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

To demonstrate the importance of **correlations**, let us imagine a person is a many-particle system. You want to determine the properties of one particle in that person by the response of that particle to an external stimulus.

This is what would happen!

So let us see what are those properties which are observed or measured and about what we will be making theoretical predictions. We will look for

A theory

which Just-describes the phenomenon,

Not under-describes and

Not over-describes !

COLLISION EQUATION

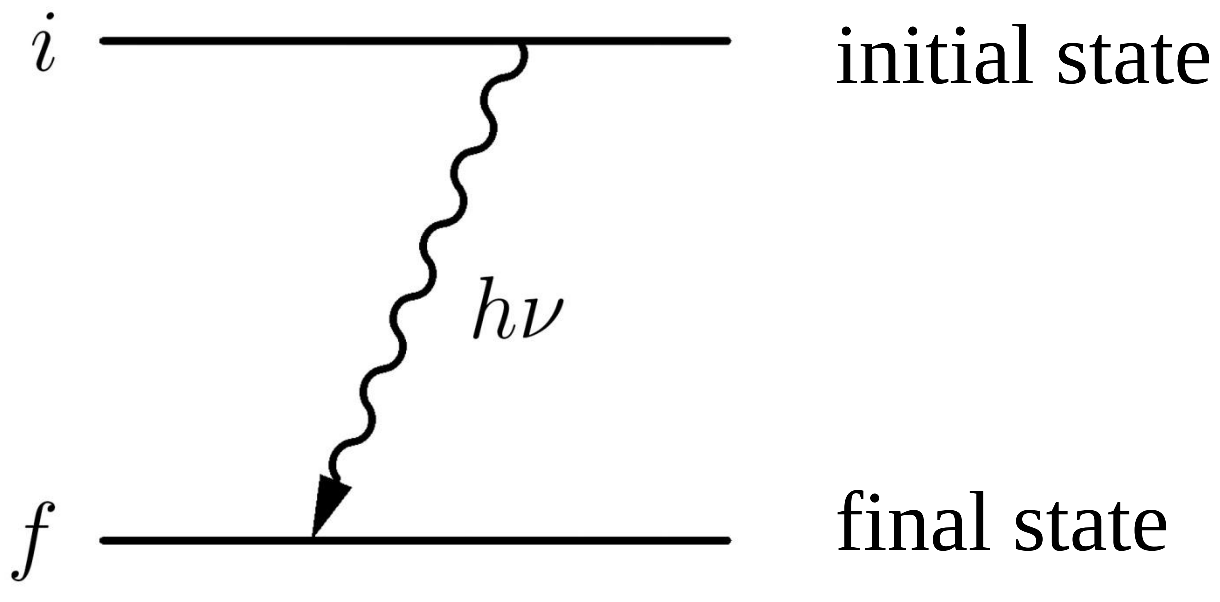
$$\rho^{(f)} = S_{fi}\,\rho^{(i)} S_{fi}^{\dagger}$$

$\rho^{(f)}$: final state

$\rho^{(i)}$: initial state

S_{fi} : Scattering-matrix

PHOTOEMISSION OF AN ATOM



COLLISION EQUATION OF PHOTOEMISSION

$$\rho_{q' q, J'_f M'_f J_f M_f} = \sum_{J'_i M'_i J_i M_i} S(q', J'_f M'_f; J'_i M'_i)\, \rho_{J'_i M'_i J_i M_i} S^*(q, J_f M_f; J_i M_i)$$

A complete description of photoemission.

