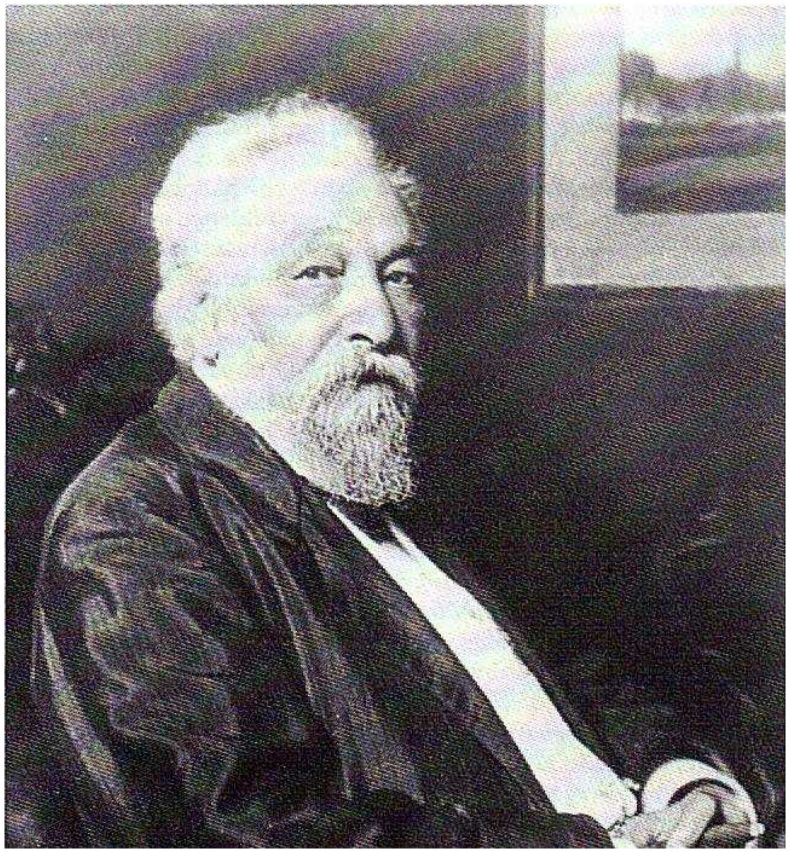
SCHRÖDINGER'S OEUVRE

This talk is not about Schrödinger's life story, interesting though it may be. I am by no means a historian, and there is a very good book about Schrödinger's life an work by Walter Moore. Here, I'll concentrate on some of Schrödinger's scientific work.

However, here are a few details about his life:

- Born in Vienna in August 1887. Father Rudolf, mother Georgine Bauer.
- Entered the university of Vienna in 1906. Principal lecturers: Franz Exner and Fritz Hasenöhrl. Supervised by Exner on conduction of electricity on surfaces in moist air.
- Military service 1908, and volunteered for one year in the fortress artillary in 1910.
- Assistantship in experimental physics with Exner in 1911, but supervised by Kohlrausch.

- Habilitation in 1914 on ‘The kinetics of dielectrics; the melting point, pyro- and piezo electricity.’
- Autumn 1913, 85th meeting of German Scientists and Physicians, in Vienna. Einstein was a speaker.



It is obviously impossible to discuss all of Schrödinger's work. Instead, I'll discuss just a number of his published articles. These are the articles articles I intend to cover:

1. Zur kinetschen Theorie des Magnetismus. (Einfluss der Leitelektronen). 1912.
2. Zur Dynamik elastisch gekoppelter Punktsysteme.
Ann. Phys. 1914.
3. Die Ergebnisse der neueren Forschung über Atom- und Molekularwärmen. Die Naturwissenschaften, 1917.

4. Über die Rotationswärme des Wasserstoffs.
Zs. für Physik, 1924.

