

Lectures on Quantum Phenomena

Public Lecture Series of the *Pacific Institute of Theoretical Physics* (PITP)

Wednesday, January 10, 2007

**At the End of the Rainbow: Optical Dispersion as the Bridge
between the Old Quantum Theory and Matrix Mechanics**

Michel Janssen

Program in the History of Science, Technology, and Medicine

University of Minnesota

Optical dispersion, observed in rainbows and prisms, was already studied seriously by Descartes and Newton. A satisfactory theory of dispersion, however, was not found until two centuries later, as part of Lorentz's elaboration of Maxwell's electrodynamics in the 1890s. Only two decades later this theory was called into question again by Bohr's quantum model of the atom. In the early 1920s the problem of dispersion took center stage. The famous *Umdeutung* (reinterpretation) paper with which Heisenberg ushered in the era of modern quantum mechanics grew directly out of a quantum theory of dispersion proposed by Kramers, Bohr's right-hand man at the time. Drawing on work by Einstein and Ladenburg, Kramers was able to reconcile Lorentz's theory of dispersion with Bohr's theory of the atom. With hindsight, it was only a small step from Kramers' theory to Heisenberg's matrix mechanics.

Heisenberg's first paper (July 1925) on what became matrix mechanics is notoriously hard to follow

“Über die quantentheoretische **Umdeutung** kinematischer und mechanischer Beziehungen.” [On the quantum-theoretical **reinterpretation** of kinematical and mechanical relations] *Zeitschrift für Physik* 33 (1925): 879–893. English translation in: B. L. van der Waerden (ed.), *Sources of Quantum Mechanics*. New York: Dover, 1968.

Steven Weinberg (*Dreams of a Final Theory*, Ch. IV): “If the reader is mystified at what Heisenberg was doing, he or she is not alone. I have tried several times to read the paper that Heisenberg wrote on returning from Helgoland, and, although I think I understand quantum mechanics, I have never understood Heisenberg's motivations for the mathematical steps in his paper.”

To understand the *Umdeutung* paper we first need to understand a paper by Kramers and Heisenberg on dispersion theory (January 1925):

“Über die Streuung von Strahlung durch Atome.” [On the Scattering of Radiation by Atoms] *Zeitschrift für Physik* 31 (1925): 681–707. Also reprinted in Van der Waerden.

Max Dresden (student and biographer of Kramers): Kramers-Heisenberg paper is “the direct, immediate, and exclusive precursor to the Heisenberg paper on matrix mechanics.”

Martin J. Klein (senior historian of modern physics): “this work was the immediate predecessor of Heisenberg’s new quantum mechanics.”

Unfortunately, the Kramers-Heisenberg paper is *also* hard to follow.

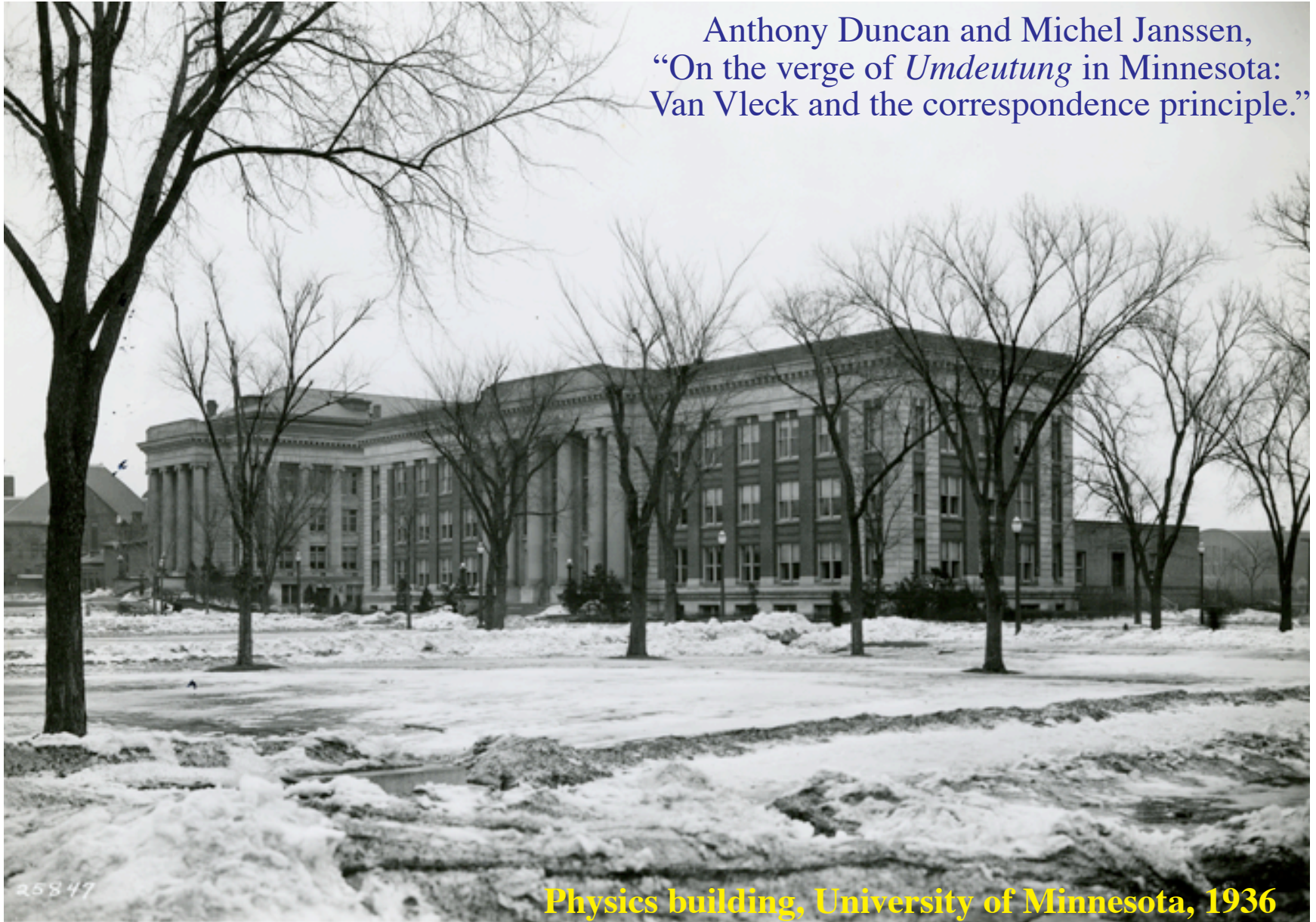
Despite:

