a 3D δ-function! Thus the integral is proportional to $< \psi^\dagger \delta^3(\mathbf{x}) \psi >$, i.e., to the square of the atomic wave function at zero distance. This means in turn that the $shift$ affects only the $2s_{1/2}$ state, while the $2p_{1/2}$ state remains unshifted, w.r.t. the Dirac theory predictions. Bethe estimated this value as 1040 MHz in amazingly good accord with the Lamb-Retherford value [1].

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Discussion

For a historical perspective on how Bethe zoomed in (like a homing pigeon) on a non-relativistic treatment, the interested reader is referred to Dyson's narrative [2] on how Bethe's previous training and experience led him to the right answer, without being led astray by irrelevant details! A lesser mortal would have been overawed by the QED infinities, so as not to think of anything but a full-fledged relativistic treatment of both the electron and photon fields. And indeed, the fuller ramifications of the Kramers renormalization idea were to extend from that of mass, to every conceivable physical quantity: mass, charge, wave function, etc., not merely in second order, but to every conceivable order in perturbation theory in a *closed* form. Dyson showed how

to do this systematically in terms of appropriate classes of Feynman diagrams [12]. And of course the treatment had to be entirely in terms of a relativistically invariant QFT, at the end of which the agreement between theory and experiment was 1 in 10^{12}! But the impetus for this drive came from Hans Bethe's pilot project which covered just two pages of the *Physical Review*.

I am grateful to Freeman Dyson for making available to me his thoughts [2] on Hans Bethe, prior to publication, which has helped put several things in this paper in perspective.

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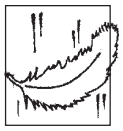

Concern for man and his fate must always form the chief interest of all technical endeavors. Never forget this in the midst of your diagrams and equations.

Albert Einstein