5. Zur Einsteinschen Gastheorie. Phys. Zs., 1926.

6. Quantisierung als Eigenwertproblem I-IV. Ann. Phys. 1926.

7. Probability Problems in Nuclear Chemistry. Proc. Royal Irish Acad. 1945.

8. The Foundation of the Theory of Probability. Proc. Royal Irish Acad., 1947.

Zur kinetischen Theorie des Magnetismus. (1912)

Here Schrödinger attempts to formulate a theory for diamagnetism of metals like Cu, Pb, Bi, and Ag. Earlier, Langevin had derived a formula for the diamagnetic susceptibility of dielectrics, in which he attributed the diamagnetism to the angular momentum of bound electrons. His formula reads:

$$\chi = -\frac{1}{6}\frac{e^2 n}{mc^2}\langle r^2\rangle,$$

where $\langle r^2\rangle$ is the average radius squared of the electron orbit, and n is the electron density.

Using the law of Biot and Savart for the induced magnetic field of a rotating charge,

$$\vec{H} = \frac{e}{r^3}\vec{v} \times \vec{r},$$

Schrödinger essentially obtains the same formula for conduction electrons:

$$\chi_f = -\frac{1}{3}\frac{e^2}{mc^2}\lambda^2 n,$$

where λ is the mean free path of the electrons. In this case, he argues that the path of the electrons is curved due to the magnetic field, giving rise to an angular velocity, which induces a magnetic field. In an an appendix, he shows that the Maxwell-Boltzmann velocity distribution is unaffected by the magnetic field, and he uses this distribution of $\langle v^2 \rangle$ to obtain the average curvature of the electron orbits. The mean free path determines the length of the arcs. His results are in general much larger than the measured values.

In fact, one year earlier (1911), Bohr, in his doctoral thesis, had derived that *classically*, an external magnetic field *cannot* induce a magnetic moment in a system of charges. This result remained virtually unnoticed, however, and was rediscovered 8 years later by Van Leeuwen. It is now known as the Bohr-Van Leeuwen Theorem. The argument is as follows: The equilibrium distribution in phase space is given by

$$d\mathbb{P}(\vec{r}_1, \ldots, \vec{r}_N; \vec{p}_1, \ldots, \vec{p}_N)$$

$$= \frac{1}{Z_N} e^{-\beta\mathcal{H}(\vec{r}_1, \ldots, \vec{r}_N; \vec{p}_1, \ldots, \vec{p}_N)} d\vec{r}_1 \ldots d\vec{r}_N d\vec{p}_1 \ldots d\vec{p}_N.$$

The kinetic part of the Hamiltonian is given by $\mathcal{H}_{\rm kin} = \sum_{i=1}^N \frac{p_i^2}{2m}$. In the presence of an external magnetic field H this changes to

$$\mathcal{H}_{\rm mag} = \sum_{i=1}^N \frac{1}{2m}\left(\vec{p}_i + \frac{e}{c}\vec{A}(\vec{r}_i)\right)^2 .$$

Since $\vec{A}$ depends only on the coordinates, however, we can make a change of variables and find that the velocity distribution is unchanged, just as Schrödinger claimed.

But, the induced field, according to Biot and Savart depends linearly on the velocities, not their squares! It follows that it is also unchanged, i.e. there is no induced field.

Diamagnetism, just like other forms of magnetism, is therefore a purely quantum mechanical phenomenon! The correct expression for the diamagnetic susceptibility was derived by Landau in 1930. It is a consequence of the quantisation of the orbits.

Note that Langevin's derivation in the case of dielectrics is also classical. Nevertheless, it is correct provided $\langle r^2 \rangle$ is computed quantum mechanically. Similarly, the reason that Schrödinger's formula yields such poor results is not the quantisation of the orbits, but the fact that the Boltzmann distribution has to be replaced by the Fermi distribution. This is analogous to the fact that that the Drude-Lorentz formula for the conductivity has to be replaced by the Sommerfeld formula.

Zur Dynamik elastisch gekoppelter Punktsysteme.