Jagdish Mehra and Helmut Rechenberg (six-volume history of quantum physics):
“the authors ... wrote in such a way that every physicist, theoretician or experimentalist, interested in the subject could understand ... the Kramers-Heisenberg paper stood out for its clarity and straightforwardness, in which the results were obtained from a few intelligible assumptions.”

Clearer earlier paper (October 1924) by Van Vleck covering similar terrain:

J. H. Van Vleck, “The absorption of radiation by multiply periodic orbits, and its relation to the correspondence principle and the Rayleigh-Jeans law.” Part I. “Some extensions of the correspondence principle.” Part II. “Calculation of absorption by multiply periodic orbits.” *Physical Review* 24 (1924): 330–346, 347–365. Part One reprinted in Van der Waerden.

Anthony Duncan and Michel Janssen,
“On the verge of *Umdeutung* in Minnesota:
Van Vleck and the correspondence principle.”



Physics building, University of Minnesota, 1936

Van the Man: John Hasbrouck Van Vleck (1899–1980).



- Born in Middletown, Connecticut
- Undergrad Madison
- 1922: Ph.D. Harvard
- **1923–1928: Minnesota**
- 1928–1934: Madison
- 1934–1969: Harvard
- 1977: Shares Nobel Prize with former graduate student Phil Anderson and Sir Nevill Mott “for their fundamental theoretical investigations of the electronic structure of magnetic and disordered systems.” Van Vleck known as the “father of modern magnetism.”

Cf. Fred Fellows, *J. H. Van Vleck: The Early Life and Work of a Mathematical Physicist*. Ph.D. Thesis, University of Minnesota, 1985.

Van Vleck commenting on his 1924 paper:

Van Vleck in 1963 in an interview with **Thomas S. Kuhn (1922–1996)** for the *Archive for the History of Quantum Physics (AHQP)* project:*

Kuhn: “You said something to me about that paper once before [...] you thought if you had been a little bit more perceptive, you might have taken off from that paper to do what Heisenberg did.”

Van Vleck: “That’s true. Perhaps I should say *considerably* more perceptive ...”

*Kuhn, author of *The Structure of Scientific Revolutions* (1962) and director of the AHQP project (1961–1964), did his Ph.D. in physics with Van Vleck right after WWII.

Autobiographical statement for the AHQP:

“In the two or three years after my doctorate ... my most significant paper was one on the correspondence principle for absorption ... It was somewhat related to considerations based on the correspondence principle that led Heisenberg to the discovery of quantum mechanics, but I did not have sufficient insight for this.”

Task of conceptual history of QM: tracing the transition from representing states by points in classical phase space to representing states by vectors in Hilbert space.

- **Old quantum theory**
(Bohr, Sommerfeld)

Retain classical phase space but only allow certain orbits, selected by quantum condition $\oint p dq = nh$ (damage control).

My focus

- **Dispersion theory / Matrix mechanics**

(Ladenburg, Reiche, Kramers, Van Vleck, Born, Heisenberg, Born, Jordan, Pauli)

- From **states** (quantized orbits in phase space) to **transitions between states** (no representation of states themselves).
- From **numbers** (functions on phase space) to **matrices** connected with transitions.
- From **Bohr-Sommerfeld quantum condition** in phase space $\oint p dq = nh$ to **commutation relation** $[q, p] = i\hbar$ for transition matrices.

- **Wave mechanics** (De Broglie, Schrödinger, Born): states represented by wave functions generating transition probabilities
- **Mathematical clean-up** (... , Dirac, Wiener, Von Neumann): states represented by vectors in Hilbert space

A closer look at second stage:

Dispersion theory / Matrix mechanics

- From **states** (quantized orbits in phase space) to **transitions between states**
- From **numbers** (functions on phase space) to **matrices** connected with transitions
 - These steps were already taken in dispersion theory.
 - Dispersion theory vs. matrix mechanics:
 - Dispersion theory: problems are first solved classically and then the solution is ‘translated’ (through inspired guesswork guided by Bohr’s correspondence principle) into an expression in terms of quantum transitions.
 - Matrix mechanics: theory formulated and problems solved in terms of quantum transitions from the get-go.
- From **Bohr-Sommerfeld quantum condition in phase space** to **commutation relation for transition matrices**.

In two steps:

- Heisenberg: Bohr-Sommerfeld quantum condition (expressed in terms of orbits) → **Thomas-Kuhn(-Reiche) sum rule** (expressed in terms of transition matrices) [by-product of dispersion theory; found independently by Van Vleck]
- Born-Jordan: from **sum rule** to **commutator**.

