Quantum Probability Theory and Measurement

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ABSTRACT

The probabilistic structure of quantum theory, basic features of quantum information, and the principle of measurement are reviewed. The fascinating interplay between quantum probability and measurement are explored in the context of reduced transition-matrix formalism.

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Quantum Statistics

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7.1 STATISTICS

A. Definition

The mathematics of the collection, organization, and interpretation of numerical data, especially, the analysis of population characteristics by inference from sampling.

B. Statistician

A person specializing in statistics is called a statistician.

We may say that a **statistician** is a number juggler who plays and makes sense out of a large collection of numbers, real or complex.

C. Information Theory

Probability theory for the transmission of messages with specific accuracy when the bits of information constituting the messages are subject to transmission failure, distortion, and accidental additions or omissions with certain probabilities.

7.2 SEQUENCE

A. Definition

A **finite** or **countably infinite sequence**, or briefly a **sequence**, is a set $\{a_n\} \equiv \{a_1, a_2, a_3, \cdots\}$ of elements a_n arranged in order such that for every positive integer n there is associated an element. Each element a_n of the sequence may be a number or a function or a certain mathematical entity. We shall refer to the subscript n of the element a_n as the **index** for

the element.

The definition of sequence may be extended to include a sequence with uncountably infinite elements, in which case the sequence is denoted by

$$\{ b(x) \mid \alpha \le x \le \beta \}$$

where the **index** x may be a real number in the interval $[\alpha, \beta]$. More generally, we may have a sequence consisting of both discrete and continuum parts:

$$\{\, a_n \,;\, b(x) \mid \alpha \le x \le \beta \,\}$$

For notational convenience, we may denote a general sequence symbolically and briefly by $\{a_n\}$ no matter how many elements the sequence has.

B. Probability Sequence

In the following of this subsection, we shall consider only sequences $\{p_i\}$ of non-negative real numbers, in which each element p_i, called the **probability mass** or **density** respectively for discrete and continuum cases, is a non-negative real numbers, *i.e.*, $p_i \geq 0$.

C. Discrete Sequence

A sequence $\{p_{\omega_i}\}$ is said to be **discrete** if the spectrum of the index ω_i is a set of discrete real numbers.

In physics, for a discrete sequence, we shall call p_{ω_i} the probability mass or simply the **probability**.

D. Continuum Sequence

A sequence $\{ D(\omega) \mid a \le \omega \le b \}$ is raid to be **continuum** if the spectrum of the index ω is an interval or intervals of real numbers.

For a continuum sequence, we shall define the probability density or simply the **density** $D(\omega)$, instead of the probability mass p_{ω_i}.

E. A General Sequence

The index ω of an arbitrary sequence may have a spectrum consisting of both **discrete** and **continuum parts**, $\{ p, D \} \equiv \{ p_{\omega_i}, D(\omega) \mid a \le \omega \le b \}$, where the index ω runs through both discrete and continuum values $\{ \omega_1, \omega_2, \omega_3, \cdots ; a \le \omega \le b \}$, and we call p and D, respectively, the probability and density.

F. Normalized Sequence

A sequence $\{p, D\}$ is said to be **normalized** if

$$\sum_i p_i + \int_{-\infty}^{\infty} d\omega\, D(\omega) = 1$$

where for ease of notation we write the probability as $p_i \equiv p_{\omega_i}$, and the density $D(\omega)$ is said to be normalized on the ω-scale.

Probability sequences considered here are always assumed to be normalized.

7.4 OBSERVABLE

A. Definition

The self-adjoint operator Ω associated with a physical quantity ω is called an observable.

For example, the three-dimensional observable $\boldsymbol{X}$ is associated with the position $\boldsymbol{x}$, and the three-dimensional observable $\boldsymbol{P}$ with the momentum $\boldsymbol{p}$, *etc*. Furthermore, the state operator $\Psi \equiv |\psi\rangle\langle\psi|$, which is associated with a pure physical state ψ, is an observable,

and the general state operator $\rho \equiv \sum_{ij} \rho_{ij} |i\rangle\langle j|$, which is commonly known as the **density operator**, is also an observable.

We shall use capital letters Ω, Λ, Σ, Γ, *etc*. to denote an arbitrary observable.

B. Pure Operator

A self-adjoint operator Ω is called a pure operator, if there exists a representation in which this operator may be expressed as the outer product of a vector $|\phi\rangle$ with itself, *i.e.*, $\Omega = |\phi\rangle\langle\phi|$.

C. Mixed Operator

A self-adjoint operator which is not a pure operator is called a mixed operator.

D. State Operator

The self-adjoint operator which provides a **complete description** of the state of a given physical system is called the state operator.

The physical system is in a **pure state** if the state operator is a pure operator and in a **mixed state** if the state operator is a mixed operator.

7.5 ORTHONORMAL BASIS

A. Eigen-Equation of an Observable

The eigen-equation of an observable Ω may be given in the canonical form,

$$\Omega\,|\,\omega_i\rangle = \omega_i\,|\,\omega_i\,\rangle$$

where real values of the set $\{\omega_i\} \equiv \{\omega_1, \omega_2, \omega_3, \cdots\}$ are called **eigenvalues** of Ω. Here the exhaustative set $\{|\,\omega_i\,\rangle\} \equiv \{|\,\omega_1\,\rangle, |\,\omega_2\,\rangle, |\,\omega_3\,\rangle, \cdots\}$ of all linearly-independent normalized vectors $|\,\omega_i\rangle$ are called **eigenvectors** of Ω and are labeled

by their respective eigenvalues ω_i. It is important to note that some of these **distinct** eigenvectors may have equal eigenvalues, in which case, called **degeneracy**, we need additional labels to distinguish different eigenvectors.

B. Degenerate Basis

A degenerate basis is a basis in which two or more linearly-independent basis-vectors have the same set $\{\omega, \lambda, \cdots\}$ of eigenvalues for a given set $\{\Omega, \Lambda, \cdots\}$ of compatible observables.

C. Non-Degenerate Basis

A non-degenerate basis, is also called specifically **distinct basis**, may be provided by the set of all co-eigenvectors $\{|\omega\lambda\sigma\cdots\rangle\}$ of a **complete set** $\{\Omega, \Lambda, \Sigma\cdots\}$ of compatible observables.

D. Distinct Basis

A non-degenerate basis for the Hilbert space is called a distinct basis if each basis-vector of this basis may be uniquely specified by a distinct set, say, $\{\omega, \lambda, \sigma, \cdots\}$ of eigenvalues.

