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Stochastic Aspects in the Theory of Spectral-Line Broadening. II. Noncommutative Cluster Expansions

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Generalizing ideas of von Waldenfels we develop a systematic procedure to define truncated n-point operators which are reminiscent of Ursell functions of statistical mechanics. The truncation procedure is adapted to factorization relations obeyed by the operators in question. The results are applied to spectral-line broadening in plasmas. We derive cluster expansions for the line-shape function in terms of these truncated operators, where the ions are treated quasistatistically. The first order approximation for the line-shape function is discussed. The results are carried over to several moving perturber species, in particular to nonquasistatic ions.

KEY WORDS: Pressure broadening; series expansions; stochastic differential equations; cluster expansions for operators.

1. INTRODUCTION

We continue our investigation of the line shape emitted by an atom in a gas (plasma) of charged classical particles. In Part I[(1)] we discussed the two-level model and the associated Schrödinger equation with a random potential arising from the gas particles (perturbers). Shielding was taken into account by a cutoff at the Debye sphere, i.e., perturbers contribute to the potential only as long as they are in this sphere. Owing to their much greater mass as compared to electrons, ions were treated quasistatistically; but it was also pointed out how to include ion motion.

Von Waldenfels[(2)] has considered a particular case of the model: a single-particle species (electrons) only, a lower velocity cutoff in the Maxwell distribution, and no static ions. In Sections II.2 and II.3 of Ref. 2 he

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introduces, somewhat *ad hoc*, truncation for four special types of n-point operators, inserts these expressions into $\langle T(t,0)\rangle$ and $(d^2/dt^2)\langle T(t,0)\rangle$, and is then able to perform the N-particle limit. From this there result two cluster expansions in terms of truncated quantities, one for $\langle T(t,0)\rangle$ and one for $(d^2/dt^2)\langle T(t,0)\rangle$.

It is in no way obvious how to include several particle species and, in particular, static ions. When we tried to include these we had to reconsider the truncated operators of von Waldenfels and found little *explicit* motivation for their introduction or for their particular form which was different for each of the four types of operators.

Our problem thus was twofold. On the one hand we had to delve deeper into the truncation notion, clarify the underlying ideas, remove the *ad hoc* nature by a systematic truncation procedure, and, in particular, find support for the belief that an expansion in quantities thus constructed possesses faster convergence properties. All this is done in Section 2. The systematic truncation procedure presented there gives von Waldenfels' truncated expressions when applied to his four types of operators (cf. the examples after Theorem 2.1), and it is clear that he was implicitly guided by the same motivation. Once one has found the general procedure, the abstract algebraic considerations of von Waldenfels in Section II.2 of Ref. 2 on the free algebra generated by intervals become very useful.

On the other hand, we had the intricate problem to find suitable n-point operators in terms of which the more general intensity operator could be expressed and to which the truncation procedure could be applied. With hindsight the form of these operators [Eq. (2.2); cf. also Ref. 3] appears quite natural when compared with the corresponding expressions of Ref. 2.

The truncated "n-point operators" of Section 2 depend on n *time* points. They are analogous to Ursell functions of statistical mechanics insofar as correlations have been partially removed. The procedure, however, is not as simple as for Ursell functions or for the truncated n-point functions of quantum field theory, because its form varies and has to be adapted to factorization properties of the operators in questions. Furthermore, time ordering has to be preserved in the operator expressions, giving rise to a noncommutative aspect.

In Section 3 the resulting expressions are fed into the intensity operator $J_i(\omega)$ of Theorem 3.1 of Part I [cf. Eqs. (1.15) and (1.16) below] and the N-perturber limit $N\to\infty$ is performed. Basically this is similar to von Waldenfels,[2] although we work directly with the intensity operator J_i instead of $\langle T(t,0)\rangle$ since this seems to make the whole treatment more transparent, avoiding convolution algebras, *-inverses of δ functions, etc., as in Ref. 2.

We obtain in this way a cluster expansion of the intensity operator in terms of the truncated quantities of Section 2, leading in a natural way to an approximation scheme, or rather two schemes which arise from the two alternative expressions for J_i in Eqs. (1.15) and (1.16) below. It is pointed out that the two approximation schemes are equivalent in each order (for a proof see Ref. 3), a fact underlining the internal consistency of the whole approach. Without ions these approximations reduce to those of von Waldenfels[2] arising from his cluster expansions of $\langle T(t,0)\rangle$ and $(d^2/dt^2)\langle T(t,0)\rangle$, their equivalence in each order not being noticed there.

In this connection we mention an interesting open problem. The convergence of the expansion is proved by means of additional technical assumptions which are somewhat *ad hoc*. It would be worthwhile to avoid them or replace them by physically motivated assumptions.

In Section 4 the first-order approximation is analyzed and brought into a simplified form. In Ref. 5 we have given a direct derivation of this first-order term without using cluster expansions. The derivation in Ref. 5 clarifies the implicit physical approximations involved and it shows that the first-order term already partially contains the overlapping of the perturbers. Also in Ref. 5 a numerical evaluation for Lyman-α is given, showing good agreement with experimental data except in the line center. The latter is presumably due to the quasistatic treatment of the ions.

At the end of Section 3 the cluster expansion is carried over to several *moving* perturber species, in particular for nonquasistatic ions. The corresponding first-order term is explicitly written out at the end of Section 4. At the moment, however, it remains unclear how good this first-order term is numerically in the case of several moving perturber species.

Notation

As in I we consider the perturber as an ideal gas and describe an individual perturber by its velocity $\mathbf{v}_\kappa$, collision time τ_κ and impact parameter $\boldsymbol{\rho}_\kappa$, where τ_κ and $\boldsymbol{\rho}_\kappa$ are time and position of closest approach to the atom sitting at the origin. The total random potential is then of the form

$$V(t) = V_i + V_e(t) = V_i + \sum_\kappa \varphi(\boldsymbol{\rho}_\kappa, \mathbf{v}_\kappa; t - \tau_\kappa) \tag{1.1}$$

where $V_i = V_{\text{ions}}$, $V_e = V_{\text{electrons}}$. κ runs from $-\infty$ to ∞. If $\kappa > 0$, the index κ refers to the κth perturber colliding after $t = 0$; if $\kappa \leqslant 0$, it refers to the $|\kappa| + 1$st perturber colliding before $t = 0$. The intercollision times

$$u_\kappa := \tau_{\kappa+1} - \tau_\kappa \tag{1.2}$$

are independent and distributed exponentially according to

$$ce^{-cu}\,du \tag{1.3}$$

where c is the mean collision frequency,

$$c = \langle u_\kappa \rangle_{\text{av}}^{-1} = \rho_D^2 \bar{v} \nu \tag{1.4}$$

($\bar{v}$ = mean velocity, ν = density).

The averaging (expectation) is decomposed into two steps, first over electrons with a fixed ion configuration, then over ions. The electron expectation is written as $\langle\ \rangle$,

$$\langle\ \rangle \equiv \langle\ \rangle_{\text{electrons}} \tag{1.5}$$

One has to solve the stochastic Schrödinger equation

$$\dot{T}(t,t') = -iV(t)T(t,t') \tag{1.6}$$

and to determine the Fourier transform of $\langle T(t,0)\rangle_{\text{av}}$. The line-shape function then results from a trace operation. As in Part I we introduce the *intensity operator* J_i for fixed ion configuration,

$$J_i(\omega) := (2\pi)^{-1} \int dt\, e^{i\omega t} \langle T(t,0) \rangle \tag{1.7}$$

We will have to consider different time-development operators simultaneously. For the solution of an equation of the form

$$\begin{aligned} \frac{d}{dt} U(t,t') &= -i\phi(t) U(t,t') \\ U(t',t') &= \mathbb{1} \end{aligned} \tag{1.8}$$

we write therefore

$$U(t,t') = U(t,t';\phi(\cdot)) \tag{1.9}$$

or, for short,

$$U(t,t') = U(t,t';\phi) \tag{1.10}$$

so that

$$T(t,t') = U(t,t';V)$$

One of the main results of I, Theorem 3.1, can then be formulated as follows.