Dispersion theory as the bridge between the old quantum theory and matrix mechanics

Important for breakthrough to matrix mechanics:

- **Bohr's frequency condition**, $h\nu_{n \rightarrow m} = E_n - E_m$
- **Einstein's quantum theory of radiation** (A & B coefficients)
- **Bohr's correspondence principle**. In the limit of high quantum numbers:
 - radiation frequencies $\rightarrow$ orbital frequencies (Bohr)
 - amplitudes $\rightarrow$ Einstein's A & B coefficients (Ladenburg)
 - derivatives $\rightarrow$ difference quotients (Kramers, Van Vleck, Born)
- **Classical mechanics**: action-angle variables, canonical perturbation theory (Epstein, Kramers, Van Vleck, Born)
- **Dispersion theory** (Ladenburg, Reiche, Bohr, Kramers, Van Vleck)

Dispersion theory as the bridge between the old quantum theory and matrix mechanics

Unimportant for breakthrough to matrix mechanics:

- **Helium** [produced Kuhnian crisis for the old quantum theory in 1923–1925]
- **Zeeman effect** [likewise produced crisis for old quantum theory]
- **Light quanta** [widely accepted after Compton (1923) but physicists continue to talk about light as a wave phenomenon]
- **Compton effect** [*pace* Roger Stuewer, *The Compton Effect: A Turning Point in Physics* (1975)]
- **Bohr-Kramers-Slater (BKS) theory** [except for ‘virtual oscillators,’ but those actually originated in dispersion theory]
- **Hamilton-Jacobi theory**

From dispersion theory to matrix mechanics

Dispersion has a venerable history (think of Descartes' rainbow and Newton's prism) but the first reasonable dispersion theory dates from the late-19th century.



The Lorentz-Drude dispersion theory (1890–1900): the index of refraction is related to polarization of groups of charged harmonic oscillators (electrons) in matter.



H. A. Lorentz (1853–1928)

Radiation (electric field E , angular frequency ω) hits harmonically-bound electron (mass m , charge $-e$, characteristic angular frequency ω_0).

Component $\Delta x_{\text{coh}}(t) = A \cos \omega t$, coherent with incident wave and superimposed on pre-existing oscillations, is responsible for (normal) dispersion (ν far from ν_0). Use $\mathbf{F} = m\mathbf{a}$, to determine amplitude A (ignoring radiation damping):

$$m\Delta \ddot{x}_{\text{coh}} = -m\omega_0^2 \Delta x_{\text{coh}} - eE \cos \omega t$$

$$-m\omega^2 A = (-m\omega_0^2 A - eE) \rightarrow A = \frac{eE}{m(\omega^2 - \omega_0^2)}$$

Dipole moment

$$p(t) = -e\Delta x_{\text{coh}}(t) = \frac{e^2 E}{m(\omega_0^2 - \omega^2)} \cos \omega t$$

The Lorentz-Drude dispersion theory (1890–1900)

Dipole moment for one dispersion electron

$$p(t) = \frac{e^2 E}{4\pi^2 m (\nu_0^2 - \nu^2)} \cos 2\pi \nu t$$

For groups of n_i dispersion electrons per unit volume with characteristic frequencies ν_i , the polarization due to field with frequency ν is **[Lorentz-Drude dispersion formula]**:

$$P(t) = \frac{e^2 E}{4\pi^2 m} \sum_i \frac{n_i}{\nu_i^2 - \nu^2} \cos 2\pi \nu t$$

Note:

- Resonance poles at characteristic frequencies ν_i .
- The number n_i of dispersion electrons per unit volume is a fraction f_i of the number N_i of atoms per unit volume. $f_i = n_i/N_i$ is called the **oscillator strength**.

The Lorentz-Drude formula is in tolerable agreement with experiment if the resonance poles are identified with frequencies of absorption lines.

Two centuries after Newton, the Lorentz-Drude theory finally gave a reasonable account of dispersion. Only two decades later, the picture of matter underlying this theory was rendered obsolete by the Bohr-Sommerfeld theory.



Quantum condition (action J is some integer multiple n of Planck's constant h) picks out allowed orbits in phase space (spanned by coordinates q and momenta p).

The Sommerfeld-Debye(-Davisson) dispersion theory (1915)

In 1915, **Arnold Sommerfeld (1868–1951)** and **Peter Debye (1884–1966)** adapt Lorentz-Drude dispersion theory to Bohr's new theory.

oscillating electrons → electrons orbiting the nucleus.

Otherwise, same story as before. Hence, Sommerfeld-Debye theory gives formula of the same form as the Lorentz-Drude theory. Polarization for groups of N_i Bohr atoms per unit volume with electrons in orbits with quantum number i and orbital frequency ν_i :

$$P(t) \propto \sum_i \frac{f_i N_i}{\nu_i^2 - \nu^2} \cos 2\pi \nu t$$

Odd feature of Sommerfeld-Debye theory: large accelerations to keep electrons in Bohr orbits do not give rise to radiation, but small deviations from such orbits do!

The big problem: orbital frequencies $\neq$ radiation frequencies → resonance poles at the wrong frequencies!

Erwin Schrödinger to H. A. Lorentz, June 6, 1926: the discrepancy between radiation frequency and orbital frequency “seems to me ... to be something so *monstrous*, that I should like to characterize the excitation of light in this way as really almost *inconceivable*.”

The Sommerfeld-Debye(-Davisson) dispersion theory (1915)

Bohr's criticism (in almost published paper in 1916): "... experiments ... show that the dispersion ... can be represented with a high degree of approximation by [the Lorentz-Drude formula] in which the characteristic frequencies ... correspond with transitions between the normal states of the atom ... we must consequently assume that the dispersion ... depends on the same mechanism as the transition between different stationary states, and that it cannot be calculated by application of ordinary electrodynamics from the configuration and motions of the electrons in these states"

and turning it around (dispersion same mechanism as transition $\rightarrow$ transition same mechanism as dispersion) in what turns out to be a prescient comment: "... if the above view is correct ... we must ... assume that this mechanism [of transition between states] shows a close analogy to an ordinary electrodynamic vibrator."