A general distinct basis may consist of both discrete and continuum parts. We however shall use $\{|i\rangle\} \equiv \{|1\rangle, |2\rangle, |3\rangle, \cdots\}$ to represent an arbitrary **distinct basis**, in which the index i denotes symbolically a distinct

set $\{\omega, \lambda, \sigma, \cdots\}$ of eigenvalues for **both** discrete and continuum basis-vectors. The distinct basis $\{|i\rangle\}$ is also assumed to be orthonormal and complete, such that we have

(i) $\langle i | j \rangle = \delta_{ij}$

(ii) $\sum_i |i\rangle\langle i| = I$

for a discrete basis, and

(i) $\langle \boldsymbol{x}' | \boldsymbol{x} \rangle = \delta^3(\boldsymbol{x}' - \boldsymbol{x})$

(ii) $\int d^3x \; |\boldsymbol{x}\rangle\langle \boldsymbol{x}| = I$

for a continuum basis such as $\{|x\rangle\}$, and

(i) $\langle \omega_i | \omega_j \rangle = \delta_{ij}$

$\langle \omega_i | \omega \rangle = 0$

$\langle \omega' | \omega \rangle = \delta(\omega' - \omega)$

(ii) $\sum_i |\omega\rangle\langle \omega_i| + \int_a^b d\omega |\omega\rangle \langle \omega_i| = I$

for a general basis composed of both discrete and continuum basis-vectors: $\{|\omega_i\rangle; |\omega\rangle\}$.

E. The ω-basis of an Observable

From the eigen-equation $\Omega|\omega_i\rangle = \omega_i|\omega_i\rangle$ of an observable Ω, we may construct a basis consisting of all its linearly-independent orthonormal eigenvectors, and we shall call this **complete basis** the eigenbasis of Ω, or simply called the **ω-basis**: $\{|\omega_i\rangle\} \equiv \{|\omega_1\rangle, |\omega_2\rangle, |\omega_3\rangle, \cdots\}$. It is obvious that the observable Ω is diagonal in the ω-basis.

The ω-basis is usually a degenerate basis, in which a single eigenvalue corresponds to more than one eigenvector. We shall group together all linearly-independent eigenvectors with same eigenvalues $\{\omega_a, \omega_b, \omega_c, \cdots\}$ into many individual sets labeled by $a, b, c, \cdots$, and the numbers of degenerate eigenvectors in respective sets are $\{n_a, n_b, n_c, \cdots\}$, *i.e.*, the set α contain n_α eigenvectors, all with the same eigenvalue ω_α.

In other words, the first n_a eigenvectors all have the same degenerated eigenvalue ω_a, the next n_b eigenvectors all have the same eigenvalue ω_b, *etc.* :

$$\omega_a = \omega_1 = \omega_2 = \cdots = \omega_{n_a}$$

$$\omega_b = \omega_{n_a+1} = \omega_{n_a+2} = \cdots = \omega_{n_a+n_b}$$

$$\cdots$$

F. Eigenspaces of an Obervable

The subspace H_a spanned by the first n_a eigenvectors $\{|\omega_1\rangle, |\omega_2\rangle, \cdots, |\omega_{n_a}\rangle\}$ is referred to as the ω_a-eigenspace, and the subspace H_b referred to as the ω_b-eigenspace is similarly defined, and so are the other subspaces.

By defining the projection operator $P_j \equiv |\omega_j\rangle\langle\omega_j|$, we may denote the projection operator P_a for the ω_a-eigenspace H_a as

$$P_a \equiv \sum_j^a P_j$$

where a signifies that the index j runs through the set $\{1,\cdots,n_a\}$. The subsequent sets *b*, *c*, *etc.* are sequentially defined:

$$b \equiv \{n_a+1, n_a+2, \cdots, n_a+n_b\}$$

$$c \equiv \{n_a+n_b+1, n_a+n_b+2, \cdots, n_a+n_b+n_c\}$$

...

Consequently, we have in general,

$$P_\alpha \equiv \sum_j^\alpha P_j \equiv \sum_j^\alpha |\omega_j\rangle\langle\omega_j|$$

where $\alpha =$ a, b, c, *etc*.

In summary, the ω-basis is subdivided into many ω_α-bases, for which we have the n_α-dimensional eigenspace H_α spanned by the ω_α-basis with the projection operator P_α, and the total Hilbert space H is a direct sum of H_a, H_b, H_c, *etc*.:

$$H = \bigoplus_\alpha H_\alpha \equiv H_a \oplus H_b \oplus H_c \oplus \cdots$$

G. Spectral Resolution of an Observable

The spectral resolution of an arbitrary observable Ω has therefore the form,

$$\begin{aligned}\Omega &\equiv \sum_j \omega_j |\omega_j\rangle\langle\omega_j| \\ &\equiv \sum_j \omega_j P_j \\ &= \sum_\alpha \omega_\alpha P_\alpha\end{aligned}$$

where the projection operator $P_j \equiv |\omega_j\rangle\langle\omega_j|$ is a **pure operator** for the one-dimensional space of $|\omega_j\rangle$, while in general the projection

operator $P_\alpha \equiv \sum_j^\alpha P_j$ is a **mixed operator** for the n_α-dimensional eigenspace H_α with $\omega_j = \omega_\alpha$ for j running through the set α.

H. The ρ-Basis of the State Operator

The state operator ρ of a physical system, usually given in an arbitrary non-degenerate **distinct basis** $\{|i\rangle\}$, may be diagonalized in the ρ-basis $\{|p_i\rangle\}$ by considering the eigen-equation of the state opertaor ρ,

$$\rho|p_i\rangle = p_i|p_i\rangle$$

Consequently, the state operator ρ has eigenvalues $\{p_i\}$ and corresponding eigenstates $\{|p_i\rangle\}$, where the eigenvalue p_i

denotes simply the **probability** for the physical system being in the eigenstate $|p_i\rangle$.

For notational convenience, we shall define $Q_i \equiv |p_i\rangle\langle p_i|$ and write the spectral resolution of the state operator ρ as

$$\rho = \sum_i p_i Q_i .$$

I. Randomness of a State Operator

The randomness R of a state operator ρ is defined to be

$$R = -\sum_i p_i \log p_i$$

where $\{p_i\}$ denotes the set of eigenvalues of the state operator ρ.

The randomness R is a dimensionless quantity and has the range, $0 \le R \le \infty$. The entropy S of a physical system in **statistical mechanics** is proportional to the randomness

R as

$$S = kR$$

where k is the Boltzmann constant.

J. Vagueness of a State Operator

The vagueness V of a state operator ρ is defined to be

$$V \equiv \prod_i (p_i^{-p_i}) = e^R$$

which has the range $1 \le V \le \infty$.

It is of interest to note that the vagueness V is proprotaional to the phase-space volume of the physical syatem in **statistical mechanics**.

7.6 RANDOM VARIABLE

A. Definition

A variable Ω which assumes a set $\{\omega_j\} \equiv \{\omega_1, \omega_2, \cdots\}$ of real values ω_j with corresponding probabilities $\{p_j\} \equiv \{p_{\omega_j}\} \equiv \{p_1, p_2, \cdots\}$ is called a random variable.