In 1914, Schrödinger considered a simple 1-dimensional system of point masses with harmonic forces between nearest-neighbours. It is described by the equations

$$m\frac{d^2\xi_n}{dt^2} = f(\xi_{n+1} - \xi_n) - f(\xi_n - \xi_{n-1}); \quad (n \in \mathbb{Z}).$$

Here, the ξ_n are the deviations from equilibrium positions at distances a. The traditional way to solve this system is by

Fourier analysis: a general solution is a linear combination of the running waves $\xi_n = a_n e^{i(\nu' t + n\varphi)}$, but Schrödinger proposed a new method. He defined new variables x_n by

$$x_{2n} = \sqrt{m}\dot{\xi}_n, \quad x_{2n+1} = \sqrt{f}(\xi_n - \xi_{n+1}).$$

Writing

$$\nu = 2\sqrt{\frac{f}{m}},$$

the equations of motion become

$$\frac{dx_{2n}}{dt} = -\frac{1}{2}\nu(x_{2n+1} - x_{2n-1}).$$

On the other hand, by definition,

$$\frac{dx_{2n+1}}{dt} = -\frac{1}{2}\nu(x_{2n+2} - x_{2n}).$$

Hence, for all n,

$$\frac{dx_n}{dt} = -\frac{1}{2}\nu(x_{n+1} - x_{n-1}).$$

He then remarked that these are precisely the recursion relations for the Bessel functions J_n. Thus, a particular solution is given by

$$x_n = x_k^0 J_{n-k}(\nu t).$$

Since k and x_k^0 are arbitrary, a general solution can be written as

$$x_n(t) = \sum_{k \in \mathbb{Z}} x_k^0 J_{n-k}(\nu t).$$

A particular example is the case where at $t = 0$ all points are at rest, and $\xi_n = 0$ for $n \neq 0$, whereas $\xi_0 = \epsilon$. Then

$$x_n = \epsilon \sqrt{f}(J_{n-1}(\nu t) - J_{n+1}(\nu t)),$$

and

$$\xi_l = \int_0^t \dot{\xi}_l dt = \epsilon J_{2l}(\nu t).$$

This shows that the initial disturbance *does not* move like a wave with a given speed, as in a continuous medium. For large times, $J_n(\nu t) \sim \sqrt{\frac{2}{\pi\nu t}} \cos\left(\nu t - \frac{2n+1}{4}\pi\right)$, so the wave is damped with a factor $1/\sqrt{t}$. Note that *all* points start moving *instantaneously* at $t = 0$, though extremely slowly for large n. Appreciable movement occurs only after a time comparable to the distance al divided by the wave velocity $\frac{1}{2}a\nu$, i.e. $2l/\nu$. Schrödinger then analyses what initial disturbances would give rise to wave solutions similar to those in a continuum. He expands the solution in a Taylor series, and using the recursion relations, finds:

$$x_n = \sum_{k=0}^{\infty} \frac{(\nu t)^k}{2^k k!} \Delta_n^{(k)},$$

where $\Delta_n^{(k)} = \Delta_{n-1}^{(k-1)} - \Delta_{n+1}^{(k-1)}$ are the finite differences, with $\Delta_n^{(0)} = x_n^0$. Rewriting this in terms of ξ_n yields a formula which is similar in form to a Taylor expansion of d'Alembert's solution of the wave equation. He concludes that the solution for the system of points is similar to that of the wave equation provided the initial disturbance varies slowly compared to the distance a between point masses. However, even in that case, the solution eventually becomes different from a wave at large times.

Further details about his life:

- Sent to the Italian front during World War I. Nevertheless managed to complete some work on Millikan's experiment.
- In 1915 he distinguished himself during more serious fighting. Became *Oberleutnant*. Transferred to Vienna in 1917 to teach meteorology.
- Married Annemarie Bertel in 1920; obtained assistantship in Jena.
- Moved to Stuttgart in 1921; then to Breslau as *Ordinarius* (full professor).

- Obtained a professorship in Zürich shortly after arriving in Breslau, but fell ill and had to recover in Arosa, near Davos.

Zur Theorie der Fall- und Steigversuche an Teilchen mit Brownscher Bewegung. Physikalische Zeitschrift 16 (1915).