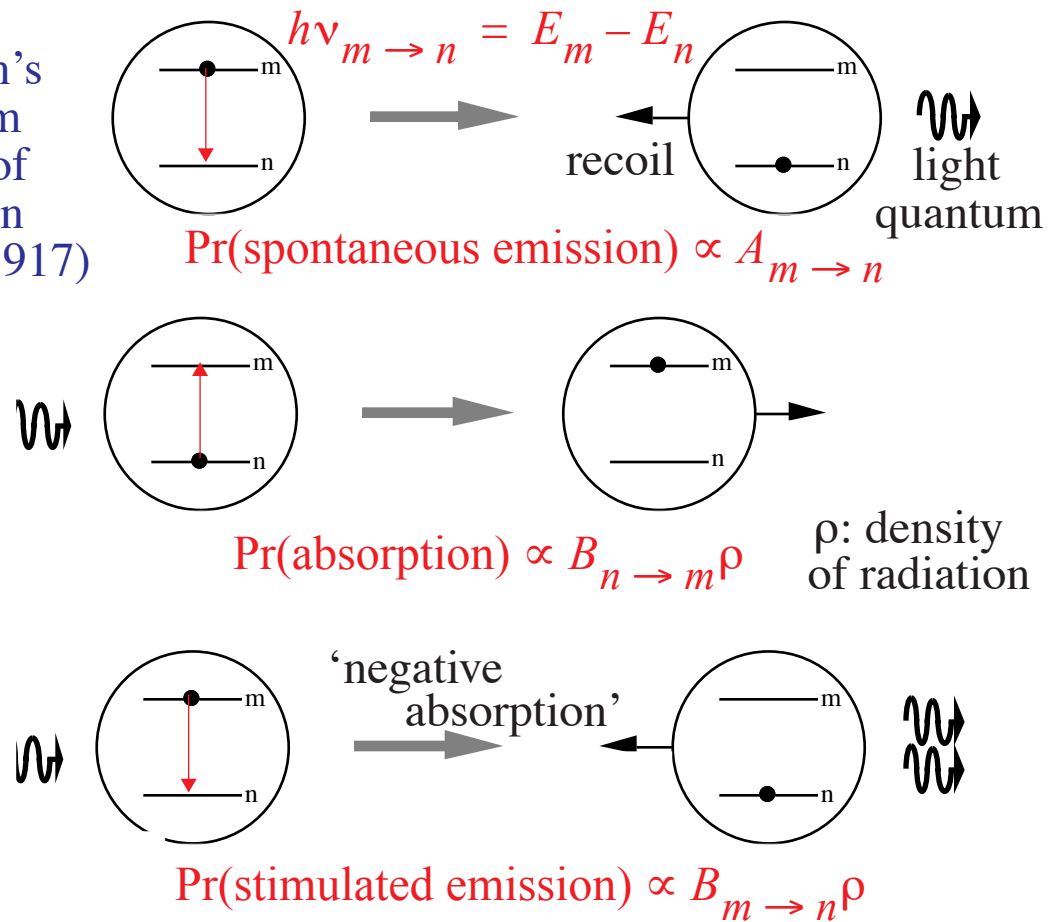
Ingredients needed to get out of impasse reached with Sommerfeld-Debye theory:

- (1) Einstein's A and B coefficients (Ladenburg)
- (2) Bohr's correspondence principle (Kramers, Van Vleck, Born)
- (3) Canonical perturbation theory in action-angle variables (Epstein, Kramers, Van Vleck, Born)

First ingredient: Einstein's A & B coefficients, transition probabilities



Einstein's
quantum
theory of
radiation
(1916/1917)



Equilibrium condition gives relation between $A_{m \rightarrow n}$ and $B_{m \rightarrow n}$

Ladenburg introducing Einstein radiation theory into dispersion theory in 1921.

Breslau physicists **Rudolf Ladenburg** (1889–1953) and **Fritz Reiche** (1883–1969).



Ladenburg dispersion theory (1921).

- (0) Just take for granted that the poles must be at the radiation frequencies.
- (1) Replace oscillator strengths f_i (number of dispersion electrons per atom, measured to be as low as 1 in 50,000) by transition probabilities. To find relation between f_i and A & B coefficients:
- Calculate energy absorption rate of **classical oscillator à la Lorentz-Drude**, resonating at absorption frequencies
 - Calculate energy absorption rate of **quantum atom à la Bohr-Einstein** with transitions between discrete levels corresponding to absorption frequencies.
 - Set the two results equal to one another.

Result: **Ladenburg dispersion formula** for group of Bohr atoms in **ground state r** :

$$\text{Polarization: } P_r \propto \sum_s \frac{A_{s \rightarrow r}}{v_{s \rightarrow r}^2 (v_{s \rightarrow r}^2 - v^2)}$$

with $h v_{s \rightarrow r} = E_s - E_r$. Measurements of line widths give decay times give transition probabilities. Formula in good agreement with experiment; still holds today.

Problem: Ladenburg's derivation is totally unconvincing.

Ladenburg dispersion theory (1921).

Bohr on Ladenburg's dispersion theory in early 1923: "when the atom is illuminated ... the total reaction ... is the same as that of a number of harmonic oscillators in the classical theory, the frequencies of which are equal to those of the radiation emitted by the atom in the possible processes of transition, and the relative number of which is determined by the probability of occurrence of such processes ... A train of thought of this kind was first followed out closely in a work by Ladenburg."

Together with Reiche, Ladenburg writes another paper on his dispersion theory (1923)

Conclusion: "the end result of a process in which a wave of frequency ν acts upon the atom should not be seen as fundamentally different from the effect that such a wave exerts on classical oscillators."