A **special case** of the random variable is the ordinary **real variable** encountered in calculus for which all probabilities vanish

except for one, such that the variable Ω assumes **only one** real value ω_n at a time with **complete certainty**, *i.e.*, $\{p_j\} = \{\delta_{jn}\}$.

If the set $\{\omega_j\}$ represents a collection of discrete values, the random variable Ω is called specially a **discrete random variable**. A **continuum random variable** is similarly defined, while in general a **random variable**

may assume both discrete and continuum values. Here corresponding to a set of

continuum values $\omega \in [a,b]$, we shall have a set of probability **densities** $\{D(\omega) \mid a \le \omega \le b\}$.

For ease of discussion, we shall treat at times only **discrete** random variables in the following, but results may be extended to both **continuum** and any general random variables.

B. Standardized Random Variable

Let $\{\mu,\sigma\}$ be the **mean** and **deviation** of the random variable Ω. We define the standardized random variable Λ as

$$\Lambda \equiv (\Omega - \mu)/\sigma$$

Consequently, a standardized random variable is dimensionless and has its mean and deviation $\{0,1\}$.

C. Quantum Random Variable Ω_ρ

In quantum mechanics, the random variable Ω_ρ for the measurement Ω of a physical system in state ρ may be defined by a pair of self-adjoint operators, or specifically one observable and one state operator: $\{\Omega, \rho\}$. Here Ω plays the role for the **present measurement**, and ρ for the **previous measurement**, *i.e.*, for the preparation of the state of the physical system, on which the

present measurement is to be performed.

The random variable Ω_ρ assumes the set $\{\omega_\alpha\}=\{\omega_j\}$ of distinct outcomes $\{\omega_\alpha\}$ with corresponding probabilities $\{p_\alpha\}$, where $p_\alpha=\mathrm{tr}\{P_\alpha\rho\}$, and P_α denoted the projection operator for the subspace H_α of the observable Ω. Let the state operator ρ be given in the ρ-basis as

$$\rho=\sum_i p_i Q_i$$

with $Q_i \equiv |p_i\rangle\langle p_i|$, and then we obtain

$$p_\alpha = \sum_i \sum_j^\alpha p_i \, |\langle p_i | \omega_j \rangle|^2$$

As a reminder, the spectral resolution of the observable Ω may be given as

$$\Omega = \sum_\alpha \omega_\alpha \, P_\alpha \equiv \sum_\alpha \omega_\alpha \sum_j^\alpha P_j \equiv \sum_\alpha \omega_\alpha \sum_j^\alpha |\omega_j\rangle\langle \omega_j|$$

7.7 DISTRIBUTION FUNCTIONS

A. Density-Distribution Function

We shall define the density-distribution function, or simply the ***d*-function**, of a **continuum** random variable $\Omega \equiv \Omega(\omega; D)$ for all ω by

$$f(\omega) = D(\omega)$$

The *d*-function of a **discrete** random variable $\Omega \equiv \Omega(\omega; p)$ is given as

$$f(\omega) = \sum_j p_j \, \delta(\omega - \omega_j)$$

where $\delta(x)$ denotes the Dirac - δ function. The d-function of a **general random variable** $\Omega \equiv \Omega(\omega\,;p\,,D)$ is therefore given in the general form as

$$f(\omega) = \sum_j p_j\, \delta(\omega - \omega_j) + D(\omega)$$

B. Mass-Distribution Function

We shall define the mass-distribution function, or simply the ***m*-function**, of a **discrete** random variable $\Omega \equiv \Omega(\omega; p)$ as

$$F(\omega) = \sum_j p_j \, \theta(\omega - \omega_j)$$

where $\theta(\omega - \omega_i)$ denotes the Heaviside function,

$$\theta(x) = \begin{cases} 1, & x \geq 0, \\ 0, & x < 0. \end{cases}$$

The m-function of a continuum random variable $\Omega \equiv \Omega(\omega; D)$ is given as

$$F(\omega) = \int_{-\infty}^{\omega} dx\, D(x)$$

Consequently, the *m*-function of a **general random variable** $\Omega \equiv \Omega(\omega; p, D)$ is give generally as

$$F(\omega) = \sum_j p_j\, \theta(\omega - \omega_j) + \int_{-\infty}^{\omega} dx\, D(x)$$

An *m*-function $F(x)$ has the following general properties:

(i) $F(x)$ is monotonically increasing on the real axis x.

(ii) $F(x)$ is continuous from the right at each point x.

(iii) $F(-\infty)=0$ and $F(\infty)=1$.

C. Relation between *d*- and *m*-Functions

The *d*-function and *m*-function of a random variable Ω are related in calculus as

(i) Density: $$f(\omega) = \frac{dF(\omega)}{d\omega} = \sum_i p_i \, \delta(\omega - \omega_i) + D(\omega)$$

(ii) Mass: $$F(\omega) = \int_{-\infty}^{\omega} dx \; f(x) = \sum_i p_i \, \theta(\omega - \omega_i) + \int_{-\infty}^{\omega} dx \; D(x)$$

7.8 CERTAINTY OF A DISTRIBUTION

A. Definition

For a discrete distribution sequence $\{p_i\}$ of probabilities p_i for N possible results of an event, we shall assign a measure called the **certainty** $C \equiv C\{p_i\}$, which refers to a clear-cut and unequivocal **statement** or **result**, admitting of no doubt or misunderstanding when $C = 1$. On the other hand, for a **completely uncertain** case, for which we

have no sure knowledge such that any one of the N possible results is equally likely, we have the certainty $C = 1/N$. In the case of N approaching infinity, we have the limit $C = 0$. For a composite event which involves two independent sub-events 1 and 2, the certainty C of the composite event is assumed to the **arithmetic product** of respective certainties, $C = C_1 C_2$.

B. Analytic Form of Certainty

For a normalized sequence $\{p_i\}$, we can prove that the **certainty** C of the sequence, which satisfies the stated postulates, is given by

$$C \equiv C\{p_i\} \equiv \prod_i (p_i{}^{p_i})$$

$$\equiv p_1{}^{p_1} p_2{}^{p_2} p_3{}^{p_3} \cdots$$

which generally has the range $0 \le C \le 1$. Here we note that

$$\lim_{p \to 0} p^p = 1$$

7.9 ACCURACY OF A DISTRIBUTION

A. Definition

The ratio of the certainty C of a probability distribution $\{p_i\}$ with respect to the certainty C_0 of a distribution with equal probabilities is defined as the **relative certainty** or simply called the **accuracy** of the distribution $\{p_i\}$,

$$A \equiv A\{p_i\} \equiv C / C_0$$

which has the range $1 \le A \le \infty$.