S-MATRIX OF PHOTOEMISSION

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

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

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

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

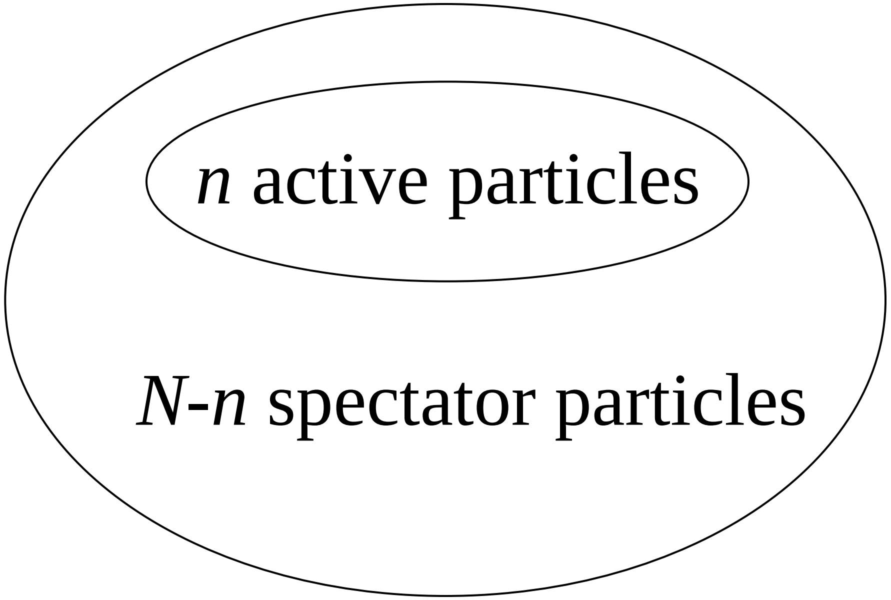
- Keh-Ning Huang,

  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

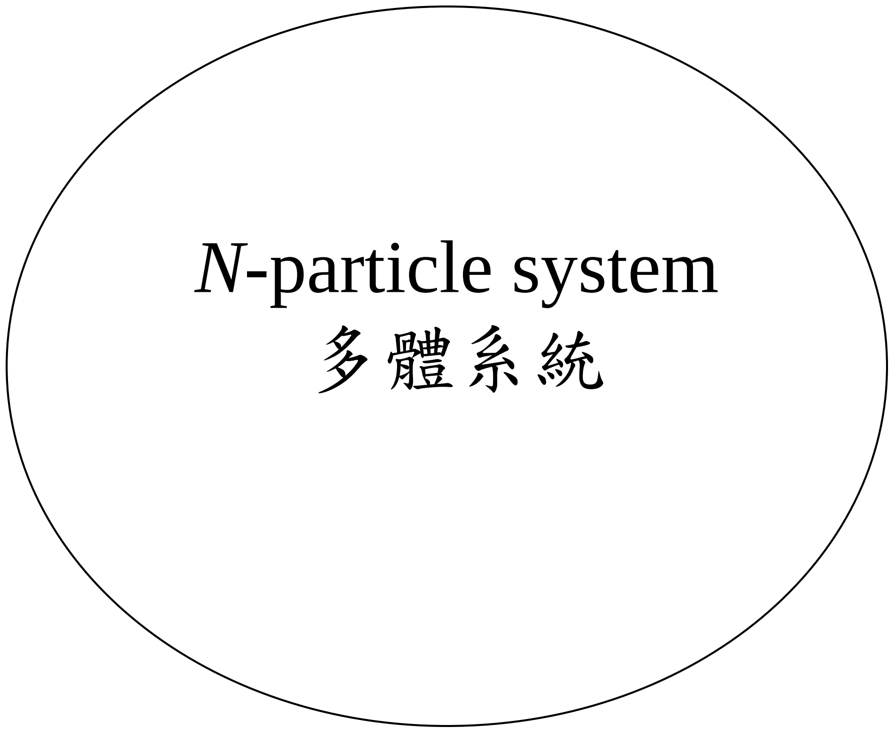
$$S_{fi}^{(2)} = \int \mathrm{d}\tau_1 \, \mathrm{d}\tau_2 \, \upsilon(12) \, \Gamma_{fi}(12; 1'2')$$