Theorem. Let the time-shifted N-electron potential in the ion interaction picture be defined by[3]

$$\phi(1 \cdots N,t) := \exp(iV_i t) \sum_{\nu=1}^{N} \varphi(t - \tau_\nu + \tau_1) \exp(-iV_i t) \tag{1.11}$$

With this potential let the random operators $\mathscr{D}(1 \ldots N;\omega)$ and

[3] The time shift is such as to have the first collision at $t = 0$. The dependence of ϕ on ρ_ν and $\mathbf{v}_\nu$ is understood.

$\mathscr{T}(1 \ldots N;\omega)$ be defined by

$$\mathscr{D}(1 \ldots N;\omega) := \int dt\, e^{i(\omega - V_i)t}\phi(1 \ldots N;t)U(t,-\infty;\phi(1 \ldots N)) \quad (1.12)$$

$$\begin{aligned}\mathscr{T}(1 \ldots N;\omega) := \int dt\, e^{i(\omega - V_i)t} \{ & U(t,-\infty;\phi(1 \ldots N)) - g(t)\mathbb{1} \\ & - [1 - g(t - u_1 - \cdots - u_N)] \\ & \times U(\infty,-\infty;\phi(1 \ldots N))\}\end{aligned} \quad (1.13)$$

where the real function g satisfies

$$\int_0^\infty |g(t)|\,dt < \infty, \qquad \int_{-\infty}^0 |1 - g(t)|\,dt < \infty \quad (1.14)$$

Then, if $\langle T(t,0)\rangle \in L^1$, one has uniformly in ω

$$J_i(\omega) = \lim_{N\to\infty} (2\pi N)^{-1} c\langle \mathscr{T}(1 \ldots N;\omega)\mathscr{T}(1 \ldots N;\omega)^*\rangle \quad (1.15)$$

and

$$\begin{aligned}&(\omega - V_i)J_i(\omega)(\omega - V_i) \\ &\quad = \lim_{N\to\infty} (2\pi N)^{-1} c\langle \mathscr{D}(1 \ldots N;\omega)\mathscr{D}(1 \ldots N;\omega)^*\rangle\end{aligned} \quad (1.16)$$

If $\langle T(t,0)\rangle \notin L^1$ the convergence is in the sense of weak convergence of measures.

2. NONCOMMUTATIVE CLUSTER DECOMPOSITIONS

Factorization Relations

We say that a set of consecutive perturbers, 1 to N, say, separates into two nonoverlapping clusters, 1 to m and $m+1$ to N, if perturbers 1 to m have already left the Debye sphere before any of the perturbers $m+1$ to N have entered. In such a situation the associated time development operator and the S-matrix factorize. For example, for t in the "support" of the second cluster, one has

$$U(t,-\infty;\phi(1 \ldots N)) = U(t,-\infty;\phi')U(\infty,-\infty;\phi(1 \ldots N)) \quad (2.1)$$

where ϕ' denotes the contribution to $\phi(1 \ldots N)$ due to perturbers $m+1$ to N. Other operators, such as $\mathscr{T}(1 \ldots N;\omega)$ or $\mathscr{D}(1 \ldots N;\omega)$, also have factorization relations, but of different form. The cluster expansions developed here will be tailored to match these relations.

Instead of $(1, \ldots, N)$ we consider general intervals in $\mathbb{N}$.

$$I := (l, l+1, \ldots, r), \qquad l, r \in \mathbb{N}$$

and define

$$\begin{aligned}
\phi(I;t) &:= \exp(iV_i t) \sum_{\nu=l}^{\tau} \varphi(t(\tau_\nu - \tau_l)) \exp(-iV_i t) \\
u(I) &:= u_l + \cdots + u_r \\
\mathscr{S}(I;\omega) &:= \exp\{i(\omega - V_i)u(I)\}\, U(\infty, -\infty; \phi(I)) \qquad (2.2) \\
\mathscr{T}(I;\omega) &:= \int dt\, e^{i(\omega - V_i)t} \{ U(t, -\infty; \phi(I)) - g(t) \\
&\qquad - [1 - g(t - u(I))] U(\infty, -\infty; \phi(I)) \} \\
\mathscr{D}(I;\omega) &:= \int dt\, e^{i(\omega - V_i)t} \phi(I;t)\, U(t, -\infty; \phi(I))
\end{aligned}$$

where $g(t)$ satisfies Eq. (1.14). We suppress the variable ω in the following. For $V_i = 0$ these expressions correspond to quantities introduced in Ref. 2 in t space with $g(t) = \theta(-t)$. Our particular choice of generalization ensures the validity of factorization relations for nonoverlapping clusters to be stated in Eqs. (2.3). We remark that already Theorem 3.1 of Part I has been tailored with this in mind. This is a central point of the paper, allowing the application of the truncation procedure.

Note that all quantities depend only on perturbers indexed by I and that they are *independent for disjoint intervals*. $\mathscr{S}$ is essentially an S matrix, $\mathscr{T}$ is the Fourier transform of a time-development operator with compensating terms to insure integrability, and $\mathscr{D}$ is related to the derivative of a time-development operator.

If the perturbers indexed by $I = (l, \ldots, r)$ separate into two *nonoverlapping* clusters indexed by $I_1 = (l, \ldots, n)$ and $I_2 = (n+1, \ldots, r)$ then explicit calculation[3] gives the factorization relations

$$\mathscr{S}(I) = \mathscr{S}(I_2)\mathscr{S}(I_1) \qquad (2.3a)$$

$$\mathscr{T}(I) = \mathscr{T}(I_2)\mathscr{S}(I_1) + \mathscr{T}(I_1) \qquad (2.3b)$$

$$\mathscr{D}(I) = \mathscr{D}(I_2)\mathscr{S}(I_1) + \mathscr{D}(I_1) \qquad (2.3c)$$

Factorization relations of the operators

$$Q_{\mathscr{T}}(I) := \mathscr{T}(I)\mathscr{T}(I)^* \qquad (2.4)$$

$$Q_{\mathscr{D}}(I) := \mathscr{D}(I)\mathscr{D}(I)^* \qquad (2.5)$$

will be derived from Eqs. (2.3a) and (2.3c) in the examples following Theorem 2.1.

We denote by $\circ$ the union of *adjoining* intervals,

$$I_1 \circ \cdots \circ I_\kappa = \bigcup_1^\kappa I_i, \qquad I_1 < \cdots < I_\kappa \tag{2.6}$$

and the intervals are nonempty *unless* explicitly stated otherwise. The ordering $I_1 < I_2$ simply means that I_1 is to the left of I_2. By the length $|I|$ of an interval $I \subset \mathbb{N}$ we denote the number of points in I.

Truncation Heuristics

The operators $\mathscr{S}(1 \ldots n)$ and their expectations are reminiscent of n-point functions in statistical mechanics and quantum field theory where the usefulness of Ursell functions and truncated n-point functions is well known. It suggests itself to carry this notion over to the operator function $\mathscr{S}(1 \ldots n)$. The general idea in the case of Ursell functions is to subtract out as many correlations as possible; in particular all Ursell functions vanish in the case of independent variables. Because of the operator nature of $\mathscr{S}(1 \ldots n)$ and the ensuing need to preserve the time order the definition has to be modified, however. It suggests itself to define the truncated operator function $\mathscr{S}[I]$ inductively by

$$\mathscr{S}(I) := \sum_{I_1 \circ \cdots \circ I_\kappa = I} \mathscr{S}[I_\kappa] \ldots \mathscr{S}[I_1] \tag{2.7}$$

a generalization of Eq. (2.3a) into a sum over all partitions of I into adjoining clusters.