B. Discrete Accuracy

For a discrete distribution $\{p_i\}$, we have the accuracy

$$A \equiv \prod_{i=1}^{N} (N p_i)^{p_i}$$

where the distribution is normalized as

$$\sum_{i=1}^{N} p_i = 1$$

C. Continuum Accuracy

For a continuum distribution $_{\{D(x)\}}$, we have the accuracy

$$A = \exp\left\{ \int_a^b dx\, D(x) \log[(b-a)\, D(x)] \right\}$$

where the distribution is normalized as

$$\int_a^b dx\, D(x) = 1$$

D. Accuracy of a General Distribution

For a general distribution $\{p_i ; D(x)\}$, we have the accuracy

$$A = \exp\Big\{ \int_a^b dx\, D(x) \log[(b-a)\, D(x)] \Big\} \prod_{i=1}^{N} (N p_i)^{p_i}$$

where the distribution is normalized as

$$\sum_{i=1}^{N} p_i + \int_a^b dx\, D(x) = 1$$

7.10 INTELLIGIBILTY OF A DISTRIBUTION

A. Definition

The difference in the randomness R of a probability distribution $\{p_i\}$ against the randomness R_0 of a distribution with equal probabilities is defined to be the intelligibility I,

$$I \equiv I\{p_i\} \equiv R_0 - R$$

which has range $0 \le I \le \infty$.

B. Discrete Intelligibility

For a discrete sequence $\{p_i\}$, we have the intelligibility,

$$I = \sum_{i=1}^{N} p_i \log(N p_i)$$

C. Continuum Intelligibility

For a continuum sequence $\{D(x)\}$, we have the intelligibility,

$$I = \int_a^b dx\, D(x) \log[(b-a)\, D(x)]$$

D. Intelligibility of a General Distribution

For a general sequence $\{p_i, D(x)\}$, we have the intelligibility,

$$C = \sum_{i=1}^{N} p_i \log(N p_i) + \int_a^b dx\, D(x) \log\left[(b-a)\, D(x)\right]$$

E. Relation between Accuracy and Intelligibility

Accuracy: $A = e^{I}$

Intelligibility: $I = \log A$

Compared with the randomness R and vagueness V of a probability distribution $\{p_i, D(x)\}$, both the accuracy A and intelligibility I are relative quantities with respect to a distribution of equal probabilities, while all four macroscopic indicators $\{R, V; A, I\}$ for the distribution $\{p_i, D(x)\}$ are dimensionless.

Relativistic Quantum Collision Theory for Many-Particle Systems

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ABSTRACT

Starting from the relativistic equation of motion governing quantum collision processes, we shall formulate the relativistic quantum collision theory in an *ab initio* manner. Quantum electrodynamic effects are however incorporated perturbatively. Because heavy projectiles or ultra-high incident energies are considered, the recoil of the target is also treated. Electron-impact ionization of uranium ion U^{91+} and proton-impact ionization of hydrogen will be given as examples.

COLLISION PROCESSES

a) **KINEMATICS**

Polarization correlations

Angular distribution

b) **DYNAMICS**

Relativistic effects

Particle-correlation effects

COLLISION EQUATION

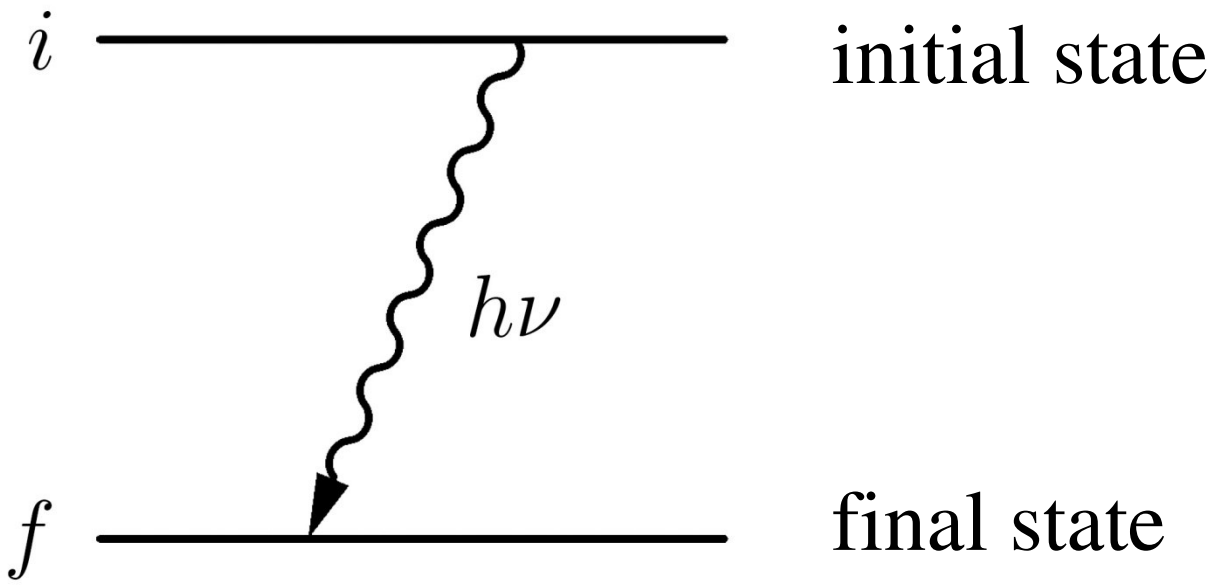
$$\rho_f = S_{fi}\,\rho_i\,S^{\dagger}_{fi}$$

ρ_f : initial state

ρ_i : final state

S_{fi} : Scattering-matrix

PHOTOEMISSION OF AN ATOM



S-MATRIX OF PHOTOEMISSION

$$S(q, J_f M_f; J_i M_i) \equiv \sqrt{\frac{\omega}{2\pi c}} \langle J_f M_f \mid \sum_{i=1}^{N} \boldsymbol{\alpha}_i \cdot \hat{\boldsymbol{\varepsilon}}_q^* \exp^{-i\boldsymbol{k}\cdot\boldsymbol{r}_i} \mid J_i M_i \rangle$$

N-Electron system

$J_f M_f$: final state

$J_i M_i$: initial state

$\boldsymbol{\alpha}_i$: Dirac matrices of the i*th* election

Emitted photon

$\hat{\varepsilon}_q$: polarization vector

$\omega, \boldsymbol{k}$: energy and momentum

ANGULAR DISTRIBUTION AND POLARIZATION OF THE PHOTON

$$\rho_{q'q} = \sum_{M_f} \rho_{q'q,\, J_f M_f J_f M_f}$$

The polarization of the residual ion may be studied in a similar manner

$$\rho_{J'_f M'_f J_f M_f} = \sum_{q} \rho_{qq,\, J'_f M'_f J_f M_f}$$

COLLISION EQUATION OF PHOTOEMISSION

$$\rho_{q'q,J'_fM'_fJ_fM_f} = \sum_{J'_iM'_iJ_iM_i} S(q', J'_fM'_f; J'_iM'_i)\,\rho_{J'_iM'_iJ_iM_i} S^*(q, J_fM_f; J_iM_i)$$

A complete description of photoemission.