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

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,

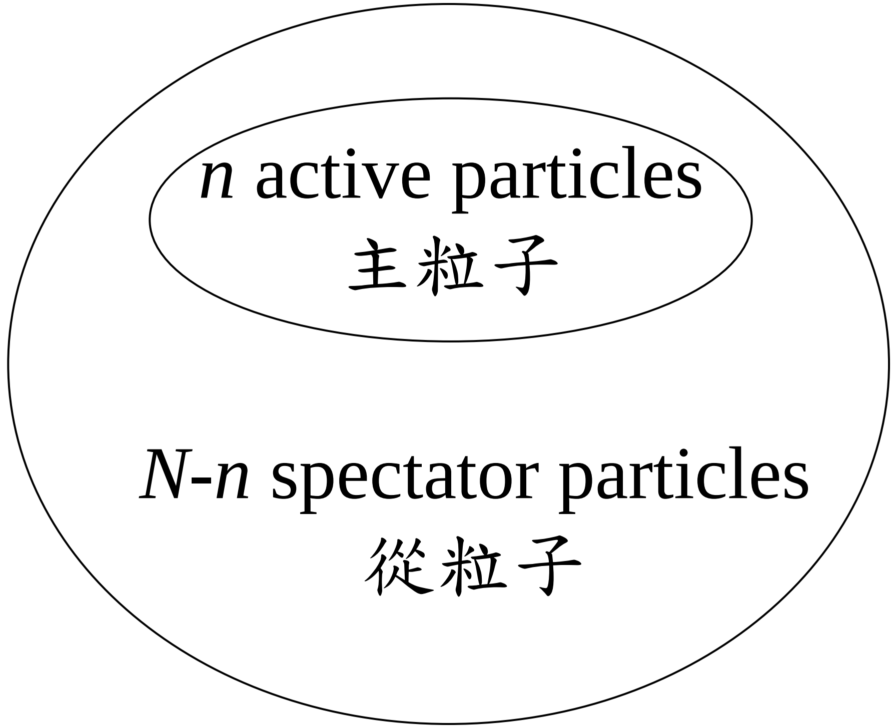
I. B Density-Matrix Description

Density matrix for *N* particles：



$$\Gamma(1 \cdots N \,,\, 1' \cdots N')$$

Reduced density matrix for *n* active particles：



$$\Gamma(1 \cdots n; 1' \cdots n') = \binom{N}{n} \int \mathrm{d}\tau_{n+1} \cdots \tau_N \Psi(1 \cdots N) \Psi^{\dagger}(1' \cdots N')$$

Ensemble average over (*N*-*n*) spectator particles

Two-Particle Operators $\mathcal{V}(12)$

a) Coulomb Interaction:

$$\frac{1}{r_{12}}$$

b) Covariant Photon Interaction:

$$(1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) \frac{e^{i\omega r_{12}}}{r_{12}}$$

c) Transverse Photon Interaction:

$$- \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 \frac{e^{i\omega r_{12}}}{r_{12}} + (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\nabla})(\boldsymbol{\alpha}_2 \cdot \boldsymbol{\nabla}) \left[\frac{e^{i\omega r_{12}} - 1}{\omega^2 r_{12}} \right]$$

d) Breit Interaction:

$$- \frac{1}{2r_{12}} \left[(\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) + \frac{(\boldsymbol{\alpha}_1 \cdot \boldsymbol{r}_{12})(\boldsymbol{\alpha}_2 \cdot \boldsymbol{r}_{12})}{r_{12}^2} \right]$$

III. C Transition Matrix

The nth-order transition matrix may also be defined in terms of field operators as

$$\Gamma_{fi}(1 \cdots n; 1' \cdots n')$$
$$= \frac{1}{n!} \langle \Psi_i | \psi^\dagger(1') \cdots \psi^\dagger(n') \psi(n) \cdots \psi(1) | \Psi_f \rangle$$

Examples:

$$\Gamma_{fi}(1\,; 1') = \langle \Psi_i | \psi^\dagger(1') \psi(1) | \Psi_f \rangle$$

$$\Gamma_{fi}(1\,2\,; 1'\,2') = \frac{1}{2} \langle \Psi_i | \psi^\dagger(1') \psi^\dagger(2') \psi(2) \psi(1) | \Psi_f \rangle$$

