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Interactive Modelling[1]

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The complementary dynamical features of two types of models are exemplified from some of Elliott Lieb's work.

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1. INTRODUCTION

1.1. Philosophical Underpinnings

My interest in the different roles models play in theoretical and mathematical physics arose when I was preparing the annotations I was asked to write for Volume 6 of Wigner's Collected Works.[59] I noticed then that Wigner had been using the word *model* in two different contexts, although he did not comment explicitly on his reasons for doing so. The difference, I argue, can be formalized in the following two definitions.

Definition 1. *H-models* explore the connections to be established between the syntactic framework—especially the physical postulates—and its physical semantic relevance: the observability of its concepts and their applicability to the "actual world" as apprehended by laboratory experiments.

Definition 2. *L-models* test the correctness and economy of the syntax: the logical consistency and independence of its axioms, the formal value of its assertions and theorems.

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I discuss in detail elsewhere[13–15, 17] how this distinction differs from the other approaches to models in the philosophy of sciences.[4, 11, 22, 24, 47, 49, 52, 53, 58] Let it suffice here to say that the present paper proposes to show how the distinction between *H-* and *L-models* helps recognize the various roles models play as active agents of change. Indeed, while operating within their own separate means, models from both classes are often designed to test their formal premises in such a way as to suggest revisions of the theoretical core and/or the consideration of new conjectures. In this paper, I situate Lieb's methodology in this perspective.

1.2. Examples of Straight H- and L-models

In order to anchor the discussion, I recall first a few examples of models in which Wigner was involved, see ref. 13. Three *H-models* in nuclear physics are reviewed there: the Heisenberg–Wigner isospin, the compound nucleus, and the random matrix depiction of the distribution of energy levels. *L-models* are also illustrated there with three examples from the foundations of quantum mechanics: superselection rules, Bell's inequalities, and models for quantum measurement processes.

Culled now from Elliott Lieb's own contributions to equilibrium statistical mechanics, another set of contrasting models obtains straightforwardly. Consider indeed for *H-models*: the imperfect Bose gas,[37] the Jellium model,[39] the Hubbard model;[31] and for *L-models*: the Lenz–Ising model,[40, 51] the X–Y model,[35] and the Pauling model for the residual entropy of ice[26] (the exact solution of which was spectacularly presented by Elliott, at the very first "Yeshiva meeting" I attended, the ancestor of today's Rutgers meetings).

2. MODELS IN MUTATION

The taxonomy of models advanced in Section 1 is stable enough to be immediately apparent in the simple cases such as the snapshots offered there. Yet, the purposes of a model may become more fluid and transient in other theories. While these mutations may be mostly a matter of mathematical rigor, they generate often—although not always—new conceptual vistas beyond the original domain of the models considered.

In this and the next Sections, two examples drawn from contributions of Lieb and collaborators—and two from other sources—will illustrate shifting of weights that occur in the modelling practice of theoretical and mathematical physicists.

The Gross–Pitaevskii equation started as a typical *H-model*;[20, 46] yet Lieb *et al.*[41] showed that most of its main predictions follow as

mathematically controllable consequences from first principles, this controllability gaining the model much of the flavor of a *L-model*. Yet, here the intended experimental domain of applicability has remained unchanged in as much as the problem is to understand the Bose–Einstein condensation of an interacting gas. For details and further refs., see ref. 17, [Section 14.2.2].

The BCS model achieved at first great successes as a *H-model* for superconductivity.[3] Further analysis evidenced a mathematical structure that converted the original model to a choice *L-model* for spontaneous symmetry breaking in algebraic quantum many-body theory[16, 21, 54]. An account of the contemporary and subsequent far-reaching avatars of the BCS model in condensed matter and elementary particle physics is sketched by Anderson,[1] who mentions also refs. 2 and 23.