EVALUATION OF *S*-MATRIX

All kinematical and dynamical effects of the collision process are contained in the scattering matrix

$$S_{fi} = \langle f \mid \Omega \mid i \rangle$$

where Ω is generally a linear combination of one- and two-particle operators.

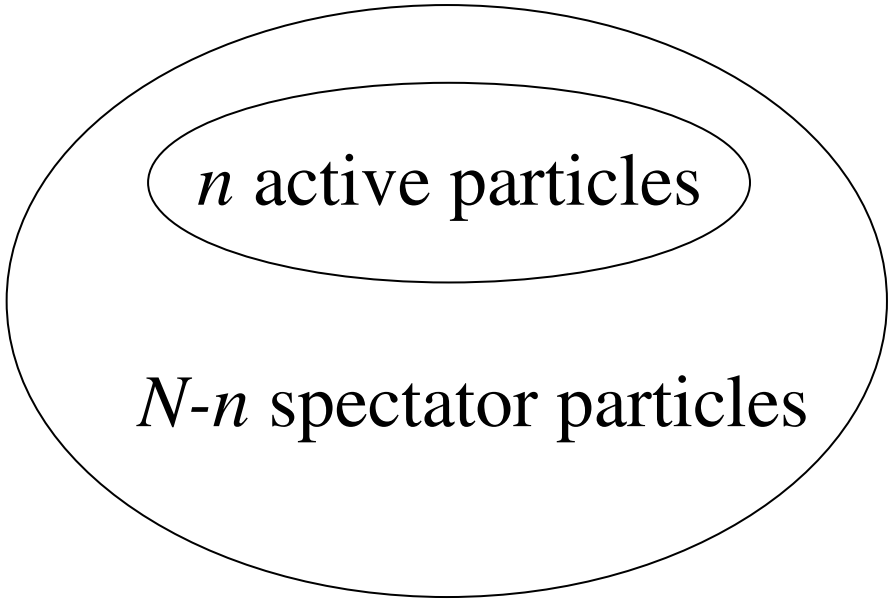
DISENTANGLE DYNAMICS from KINEMATICS by a GRAPHICAL METHOD

- Keh-Ning Huang,
  Review of Modern Physics **51**, 215 (1979).
- All dynamics are expressed in terms of Dynamical Parameters

MANY-PARTICLE SYSTEM

$$S_{fi} = \langle f \mid \Omega \mid i \rangle$$

N-particles system



Active particles : Particles connected by Ω .
Spectator particles : All other particles

The number of active particles in the *S*-matrix is at most two.

S-Matrix for One Active Particle

$$S_{fi}^{(1)} \equiv \langle f \mid \Omega^{(1)} \mid i \rangle = \int \mathrm{d}\tau_1 \, \upsilon(1) \, \Gamma_{fi}(1;1')$$

$$\Omega^{(1)} = \sum_{i=1}^{N} \upsilon(i)$$

where $\mathrm{d}\tau_1 \equiv \mathrm{d}^3 r_1$ with the spin variable included implicitly.

To evaluate $S_{fi}^{(1)}$, it suffices to know the one-particle transition matrix $\Gamma_{fi}(1;1')$.

One-Particle Transition Matrix

$$\Gamma_{fi}(1;1') = \binom{N}{1} \int \mathrm{d}\tau_2 \cdots \mathrm{d}\tau_N \langle 12\ldots N \mid f \rangle\langle i \mid \langle 1'2' \ldots N' \rangle$$

$$\equiv \binom{N}{1} \int \mathrm{d}^3 r_2 \cdots \mathrm{d}^3 r_N \, \Psi_f(\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N)\Psi_f^{\dagger}(\mathbf{r}_1, \mathbf{r}_2, \cdots \mathbf{r}_N)$$

where integrations over spectator particles { 2,...,*N* } corresponds physically to the ensemble average over spectator particles.

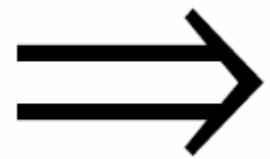
S-Matrix for Two Active Particles

$$S_{fi}^{(2)} = \int \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 \, \upsilon(12) \, \Gamma_{fi}(12; 1'2')$$

$$\Omega^{(2)} = \sum_{i<j}^{N} \upsilon(ij)$$

Knowing $\Gamma_{fi}(1;1')$ and $\Gamma_{fi}(12;1'2')$ is all that is needed to evaluate the *S*-matrix S_{fi} for any collision process,

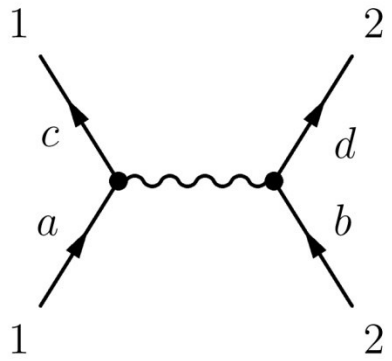
Optimizing
***N*-particle wave functions**



reduced to

Optimizing
***2*-particle transition Matrix**

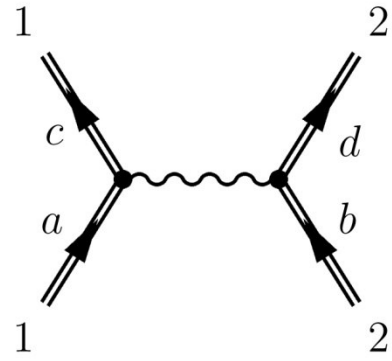
BARE STATES：



initial state

final state

DRESSED STATES：



initial state

final state

How to dress a state?

ACTIVE PARTICLES
dressed by Spectator Particles

The dressing of active particles is performed formally by taking ensemble average over Spectator Particles：

$$\Gamma_{fi}(1\cdots n;1'\cdots n')$$

$$= \binom{N}{n}\int \mathrm{d}\tau_{n+1}\cdots\mathrm{d}\tau_N \langle 12\ldots N \mid f\rangle\langle i \mid \langle 1'2'\ldots N'\rangle$$

$$\equiv \binom{N}{n}\int \mathrm{d}^3 r_{n+1}\cdots\mathrm{d}^3 r_N \Psi_f(\mathbf{r}_1,\mathbf{r}_2,\cdots\mathbf{r}_N)\Psi_f^{\dagger}(\mathbf{r}_1,\mathbf{r}_2,\cdots\mathbf{r}_N)$$

RELATIVISTIC EQUATION OF MOTION

$$i\frac{\partial}{\partial t}\Gamma_{fi}(1;1') = \omega_{fi}\Gamma_{fi}(1;1')$$

for the one-particle transition matrix

TIME-INDEPENDENT FORM of the Equation of Motion

$$h(1)\Gamma_{fi}(1;1') - \Gamma_{fi}(1;1')h(1')$$
$$+ 2\int d\tau_2[v(12) - v(1'2')]\Gamma_{fi}(12;1'2') = \omega_{fi}\Gamma_{fi}(1;1')$$

where $h(1)$ and $v(12)$ denote one-particle and two-particle operators in the total Hamiltonian.