An interesting application of Brownian motion to the Millikan experiment to determine the electron charge. Some doubt had been raised by other experimenters, but Schrödinger argues that they had underestimated the errors due to Brownian motion. The distribution of the position of a particle under

Brownian motion is of course Gaussian:

$$\rho(x,t) = \sqrt{\frac{\alpha}{\pi t}} e^{-\frac{\alpha x^2}{t}} dx.$$

But during the experiment, the distance is fixed and the time crossing it is measured. With average velocity v, Schrödinger shows that the correct solution of the diffusion equation

$$\frac{1}{4\alpha}\frac{\partial^2 \rho}{\partial x^2} = \frac{\partial \rho}{\partial t}$$

is:

$$4\rho_w(x,t) = N\sqrt{\frac{\alpha}{\pi t}}\left(e^{-\frac{\alpha x^2}{t}} - e^{4\alpha l v}e^{-\frac{\alpha(x-vt)^2}{t}}\right).$$

This is the probability distribution of the particles that have not yet reached $x = l$, and satisfies the boundary condition $\rho_w(l-vt,t) = 0$. Integrating from $-\infty$ to $l-vt$ we get

$$\frac{N}{\sqrt{\pi}}\left[\int_{-\infty}^{(l-vt)\sqrt{\alpha/t}} e^{-y^2}dy - e^{4\alpha l v}\int_{-\infty}^{-(l+vt)\sqrt{\alpha/t}} e^{-y^2}dy\right].$$

Differentiating, we get the probability of first passage between t and $t + dt$:

$$p(t)dt = l\sqrt{\frac{\alpha}{\pi}}e^{-\frac{\alpha(l-vt)^2}{t}}t^{-\frac{3}{2}}dt.$$

Schrödinger then derives expressions for the most probable α and v given a series of measurements $t_1, \ldots, t_n$, as well as their standard deviations. They show that one needs a considerable number of observations to reduce the error.

Die Ergebnisse der neueren Forschung über Atom- und Molekularwärmen. Die Naturwissenschaften, 1917.

This is Schrödinger's first article about quantum theory. It concerns the problem of the decrease of the specific heat at low temperatures. He came back to this problem in several subsequent articles. (In particular a review article in Handbuch der Physik 10, 1926: "Spezifische Wärme".) This article is basically a review article about the work of Einstein and Debye. It concerns the variation of the heat capacity of solids with the temperature. It follows from the kinetic theory of gases that the energy of a system in equilibrium divides equally over all degrees of freedom. For an ideal gas,

$$p = \frac{1}{3} n m v^2 = \frac{2}{3} \frac{N}{V} \epsilon_{\mathrm{kin}} = 2 \frac{N}{V} f(T),$$

if $f(T)$ is the energy per degree of freedom. It follows that $f(T) = \frac{1}{2} \frac{R}{N} T$. For a solid, there are also potential energy degrees of freedom, and the specific heat is therefore

$$c_V = 3\, R.$$

This is known as the Law of Dulong and Petit. It is roughly correct for many solids, but fails for the lighter solids, e.g. Carbon, Beryllium, Boron. Einstein reasoned that one can apply Planck's quantisation rule to the degrees of freedom of a solid in the same way as Planck did for black-body radiation. The energy per degree of freedom is then reduced to

$$\frac{RT}{N}\frac{\Theta/T}{e^{\Theta/T}-1},$$

where $\Theta = \frac{Nh\nu}{R}$. Thus high-frequency degrees of freedom are suppressed. Assuming a single dominant frequency for a given solid, Einstein obtained, by differentiation,

$$c_V = 3R\frac{(\Theta/T)^2 e^{\Theta/T}}{(e^{\Theta/T} - 1)^2}.$$

Adjusting the value of Θ leads to reasonable agreement with experiment. A further improvement was made by Debye, and in a different way by Born and Karman, introducing a spectrum of frequencies.

Über die Rotationswärme des Wasserstoffs.