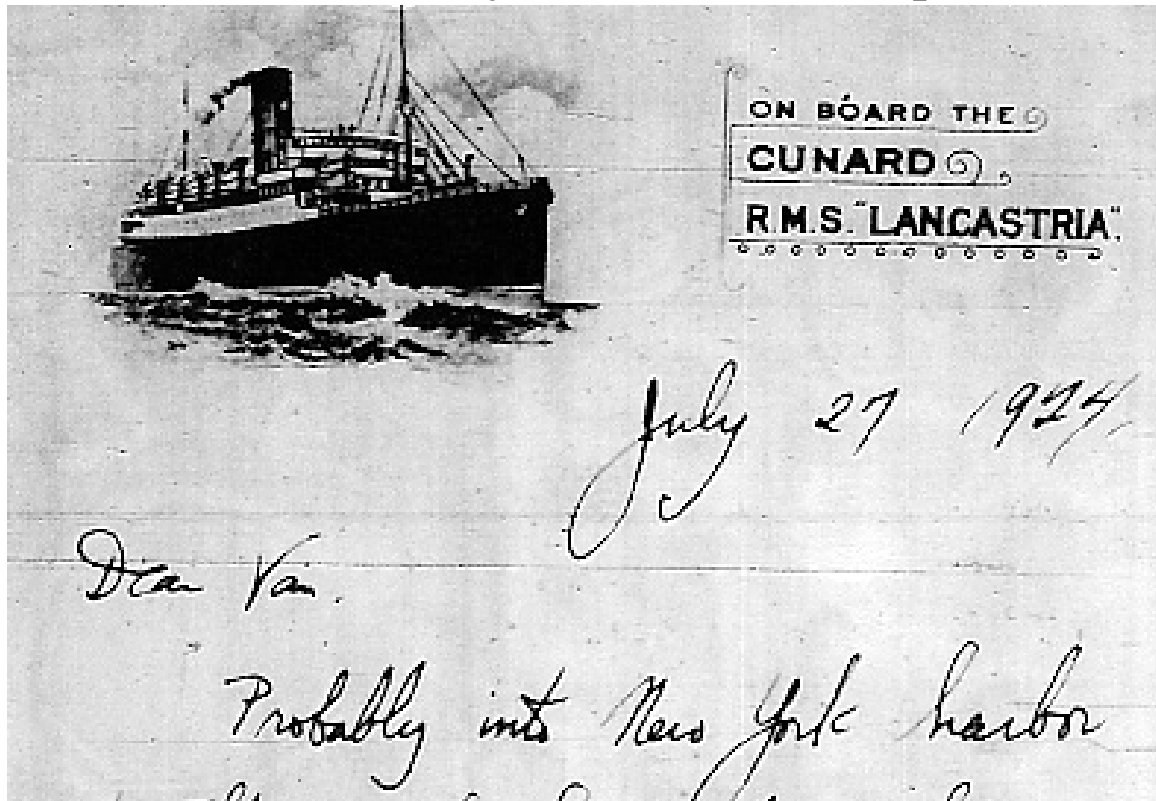
Feynman lectures (1964, Vol. 1, Sec. 31-4): "we will assume that the atoms are little oscillators, that is that the electrons are fastened elastically to the atoms ... You may think that this is a funny model of an atom if you have heard about electrons whirling around in orbits. But that is just an oversimplified picture. The correct picture of an atom, which is given by the theory of wave mechanics, says that, so far as problems involving light are concerned, the electrons behave as though they were held by springs"

Ladenburg-Reiche dispersion theory (1923).

Ladenburg and Reiche introduce the notion of ‘substitute oscillators’ [*Ersatzoszillatoren*], crediting Bohr with the basic idea.

The ‘**substitute oscillators**’ of the 1923 Ladenburg-Reiche dispersion theory became popular as the ‘**virtual oscillators**’ of the 1924 Bohr-Kramers-Slater (BKS) theory.

Slater to Van Vleck, July 27, 1924, on the ship back from Copenhagen to the US



PS We passed Nantucket light in the middle of the letter.

The Bohr-Kramers-Slater theory (1924) and virtual oscillators

Slater to Van Vleck, July 27, 1924



“Don’t remember just how much I told you about my stay in Copenhagen. The paper with Bohr and Kramers [proposing BKS] was got out of the way the first six weeks or so—written entirely by Bohr and Kramers. That was very nearly the only paper that came from the institute at all the time I was there; there seemed to be very little doing. Bohr does very little and is chronically overworked by it.”



The Bohr-Kramers-Slater theory (1924) and virtual oscillators

Slater (in follow-up paper in *Physical Review* in 1925) on BKS: “[i] the stationary state is the time during which the atom is radiating or absorbing [ii] The radiation ... is further not merely of the particular frequency connected with the transition which the atom is going to make; it includes all the frequencies connected with all the transitions which the atom could make ... [iii] Although the atom is radiating or absorbing during the stationary states, its own energy does not vary, but changes only discontinuously at transitions ... It is quite obvious that the mechanism becomes possible only by discarding conservation.”

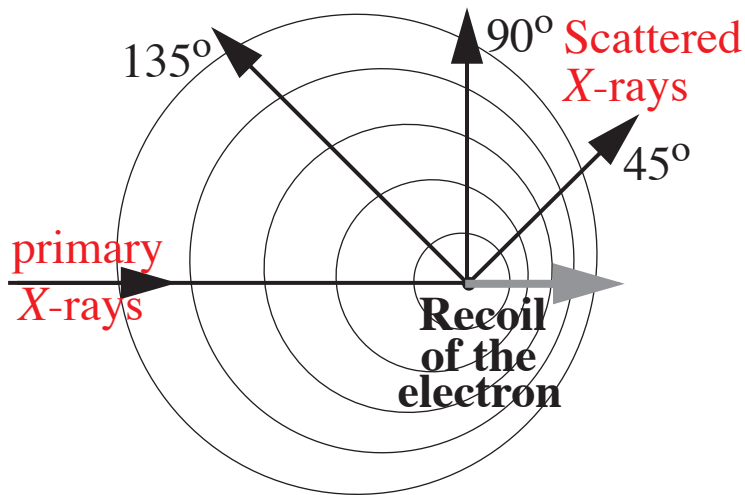
The violation of energy conservation (for which BKS is infamous) was experimentally refuted within a year (Bothe-Geiger, Compton-Simon experiments) and is unimportant for the genesis of matrix mechanics.