Multiconfiguration Relativistic Random-Phase-Approximation (MCRRPA)

The *exact* hierarchy equations may be solved independently by expressing the two-particle transition matrix $\Gamma_{fi}(12;1'2')$ in terms of the one-particle transition matrix $\Gamma_{fi}(1;1')$,

$$\Gamma_{fi}(12;1'2') = \frac{1}{2}(1 - P_{12})(1 - P_{1'2'})\Gamma_0(1;1')\Gamma_{fi}(2;2')$$

P_{ij} : exchange operator for particles i and j

$\Gamma_0(1;1')$: one-particle density-matrix for the Fermi vacuum.

RELATIVISTIC EQUATION OF MOTION for the *2*-Particle Correlation Function

$$i\frac{\partial}{\partial t}\Gamma_{fi}(12;1'2') = \omega_{fi}\Gamma_{fi}(12;1'2')$$

Time-Independent Form

$$[h(1)+h(2)]\Gamma_{fi}(12;1'2') - \Gamma_{fi}(12;1'2')[h(1')+h(2')]$$

$$+ [v(12) - v(1'2')]\Gamma_{fi}(12;1'2')$$

$$+ 3\int d\tau_3[v(13)+v(23)-v(1'3')-v(2'3')]\Gamma_{fi}(123;1'2'3')$$

$$= \omega_{fi}\Gamma_{fi}(12;1'2')$$

This equation may be solved independently by making the approximation

$$
\begin{aligned}
&\Gamma_{fi}(123;1'2'3') \\
&\cong\frac{1}{6}(1+P_{12}P_{13}+P_{23}P_{13}-P_{12}-P_{23}-P_{13}) \\
&\times(1+P_{1'2'}P_{1'3'}+P_{2'3'}P_{1'3'}-P_{1'2'}-P_{2'3'}-P_{1'3'}) \\
&\times\Gamma_0(1;1')\Gamma_{fi}(23;2'3')
\end{aligned}
$$

ONE-PARTICLE TRANSITION MATRIX

$$\Gamma_{fi}(1;1') = \Gamma_{fi}^{(+)}(1;1') + \Gamma_{fi}^{(-)}(1;1')$$

Positive-frequency part : final-state correlations

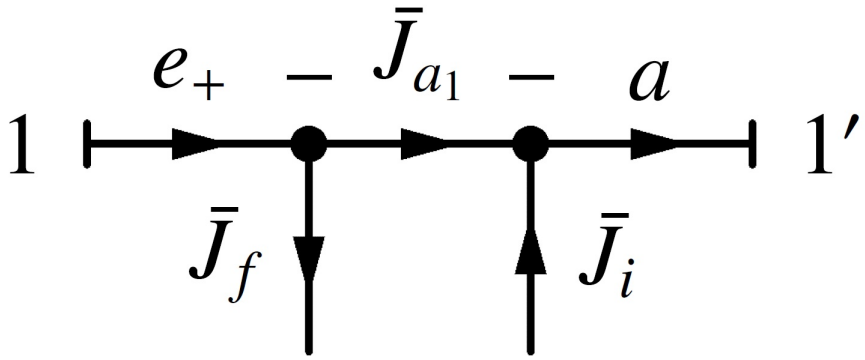
$$\Gamma_{fi}^{(+)}(1;1') = \Gamma_{fi}^{(1)}(1;1') + \Gamma_{fi}^{(2)}(1;1')$$

Negative-frequency part : initial-state correlations

$$\Gamma_{fi}^{(-)}(1;1') = \Gamma_{fi}^{(3)}(1;1') + \Gamma_{fi}^{(4)}(1;1')$$

ANGULAR-MOMENTUM-COUPLING DIAGRAM

$$\Gamma^{(1)}_{fi}(1;1') = \sum_{e\alpha_{a_1} J_{a_1} \alpha_i}$$



Graphical notations in
K.-N. Huang, Rev. Mod. Phys. 51, 215 (1979).

TWO-PARTICLE TRANSITION MATRIX

$$\Gamma_{fi}(12;1'2') = \Gamma_{fi}^{(+)}(12;1'2') + \Gamma_{fi}^{(-)}(12;1'2')$$

Positive-frequency part：

$$\Gamma_{fi}^{(+)}(12;1'2') = \Gamma_{fi}^{(1)}(12;1'2') + \Gamma_{fi}^{(2)}(12;1'2')$$

Negature-frequency part：

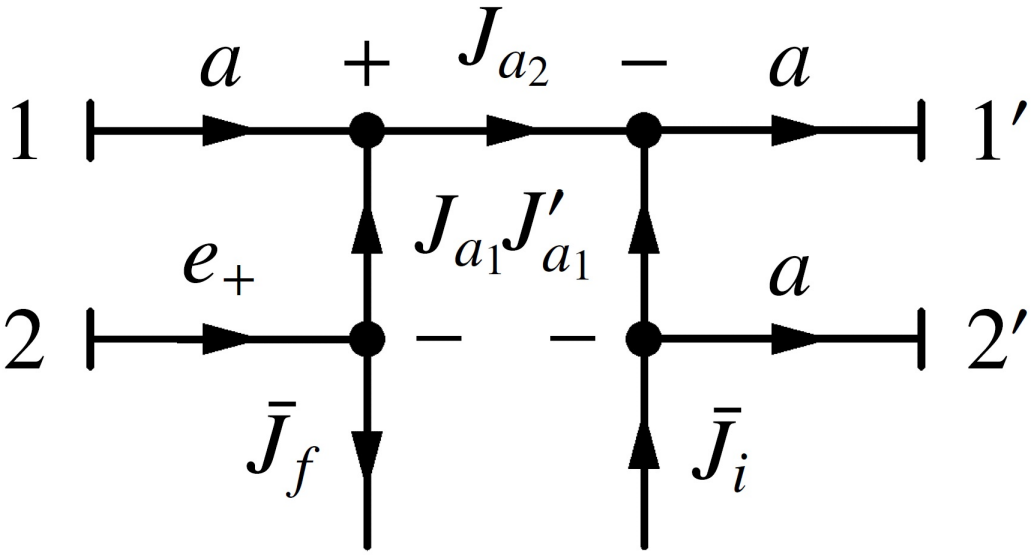
$$\Gamma_{fi}^{(-)}(12;1'2') = \Gamma_{fi}^{(3)}(12;1'2') + \Gamma_{fi}^{(4)}(12;1'2')$$

For example,

$$\Gamma_{fi}^{(1)}(12;1'2') = \frac{1}{2}(1-P_{12})(1-P_{1'2'})\Gamma_c(1;1')\Gamma_{fi}^{(1)}(2;2') + \frac{1}{2}(1-P_{12}) \sum_{e\alpha_{a_1}J_{a_1}\alpha_i\alpha'_{a_1}J'_{a_1}\alpha_{a_2}J_{a_2}} A\Gamma_{ae,aa}(12;1'2')$$

DIAGRAMMATICAL FORM

$\Gamma_{ae,aa}(12;1'2') =$



$$A = (2J_{a_1}+1)\sqrt{2J'_{a_1}+1}(N_a-1)[(a^{N_a-1})\alpha_{a_1}J_{a_1}a|\alpha_i J_i]^{-1}$$
$$\times[(a^{N_a-1})\alpha'_{a_1}J'_{a_1}a|\alpha_i J_i][(a^{N_a-2})\alpha_{a_2}J_{a_2}a|\alpha_{a_1}J_{a_1}][(a^{N_a-2})\alpha_{a_2}J_{a_2}a|\alpha'_{a_1}J'_{a_1}]$$

$[(j^N)\alpha' J'|\alpha J]$: coefficient of fractional parentage.

