Quantum Transport Theory for Fusion Plasmas

Keh-Ning Huang (黃克寧)[1,2] , Hsiao-Ling Sun (孫曉鈴)[2], Sheng-Fan Lin (林聖凡)[2] and Hao-Tse Shiao (蕭鎬澤)[1,2]

[1]*Department of Physics, National Taiwan University, Taipei, Taiwan 106, Republic of China*
[2]*Institute of Atomic and Molecular Sciences, Academia Sinica, P.O. Box 23-166, Taipei, Taiwan, 106, Republic of China*

國立台灣大學 物理學系
中央研究院 原子與分子科學研究所

ABSTRACT

Quantum transport equation for impact-ionization processes are formulated in the actor-spectator description. The density-matrix formalism is adopted to treat both coherent and incoherent effects. Quantum electrodynamic effects are also considered for high-temperature scenarios. Electron-impact ionization of U^{91+} and proton-impact ionization of H are given as examples.

1. Introduction

We start from the relativistic equations of motion governing quantum collision processes in many-particle systems [1] and formulate the relativistic quantum transport theory in an ***ab initio*** manner.

To demonstrate the importance of correlations in a many-particle system, let us imagine a person is such a system. We want to determine the properties of one particle in that person by the response of that particle to an external stimulus. Fig. 1 shows what would happen.

Fig. 1 Actor-Spectator Description

Those parts of the many-particle system which are observed or measured will be called the ***active particles*** while the rest called the ***spectator particles***. Our equation of motion is in a sense the ***quantum-version of the Boltzmann transport equation***.

In the present approach, active particles are modulated by spectator particles such that the ***bare*** propagator for active particles becomes the ***dressed*** propagator. In other words, equations of motion are then derived for the ***dressed propagator***. Bare and dressed propagators are presented symbolically in Fig. 2.

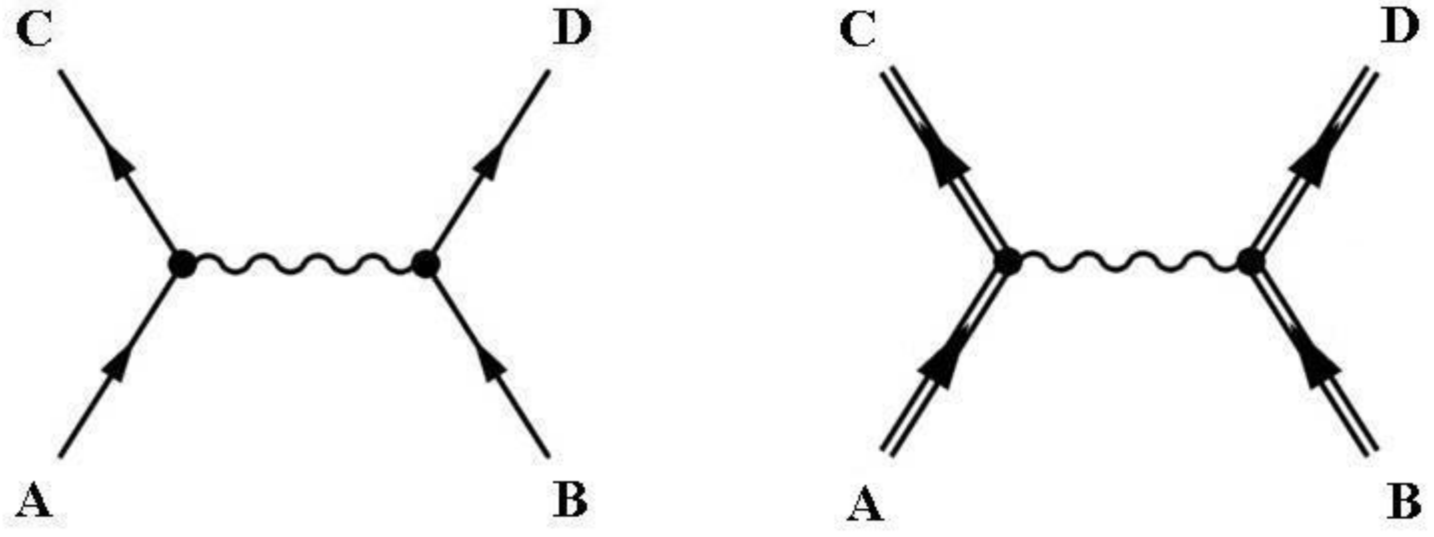

Fig. 2 Bare and Dressed Propagators

2. Collision Equation

Any reaction, such as

$$A + B + C + \cdots \longrightarrow E + F + G + \cdots \qquad (1)$$

may be formulated by a collision equation as

$$\boldsymbol{\rho}^{(f)} = \boldsymbol{S}_{fi}\,\boldsymbol{\rho}^{(i)}\,\boldsymbol{S}^{\dagger}_{fi} \qquad (2)$$

