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Dirac (1926) On the Theory of Quantum Mechanics

- Dirac extended his algebraic approach, designed to exploit the Poisson bracket structure of QM

c-numbers Vs q-numbers

(classical, commuting) (quantum, queer)

$ab = ba$ $ab \neq ba$.

- In 1926 had reached a dead end. Clear he had stuck too closely to classical theory (see §3).
- Schrödinger's theory showed the way forward.
- Dirac was unencumbered by overattachment to matrix mechanics — q-numbers more general / abstract.
- Quickly made progress by forging links with his Poisson bracket approach.

<u>In this paper</u>

§2 Time-dependent Schrödinger equation (a first)
Matrix representation of dynamical variables / solutions.

§3 Many particle systems

§4 Antisymmetric (Fermi-Dirac) Vs Symmetric (Bose-Einstein)

§5 Permutation Theory
Application to absorption ⇒ B coefficients.
(Prelude to Emission & Absorption)

The transformation:

q-numbers defined algebraically
having matrix representations $x(mn)$
become functions operating on solutions
to a wave equation $F\psi = 0$.

$$x(mn) \longrightarrow \quad x\psi_n = \sum_m x_{mn}\psi_m .$$

The crucial realisation:

conjugate variables p_r, $-W$ are <u>differential operators</u>.

$$p_r = -i\hbar\frac{\partial}{\partial q_r}, \quad -W = i\hbar\frac{\partial}{\partial t}. \qquad (2)$$

These operate from the left. Only in special cases do identities hold i.e. the commutation relations.

$$(q_r p_s - p_s q_r)X = i\hbar\delta_{rs}X \quad \text{for any } X.$$

In general, $a=b \Rightarrow [a,X] = [b,X]$.

So we preserve the results of the previous theory.

Dirac proceeds to build something that closely resembles modern quantum theory.

linear operator $\rightarrow F\psi = 0$ (5)

$$\left[\left\{ H\left(q_r, i\hbar\frac{\partial}{\partial q_r}\right) - W \right\} \psi = 0 \quad (1) \right]$$

$$\psi = \sum c_n \psi_n$$ ← linear in ψ_n's (eigenfunctions)

Notes that eigenfunctions may be continuously indexed $\psi(a)$

$$\Rightarrow \psi = \int c_a \psi(a)\, da$$

(Hints at Dirac delta in footnote - "limit of quantities")

Let $[a, F] = 0$ (so that a is constant of motion)

$$[a, F]\psi_n = 0$$

$$\Rightarrow F a \psi_n = a F \psi_n$$ i.e.

Since we can bring a inside the operator F, $a\psi_n$ is also a solution

$$\Rightarrow a\psi_n = \sum_m \psi_m a_{mn}$$ ← linear decomposition of a.

$$ab\psi_n = a\sum_m \psi_m b_{mn} = \sum_{mk} \psi_k a_{km} b_{mn}$$ ← matrix element of ab.

$$ab(kn) = ab(km; mn)$$ ← Old rule

becomes $(ab)_{kn} = \sum_m a_{km} b_{mn}$ since $ab\psi_n = \sum_k \psi_k (ab)_{kn}$

Heisenberg's theory :

F is time independent, $[W,F]=0$.

$$W\psi_n = W_n \psi_n \qquad \text{diagonal matrix elements} \qquad (7)$$

Expand $x(q_r, p_s)$ in terms of eigenfunctions

$$x\psi_n = \sum_m x_{mn}\psi_m \qquad x_{mn} \text{ are complex functions of } t$$

$$\begin{aligned} W x\psi_n &= \textstyle\sum_m W x_{mn}\psi_m \qquad \text{Heisenberg eqn. of motion for } x. \\ &= \textstyle\sum_m (W x_{mn} - x_{mn}W)\psi_m + \sum_m x_{mn} W\psi_m \\ &= \textstyle\sum_m i\hbar \dot{x}_{mn}\psi_m + \underbrace{\sum_m x_{mn} W_m \psi_m}. \qquad (9) \end{aligned}$$

$$\qquad \qquad \qquad \qquad \parallel$$

$$W_n \sum_m x_{mn}\psi_m. \qquad \text{l.h.s above}$$

$$\Rightarrow \sum_m i\hbar \dot{x}_{mn}\psi_m = W_n \sum_m x_{mn}\psi_m - W_m \sum_m x_{mn}\psi_m$$

$$\Rightarrow \quad i\hbar \dot{x}_{mn} = x_{mn}(W_n - W_m)$$

$$\Rightarrow i\hbar \frac{d}{dt}\left(a_{mn} e^{i(W_m - W_n)t/\hbar}\right) = a_{mn} e^{i(W_m - W_n)t/\hbar}(W_n - W_m)$$

In order to ensure that matrix elements are "Hermitic" (Hermitian) we need to restrict the form of the expansion.
(Dirac has already noted that this is arbitrary)

Satisfied in case at hand since :

$$\psi_n = u_n e^{-iW_n t/\hbar}$$

bounded $\quad$ not bounded if $W_n^\dagger \neq W_n$.