The specific heat of molecular hydrogen is particularly puzzling. Schrödinger quotes Eucken, Scheel and Heuse, who found that the specific heat of gaseous hydrogen falls from $5R/2$ at room temperature, to $3R/2$ at 60 K. This is clearly due to the 'freezing out' of rotational degrees of freedom. Indeed, for any diatomic gas, the partition function can be written as

$$Z = Z_{\rm trans} Z_{\rm rot} Z_{\rm vib} Z_{\rm elec}.$$

The electronic contribution is negligible in most gases. The vibrational contribution is given by

$$Z_{\text{rot}} = \sum_{l=0}^{\infty} (2l + 1) \exp[-l(l + 1)\Theta/T].$$

For all gases except hydrogen, $\Theta \ll T$ for all available temperatures, so the sum can be replaced by an integral. Writing

$y = l(l+1)$ we get

$$Z_{\mathrm{rot}} \approx \int_0^\infty e^{-y\Theta/T} dy = \frac{\Theta}{T}.$$

This gives a contribution $C_{rmrot} = R$ to the specific heat, in addition to the normal $\frac{3}{2}R$ due to translational motion. In hydrogen, however, $\Theta \approx 84$ K, so for low temperatures, Z_{rot} reduces to the first term $(l = 0)$ and there is no rotational contribution. In the intermediate regime, however, the agreement with experiment is poor! Schrödinger suggested a partial solution to this problem. It had been proposed by Kratzer (1922) and Kramers and Pauli (1923), that the electrons in hydrogen contribute a half-integer times $\hbar$ to the angular momentum. The total angular momentum J would then replace l and $J = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots$. This leads him to

$$Z = g_1 e^{-\Theta'/T} + g_2 e^{-9\Theta'/T} + g_3 e^{-25\Theta'/T} + \ldots$$

He leaves the multiplicities arbitrary, but $g_1 : g_2 : g_3 = 1 : 2 : 4$ seems to give reasonable agreement with experiment.

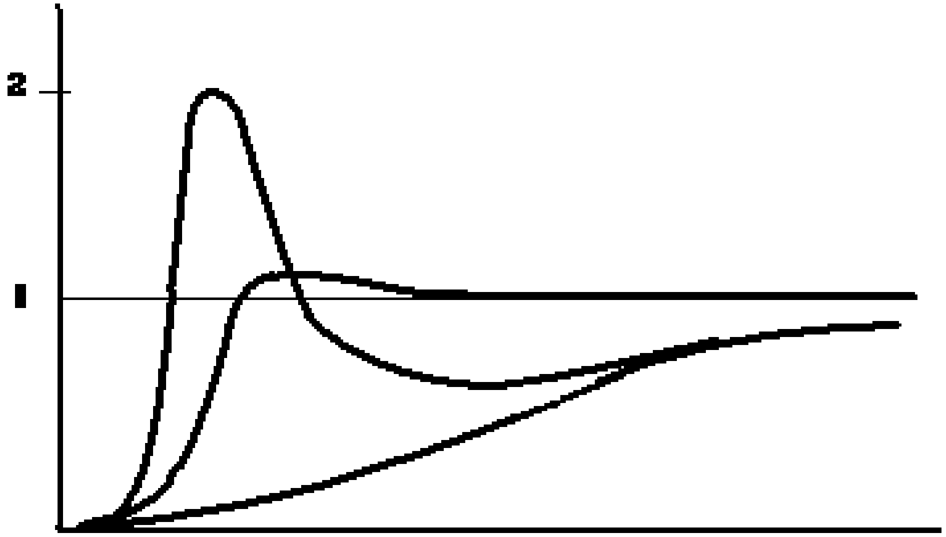
Of course, this theory is wrong. The electron spin was only properly understood in 1925. It is independent of the rotational angular momentum and gives a negligible contribution as remarked above. However, the nuclear spins do have an important effect however, due to the Pauli exclusion principle. The two spins of the hydrogen nuclei can be aligned or anti-aligned. The singlet state is anti-symmetric, and has to be combined with a symmetric rotational state, i.e. $j = 0, 2, 4, \ldots$. The triplet states are symmetric and combine with $j = 1, 2, 3, \ldots$.