In terms of *N*-particle wave functions, we have

Transition Matrix

$$\Gamma_{fi}(1 \cdots N\,;\, 1' \cdots N') \equiv \Psi_f(1 \cdots N)\Psi_i^{\dagger}(1' \cdots N')$$

$$\equiv \langle 1 \cdots N \,|\Psi_f\rangle \, \langle \Psi_i|\, 1' \cdots N'\rangle$$

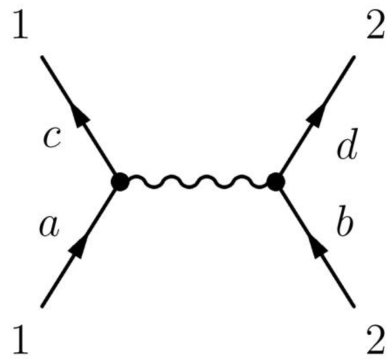
Reduced Transition Matrix

$$\Gamma_{fi}(1 \cdots n; 1' \cdots n') = \binom{N}{n} \int \mathrm{d}\tau_{n+1} \cdots \mathrm{d}\tau_N \Psi_f(1 \cdots N)\Psi_i^{\dagger}(1' \cdots N')$$

Recurrence Relation

$$\Gamma_{fi}(1 \cdots n; 1' \cdots n') = \left(\tfrac{n+1}{N-n}\right) \int \mathrm{d}\tau_{n+1} \Gamma(1 \cdots n{+}1\,;\, 1' \cdots n{+}1')$$

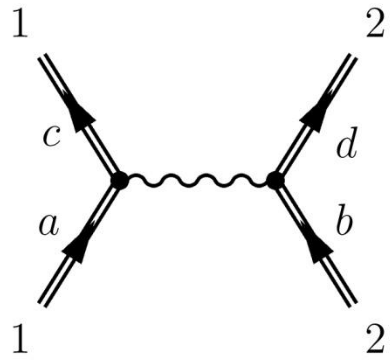
BARE STATES：



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：

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

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

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

III. D Relativistic Equations of Motion

Assuming $|\Psi_f\rangle$ and $|\Psi_i\rangle$ are energy eigenstates, we get

$$i\frac{\partial}{\partial t}\langle 1\cdots N\,|\Psi_f\rangle = E_f\,\langle 1\cdots N\,|\Psi_f\rangle$$

$$i\frac{\partial}{\partial t}\langle 1\cdots N\,|\Psi_i\rangle = E_i\,\langle 1\cdots N\,|\Psi_i\rangle$$

Consequently, we may derive

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

with $\omega_{fi} \equiv E_f - E_i$. By using the recurrence relation, we obtain in general

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

This is our **Relativistic Equation of Motion** for the **nth-order transition matrix**.

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

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

where $h(1)$ and $\upsilon(12)$ 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

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

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

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

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

This equation may be solved independently by making the approximation

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

III. E Calculation of Transition Matrix

(*i*) $$\Gamma_{fi}(1\,;1') = \sum_{(ab)} (-)^{P_{ab}} \sqrt{N_a N_b'}\, |q(a)\rangle\, \langle q'(b)|$$

where the summation is over all non-vanishing pairs.

(*ii*) $$\Gamma_{fi}(12\,;1'2') = \sum_{(ab,cd)} \tfrac{1}{2}(1-\delta_{ab}-P_{12})(1-\delta_{cd}-P_{1'2'})$$

$$\times\, (-)^{P_{ab,cd}} \sqrt{N_a(N_b-\delta_{ab})N_c'(N_d'-\delta_{cd})}\, |q(ab)\rangle\, \langle q'(cd)|$$

where the summation is over all distinct

non-vanishing pairs with $a \le b$ and $c \le d$.

See notations in

K.-N. Huang, Rev. Mod. Phys. **51**, 215 (1979).