The Dyson model was advanced as a *L-model*[12] to delineate the boundaries outside of which the van Hove–Ruelle theorems[48, 56] do not apply. After having performed well in that capacity, its exact solvability can be exploited most profitably[6, 7, 9] to obtain an instructive *L-model* for a much later stage in the theory of phase transitions, namely the Kadanoff–Wilson–Fisher scaling program that offers a rich collection of computationally challenging *H-models,* see, e.g., ref. 8.

3. THE THOMAS–FERMI MODEL

The changing status of the Thomas–Fermi model is even more interesting as it occurs in contexts where the arena for which it was intended has changed drastically: from the quantum description of the properties of a single atom with a few electrons, to the understanding of the stability of matter in bulk, e.g., stars.

The Thomas–Fermi model[19, 55] saw the light of day as a *H-model* in 1927—i.e., in the beginning of the second phase in the development of quantum theory—when it was realized that the quantum mechanical problem of determining the energy spectrum of the hydrogen atom could not receive a similarly simple and yet exact solution for the higher elements. Thus, the model designed by Thomas and Fermi is a *H-model* that describes an atom as a cloud of electrons surrounding the nucleus. This simple picture is approximate by design in order to avoid the then insurmountable complications that a rigorous treatment of the Schrödinger equation would have entailed.

Specifically, the initial aims of the model were: to compute the electronic distribution and the ionization energy; to determine how the electrostatic potential varies as a function of the distance from the nucleus; and to understand the onset of the periodic system of elements. Fermi points

out explicitly that, in order to take into account the Pauli exclusion principle, the cloud of electrons must obey the quantum statistics he had proposed *only the previous year*;[18] we would talk today of the Fermi–Dirac statistics, and thus of the cloud of electrons as a Fermi gas.

The model certainly did not go unnoticed. Within a few years, its predictions, its theoretical justification and some improvements on it were widely discussed, e.g., by Frenkel (1928), Dirac (1930), Lenz (1932), Fock (1932), Jensen (1933), von Weizsäcker (1935). By the middle of the twentieth century, the model had become a routine staple in the quantum mechanics curriculum, see, e.g., ref. 50 [pp. 281–283], ref. 25 [pp. 235–240], and ref. 45 [pp. 524–528].

To emphasize its *heuristic* character, I sketch first the model's original version. Its two ingredients are: $\rho(r)$, the spherically symmetric ground state one-particle electron density, with the normalization

$$4\pi \int_o^\infty dr\, r^2 \rho(r) = Z; \tag{3.1}$$

and the average electric potential $\Phi(r)$ in the atom, due to (a) the nucleus, assumed to be a point at 0 with charge eZ, and (b) the continuous electric distribution $e\rho(r)$.

The model is semi–classical in the following sense.

The classical aspect is that Φ is to satisfy the Poisson equation

$$\Delta\Phi \equiv \frac{1}{r}\frac{d^2}{dr^2}(r\Phi) = 4\pi e\rho \qquad \text{with} \quad \lim_{r\to 0} \Phi(r) = eZ. \tag{3.2}$$

The quantum aspect of the model is that ρ is obtained from

$$n(r, p) = \begin{cases} 2h^{-3} & \text{if} \quad \epsilon \equiv \frac{1}{2m} - e\Phi < \epsilon_o \\ 0 & \text{if} \quad \epsilon > \epsilon_o \end{cases} \tag{3.3}$$

by integration over p (upon putting $\epsilon_o = 0$):

$$\rho(r) = \begin{cases} \frac{8\pi}{3h^3}(2me\Phi)^{3/2} & \text{if} \quad \Phi > 0 \\ 0 & \text{if} \quad \Phi < 0. \end{cases} \tag{3.4}$$