Hence,

$$Z_{\text{rot}} = \sum_{l=0,2,4,\ldots} (2l+1)e^{-l(l+1)\Theta/T} + 3 \sum_{l=1,2,3,\ldots} (2l+1)e^{-l(l+1)\Theta/T}.$$

Remarkably, this result does not agree with experiment either! In fact, the two spin states do not exchange in collisions, and the contributions to the specific heat are independent:

$$C_{\text{V,rot}} = \frac{3}{4}C_{\text{V,ortho}} + \frac{1}{4}C_{\text{V,para}}.$$



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Zur Einsteinschen gastheorie.

This article was published in December 1925, the year before Schrödinger formulated his famous wave equation. It contains an alternative derivation of the thermodynamics of the Bose-Einstein gas. Working in the canonical ensemble, he uses Fowler's method of contour integration to take account of the fixed particle number. The partition function is

$$Z = \prod_{s=1}^{\infty} \sum_{n_s=0}^{\infty} e^{-n_s \epsilon_s/(kT)} = \prod_{s=1}^{\infty} \frac{1}{1 - e^{-\frac{\epsilon_s}{kT}}}.$$

(Here s enumerates the 1-particle energy levels.) The total number of particles is $n = \sum_s n_s$. Schrödinger then writes

$$Z = \frac{1}{2\pi i} \oint_{z=0} \prod_{s=1}^{\infty} \frac{1}{1 - z x_s} \frac{dz}{z^{n+1}},$$

where $x_s = \exp[-\frac{\epsilon_s}{kT}]$. He then calculates the integral by the method of stationary phase.

In fact, Schrödinger is doubtful about the predicted phenomenon of Bose-Einstein condensation. Similar doubts were expressed later by Uhlenbeck, but they were eventually resolved by a careful consideration of the thermodynamic limit. More interestingly, he argues that it is not in fact the particles, but rather the degrees of freedom of the matter waves, as introduced by De Broglie, that are quantised. This seems to be a clear prelude to his wave equation. This was an attempt to make waves the basic entities of physics and consider particles simply as “wavecrests” without a true existence by themselves. Max Born resisted this interpretation, insisting that particles were real, and interpreting the waves as probability amplitudes. Schrödinger has never accepted this Copenhagen formulation of quantum mechanics.

More about his life:

- Moved to Berlin in 1927 to succeed Planck.
- Speaks at the famous Fifth Solvay Conference in Brussels. Extensive debate about his interpretation vs. the Copenhagen interpretation. Here Einstein presents his own critique of quantum mechanics and Bohr gives his rebuttal.
- Became a member of the Prussian Academy of Sciences, 1929.
- "Über die kräftefreie Bewegung in der relativistischen Quantenmechanik."
- January 1933, Hitler comes to power. Einstein is in US and

vows never to return to Germany. He becomes professor at the Institute for Advanced Study created by Abraham Flexner.

• F.A. Lindemann in Oxford sets up a fund for Jewish refugees. Schrödinger hears about this and says he would like to come.

• November 1933: arrival in Oxford; Fellow of Magdalen College. News of Nobel Prize with Dirac.

• In May 1934, Hilde March gives birth to his first daughter, Ruth.

• The EPR paper appears in Phys. Rev. prompting Schrödinger to write his extensive review of the current status of quantum mechanics.

• Becomes professor in Graz from March 1936. • Foundation member of the Pontifical Academy of Sciences, 1936.

• In March 1938, *Anschluss* came, and thousands of arrests are made, and lecturers and professors are sacked, among whom his good friend Hans Thirring. Schrödinger is not in immediate danger, but writes a "Confession to the Führer". In August he is dismissed anyway.

• De Valera sends a letter via Whittaker and Born in Edinburgh, inviting him to become Senior Professor at the institute he wants to found in Dublin.