ONE-PARTICLE TRANSITION MATRIX

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

Positive-frequency part : final-state correlations

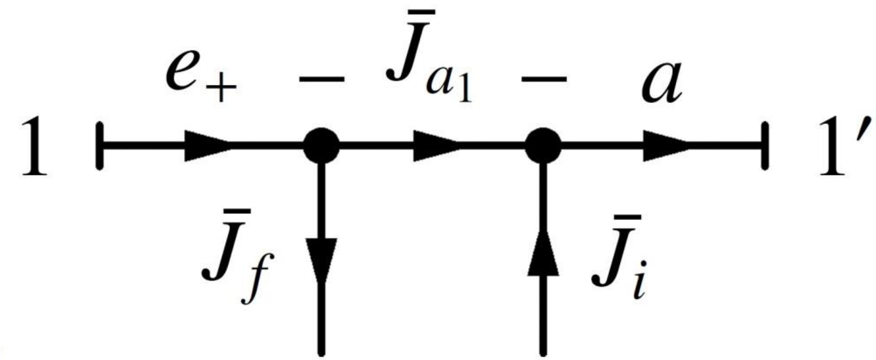
$$\Gamma_{fi}^{(+)}(1;1') = \Gamma_{fi}^{(1)}(1;1') + \Gamma_{fi}^{(2)}(1;1')$$

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：

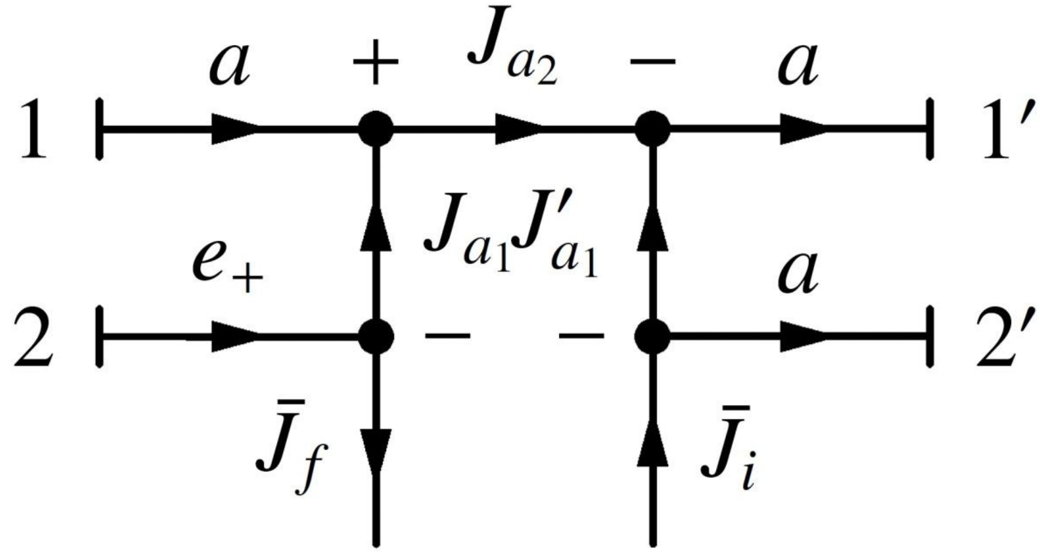
$$\Gamma_{fi}^{(-)}(12;1'2') = \Gamma_{fi}^{(3)}(12;1'2') + \Gamma_{fi}^{(4)}(12;1'2')$$

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.