The one important idea of BKS comes from dispersion theory: Dual representation of atoms:

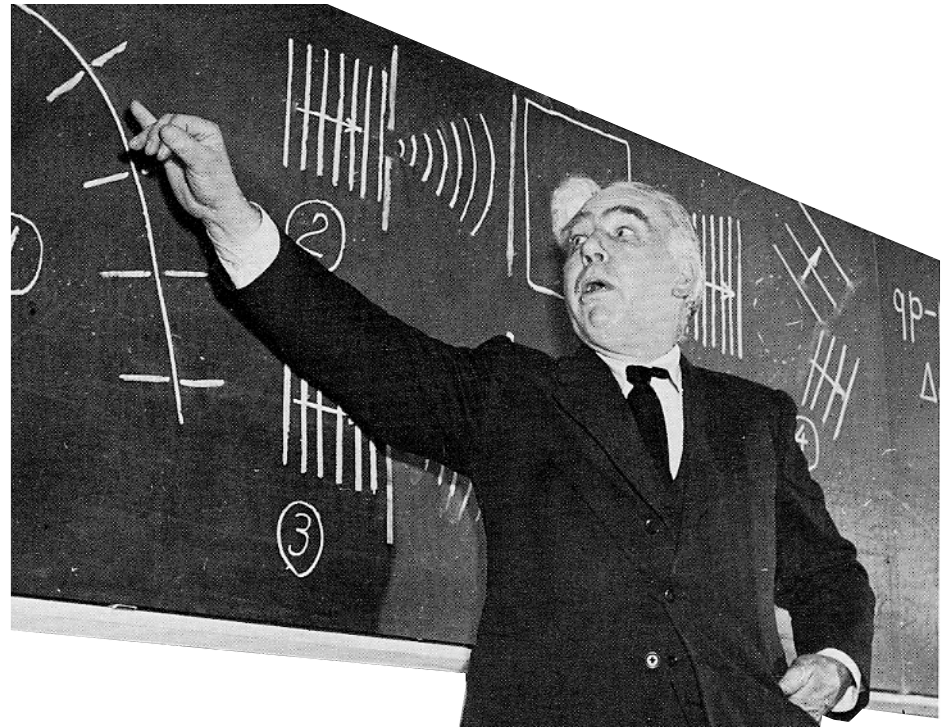
- (1) Set of quantized orbits of Bohr-Sommerfeld theory;
- (2) “**Orchestra of virtual oscillators**” associated with transitions between orbits, emitting and absorbing radiation while electron stays in the same orbit.

*Term by Alfred Landé (1888–1976)

The BKS explanation of the Compton effect: Doppler shift of X-ray waves



Measured wave-length increases going from 0° to 180°



- For **Doppler effect** on the X-rays to come out right, the virtual orchestra must have the right velocity $v_{\text{orchestra}}$.
- For **momentum conservation** (averaged over many electrons interacting with the X-rays), the electron must have the right velocity v_{electron} .
- **Problem:** $v_{\text{orchestra}} \neq v_{\text{electron}}$! BKS: "That in this case the virtual oscillator moves with a velocity different from that of the illuminated electrons themselves is certainly a feature strikingly unfamiliar to the classical conceptions."

The Kramers dispersion formula (1924)

Next step after Ladenburg-Reiche but before BKS: Bohr's first lieutenant, **H. A. Kramers**



Correspondence principle requires dispersion formula with two terms:

Result: Kramers dispersion formula for group of Bohr atoms in arbitrary state r :

$$P_r \propto \sum_{s > r} \frac{A_{s \rightarrow r}}{\nu_{s \rightarrow r}^2 (\nu_{s \rightarrow r}^2 - \nu^2)} - \sum_{t < r} \frac{A_{r \rightarrow t}}{\nu_{r \rightarrow t}^2 (\nu_{r \rightarrow t}^2 - \nu^2)}$$

(sums over s and t refer to states higher and lower than r , respectively)

Kramers formula reduces to Ladenburg formula if r is the ground state (no second term).

The second ('negative dispersion') term is verified experimentally in a series of investigations by Ladenburg and his collaborators published between 1926 and 1934.

Hans Kramers (1894–1952)

The Kramers dispersion formula (1924)

The Kramers dispersion formula, like Ladenburg's, is interpreted in terms of *substitute* or *virtual oscillators*:

Van Vleck in his 1924 paper: the Kramers formula “assumes the dispersion to be due not to the actual orbits but to Slater's [in fact: Ladenburg and Reiche's] ‘virtual’ or ‘ghost’ oscillators having the spectroscopic rather than orbital frequencies ... The introduction of these virtual resonators is, to be sure, in some ways very artificial, but is nevertheless apparently the most satisfactory way of combining the elements of truth in both the classical and quantum theories. In particular this avoids the otherwise almost insuperable difficulty that it is the spectroscopic rather than the orbital frequencies [which give the positions of the poles in the dispersion formula].”

Kramers already had his dispersion formula around Christmas 1923 when Slater arrived in Copenhagen; only published two short notes on it in 1924 (in *Nature*); his first complete treatment is the Kramers-Heisenberg paper, written over the 1924 Christmas break. Meanwhile Born and Van Vleck had already published a detailed derivation.