Examples. One has

$$\mathscr{S}[i_1] = \mathscr{S}(i_1)$$

$$\mathscr{S}[i_1 i_2] = \mathscr{S}(i_1 i_2) - \mathscr{S}(i_2)\mathscr{S}(i_1)$$

$$\mathscr{S}[i_1 i_2 i_3] = \mathscr{S}(i_1 i_2 i_3) - \mathscr{S}(i_2 i_3)\mathscr{S}(i_1) - \mathscr{S}(i_3)\mathscr{S}(i_1 i_2) + \mathscr{S}(i_3)\mathscr{S}(i_2)\mathscr{S}(i_1)$$

For Ursell functions one would also have a term of the form (13)(2); but because of the time ordering such a term does not appear here.

An important consequence of our definition and of the factorization relation, Eq. (2.3a), is that if the perturbers indexed by I decompose into two nonoverlapping clusters then

$$\mathscr{S}[I] = 0 \tag{2.8}$$

Indeed, let the clusters be indexed by I_1, I_2 and assume the statement for all intervals of length less than that of I as induction hypothesis. Then in Eq.

(2.7) only partitions contribute which are also partitions of I_1 and I_2, hence

$$\mathscr{S}(I) = \mathscr{S}[I] + \sum_{I'' \circ \cdots I''_l = I_2} \mathscr{S}[I''_l] \ldots \mathscr{S}[I''_1]$$
$$\times \sum_{I'_1 \circ \cdots I'_m = I_1} \mathscr{S}[I'_m] \ldots \mathscr{S}[I'_1] \tag{2.9}$$

The last term is $\mathscr{S}(I_2)\mathscr{S}(I_1)$ which is just $\mathscr{S}(I)$ for nonoverlapping clusters, by Eq. (2.3a). Hence $\mathscr{S}[I] = 0$ follows.

This property suggests that not only should $\langle \mathscr{S}[1, \ldots, N] \rangle$ be small compared to the untruncated quantity but that it should go to 0 for $N \to \infty$ since for large N the probability for two nonoverlapping clusters increases. In view of Theorem 3.1 of Part I it is this large N limit we are after, and we therefore try to define $\mathscr{T}[I]$ and $\mathscr{D}[I]$ in a similar way.

To this end we generalize Eqs. (2.3b) and (2.3c) to a sum over all ordered partitions by

$$\mathscr{T}(I) =: \sum_{I_1 \circ \cdots \circ I_\kappa \circ I_{\kappa+1} = I} \mathscr{T}[I_\kappa]\mathscr{S}[I_{\kappa-1}] \cdots \mathscr{S}[I_1] \tag{2.10}$$

with $\kappa \geqslant 1$, $I_1 < \cdots < I_\kappa$ and with $I_{\kappa+1}$ either empty or $I_\kappa < I_{\kappa+1}$; for $\kappa = 1$ the $\mathscr{S}$ factors are absent. The definition of $\mathscr{D}[I]$ is analogous. If I indexes two *nonoverlapping* clusters then again

$$\mathscr{T}[I] = \mathscr{D}[I] = 0 \tag{2.11}$$

This is proved by Eqs. (2.3b) and (2.3c) similarly as before.

Now one might try to insert the expansion Eq. (2.10) into the quadratic expressions

$$Q_{\mathscr{T}}(1 \ldots N) := \mathscr{T}(1 \ldots N)\mathscr{T}(1 \ldots N)^*$$
$$Q_{\mathscr{D}}(1 \ldots N) := \mathscr{D}(1 \ldots N)\mathscr{D}(1 \ldots N)^*$$

which are related to the intensity operator J_i through Eqs. (1.12) and (1.13). The resulting sum, however, contains a large number of products of statistically dependent factors and one would have to rearrange the sum to be able to perform the limit $N \to \infty$. It is not quite obvious how to do this directly, and we will therefore obtain this rearrangement by introducing a truncated quantity $Q[I]$ with the same property as before, i.e., $Q[I] = 0$ for nonoverlapping clusters. The form of $Q[I]$ is not so easy to guess, and it is therefore advisable to systematize the procedure for defining truncated quantities.

General Truncation Procedure

To arrive at this we express $\mathscr{S}[I]$ and $\mathscr{T}[I]$ in terms of untruncated quantities. In Eq. (2.7) we keep I_κ fixed and perform the remaining sum.

This yields

$$\mathscr{S}(I) = \mathscr{S}[I] + \sum_{I_1 \circ I_2 = I} \mathscr{S}[I_2]\mathscr{S}[I_1] \tag{2.12}$$

Using this it is straightforward to show by induction on the length of I that

$$\mathscr{S}[I] = \sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} \mathscr{S}(I_\kappa) \ldots \mathscr{S}(I_1) \tag{2.13}$$

With the notation

$$\mathscr{S}(I_1 I_2 \ldots I_\kappa) := \mathscr{S}(I_\kappa) \ldots \mathscr{S}(I_1) \tag{2.14}$$

this reads

$$\mathscr{S}[I] = \sum_{I_1 \circ \circ I_\kappa = I} (-1)^{\kappa-1} \mathscr{S}(I_1 \ldots I_\kappa) \tag{2.15}$$

In a similar way one has from Eq. (2.10)

$$\mathscr{T}(I) = \mathscr{T}[I] + \sum_{\substack{I_1' \circ I_2' \circ I_3' = I \\ I_2' \neq I}} \mathscr{T}[I_2']\mathscr{S}(I_1') \tag{2.16}$$

where I_3' may be empty. By induction one shows

$$\mathscr{T}[I] = \sum_{I_1 \circ \circ I_\kappa = I} (-1)^{\kappa-1} \sum_{\nu=1}^{\kappa} \mathscr{T}(I_\nu)\mathscr{S}(I_1 \ldots I_{\nu-1}) \tag{2.17}$$

where for $\nu = 1$ the $\mathscr{S}$ factor is to be omitted. We now introduce the quantity $\mathscr{T}(I_1 \ldots I_\nu)$ defined inductively by

$$\mathscr{T}(I_1 \ldots I_\kappa) := \mathscr{T}(I_\kappa)\mathscr{S}(I_1 \ldots I_{\kappa-1}) + \mathscr{T}(I_1 \ldots I_{\kappa-1}) \tag{2.18}$$

for $\kappa \geqslant 2$. Then it is straightforward to see that

$$\mathscr{T}[I] = \sum_{I_1 \circ \circ I_\kappa = I} (-1)^{\kappa-1} \mathscr{T}(I_1 \ldots I_\kappa) \tag{2.19}$$

In Ref. 2, Eqs. (2.15) and (2.19) were introduced with little explicit motivation directly as definitions in the case $V_i = 0$. Here we have defined our quantities $\mathscr{S}$, $\mathscr{T}$, and $\mathscr{D}$ so as to retain the same formal relationships.

Compare now the definitions of $\mathscr{S}(I_1 \ldots I_\kappa)$ and $\mathscr{T}(I_1 \ldots I_\kappa)$, Eqs. (2.14) and (2.19), with the factorization relations of $\mathscr{S}(I)$ and $\mathscr{T}(I)$ for nonoverlapping clusters, Eqs. (2.3). The similarity suggests a general mechanism to obtain truncated quantities which vanish for nonoverlapping clusters as in Eqs. (2.8) and (2.11). This is our next result, which is new.