ELECTRON-IMPACT IONIZATION OF U^{91+}

The electromagnetic interaction $v(\mathbf{r}_{12})$ between charged particles arising from the exchange of one photon may be summarized in the QED theory as the Coulomb interaction plus transverse-photon interaction,

$$v(\mathbf{r}_{12}) = \frac{1}{r_{12}} - (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 \frac{e^{i\omega r_{12}}}{r_{12}}) + (\boldsymbol{\alpha}_1 \cdot \nabla_1)(\boldsymbol{\alpha}_2 \cdot \nabla_2)\left[\frac{e^{i\omega r_{12}} - 1}{\omega^2 r_{12}}\right]$$

The QED cross sections of electron-impact ionization for the hydrogenlike U^{91+} have been calculated.

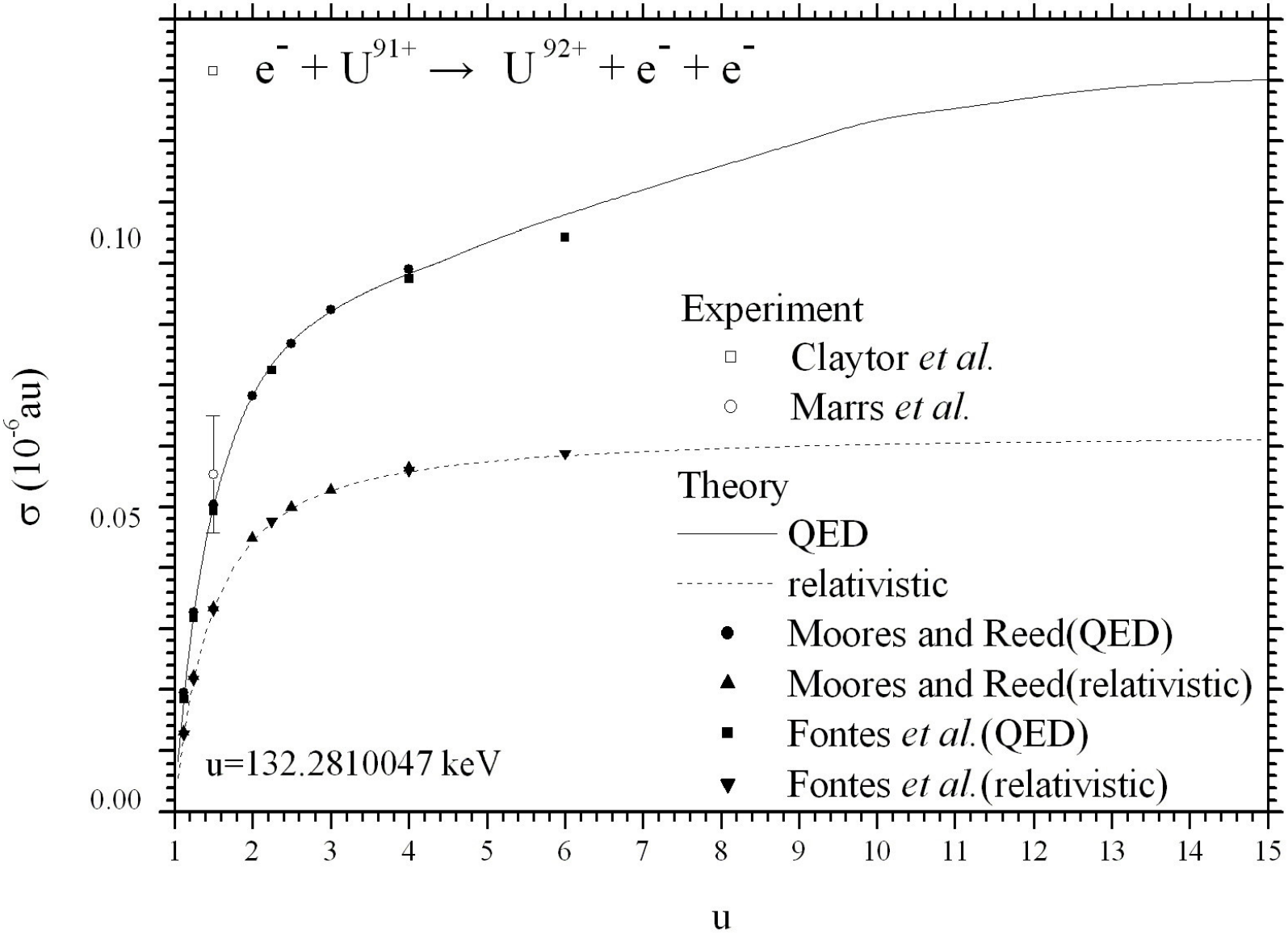


FIG. 1. Huang *et al.*

PROTON-IMPACT IONIZATION OF HYDROGEN

In the LAB frame

projectile : $z\ ,\ m_p\ ,\ \boldsymbol{R}_p$

target election : $-e\ ,\ m_e\ ,\ \boldsymbol{R}_e$

target nucleus : $Ze\ \ ,\ m_n\ ,\ \boldsymbol{R}_n$

In the CM frame

projectile : $ze\ ,\ \mu = (m_p m_n)/(m_p + m_n)\ ,\ \boldsymbol{R} = \boldsymbol{R}_p - \boldsymbol{R}_n$

target election : $-e\ ,\ m = (m_e m_n)/(m_e + m_n)\ \ ,\ \boldsymbol{R} = \boldsymbol{R}_e - \boldsymbol{R}_n$

collision in the field of a Fixed charge Z.