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

$\Longrightarrow$ reduced to

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

ELECTRON-IMPACT IONIZATION OF U^{91+}

The electromagnetic interaction $\upsilon(\mathbf{r}_{12})$ 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,

$$\upsilon(\mathbf{r}_{12}) = \frac{1}{r_{12}} - (\alpha_1 \cdot \alpha_2 \frac{e^{i\omega r_{12}}}{r_{12}}) + (\alpha_1 \cdot \nabla_1)(\alpha_2 \cdot \nabla_2)\left[\frac{e^{i\omega r_{12}} - 1}{\omega^2 r_{12}}\right]$$

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

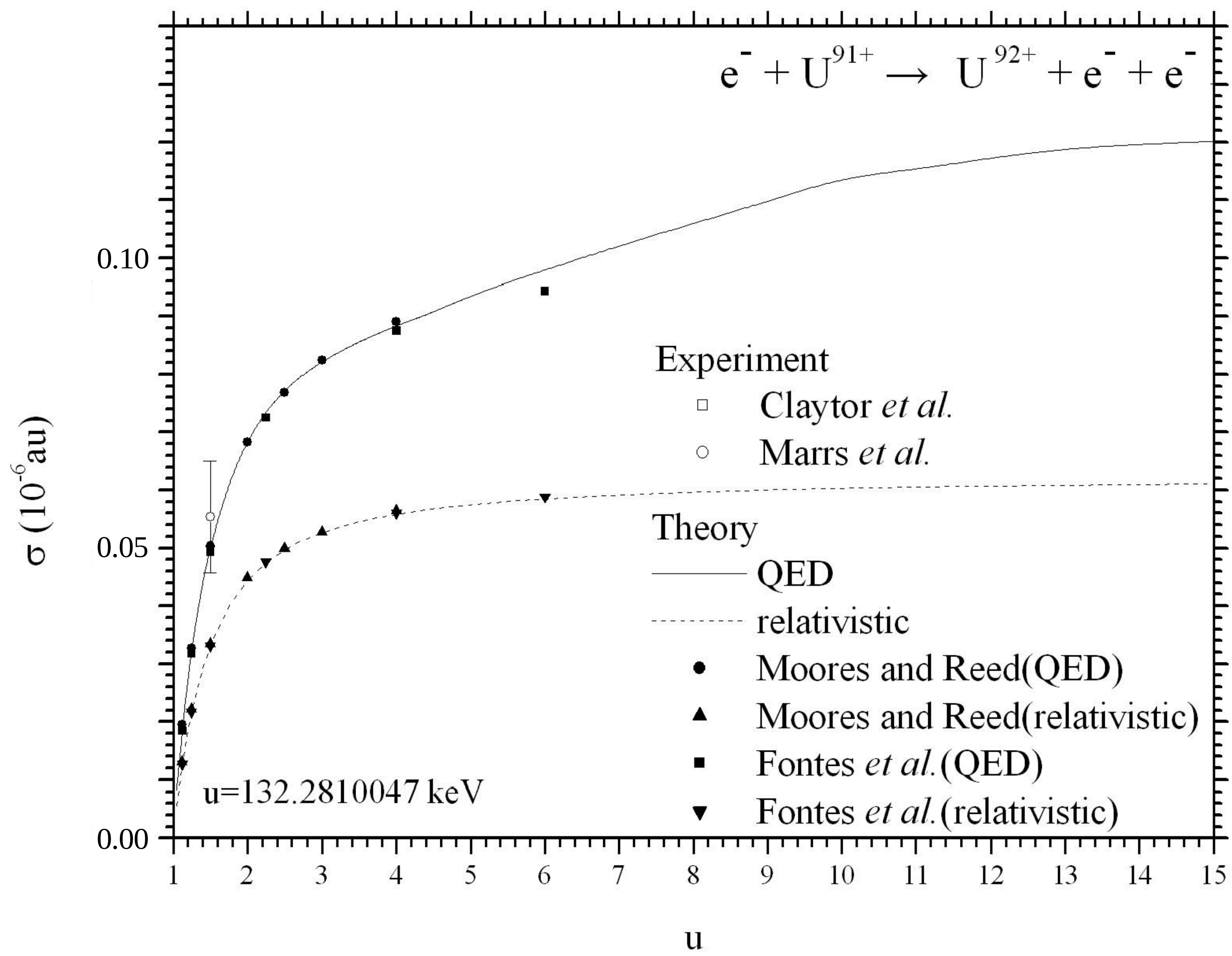


FIG. 1. Huang *et al.*

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*.