Only some expansions will satisfy Hermetic property (later self-adjoint operators)

In stationary states:

$$a\psi_n = a_n \psi_n \quad , \quad b\psi_n = b_n \psi_n$$

annotated values (eigenvalues)

We can say that systems in such a state have
<u>definite</u> values for these quantities

[We are remarkably close to the finished form of quantum theory:

1. Eqn. of motion Schrödinger $\Leftrightarrow$ Heisenberg
2. Time dependence $\psi = \psi(0)e^{-iHt}$
3. Observables $A\psi = \sum_n a_n \psi_n$.

What is missing is a way to relate the various expansions.

↳ Dirac and Jordan's "transformation theories" (1927)

Find a way to represent canonical transformations as (what will turn out to be) unitary operators.

Many Particle Systems

- In the old quantum theory (i.e. Dirac's) probabilities are given for particular transitions $m \to n$.
- In a system with two indistinguishable particles, how should the same transition involving <u>different</u> particles be treated?

<u>Either</u> (i) $(mn) \to (m'n') = (nm) \to (n'm')$ (one matrix element)

<u>or</u> (ii) $(mn) \to (m'n') \neq (nm) \to (n'm')$ (two matrix elements)

Dirac rejects (ii) since the theory should "enable one to calculate only observable quantities".

$$\text{But (i)} \Rightarrow x_1(mn; m'n') = x_2(nm; n'm')$$

$$\Rightarrow x_1 = x_2.$$

However, this can't be right since (in general) $x(nm) \neq x(mn)$

$\Rightarrow$ "unsymmetrical functions ... cannot be represented by matrices"

Dirac's "theory of uniformizing variables" can't apply.

$$(mn) \xrightarrow{e^{i(\alpha w)}} (m'n') \xrightarrow{e^{i(\alpha w)}} (m''n'')$$

$$\Rightarrow m'' - m' = m' - m, \quad n'' - n' = n' - n$$

But could have had (since $mn = nm$ (i)

$$m'' - n' = n' - m, \quad n'' - m' = m' - n.$$

Wave mechanics to the rescue:

$$\psi_m(x_1,y_1,z_1,t)\,\psi_n(x_2,y_2,z_2,t) = \psi_m(1)\psi_n(2).$$

[What has changed? Less of a reliance on transitions allowed by system; now imbue electrons with individual properties.]

only one of these

$$\psi_{mn} = a_{mn}\psi_m(1)\psi_n(2) + b_{mn}\psi_m(2)\psi_n(1)$$

$\psi_{mn} = \psi_{nm}$.

Key decision:

Either $\psi_m(1)\psi_n(2) = \psi_m(2)\psi_n(1)$

symmetric

or $\psi_m(1)\psi_n(2) = -\psi_m(2)\psi_n(1)$

antisymmetric

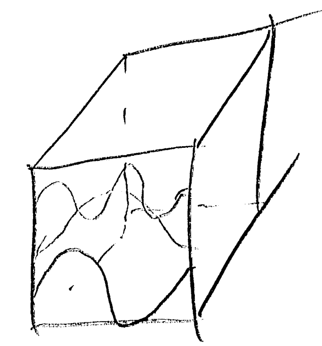
If antisymmetric then $\psi_m(1)\psi_n(2) - \psi_m(2)\psi_n(1) = 0$, so no two particles in the same state.

Application to Ideal Gas

General Solution $\psi_{\alpha_1 \alpha_2 \alpha_3} = e^{i(\alpha_1 x + \alpha_2 y + \alpha_3 z - Et)/\hbar}$

Impose periodic boundary conditions

$$x(0) = x(2\pi) \quad \text{etc.}$$



$$\Rightarrow \quad f(x) = \sum_n a_n e^{inx}.$$

$$f(x))\ \psi_{\alpha_1 \alpha_2 \alpha_3} = \sum_n a_n e^{i(nx + ny + nz - Et)/\hbar}$$

Density of states E to $E + dE$

$$\frac{2\pi}{h^3} (2m)^{3/2} E^{1/2} \, dE$$

(Assume equal a priori probability)

no. molecules, no. waves

symmetric $\Rightarrow$ $N_s = \dfrac{A_s}{e^{\alpha + E/kT} - 1}$ Bose-Einstein

antisymmetric $\Rightarrow$ $N_s = \dfrac{A_s}{e^{\alpha + E/kT} + 1}$ Dirac-Fermi

Second option leads to no Bose-Einstein condensate.