Theorem 2.1 (Truncation Theorem). Let $A_\nu(I)$, $\nu = 0, \ldots, N$, be (operator-valued) functions of the perturbers indexed by the interval I. Let $A_0(I) \equiv \mathbb{1}$. Suppose that for two nonoverlapping clusters of perturbers,

indexed by I_1 and I_2 with $I = I_1 \circ I_2$, one has

$$A_\nu(I) = c_\nu^{\alpha\beta} A_\alpha(I_1) A_\beta(I_2) + d_\nu^{\alpha\beta} A_\alpha(I_2) A_\beta(I_1), \qquad \nu = 0, 1, \ldots N \quad (2.20)$$

with suitable constants $c_\nu^{\alpha\beta}, d_\nu^{\alpha\beta}$ and with the usual sum convention over repeated indices. For formal products $I_1 \ldots I_\kappa$ of intervals define inductively

$$A_\nu(I_1 \ldots I_\kappa) = c_\nu^{\alpha\beta} A_\alpha(I_1 \ldots I_{\kappa-1}) A_\beta(I_\kappa) + d_\nu^{\alpha\beta} A_\alpha(I_\kappa) A_\beta(I_1 \ldots I_{\kappa-1}),$$
$$\nu = 0, 1 \ldots N \quad (2.21)$$

Assume Eq. (2.21) holds also with I_κ replaced by (the formal product) $I_\kappa I_{\kappa+1}$ on both sides ("weak associativity"). Now define truncation inductively by

$$A_\nu[I] = \sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} A_\nu(I_1 \ldots I_\kappa) \quad (2.22)$$

Then, if I indexes two nonoverlapping clusters, one has

$$A_\nu[I] = 0, \qquad \nu = 1, \ldots, N \quad (2.23)$$

The proof will be given in the Appendix. A possible dependence of A_ν on ω and other variables has not been written out explicitly. We illustrate the theorem by some examples which are relevant for the following.

Example 1. $N = 1$ and

$$A_1(I) = \mathscr{S}(I) \quad (2.24)$$

Equation (2.20) becomes Eq. (2.3a), and Eqs. (2.21) and (2.22) become Eqs. (2.14) and (2.15).

Example 2. $N = 2$, A_1 as before and

$$A_2(I) = \mathscr{T}(I) \quad (2.25)$$

Equations (2.20) and (2.21) become Eqs. (2.3b) and (2.18). Weak associativity is easily checked.

Example 3. $N = 2$, A_1 as before and

$$A_2(I) = \hat{\mathscr{T}}(I) := \mathscr{S}(I)\mathscr{T}(I)^* \quad (2.26)$$

For two nonoverlapping clusters one has from Eq. (2.3)

$$\hat{\mathscr{T}}(I) = \hat{\mathscr{T}}(I_2) + \mathscr{S}(I_2)\hat{\mathscr{T}}(I_1) \quad (2.27)$$

Thus Eq. (2.21) reads

$$\hat{\mathscr{T}}(I_1 \ldots I_\kappa) = \hat{\mathscr{T}}(I_\kappa) + \mathscr{A}(I_\kappa)\hat{\mathscr{T}}(I_1 \ldots I_{\kappa-1}) \tag{2.28}$$

and weak associativity is easily checked. Hence $\hat{\mathscr{T}}[I]$ defined through Eq. (2.22) satisfies $\hat{\mathscr{T}}[I] = 0$ for nonoverlapping clusters.

Example 4. $N = 6, A_1 = \mathscr{A}, A_2 = \mathscr{T}, A_3 = \mathscr{T}^*, A_4 = \hat{\mathscr{T}}, A_5 = \hat{\mathscr{T}}^*$, and

$$A_6(I) = Q_{\mathscr{T}}(I) := \mathscr{T}(I)\mathscr{T}(I)^* \tag{2.29}$$

For two nonoverlapping clusters one has from Eq. (2.3)

$$Q_{\mathscr{T}}(I) = Q_{\mathscr{T}}(I_1) + Q_{\mathscr{T}}(I_2) + \hat{\mathscr{T}}(I_1)^*\mathscr{T}(I_2)^* + \mathscr{T}(I_2)\hat{\mathscr{T}}(I_1) \tag{2.30}$$

so that for $\nu = 6$ Eq. (2.21) reads

$$\begin{aligned} Q_{\mathscr{T}}(I_1 \ldots I_\kappa) = {} & Q_{\mathscr{T}}(I_1 \ldots I_{\kappa-1}) + Q_{\mathscr{T}}(I_\kappa) + \hat{\mathscr{T}}(I_1 \ldots I_{\kappa-1})^*\mathscr{T}(I_\kappa)^* \\ & + \mathscr{T}(I_\kappa)\hat{\mathscr{T}}(I_1 \ldots I_{\kappa-1}) \end{aligned} \tag{2.31}$$

Weak associativity follows from that of $\mathscr{T}$ and $\hat{\mathscr{T}}$. Hence the truncated quantity $Q_{\mathscr{T}}[I]$ defined through Eq. (2.22),

$$Q_{\mathscr{T}}[I] = \sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} Q_{\mathscr{T}}(I_1 \ldots I_\kappa) \tag{2.32}$$

satisfies $Q_{\mathscr{T}}[I] = 0$ for nonoverlapping clusters.

For $Q_{\mathscr{D}}$ of Eq. (2.5) one has analogous expressions with $\mathscr{T}$ replaced by $\mathscr{D}$ and $\hat{\mathscr{D}}$ by

$$\hat{\mathscr{D}}(I) = \mathscr{A}(I)\mathscr{D}(I)^* \tag{2.33}$$

The decomposition of $A_\nu(I)$ for nonoverlapping clusters in Eq. (2.20) was assumed to be bilinear. More general situations may be envisaged, for instance, expressions cubic or quartic in $\mathscr{T}$. It is clear how one should try to generalize Theorem 2.2 in such cases.

Example 4 gives us the truncated quantities for the problem under consideration. It remains to express, conversely, $Q_{\mathscr{T}}(I)$ and $Q_{\mathscr{D}}(I)$ in terms of truncated quantities. In the Appendix we prove

$$\begin{aligned} Q_{\mathscr{T}}(I) = \sum_{\substack{I^{(0)} \circ I^{(1)} \circ I^{(2)} \\ |I^{(0,2)}| \geqslant 0}} \Bigg\{ & Q_{\mathscr{T}}[I^{(1)}] + \sum_{\substack{I_1 \circ \cdots \circ I_\kappa = I^{(1)} \\ \kappa \geqslant 2}} \\ & (\mathscr{T}[I_\kappa]\mathscr{A}[I_{\kappa-1}] \ldots \mathscr{A}[I_2]\hat{\mathscr{T}}[I_1] + \text{h.c.}) \Bigg\} \end{aligned} \tag{2.34}$$

where I_0, I_2 may be empty and where for $\kappa = 2$ there are no $\mathscr{S}$ factors in the inner sum. By h.c. we denote hermitian conjugate. An analogous equation holds for $Q_{\mathscr{D}}$. We note that the second sum can be rewritten, by Eq. (2.7), to yield

$$Q_{\mathscr{T}}(I) = \sum_{\substack{I^{(0)} \circ I^{(1)} \circ I^{(2)} \\ |I^{(1)}| \geqslant 0}} \Big\{ Q_{\mathscr{T}}[I^{(1)}] + \sum_{I_1 \circ I_2 \circ I_3 = I^{(1)}} (\mathscr{T}[I_3]\mathscr{S}(I_2)\hat{\mathscr{T}}[I_1] + \text{h.c.}) \Big\} \tag{2.35}$$

and analogously for $Q_{\mathscr{D}}(I)$. For I_2 empty, the $\mathscr{S}$ term is put equal to 1. An expression formally the same as in Eq. (2.34) appears in Lemma 10 of Ref. 2.