where $\boldsymbol{\rho}^{(f)}$ denotes the final state, $\boldsymbol{\rho}^{(i)}$ the initial state, and $\boldsymbol{S}_{fi}$ represents the ***scattering-matrix*** of this reaction.

3. Actor-Spectator Description of Many-Particle Systems

In the ***actor-spectator description***, an *N*-particle system is formally devided into two parts: *n* active particles and *N*-*n* spectator particles. Therefore, $\boldsymbol{S}_{fi}$ is in fact a summation over matrix elements of operators $\Lambda^{(n)}$ between configurations $|\phi_k\rangle$ and $|\psi_j\rangle$, denoted symbolically as

$$\begin{aligned} \boldsymbol{S}_{fi} &= \langle\, f \,|\, \Omega \,|\, i \,\rangle \\ &= \sum_{jk} \langle\, \psi_j \,|\, \Lambda^{(1)} \,|\, \phi_k \,\rangle + \sum_{jk} \langle\, \psi_j \,|\, \Lambda^{(2)} \,|\, \phi_k \,\rangle \\ &= \boldsymbol{S}_{fi}^{(1)} + \boldsymbol{S}_{fi}^{(2)} \end{aligned} \tag{3}$$

where $\Omega = \Lambda^{(1)} + \Lambda^{(2)}$ is a sum of one-particle operator $\Lambda^{(1)}$ and two-particle operator $\Lambda^{(2)}$. For symmetric cases, operators $\Lambda^{(1)}$ and $\Lambda^{(2)}$ have the general forms,

$$\Lambda^{(1)} = \sum_{i=1}^{N} v(i) \quad ; \qquad \Lambda^{(2)} = \sum_{i<j}^{N} v(ij) \tag{4}$$

4. Transition Matrices

In terms of *N*-particle wave functions, we have the full transition matrix for the *N*-particle system defined as

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

$$\equiv \langle 1\cdots N|\,\Gamma_{fi}|\,1^{'}\cdots N^{'}\,\rangle \qquad (5)$$

wher $\Gamma_{fi} \equiv |\,\Psi_f\,\rangle\langle\Psi_i|.$

The ***reduced transition matrix***, or called specifically the *n*th-order transition matrix, is in turn defined as

$$\Gamma_{fi}(1\cdots n;1^{'}\cdots n^{'}) \equiv \binom{N}{n}\mathsf{Tr}^{(N-n)}\{\Gamma_{fi}\}$$

$$=\binom{N}{n}\int d\tau_{n+1}\cdots d\tau_N \qquad (6)$$

$$\times\,\Psi_f(1,\cdots,n,n+1,\cdots,N)\times\Psi_i^{\dagger}(1^{'},\cdots,n^{'},n+1,\cdots,N)$$

where $d\tau_1 \equiv d^3\boldsymbol{r}_1$ with intrinsic variables, such as spin, included implicitly.

Here $\mathsf{Tr}^{(k)}\{\Omega\}$ denotes taking the trace of the operator Ω in any specific representation over *k* particle variables. The *n*th-order transition matrix $\Gamma_{fi}(1\cdots n;1'\cdots n')$ is the ***dressed*** propagator for *n* active particles, and the ***dressing*** of the propagator for *n* active particles is carried out formally by taking ensemble average over *N*-*n* spectator particles.

5. Evaluation of the S-Matrix

$$S_{fi}^{(1)} \equiv \langle f \,|\, \Lambda^{(1)} \,|\, i \rangle \equiv \mathsf{Tr}^{(N)} \left\{ \Lambda^{(1)} \Gamma_{fi} \right\}$$

$$= \int d\tau_1 \upsilon(1) \Gamma_{fi}(1;1^{'}) \tag{7}$$

$$S_{fi}^{(2)} \equiv \langle f \,|\, \Lambda^{(2)} \,|\, i \rangle \equiv \mathsf{Tr}^{(N)} \left\{ \Lambda^{(2)} \Gamma_{fi} \right\}$$

$$= \int d\tau_1 d\tau_2 \upsilon(12) \Gamma_{fi}(12;1^{'}2^{'}) \tag{8}$$

In summary, 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.