Slater to Van Vleck, July 27, 1924: “Kramers hasn't got much done, either. You perhaps noticed his letter to *Nature* on dispersion; the formulas & that he had before I came [and thus before BKS] ... and except for that he hasn't done anything.”

The Kramers dispersion formula (1924)

Van Vleck to Kramers, September 22, 1924: “[my] article was ready to send to the printer about the time we received the copy of Nature containing your dispersion formula. In your note I did not understand you to state how generally you had verified [that the quantum dispersion formula merges with the classical one for high quantum numbers], and it immediately occurred to me that this question could easily be investigated by the perturbation theory method I had previously developed in connection with what I call the “correspondence principle for absorption.” I therefore inserted two sections ... showing that your formula merged into the classical one”

Kramers to Van Vleck, November 11, 1924: “Your note on absorption made me much pleasure and I think it very just of Providence that you got it published before hearing of our work.”

Van Vleck's derivation of the Kramers dispersion formula (1924)

Classical part: perturbation theory in action-angle variables.

Action-angle variables. In general coordinates (x_i, p_i) , Hamilton's equations are:

$$\dot{q}_i = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = -\frac{\partial H}{\partial q_i}.$$

Given the Hamiltonian of a system, one can often find special coordinates (w_i, J_i) (**J : action; w : angle**) such that Hamilton's equations take on the simple form:

$$\dot{w}_i = \frac{\partial H}{\partial J_i} = \nu_i, \quad \dot{J}_i = -\frac{\partial H}{\partial w_i} = 0.$$

$w_i = \nu_i t$ gives the characteristic frequencies of the system; $J_i = H/\nu_i$ is subject to the Bohr-Sommerfeld quantization condition: $J_i = \int p_i dq_i = n_i h$.

Consider some periodic system (example: charged harmonic oscillator) perturbed by a weak electromagnetic field. Hamiltonian: $H = H_0 + H_{\text{int}}$ with $H_{\text{int}} = eEx \cos 2\pi \nu t$. Calculate the coherent part of the displacement Δx caused by the perturbation (the part responsible for dispersion).

Van Vleck's derivation of the Kramers dispersion formula (1924)

Classical part (continued): Calculate the coherent part of the displacement Δx caused by the perturbation $H_{\text{int}} = eEx \cos 2\pi \nu t$

1. Assume that the *unperturbed* system can be solved in action-angle variables:

Fourier expansion: $x(t) = \sum_{\tau} A_{\tau}(J) e^{2\pi i w} \quad [\text{recall: } w_i = \nu_i t]$

2. Use Hamilton's equations in action-angle variables (for H_{θ}) to calculate Δw and ΔJ :

$$\Delta w = \int \dot{\Delta w} dt = \int \frac{\partial H_{\text{int}}}{\partial J} dt, \quad \Delta J = \int \Delta \dot{J} dt = - \int \frac{\partial H_{\text{int}}}{\partial w} dt.$$

3. Insert Δw and ΔJ into $\Delta x = (\partial x / \partial w) \Delta w + (\partial x / \partial J) \Delta J$ and focus on coherent terms (i.e., terms with factor $e^{2\pi i \nu t}$).

Result: $\Delta x_{\text{coh}}(t) = 2eE \frac{\partial}{\partial J} \left(\frac{\nu_0}{\nu^2 - \nu_0^2} |A_{\tau}(J)|^2 \right) \cos 2\pi \nu t.$

Reduces to simple expression for charged harmonic oscillator found earlier:

Van Vleck's derivation of the Kramers dispersion formula (1924)

Quantum part: translate classical formula into quantum formula using the correspondence principle.

(i) **derivatives $\rightarrow$ difference quotients:** $\left. \frac{\partial F}{\partial J} \right|_{J=r\hbar} \rightarrow \frac{1}{\hbar}(F(r+1) - F(r))$

- Called 'Born correspondence rule' but found earlier by both Kramers and Van Vleck.

- Earliest example: Bohr frequency condition: $\nu_r = \left. \frac{\partial H}{\partial J} \right|_{J=r\hbar} \rightarrow \nu_r = \frac{1}{\hbar}(E_{r+1} - E_r)$

(ii) **amplitudes $\rightarrow$ transition probabilities:** $|A^{r+1}|^2 \rightarrow A_{r+1 \rightarrow r}$
(Einstein coefficients introduced by Ladenburg)

(iii) **orbital frequencies $\rightarrow$ transition frequencies:** ν_0 (ν_i in general) $\rightarrow \nu_{n \rightarrow m}$.

Basic idea: Formulae are constructed so that they merge with their classical counterparts for *large* quantum numbers. Take the leap of faith that the formulae constructed this way will hold *for all* quantum numbers!

Van Vleck's derivation of the Kramers dispersion formula (1924)

Quantum part (continued):

- (i) derivatives $\rightarrow$ difference quotients:
- (ii) amplitudes $\rightarrow$ transition probabilities:
- (iii) orbital frequencies $\rightarrow$ transition frequencies

Classical formula: $\Delta x_{\text{coh}}(t) = 2eE \frac{\partial}{\partial J} \left(\frac{\nu_0}{\nu^2 - \nu_0^2} |A_{\tau}(J)|^2 \right) \cos 2\pi \nu t.$

Quantum formula (special case of charged harmonic oscillator):

$$P_r \propto \frac{A_{r+1 \rightarrow r}}{\nu_{r+1 \rightarrow r}^2 (\nu_{r+1 \rightarrow r}^2 - \nu^2)} - \frac{A_{r \rightarrow r-1}}{\nu_{r \rightarrow r-1}^2 (\nu_{r \rightarrow r-1}^2 - \nu^2)}$$

Quantum formula (general case: charged non-degenerate multiply-periodic system):

$$P_r \propto \sum_{s > r} \frac{A_{s \rightarrow r}}{\nu_{s \rightarrow r}^2 (\nu_{s \rightarrow r}^2 - \nu^2)} - \sum_{t < r} \frac{A_{r \rightarrow t}}{\nu_{r \rightarrow t}^2 (\nu_{r \rightarrow t}^2 - \nu^2)}$$

From Kramers dispersion formula to Heisenberg's Umdeutung

Kramers dispersion formula

$$P_r \propto \sum_{s > r} \frac{A_{s \rightarrow r}}{v_{s \rightarrow r}^2 (v_{s \rightarrow r}^2 - v^2)} - \sum_{t < r} \frac{A_{r \rightarrow t}}{v_{r \rightarrow t}^2 (v_{r \rightarrow t}^2 - v^2)}$$

only depends on transition quantities such as $A_{i \rightarrow f}$ and $v_{i \rightarrow f}$.