3. CLUSTER EXPANSION OF THE INTENSITY OPERATOR. THE LIMIT $N \to \infty$

We are going to express the intensity operator $J_i(\omega)$ of the Introduction in terms of truncated quantities. The limit $N \to \infty$ in Eqs. (1.16) and (1.17) will be performed and the factor $1/N$ in those equations will disappear. Basically the procedure is the same as that of von Waldenfels.[2]

Our motivation is the fact that the truncated quantities vanish for nonoverlapping clusters. One can therefore expect that in general the expectations of truncated quantities go to zero with increasing perturber numbers since the probability for two nonoverlapping clusters increases, i.e., one expects for $n \to \infty$

$$\langle \mathscr{T}[1 \ldots n] \rangle \to 0, \qquad \langle Q_{\mathscr{T}}[1 \ldots n] \rangle \to 0 \tag{3.1}$$

etc.

We insert now Eq. (2.34) or, rather, Eq. (2.35) for $Q_{\mathscr{T}} = \mathscr{T}\mathscr{T}^*$ and for $Q_{\mathscr{D}} = \mathscr{D}\mathscr{D}^*$ into Eqs. (1.15) and (1.16) for the intensity operator J_i. Putting $I^{(1)} = (l, \ldots, r)$ in Eq. (2.34) and using independence we obtain from Eq. (2.15)

$$J_i = \lim_{N\to\infty} \frac{c}{2\pi N} \sum_{1<l<r<N} \Big\{ \langle Q_{\mathscr{T}}[l \ldots r] \rangle + \sum_{I_1 \circ I_2 \circ I_3 = (l \ldots r)} (\langle \mathscr{T}[I_3]\mathscr{S}(I_2)\hat{\mathscr{T}}[I_1] \rangle + \text{h.c}) \Big\}$$

Let $n_\alpha = |I_\alpha|$ and $n = r - l + 1$. Then, by stationarity, I_α can be replaced by $(1, \ldots, n_\alpha)$ and $(l, \ldots, r)$ by $(1, \ldots, n)$. For fixed N and n there are

$N - n + 1$ intervals of the form $(l, \ldots, r)$. Hence

$$J_i = \lim_{N\to\infty} \frac{c}{2\pi} \sum_{n=1}^{N} \frac{N-n+1}{N}$$
$$\times \left\{ \langle Q_{\mathscr{T}}[1, \ldots, n] \rangle + \sum_{\substack{n_1+n_2+n_3=n \\ n_1,n_2 \geqslant 1}} (\langle \mathscr{T}[1 \ldots n_3] \rangle \langle \mathscr{S}(1 \ldots n_2) \rangle \right.$$
$$\left. \times \langle \hat{\mathscr{T}}[1 \ldots n_1] \rangle + \text{h.c}) \right\} \tag{3.2}$$

Under an additional technical assumption the limit can now be performed explicitly. We assume essentially that the vanishing of the truncated expectations in Eq. (3.1) for $n \to \infty$ is sufficiently fast.

Theorem 3.1. Let $\sum_n \langle \mathscr{S}[1, \ldots, n](\omega) \rangle$ be absolutely convergent to an operator with norm less than 1. (a) Let

$$\begin{gathered} \sum_n \langle \mathscr{T}[1 \ldots n](\omega) \rangle \\ \sum_n \langle \hat{\mathscr{T}}[1 \ldots n](\omega) \rangle \\ \sum_n \langle Q_{\mathscr{T}}[1 \ldots n](\omega) \rangle \end{gathered} \tag{3.3}$$

be absolutely convergent. Then one has, with absolute convergence,

$$J_i = \frac{c}{2\pi} \sum_1^{\infty} \langle Q_{\mathscr{T}}[1 \ldots n] \rangle$$
$$+ \frac{c}{2\pi} \left\{ \sum_1^{\infty} \langle \mathscr{T}[1 \ldots n] \rangle \left(1 - \sum_1^{\infty} \langle \mathscr{S}[1 \ldots n] \rangle\right)^{-1} \right.$$
$$\left. \times \sum_1^{\infty} \langle \hat{\mathscr{T}}[1 \ldots n] \rangle + \text{h.c} \right\} \tag{3.4}$$

(b) Let

$$\begin{gathered} \sum_n \langle \mathscr{D}[1 \ldots n](\omega) \rangle \\ \sum_n \langle \mathscr{D}[1 \ldots n](\omega) \rangle \\ \sum_n \langle Q_{\mathscr{D}}[1 \ldots n](\omega) \rangle \end{gathered} \tag{3.5}$$

be absolutely convergent. Then one has, with absolute convergence,

$$(\omega - V_i)J_i(\omega)(\omega - V_i) = \frac{c}{2\pi}\sum_1^\infty \langle Q_{\mathscr{D}}[1 \ldots n]\rangle + \frac{c}{2\pi}\left\{\sum_1^\infty \langle \mathscr{D}[1 \ldots n]\rangle \times \left(1 - \sum_1^\infty \langle \mathscr{S}[1 \ldots n]\rangle\right)^{-1} \times \sum_1^\infty \langle \hat{\mathscr{D}}[1 \ldots n]\rangle + \text{h.c.}\right\} \quad (3.6)$$

We first note a well-known fact.

Lemma 3.1. If $\sum a_n$ is absolutely convergent then

$$\lim_{N\to\infty} \sum_{n=1}^{N} \frac{n}{N} a_n \to 0 \quad (3.7)$$

In view of this it suffices to prove absolute convergence of the right-hand side of Eq. (3.2) without the factor $(N - n + 1)/N$.

Proof of Theorem 3.1a. We will show below that $\sum\langle \mathscr{S}(1 \ldots n)\rangle$ converges absolutely. Now, the points (n_1, n_2, n_3) in $\mathbb{R}^3$ satisfying $n_1 + n_2 + n_2 = n$, $n_i \geqslant 0$, lie on the triangle with corners in $(n, 0, 0)$, $(0, n, 0)$ and $(0, 0, n)$. Thus the second sum in Eq. (3.2) is over such a triangle, and the sum over n results in a sum over the positive quadrant when N goes to infinity (except for the points with $n_1 = 0$ or $n_2 = 0$). By absolute convergence the second term therefore becomes, for $N \to \infty$,

$$\sum_{n=1}^{\infty} \langle \mathscr{T}[1 \ldots n]\rangle \left(1 + \sum_{n=1}^{\infty} \langle \mathscr{S}(1 \ldots n)\rangle\right) \sum_{n=1}^{\infty} \langle \hat{\mathscr{T}}[1 \ldots n]\rangle \quad (3.8)$$

The proof will be completed by the following.

Lemma 3.2. Let $\sum\langle \mathscr{S}[1 \ldots n](\omega)\rangle$ be absolutely convergent to an operator of norm less than 1. Then

$$1 + \sum_1^\infty \langle \mathscr{S}(1 \ldots n; \omega)\rangle = \left(1 - \sum_1^\infty \langle \mathscr{S}[1 \ldots n](\omega)\rangle\right)^{-1} \quad (3.9)$$

where the convergence is absolute.