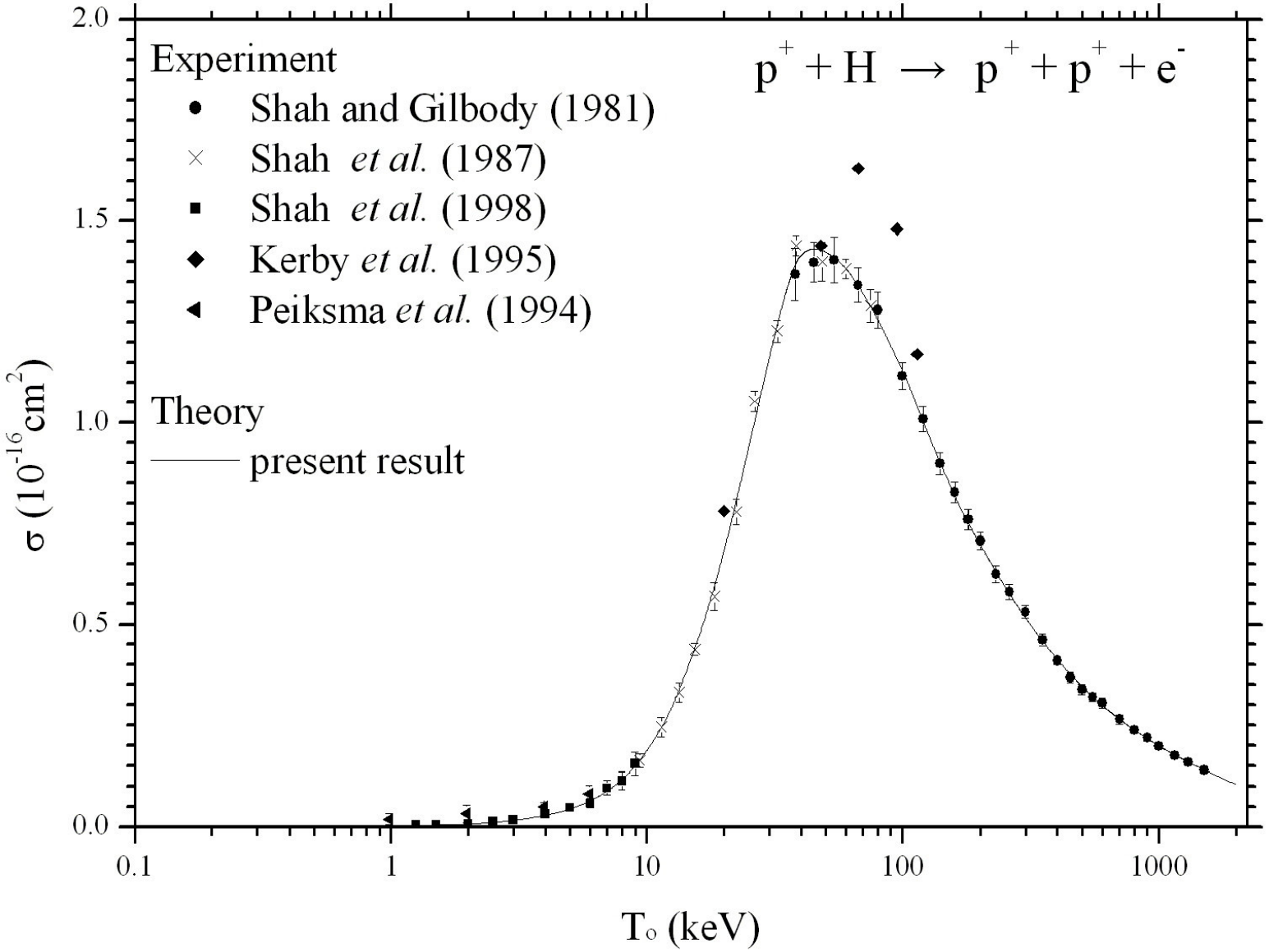


FIG. 2 Lin *et al.*

SUMMARY

(i) A relativistic quantum collision theory for many-particle systems has been proposed to treat relativistic and particle-correlation effects in an *ab initio* manner.

(ii) The ensemble average over spectator particles of the many-particle system is formally carried out from the outset to reduced the problem to that of active particles only.

(iii) This approach, called MCRRPA, has been applied to photoexcitation and photoionization with great success.

SUMMARY (continued)

(iv) We have further incorporated quantum electrodynamic effects perturbatively in the formulation.

(V) Our results for the electron-impact ionization of U^{91+} agree well with existing experimental and theoretical data.

(Vi) The proton-impact-ionization cross sections of hydrogen are calculated including recoil effects and are in excellent agreement

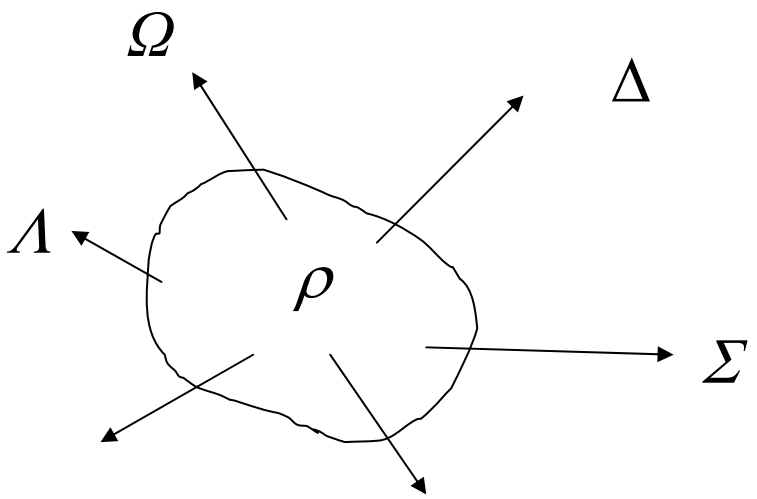
Complexization

Yin-Yang

陰 - 陽

Complementarity

Quantum measurement



$$\Omega_\rho = \{\ w;\ \ p_w,\ \ D(w)\}$$

$$\Lambda_\rho = \{\ \lambda;\ \ p_\lambda,\ \ D(\lambda)\}$$

$$\Sigma_\rho = \{\ \sigma;\ \ p_\sigma,\ \ D(\sigma)\}$$

$$\Delta_\rho = \{\ \delta;\ \ p_\delta,\ \ D(\delta)\}$$

$$\vdots$$

Measurement of Ω on ρ

$$< w^n > \;=\; \mathrm{tr}\{\rho\Omega^n\}$$

Spectral Resolution

$$\rho = \sum_i p_i Q_i \qquad ; \;\; Q_i \equiv |\, p_i >< p_i \,|$$

$$\Omega = \sum_\alpha w_\alpha P_\alpha \qquad ; \;\; P_\alpha \equiv \sum_j^\alpha P_j, \;\; P_j \equiv |\, w_j >< w_j \,|$$

$$\Omega^n = \sum_\alpha w_\alpha^n P_\alpha \,`$$

Correlations - beyond mean field

- Kinematic and Dynamic
- Initial and Final
- Discrete and Continuum
- Core and Valence
- Creation and Annihilation
- Shielding and Polarization
- Symmetrization and Relativisitic

Key words

Coherent Ensemble

Incoherent Ensemble

Transition Matrix

Density Matrix

Full and Reduced

Kinematic correlations

Dynamical correlations

Life is a quantum phenomena

Human brain is a quantum computer