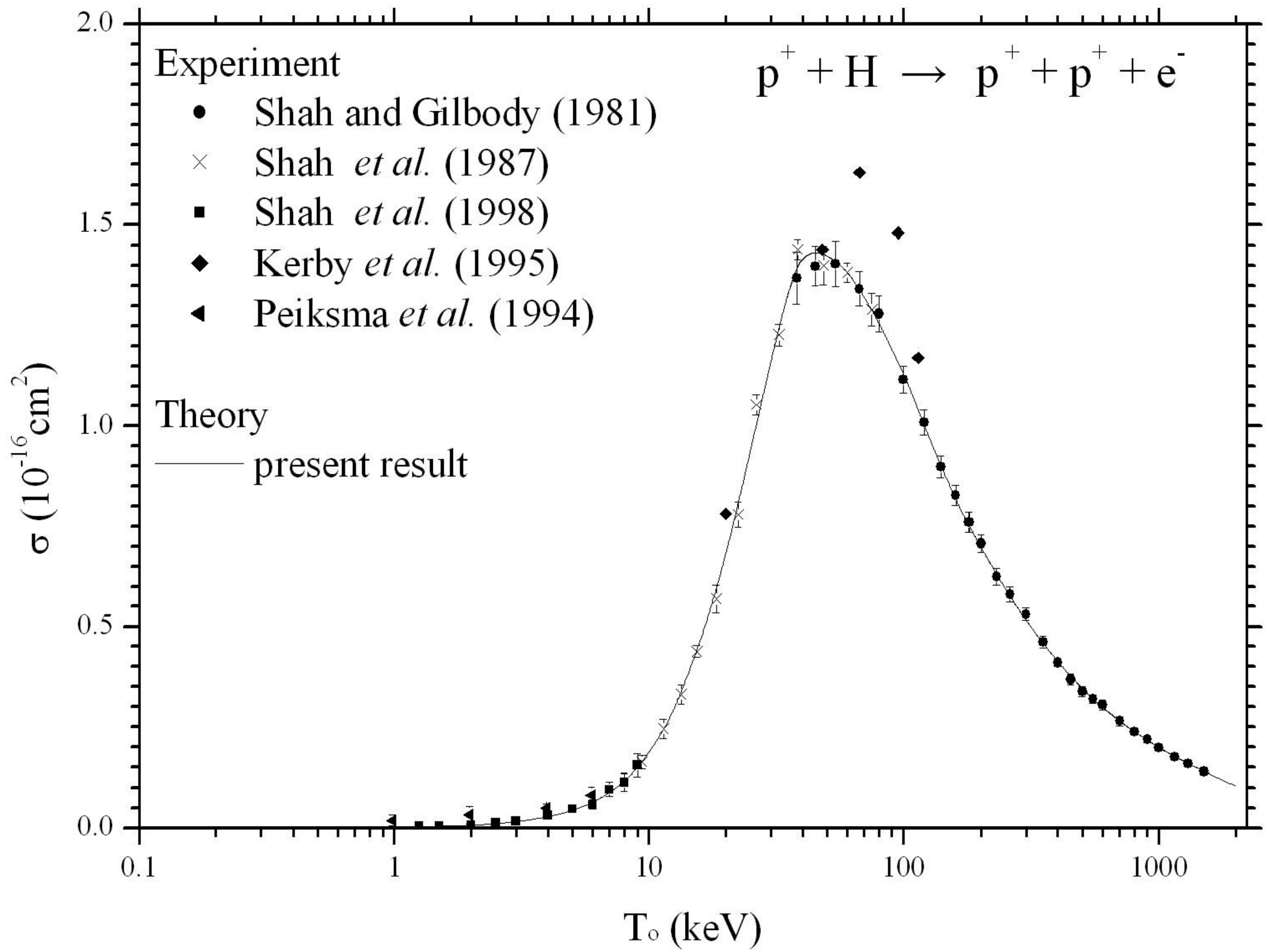


FIG. 2 Lin *et al.*

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