Proof. The Neumann series for the right-hand side gives

$$1 + \sum_{\kappa=1}^{\infty} \sum_{n_1, \ldots, n_\kappa = 1}^{\infty} \langle \mathscr{S}[1 \ldots n_\kappa]\rangle \cdots \langle \mathscr{S}[1 \ldots n]\rangle \quad (3.10)$$

By absolute convergence we can replace this by a threefold sum, first over $n_1 + \cdots + n_\kappa = n$ with $n_i \geqslant 1$, then over $\kappa = 1, \ldots, n$ and then over $n = 1, \ldots$. Introducing κ intervals such that $I_1 \circ \cdots \circ I_\kappa = (1, \ldots, n)$ and $|I_\alpha| = n_\alpha$, Eq. (3.10) can then be written as

$$1 + \sum_{n=1}^{\infty} \sum_{\kappa=1}^{n} \sum_{I_1 \circ \cdots \circ I_\kappa = n} \langle \mathscr{A}[I_\kappa] \cdots \mathscr{A}[I_1] \rangle$$

By Eq. (2.7) this is the left-hand side of Eq. (3.9). ■

The proof of part (b) of Theorem 3.1 is analogous.

Remark. It is an interesting open problem of how to get rid of the technical assumptions of Theorem 3.1, either by actually proving them or replacing them by more physical assumptions. In Ref. 2 a special case of the formula in Eq. (3.4) was derived under rather restricted assumptions. If there are no ions present and if one assumes a lower velocity cutoff which is related in a special way to the electron density then the Fourier transform of J_i was shown to converge in a certain measure theoretic norm as $N + \infty$.

Approximation Scheme

The expressions for the intensity operator $J_i(\omega)$ in Theorem 3.1 lend themselves to obvious approximations by terminating the sum over the truncated quantities at some given N. Let us denote the resulting expressions by $J_{i\mathscr{T}}^{(N)}$ and $J_{i\mathscr{D}}^{(N)}$. These contain all correlations up to N particles.

It is reassuring for the soundness of the approximation scheme that both approximations coincide in each order although $J_{i\mathscr{T}}^{(N)}$ contains the unspecified function $g(t)$ from Eq. (1.13) while $J_{i\mathscr{D}}^{(N)}$ does not.

Theorem 3.2. For each N one has

$$J_{i\mathscr{T}}^{(N)} = J_{i\mathscr{D}}^{(N)} \tag{3.11}$$

For the proof we refer to the thesis.[3] This result shows in fact that $J_{i\mathscr{T}}^{(N)}$ is independent of the particular choice of the function g. Without loss of generality one may take $g(t) = \theta(-t)$. The freedom in the choice of $g(t)$ remained unnoticed in Ref. 2, only $\theta(-t)$ was introduced there. This freedom, however, might be useful in numerical evaluations.

Several Perturber Species

The results of this section can be easily carried over to the situation where one has several moving perturber species. This is achieved by a simple observation on Poisson processes: the sum of two Poisson processes is again a Poisson process. In our situation this means the following. The

κth collision can now be by any of the perturber species, and the intercollision times

$$u_\kappa = \tau_{\kappa+1} - \tau_\kappa$$

are distributed according to

$$ce^{-cu}\,du$$

where c is the sum of the collision frequencies for the individual perturber species,

$$c = c_1 + \cdots + c_r \tag{3.12}$$

A perturber is characterized, in addition to ρ_κ, $\mathbf{v}_\kappa$, and τ_κ, by a parameter α, $\alpha = 1, \ldots, r$, which distinguishes the different perturber species and over which one also has to average with weight c_α/c. The distribution for $\rho_\kappa, \mathbf{v}_\kappa$ depends of course on the species in question. For the first-order approximation this is spelled out explicitly at the end of the next section.

4. THE FIRST-ORDER APPROXIMATION FOR THE INTENSITY OPERATOR

Let $V_I(t)$, $U_I(t)$, and S_I be the one-electron potential, time-development operator from $-\infty$ to t and S matrix, respectively, in the ion interaction picture,

$$\begin{aligned} V_I(t) &:= \phi(1,t) = e^{iV_i t}\varphi(\rho, \mathbf{v}; t)e^{-iV_i t} \\ U_I(t) &:= U(t, -\infty; V_I) \\ S_I &:= U_I(\infty) \end{aligned} \tag{4.1}$$

Since

$$\langle e^{i(\omega - V_i)u}\rangle = c\int_0^\infty du\, e^{-cu + i(\omega - V_i)u} = c\{c - i(\omega - V_i)\}^{-1} \tag{4.2}$$

we have, from Eq. (2.3) and from the independence of u and S_I,

$$\langle \mathscr{S}[1]\rangle = \langle \mathscr{S}(1)\rangle = c\{c - i(\omega - V_i)\}^{-1}\langle S_I\rangle$$

and

$$\{1 - \langle \mathscr{S}[1]\rangle\}^{-1} = \{-i(\omega - V_i) + c(1 - \langle S_I\rangle)\}^{-1}\{c - i(\omega - V_i)\} \tag{4.3}$$

We define $\mathscr{T}_R(1)$ by

$$\mathscr{T}_R(1;\omega) := \int dt\, e^{i\omega t}e^{-iV_i t}\{U_I(t) - g(t) - (1 - g(t))S_I\} \tag{4.4}$$

where the index R stands for "reduced" (no shift by u_1). Then we can write

by Eq. (4.3)

$$\mathscr{T}[1] = \mathscr{T}(1) = \mathscr{T}_R(1) + \mathscr{F}\{e^{-iV_i\cdot}(g(\cdot - u) - g)\}S_I \tag{4.5}$$

where $\mathscr{F}$ denotes Fourier transform. We use partial integration and set $\widetilde{g'} = \mathscr{F}g'$. Then

$$\mathscr{T}(1,\omega) = \mathscr{T}_R(1,\omega) + i\{\omega - V_i\}^{-1}\{e^{i(\omega - V_i)u} - 1\}\widetilde{g'}(\omega - V_i)S_I \tag{4.6}$$

From $\hat{\mathscr{T}} = \mathscr{S}\mathscr{T}$ one then has

$$\hat{\mathscr{T}}[1](\omega) = \hat{\mathscr{T}}(1;\omega) = e^{i(\omega - V_i)u}S_I\mathscr{T}_R(1;\omega)^* + i\{\omega - V_i\}^{-1}\{e^{i(\omega - V_i)u} - 1\}\widetilde{g'}(-\omega + V_i) \tag{4.7}$$

Taking expectations and using Eq. (4.2) gives

$$\langle\mathscr{T}[1](\omega)\rangle = \langle\mathscr{T}(1;\omega)\rangle = \langle\mathscr{T}_R(1;\omega)\rangle - \{-i(\omega - V_i) + c\}^{-1}\widetilde{g'}(\omega - V_i)\langle S_I\rangle \tag{4.8}$$

and

$$\langle\hat{\mathscr{T}}[1](\omega)\rangle = \{-i(\omega - V_i) + c\}^{-1}\{c\langle S_I\mathscr{T}_R(1;\omega)^*\rangle - \widetilde{g'}(\omega - V_i)^*\} \tag{4.9}$$

From Eq. (4.6) one finds

$$\begin{aligned}\langle Q_{\mathscr{T}}[1](\omega)\rangle &= \langle\mathscr{T}(1;\omega)\mathscr{T}(1;\omega)^*\rangle \\ &= \langle\mathscr{T}_R(1;\omega)\mathscr{T}_R(1;\omega)^*\rangle \\ &\quad - \{c - i(\omega - V_i)\}^{-1}\widetilde{g'}(\omega - V_i)\langle S_I\mathscr{T}_R(1;\omega)^*\rangle \\ &\quad - \langle\mathscr{T}_R(1;\omega)S_I^*\rangle\{c + i(\omega - V_i)\}^{-1}\widetilde{g'}(\omega - V_i)^* \\ &\quad + 2\{c^2 + (\omega - V_i)^2\}^{-1}\widetilde{g'}(\omega - V_i)\widetilde{g'}(\omega - V_i)^*\end{aligned} \tag{4.10}$$