The substitutions

$$r = Z^{-\frac{1}{3}} bx; \qquad \Phi = \frac{Ze}{r}\chi; \qquad b = \frac{1}{2}\left(\frac{3\pi}{4}\right)^{\frac{2}{3}} \frac{\hbar^2}{me^2} \tag{3.5}$$

introduce the dimensionless quantities χ and x, in terms of which the basic equations (4.2) and (4.4) combine to

$$\chi''(x) = \left\{ \begin{matrix} x^{-\frac{1}{2}}\chi^{3/2}(x) & \text{if} \quad \chi > 0 \\ 0 & \text{if} \quad \chi < 0 \end{matrix} \right\} \qquad \text{with} \quad \chi(0) = 1. \tag{3.6}$$

(4.6) entails $\chi(x_o) = 0$ for exactly one $x_o \in (0, \infty]$, and thus

$$1 = \int_0^{x_o} dx\, x^{\frac{1}{2}}\chi^{\frac{3}{2}} = \int_0^{x_o} dx\, x\chi'' = x_o\chi'(x_o) + 1 \tag{3.7}$$

so that $\chi'(x_o) = 0$ and thus $x_o = \infty$; hence (4.6) reads

$$\chi''(x) = x^{-\frac{1}{2}}\chi^{3/2}(x) \qquad \text{with} \quad \chi(0) = 1 \quad \text{and} \quad \chi(\infty) = 0 \tag{3.8}$$

The solution of this equation obtains numerically, allowing to plot the graph of the functions $\rho(r)$ and $\Phi(r)$. The solution of the model is hereby completed. Note that the analytic simplicity of the model permits the conclusion (4.8) to be an exact consequence of the basic assumptions (4.2) and (4.4). Nevertheless, this fact by itself does *not* suffice to qualify the model as a *L-model* since it is *a priori* inconsistent: it is *semi-classical* as its assumptions borrow from both classical and quantum theories.

This calls for two questions: (1) how experimentally accurate are the model's predictions; and (2) how much of the model can be justified from the basic principles of quantum theory alone.

Scholium 1. Let R_α be the radius of the sphere centered at the nucleus and containing the fraction $(1-\alpha)$ of the Z electrons, i.e.,

$$(1-\alpha)\, Z = \int_0^{R_\alpha} dr\, r^2\rho(r). \tag{3.9}$$

Then

$$R_\alpha = Z^{-\frac{1}{3}} b X_\alpha \tag{3.10}$$

where X_α is the unique solution of

$$\chi(X_\alpha) - X_\alpha\, \chi'(X_\alpha) = \alpha. \tag{3.11}$$

Corollary 3.1. If one takes the same value of α to define the radius of all atoms, R_α decreases as $Z^{-\frac{1}{3}}$.

Corollary 3.2. Define the radius of the atom as the radius of the sphere that contains all the electrons but one, i.e., $R(Z) \equiv R_{\alpha = Z^{-1}} = Z^{-\frac{1}{3}} b\, X_{Z^{-1}}$, where $X_{Z^{-1}}$ is the numerical solution of (4.11) for $\alpha = Z^{-1}$, and $b \approx 0.5 \times 10^{-8}$ cm is the constant b defined in (4.5). Then $R(Z)$ increases monotonically from 2.2×10^{-8} cm for $Z = 25$ to 2.8×10^{-8} cm for $Z = 100$.

Remarks. The order of magnitude is correct. However: (1) the largest atom is cesium ($Z = 55$); afterwards $R(Z)$ decreases, albeit slowly; (2) the model yields an electron density with unreasonable properties very close and very far from the nucleus; (3) the natural extension of the model to the case of several nuclei does not allow for the existence of stable molecules; (4) its extension to the relativistic domain does present serious challenges.

These problems are corrected in the modern versions of the Thomas–Fermi model devised by Lieb and co-workers, and explained in refs. 5, 27, 29, 30, and 42. The results cover two corrections proposed early in the game, the first by Dirac[10] to include the exchange term, and the second by von Weizsäcker;[57] as indicated already by the titles of refs. 5, 29, 30, and 42, the domain of applicability of this circle of ideas is thus extended from atoms to molecules, solids, and stars. The proofs depend on the technical refinements developed in refs. 36, 44, and 43 for the thermodynamical limit of Coulomb systems, the stability of matter, and the Hartree–Fock method.