Heisenberg's *Umdeutung* [reinterpretation]. Get rid of orbits, focus on transitions.

1. Apply correspondence principle* to the starting point of the classical calculation (Fourier expansion of x)** rather than to its end result (classical dispersion formula).

*Three replacements: (i) derivatives $\rightarrow$ difference quotients; (ii) amplitudes $\rightarrow$ transition probabilities; (iii) orbital frequencies $\rightarrow$ transition frequencies.

** $x(t) = \sum_{\tau} A_{\tau} e^{2\pi i \omega_{\tau} t} \rightarrow$ array of numbers involving $A_{i \rightarrow f}$ and $v_{i \rightarrow f}$

2. Replace position x in classical mechanics by array of numbers representing position in the new theory.
3. Apply correspondence principle to Bohr-Sommerfeld condition to find new quantum condition. Result: **Thomas-Kuhn(-Reiche) sum rule** (high-frequency limit of the Kramers dispersion formula). Born and Jordan subsequently extracted the familiar position-momentum commutation relations, $[x, p] = i\hbar$, from the sum rule.

From Kuhn's AHQP interview with Heisenberg



Kuhn (talking about virtual oscillators in BKS but those are just the substitute oscillators of Ladenburg and Reiche): “... one transforms one's idea of the atom [from a system of quantized orbits] into a collection of virtual oscillators that operate between states.”

Heisenberg: “Yes, that was it ... this idea of an atom being a collection of oscillators was in some way contrary to the idea of an electron moving around a nucleus. The obvious connection, the only possible connection, was that the Fourier components of this motion in some way corresponded, as Bohr said, to the oscillators. But certainly this paper [BKS] then prepared the way for this later idea that the assembly of oscillators is nothing but a matrix ... In this way, you can say that matrix mechanics was already contained in this paper [BKS].”

Werner Heisenberg (1901–1976)

**Ernst Zimmer, *Umsturz im Weltbild der Physik* [The revolution in physics] (1934):
Matrix mechanics as a theory about virtual oscillators**



“The state of an atom should no longer be described by the unobservable position and momentum of its electrons, but by the measurable frequencies and intensities of its spectral lines ... Regardless of the nature of the real musicians who play the optical music of the atoms for us, Heisenberg imagines auxiliary musicians [*Hilfsmusiker*]: every one plays just one note at a certain volume. Every one of these musicians is represented by a mathematical expression, q_{mn} , which contains volume and frequency of the spectral line as in expressions in acoustics familiar to physicists. These auxiliary musicians are lined up in an orchestra [*Kapelle*] according to the initial and final states n and m of the transition under consideration. The mathematician calls such an arrangement a “matrix.””

Werner Heisenberg (1901–1976)

From Kuhn's AHQP interview with Heisenberg



Kuhn: “Using the Kuhn-Thomas [sic] rule is a stroke of genius but one supposes that there were a lot of other intermediate attempts.”

Heisenberg: “No, I would say it was rather trivial for the following reasons: ... I felt that perhaps only the difference of integral pdq between one quantum state and the next quantum state is an important thing [cf. the Bohr-Sommerfeld condition $\oint pdq = nh$]. So I actually felt, “Well, perhaps I should write down integral pdq in one state minus integral pdq in the neighboring state.” Then I saw that if I write down this and try to *translate it according to the scheme of the dispersion theory*, then I get the Thomas-Kuhn sum rule. And that is the point. Then I thought, “Well, that is apparently ... how it is done.”” [my emphasis]

Werner Heisenberg (1901–1976)

Conclusions

At the End of the Rainbow: Optical Dispersion as the Bridge between the Old Quantum Theory and Matrix Mechanics

- Matrix mechanics grew directly out of dispersion theory; the Bohr-Kramers-Slater theory was only a sideshow.
- The ‘virtual oscillators’ of BKS are just the ‘substitute oscillators’ of the dispersion theory of Ladenburg and Reiche.
- Dispersion theory could play such a central role in the transition from the old quantum theory to matrix mechanics because the discrepancy between orbital frequencies and radiation frequencies in the Bohr model manifested itself glaringly and unavoidably in this area.

Take-home lesson: why did Van Vleck not do what Heisenberg did? He had the Kramers dispersion formula and the Thomas-Kuhn sum rule in the summer of 1924.



Van Vleck (biographical note accompanying his Nobel lecture): “I was fortunate in being offered an assistant professorship at the University of Minnesota [Fall 1923]... with purely graduate courses to teach. This was an unusual move by that institution, as at that time, posts with this type of teaching were usually reserved for older men, and recent Ph.D.’s were traditionally handicapped by heavy loads of undergraduate teaching which left little time to think about research.”

Q: What did Van Vleck do with all this research time?

A: He wrote a 300-page review article on the old quantum theory.

J. H. Van Vleck, *Quantum Principles and Line Spectra*. Bulletin of the National Research Council 10, Part 4. Washington, D.C.: National Research Council, 1926.