To obtain the first-order approximation for the line-shape function we insert these expressions into Eq. (3.4) and terminate the sum at $n = 1$. A little algebra shows that this yields

$$\begin{aligned}J_i^{(1)} &= \frac{c}{2\pi}\langle\mathscr{T}_R(1)\mathscr{T}_R(1)^*\rangle \\ &\quad + \frac{1}{2\pi}\{[c\langle\mathscr{T}_R(1)\rangle - \widetilde{g'}(\omega - V_i)][-i(\omega - V_i) + c(1 - \langle S_I\rangle)]^{-1} \\ &\quad \times [c\langle S_I\mathscr{T}_R(1)^*\rangle - \widetilde{g'}(\omega - V_i)^*] + \text{h.c.}\}\end{aligned} \tag{4.11}$$

We note that the first term is positive and still depends on the choice of g while the whole right-hand side is independent of g. This might be used

to look for an "optimal" choice of g but we have found no natural candidate.

If one chooses $g(t) = \theta(-t)$ then

$$\widetilde{g'} = -1$$

We insert this and Eqs. (4.1) and (4.5) into $J_i^{(1)}$. With Eq. (1.13) we then obtain the following:

Theorem 4.1. Let $V_I(t)$, $U_I(t)$ and S_I be the one-electron potential, time-development operator from $-\infty$ to t and the S matrix, respectively, in the ion interaction picture. The intensity operator in first order is then given by

$$\begin{aligned} J_i^{(1)}(\omega) = \frac{c}{2\pi} \left\langle \left| \int dt\, e^{i(\omega - V_i)t} \left(U_I(t) - \theta(-t) - \theta(t) S_I \right) \right|^2 \right\rangle \\ + \frac{1}{2\pi} \left\{ 1 + c \int dt\, e^{i(\omega - V_i)t} \left\langle U_I(t) - \theta(-t) - \theta(t) S_I \right\rangle \right\} \\ \times \left\{ -i(\omega - V_i) + c\langle 1 - S_I \rangle \right\}^{-1} \\ \times \left\{ 1 + c \int dt\, e^{i(\omega - V_i)t} \left\langle U_I(t) S_I^* - \theta(-t) S_I^* - \theta(t) \right\rangle \right\}^* + \text{h.c.} \end{aligned} \tag{4.12}$$

where h.c. stands for the Hermitian conjugate of the second summand and where $|A|^2$ is defined as AA^*. An equivalent form is

$$\begin{aligned} J_i^{(1)}(\omega) = \frac{c}{2\pi} (\omega - V_i)^{-1} \Bigg[\left\langle \left| \int dt\, e^{i(\omega - V_i)t} V_I(t) U_I(t) \right|^2 \right\rangle \\ + c \int dt\, e^{i(\omega - V_i)t} \left\langle V_I(t) U_I(t) \right\rangle \\ \times \left\{ -i(\omega - V_i) + c\langle 1 - S_I \rangle \right\}^{-1} \\ \times \left\{ \int dt\, e^{i(\omega - V_i)t} \left\langle V_I(t) U_I(t) S_I^* \right\rangle \right\}^* \\ + \text{h.c.} \Bigg] (\omega - V_i)^{-1} \end{aligned} \tag{4.13}$$

The proof of the last statement starts from Theorem 3.1(b) and runs along the same lines as that of Eq. (4.12). It can also be derived from the latter by a straightforward partial integration (see below).

Remark. (i) The line-shape function in first order is obtained from Part I, Eq. (1.21),

$$L^{(1)}(\omega) = \mathrm{Tr}\, D \left\langle J_i^{(1)}(\omega - \omega_0) \right\rangle_{\text{ions}} \tag{4.14}$$

where the operator D is given by Part I, Eq. (1.5), and ω_0 is the frequency of the unperturbed line.

(ii) In the "impact approximation" of spectral-line broadening[4] the electron collisions are taken as infinitesimally short and hence as nonoverlapping. Then the first-order expression for the line-shape function becomes exact since all truncated quantities now vanish for $n \geqslant 2$. The time-development operator $U_I(t)$ becomes a step function,

$$U_I(t) = \begin{cases} \mathbb{1} & \text{for } t < 0 \\ S_I & \text{for } t > 0 \end{cases}$$

and all integrands in Eq. (4.12) are identically zero. Hence in the impact approximation for the electrons

$$\begin{aligned} L(\omega_0 + \omega) &\equiv L^{(1)}(\omega + \omega_0) \\ &= \frac{1}{2\pi} \mathrm{Tr}\, D \left\langle \{ -1(\omega - V_i) + c\langle 1 - S_I \rangle \}^{-1} + \text{h.c.} \right\rangle_{\text{ions}} \end{aligned} \tag{4.15}$$

For $V_i = 0$ this reduces to the usual result.[4]

(iii) The equivalence of the two forms for $J_i^{(1)}$ can be shown directly in a simple way. By partial integrations one has

$$\begin{aligned} &\int dt\, e^{i(\omega - V_i)t} \{ U_I(t) - \theta(-t) - \theta(t) S_I \} \\ &\quad = i(\omega - V_i)^{-1} \left\{ 1 - S_I + \int dt\, e^{i(\omega - V_i)t} V_I U_I \right\} \end{aligned}$$

If one inserts this into Eq. (4.12) one obtains Eq. (4.13) by straightforward algebra.

(iv) The two forms of $L^{(1)}$ have their merits in different regions of ω. For large ω the first term in Eq. (4.13) becomes dominant since the remaining ones fall off with a higher power of ω. For small ω it turns out in applications that all integrals in Eq. (4.12) can be neglected. This leads to the impact approximation, Eq. (4.15).

(v) A direct derivation of $L^{(1)}$ has been given by us in Ref. 5. Starting from Eq. (1.16) one can approximate in $\phi(1 \ldots N; t) U(t, -\infty; \phi(1 \ldots N))$ the second factor while retaining the first factor $\phi(1 \ldots N; t)$ in full. The second factor is approximated by considering the collisions as nonoverlapping. Then the N-perturber limit in Eq. (1.16) can be performed explicitly, a very instructive exercise. In a similar way one can also start

from Eq. (1.15).[3] This analysis shows that the first-order approximation takes perturber overlapping partially into account.

(vi) An application of our results for $L^{(1)}$ to Lyman-α has been given in Ref. 5. The agreement with experiment is good for the line wing. In the line center the agreement is not so good. This may be due to the quasistatic treatment of the ions.

Several Perturber Species

For simplicity we consider two moving particle species, ions and electrons, say, and no quasistatic potential. According to Eq. (3.12),

$$c = c_e + c_i \tag{4.16}$$

and in Theorem 4.1 the averaging $\langle\ \rangle$ is now an averaging $\langle\ \rangle_e$ over velocity and impact parameter of a single electron, with weight c_e/c, as well as an averaging $\langle\ \rangle_i$ over velocity and impact parameter of a single ion, with weight c_i/c. In obvious notation and with the abbreviations

$$B_e(\omega) = \int dt\, e^{i\omega t}\big(U_e(t) - \theta(t) - \theta(t)S_e\big) \tag{4.17}$$

and similarly for B_i, Eq. (4.12) now becomes

$$\begin{aligned} 2\pi J^{(1)} = {} & c_e\langle B_e B_e^*\rangle_e + c_e\langle B_i B_i^*\rangle_i \\ & + \Big[\{1 + c_e\langle B_e\rangle_e + c_i\langle B_i\rangle_i\}\{-i\omega + c - c_e\langle S_e\rangle_e - c_i\langle S_i\rangle_i\}^{-1} \\ & \times \{1 + c_e\langle S_e B_e^*\rangle_e + c_i\langle S_i B_i^*\rangle_i\} + \text{h.c.}\Big] \end{aligned} \tag{4.18}$$

In a similar, but more complicated way, one can write down the higher-order approximations. For ions these are expected to play a more important role.