6. Relativistic Equations of Motion for Transition Matrices

By taking ensemble average over spectator particles, we obtain in general

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

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

$$\hbar\omega_{fi}\equiv E_f-E_i$$

were

This is our relativistic equation of motion for the *n*th-order transition matrix [1]

The relativistic equation of motion for the first-order transition matrix is

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

(10)

which may be given in time-

i $h(1)\Gamma_{fi}(1;1^{'}) - \Gamma_{fi}(1;1^{'})h(1^{'})$

$$+ 2\int d\tau_2 \left[v(12) - v(1^{'}2^{'})\right]\Gamma_{fi}(12;1^{'}2^{'})$$

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

(11)

Here $h(1)$ and $v(12)$ denote one-particle and two-particle operators in the total Hamiltonian of the *N*-particle system,

$$H = \sum_{i=1}^{N} h(i) + \sum_{i<j}^{N} v(ij) \tag{12}$$

The relativistic equation of motion for the second-order transition matrix $\Gamma_{fi}(12;1^{'}2^{'})$ is

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

(13)

which has the time-independent form

$$
\begin{aligned}
&[h(1) + h(2)]\,\Gamma_{fi}(12;1'2') - \Gamma_{fi}(12;1'2')[h(1') + h(2')] \\
&+ [v(12) - v(1'2')]\Gamma_{fi}(12;1'2') \\
&+ 3\int d\tau_3 \left[v(13)+v(23)-v(1'3')-v(2'3')\right]\Gamma_{fi}(123;1'2'3') \\
&= \omega_{fi}\Gamma_{fi}(12;1'2')
\end{aligned}
\tag{14}
$$

7. Applications

The election-impact ionization of the hydrogen-like U^{91+} is described by the reaction

$$e^- + \mathrm{U}^{91+} \longrightarrow \mathrm{U}^{92+} + e^- + e^-$$

(15)

The electromagnetic interaction between charged particles arising from the exchan-ge of one photon may be summarized in the QED theory as the Coulomb interacti-on plus ***transverse-***

$$v(\mathbf{r}_{12}) = \frac{1}{r_{12}} - (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 \frac{e^{i\omega r_{12}}}{r_{12}}) + (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\nabla})(\boldsymbol{\alpha}_2 \cdot \boldsymbol{\nabla}) \left[\frac{e^{i\omega r_{12}} - 1}{\omega^2 r_{12}} \right] \tag{16}$$

The QED cross sections of electron-impact ionization for hydrogen-like U^{91+} have been calculated, and is shown in Fig. 3. Our results agree quite will with experiment [3, 4] and with available theoretical data [5, 6].