In the context of the present section, the main feature of these results is that reasonable answers, developed to justify the models from first principles, have put on a firm footing their *asymptotic* validity. In the sequel, to focus on the latter aspect, it is sufficient to review the simplest case where the von Weizsäcker and Dirac corrections are not yet taken into account; references are cited below together with the statement of the results.

The original problem demands a reliable estimate for the ground state energy $E = (\Psi, H\Psi)$ of an atom consisting of N electrons and a point nucleus of charge $Z = N$. The Hamiltonian is then $H = T + A + B$ where T is the kinetic energy of the electrons; A is the contribution to the potential due to the interaction between the electrons and the nucleus; and B is the contribution to the potential due to the interaction between the electrons:

$$H \equiv \sum_{j=1}^{N} \nabla_j^2 + Z \sum_{j=1}^{N} |x_j|^{-1} + \sum_{1 \leqslant i < j \leqslant N} |x_i - x_j|^{-1} \tag{3.12}$$

where the units have been chosen such that $\frac{\hbar^2}{2m} = 1$; $e = 1$.

Lemma 3.1 [The 5/3 law[44]]. For all $\Psi \in L^2(R^{3N})$ antisymmetric with $\|\Psi\| = 1$, and all positive integer N, let

$$T_\Psi \equiv \sum_{j=1}^{N} \int_{R^{3N}} dx_1\, dx_2 \cdots dx_N\, |\nabla_{x_j} \Psi(x_1, x_2, \ldots, x_N)|^2, \tag{3.13}$$

and

$$\rho_\Psi(x) \equiv N \int_{R^{3(N-1)}} dx_2 \cdots dx_N\, |\Psi(x, x_2, \ldots, x_N)|^2. \tag{3.14}$$

Then there exists a universal constant $K > 0$ such that

$$T_\Psi \geqslant 2^{2/3} K \int_{R^3} dx\, \rho_\Psi(x)^{5/3}. \tag{3.15}$$

Remarks. (1) The factor $2^{2/3}$ disappears when the spin of the electrons is taken into account, i.e., when $\Psi \in L^2(R^{3N}; C^{2^N})$. (2) The numerical value of K is not important; one knows $K \geqslant (2.7709)\, 2^{-2/3} = 1.7455$, and one conjectures that $K^c = 3(3\pi^2)^{2/3}/5 = 5.7425$. (3) The power $5/3$ is the main point; it reflects the dimensionality of the system. (4) The bosonic version of the $5/3$ law is discussed in ref. 28.

Definition 3. With $K^c = 3(3\pi^2)^{2/3}/5 = 5.7425$, the Thomas–Fermi functional $\mathscr{E}^{TF}(\rho)$ for $\rho \in L^{5/3}(R^3) \cap L^1(R^3)$ is:

$$\left.\begin{aligned} \mathscr{E}^{TF}(\rho) \equiv\ & K^c \int_{R^3} dx\, \rho(x)^{5/3} \\ & - Z \int_{R^3} dx\, |x|^{-1} \rho(x) \\ & + \tfrac{1}{2} \int_{R^3} \int_{R^3} dx\, dy\, \rho(x)\, \rho(y)\, |x-y|^{-1}. \end{aligned}\right\} \tag{3.16}$$

The Thomas–Fermi ground state energy is:

$$E^{TF} \equiv E^{TF}(N, z) \equiv \inf \left\{ \mathscr{E}^{TF}(\rho) \;\middle|\; \int dx\, \rho = 1 \right\}. \tag{3.17}$$