• Erwin and Anny flee to Italy, and stay in the Vatican. From there they go to Geneva with De Valera's help, and then via

Spain back to Oxford.

- Visiting position in Gent (Belgium).
- October 1939, Erwin, Anny, Hilde and Ruth arrive in Dublin and buy a house in Clontarf.

- Temporary professorship at the Royal Irish Academy.

- In 1940, the bill establishing DIAS passes the Dail. Refurbishment of the offices at 64-65 Merrion Square is completed in October.

- First meeting of the Board, November 1940. Schrödinger is elected Director and Heitler is invited to an assistant professorship.

- Starts research on Unified Field Theory, 1942.

Gives statutory public lecturers on “What is Life?”.

- Debacle with Einstein, 1946.

- Visited Innsbruck to get a position in Austria, but this fell through. Vienna was still too dangerous.
- Returned to Vienna in March 1956.
- Died in Alpbach, January 1961.

Probability Problems in Nuclear Chemistry.

(Proc. Royal Irish Acad., Nov. 1945.)

In this curious article, Schrödinger analyses a probabilistic aspect of the atomic bomb. He considers the question when a chance fission would peter out. If each fission gives rise to a neutrons, and the probability of a neutron being removed is η, then on average, the reaction will continue if $a(1-\eta) > 1$ and it will stop if $a(1-\eta) < 1$. However, we need to be *certain* that the reaction will stop! To determine the probability that the reaction stops, call it τ. The probability that exactly s neutrons score hits is

$$\binom{a}{s}(1-\eta)^s\eta^{a-s}.$$

The probability that all these secondary fissions die out is τ^s, and summing over s should give τ:

$$\tau=\sum_{s=0}^{a}\binom{a}{s}(1-\eta)^s\eta^{a-s}\tau^s=[(1-\eta)\tau+\eta]^a.$$

Setting $x = \tau^{1/a}$ and $\zeta = 1 - \eta$, this reads

$$1 - x = \zeta(1 - x^a).$$

This equation has only one solution, $x = 1$ and hence $\tau = 1$ if $\zeta = 1-\eta \leq \frac{1}{a}$, so in that case, the reaction stops with certainty! For $1 - \eta = \frac{1}{a}(1 + \delta)$ with $\delta > 0$ small, he finds

$$\tau \approx 1 - \frac{2a}{a-1}\delta.$$

Next, he remarks that η will in fact depend on the position within the reacting body where the neutron is produced. He therefore generalises the above equations to

$$1 - x(\vec{r}) = \int f(\vec{r}, \vec{r}')(1 - x(\vec{r}')^a)dv',$$

where $f(\vec{r}, \vec{r}')dv'$ is the probability that a neutron produced at $\vec{r}$ scores a hit in a volume dv' around $\vec{r}'$. Assuming that f is symmetric, this equation has as only solution $\tau(\vec{r}) = 1$ if $a \leq \lambda$, where λ is the lowest eigenvalue of the equation

$$\rho(\vec{r}') - \lambda \int \rho(\vec{r}) f(\vec{r}, \vec{r}') dv = 0.$$

Irreversibility. (Proc. RIA 53, 1949.)

In this article Schrödinger argues that irreversibility can be explained on entirely probabilistic grounds, and does not need quantum mechanics, as suggested by Max Born. He illustrates this with a curious example of a prisoner serving a long sentence, who is being offered a chance to be set free, but with on the other hand a chance of being put to death. An urn contains 91 counters, 81 of which have a 4 on one side and a 3 on the other, 9 have a 3 on one side and a 2 on the other, and one has a 2 on one side and a 1 on the other. He has to pick one at random and toss it up in the air. Whatever number comes up, he has to guess the number on the reverse side. If he guesses right, he is set free, otherwise he is executed. But at every stage, he is allowed to quit. He agrees to play, and a 2 comes up. He is just about to shout 3, when the gaol keeper advises him to think first. Then it occurs to him that if it is indeed a 2/3 counter, it could equally well have landed on the 3 side, so he might be wrong with probability 1/2. He therefore declines to answer.