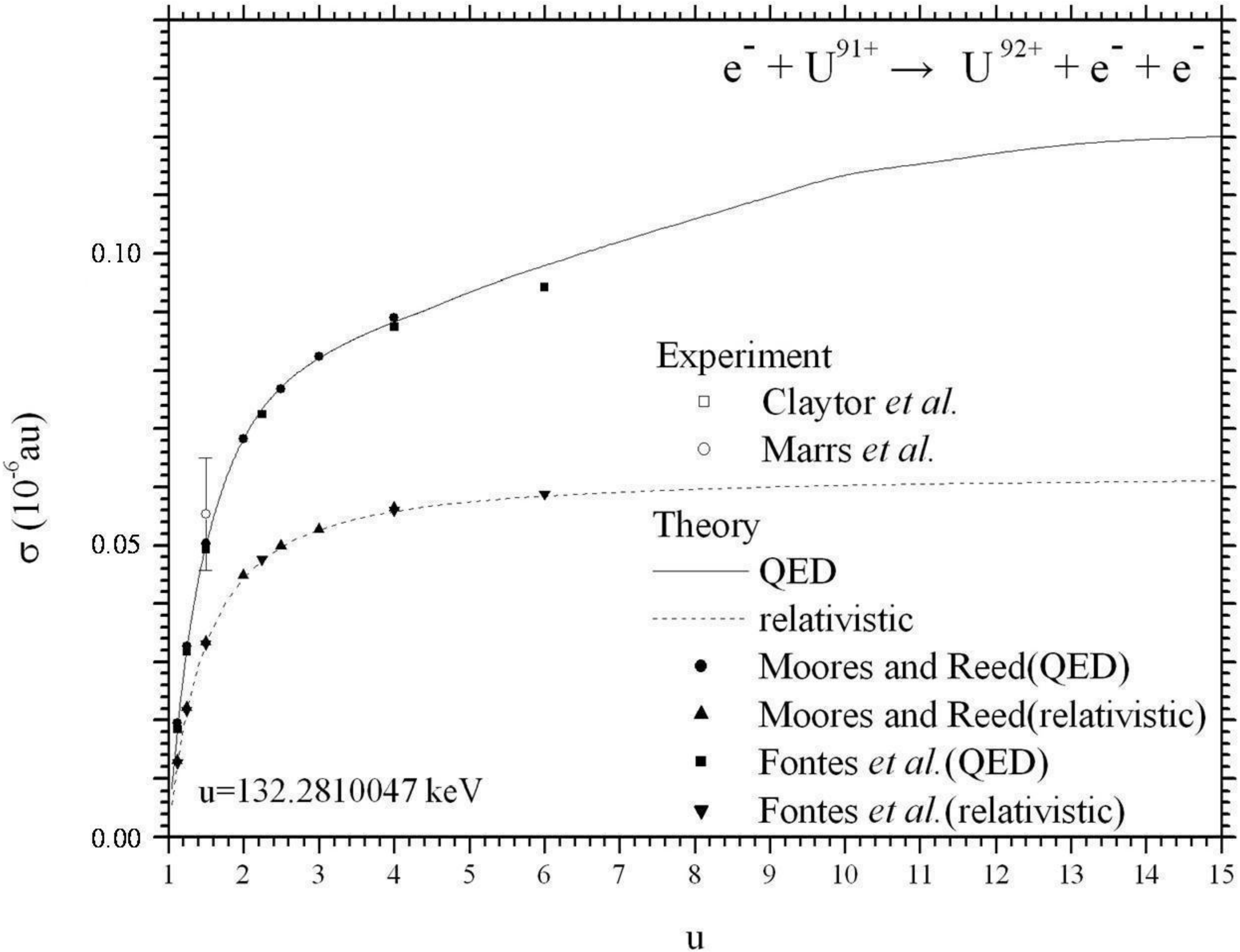

Fig. 3 Electron-Impact Ionization of U^{91+}

The proton-impact ionization of hydrogen has been calculated in the present formulation, and the results are presented in Fig. 4. There is an excellent agreement with experiment [7, 8, 9].