Theorem 3.1 (TF is asymptotically exact;[30] see also the earlier papers[29, 42]). Let $0 < \lambda \leqslant 1$; $z_N = N/\lambda$ for $N = 1, 2, \ldots$; $E(N, z_N)$ be the Schrödinger ground state energy for an atom with nuclear charge z_N and

N electrons; $\rho_N(x)$ be, as in (4.14), the density of any ground state Ψ_N; $E^{TF}(N, z_n)$ be the corresponding Thomas–Fermi energy; and $\rho^{TF}{}_N$ be the corresponding Thomas–Fermi density. Then

$$\lim_{N\to\infty} \frac{E(N, z_N)}{E^{FT}(N, z_N)} = \lim_{N\to\infty} \frac{E(N, z_N)}{z^{7/3}E^{TF}(\lambda, 1)} = 1. \tag{3.18}$$

In the sense of weak $L^1(R^3)$ convergence on compact sets,

$$\lim_{N\to\infty} z^{-2}\rho_N(z^{-1/3}x) = \lim_{N\to\infty} z^{-2}\rho^{TF}{}_N(z^{-1/3}x) = \tilde{\rho}(x) \tag{3.19}$$

where $\tilde{\rho}(x)$ is the TF minimizer for $z = 1$ and $N = \lambda$.

There is also a result for $\lambda > 1$, but the above theorem is enough for what I want to illustrate.

Recall that the Thomas–Fermi model was devised for atoms with several electrons, a situation where the Schrödinger eigenvalue equation for the ground state cannot be solved explicitly. Theorem 4.1 gives the precise sense in which the Thomas–Fermi model is an *asymptotic L-model* for large atoms, i.e., precisely for the situation where the Schrödinger equation itself cannot be solved explicitly. This theorem admits generalizations—to the TFW, TFD, and TFDW models—wide enough to prompt the upbeat concluding comment of Lieb's Gibbs lecture.[30]

For the commentary on method pursued in the present paper, the Thomas–Fermi model is a prime example of a *H-model* evolving to a *L-model* and suggesting further *H-models* and the rigorous delineation of their asymptotic domain of applicability.

4. CONCLUSIONS

When asked for his guiding precepts, Elliott succinctly responded: "*the pursuit of a consistent explanation of phenomena*,"[34] a lapidary statement by which most theoretical physicists would want to abide, albeit in a variety of ways.

Some, like von Neumann or Wightman and Haag, focus on boiling essential experience of phenomena down to concise axioms, and/or rich abstract theories.

Others, like Lenz (with the Ising model) or Dyson (with his hierarchical model), advance concrete explanatory models that are simple enough to obtain rigorously from the general doctrine some specific conclusions that cannot be changed without modifying the core of the doctrine from which they derive. These are *L-models*.

Still other physicists, like Wigner (especially when he wears his nuclear physicist's hat), Bardeen *et al.*, Gross and Pitaevskii, or Thomas and Fermi, concentrate on specific laboratory experiments to identify the phenomena, and their theoretical explanations usually propose *H-models*.

In the rich multiplicity of the models that bear Lieb's indelible mark, I had to select here only a few representatives, those that help most in tracing his general methodology.

Firstly, pure *L-models,* the most spectacular of which was the ice model, which he solved exactly, disproving beyond doubt the Nernst conjecture that the entropy must vanish when the temperature approaches the absolute zero. Among the other *L-models* he considered, several others focus on the essential features that delineate the nature of phase transitions, rather than presenting detailed prescriptions on how to compute critical coefficients for specific fluids of ferromagnetic substances.

Secondly, Lieb may be at his best when he takes a *H-model*, such as Thomas–Fermi's, reformulates it in terms of first principles, and then proceeds to study the asymptotic regime in which it can be solved exactly, thus producing a reliable *L-model*. The mathematical structures he brings to light in so doing often results in considerable broadenings of the original domain of applicability of the models from which he started. This is indeed one of the most instructive methodological lessons a physicist may draw from Elliott's work.

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