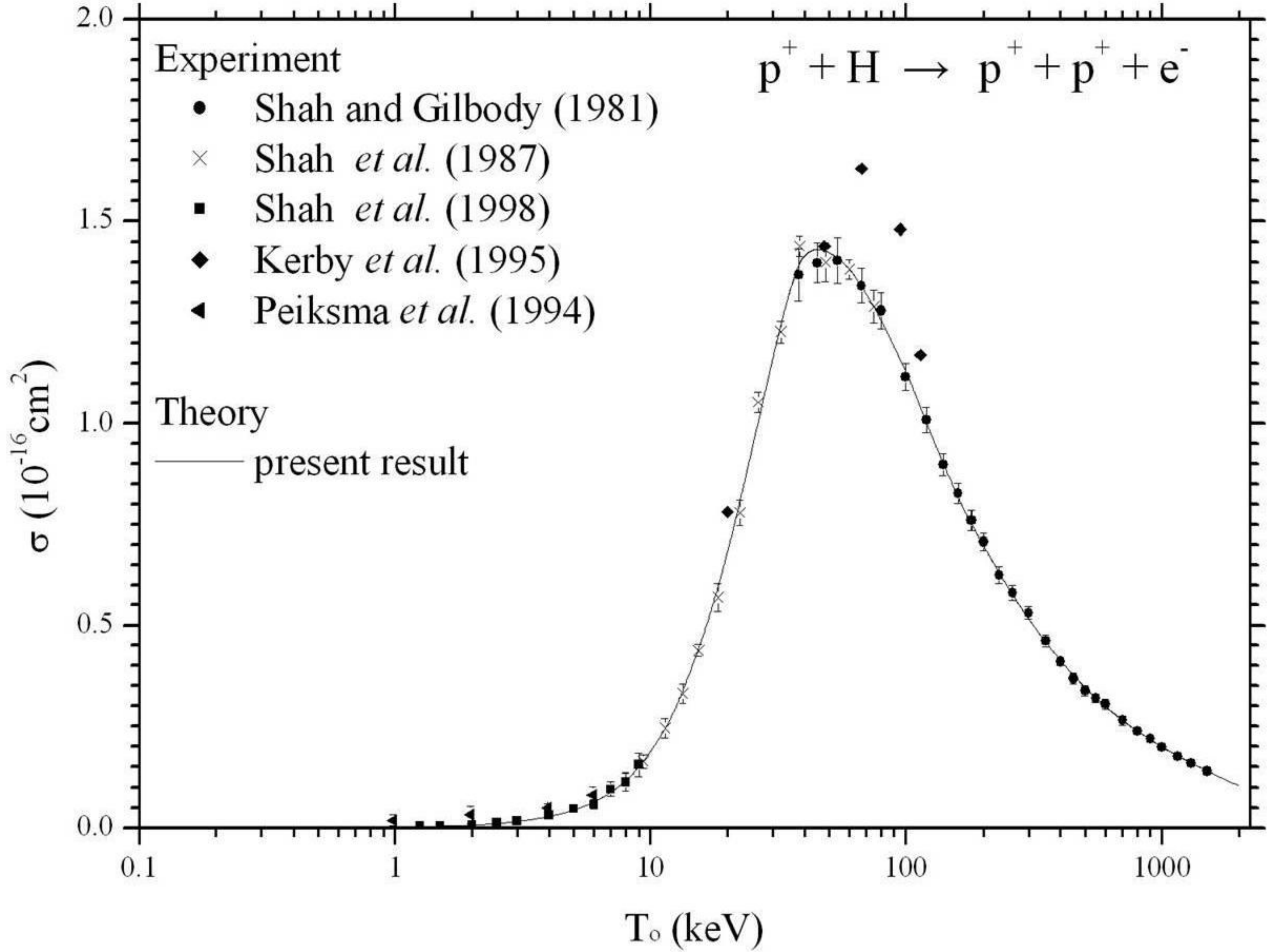

Fig. 4 Proton-Impact Ionization of Hydrogen

8. Conclusion

A relativistic quantum transport theory for many-particle systems has been proposed to treat particle-correlation and relativistic effects in an ***ab initio*** manner. The ensemble average over spectator particles of the many-particle system is formally carried out from the outset to reduced the problem only to that of active particles.

Important characteristics of this approach may be summarized as follows.

1. Applicable to both closed- and open-shell many-particle systems.
2. Gauge independent for radiative transitions.
3. Fine structures and spin polarizations are built in.

4. Both discrete- and continuum-state correlations are dealt with.
5. Multi-electron excitations are incorporated.
6. Initial- and final-state correlations are treated on an equal footing.
7. Core polarization and shielding effects are included self-consistently.

An approximation to the present approach, called the multiconfiguration relativistic random-phase approximation (MCRRPA), has been applied to photoexcitation and photoionization with great success. We have further incorporated quantum electrodynamic effects perturbatively in the formulation.

Our results for the electron-impact ionization of U^{91+} agree well with existing experimental and theoretical data. The proton-impact-ionization cross sections of hydrogen are calculated including recoil effects and are in excellent agreement with available data.

References

1. K.-N. Huang, Phys. Rev. A 26, (1982) 734.
2. K.-N. Huang, Phys. Rev. A 18, (1978) 1119.
3. N. Claytor, B. Feinberg, H. Gould, C. E. Bemis, Jr., J. Gomez Del Campo, C. A. Ludemann, and C. R. Vane, Phys. Rev. Lett. 61, (1988) 2081.
4. R. E. Marrs, S. R. Elliott, and D. A. Knapp, Phys. Rev. Lett. 72, (1994) 4082.

5. D. L. Moores and K. J. Reed, Phys. Rev. A 51, (1995) R9.
6. C. J. Fontes, D. H. Sampson, and H. L. Zhang, Phys. Rev. A 59}, (1999) 1329.
7. M. B. Shah and H. B. Gilbody, J. Phys. B 14, (1981) 2361.
8. M. B. Shah, D. S. Elliott, and H. B. Gilbody, J. Phys. B 20, (1987) 2481.

9. M. B. Shah, J. Geddes, B. M. Mclaughlin, and H. B. Gilbody, Phys. B 31, (1998). L757
10. M. Pieksma, S. Y. Ovchinnikov, J. van Eck, W. B. Westerveld, and A. Niehaus, *Phys. Rev. Lett.* 73, (1994) 46.
11. G. E. Kerby, III *et al.*, *Phys. Rev.* A 51, (1995) 2256.