APPENDIX: PROOF OF THEOREM 2.1 (TRUNCATION THEOREM)

Under the assumptions of Theorem 2.1 we first prove the following.

Lemma A1. Let $I = I_1 \circ \ldots \circ I_\kappa$, let $I_i = I_i^1 \circ I_i^2$ for some $i \leqslant \kappa$, and let the perturbers indexed by I decompose into two nonoverlapping clusters according to $I_1 \circ \cdots \circ I_i^1$ and $I_i^2 \circ \cdots \circ I_\kappa$. Then, for $\nu = 1, \ldots, N$

$$A_\nu(I_1 \ldots I_i \ldots I_\kappa) = A_\nu(I_1 \ldots I_i^1 I_i^2 \ldots I_\kappa) \tag{A1}$$

Proof. We proceed by induction on κ. For $\kappa = 1$, Eq. (A.1) reduces to Eqs. (2.20) and (2.21). Assume the statement to be true for all $\kappa \leqslant n - 1$.

To prove it for $\kappa = n$, we distinguish the cases $i = n = \kappa$ and $i < n = \kappa$ in Eq. (A.1). For $i = n = \kappa$ we have from Eqs. (2.20) and (2.21)

$$A_\nu(I_1 \ldots I_\kappa) = C_\nu^{\alpha\beta} A_\alpha(I_1 \ldots I_{\kappa-1}) A_\beta(I_\kappa^1 I_\kappa^2) + d_\nu^{\alpha\beta} A_\alpha(I_\kappa^1 I_\kappa^2) A_\beta(I_1 \ldots I_{\kappa-1})$$

By weak associativity the right-hand side equals $A_\nu(I_1 \ldots I_\kappa^1 I_\kappa^2)$.

For the case $i < n = \kappa$ we have, by induction hypothesis,

$$A_\nu(I_1 \ldots I_\kappa) = C_\nu^{\alpha\beta} A_\alpha(I_1 \ldots I_i^1 I_i^2 \ldots I_{\kappa-1}) A_\beta(I_\kappa) + d_\nu^{\alpha\beta} A_\alpha(I_\kappa) A_\beta(I_1 \ldots I_i^1 I_i^2 \ldots I_{\kappa-1})$$

By Eq. (2.21) this equals $A_\nu(I_1 \ldots I_i^1 I_i^2 \ldots I_\kappa)$. ■

In order to handle the combinatorics it is convenient at this point to consider arbitrary formal products of intervals as in Section II.2 of Ref. 2, not only subsequent ones. We use Eq. (2.21) and linearity to extend the definition of A_ν to all formal linear combinations of such formal products. In this way A_ν is defined on the free algebra, $\mathscr{A}\{I\}$, generated by the intervals. Eq. (2.22) then reads

$$A_\nu[I] = A_\nu\left(\sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} I_1 \ldots I_\kappa \right) \tag{A2}$$

This motivates the introduction of a formal truncated quantity $[I]$ for an interval I by

$$[I] := \sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} I_1 \ldots I_\kappa \tag{A3}$$

Then I, as an element of the free algebra, can be expressed as[2]

$$I = \sum_{I_1 \circ \cdots \circ I_\kappa = I} [I_1] \ldots [I_\kappa] \tag{A4}$$

This is easily proved by induction on the length of I by means of the next lemma.

Lemma A2[2]**.** Let $I = (i_1 \ldots i_N)$. If $N = 1$, then[4]

$$[i_1] = (i_1) \tag{A5}$$

Furthermore,

$$I = [I] + (i_1)[i_2 \ldots i_N] + \cdots + (i_1 \ldots i_{N-1})[i_N] \tag{A6}$$

and also

$$I = [I] + [i_1 \ldots i_{N-1}](i_N) + \cdots + [i_1](i_2 \ldots i_N) \tag{A7}$$

[4] For intervals we use round brackets. Instead of $[(i_1 \ldots i_N)]$ we write $[i_1 \ldots i_N]$.

Proof. Equation (A.5) is obvious. Equation (A.6) is proved from the definition,

$$\begin{aligned} I &= I + \sum_{k\geqslant 2} (-1)^{\kappa-1} \sum_{I_1 \circ \ldots I_\kappa = I} I_1 \ldots I_\kappa \\ &= I - \sum_{l=1}^{N-1} (i_1 \ldots i_l) \sum_{\kappa \geqslant 1} (-1)^{\kappa-1} \sum_{I_1 \circ \cdots \circ I_\kappa = (i_{l+1}, \ldots, i_N)} I_1 \ldots I_\kappa \\ &= I - \sum_{l=1}^{N-1} (i_1 \ldots i_l)[i_{l+1} \ldots i_N] \end{aligned}$$

Equation (A.7) is proved similarly. ■

We also need the following combinatorical fact.

Lemma A3[2]. For given integer m let the partition operator p_m on $\mathscr{A}[I]$ be defined by

$$p_m(i_1 \ldots i_N) := \begin{cases} (i_1 \ldots m)(m+1 \ldots i_n), & \text{if } i_1 \leqslant m < i_N \\ (i_1 \ldots i_N), & \text{otherwise} \end{cases} \tag{A8}$$

$$p_m(I_1 \ldots I_\kappa) := p_m I_1 \ldots p_m I_\kappa \tag{A9}$$

and by linearity. If I and m are such that $p_m I \neq I$, then

$$p_m[I] = 0 \tag{A10}$$

Proof. We use Lemma A.2 and induction on the length of I. For intervals with a single point the statement is trivially true. Assume it to hold for all intervals of length less than that of I. By Eq. (A.6) we then have

$$\begin{aligned} (i_1 \ldots m)(m+1 \ldots i_N) &= p_m(i_1 \ldots i_N) \\ &= p_m[i_1 \ldots i_N] + (i_1 \ldots m)[m+1 \ldots i_N] \\ &\quad + (i_1 \ldots m)(m+1)[m+2 \ldots i_N] + \cdots \\ &\quad + (i_1 \ldots m)(m+1 \ldots i_{N-1})[i_N] \\ &= p_m[i_1 \ldots i_n] + (i_1 \ldots m)(m+1 \ldots i_N) \end{aligned}$$

This implies Eq. (A.10). ■

Proof of Theorem 2.1. If the perturbers indexed by I decompose into two nonoverlapping clusters according to $(i_1 \ldots m)$ and $(m \ldots i_N)$ we have from Lemma A.1 for $I_1 \circ \cdots \circ I_\kappa = I$,

$$A_\nu(I_1 \ldots I_\kappa) = A_\nu(p_m(I_1 \ldots I_\kappa))$$

Hence, by linearity,

$$\begin{aligned} A_\nu[I] &= \sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} A_\nu(p_m(I_1 \ldots I_\kappa)) \\ &= A_\nu(p_m[I]) \\ &= 0 \end{aligned}$$

by Lemma A.3. ■

We now turn to the proof of Eq. (2.34) where we follow Ref. 2. We first prove the little combinatorial identity

$$\sum_{I_1 \circ \cdots \circ I_\kappa = I} (-1)^{\kappa-1} = \delta_{1|I|} := \begin{cases} 1, & \text{if } I = (i_1) \\ 0, & \text{otherwise} \end{cases} \tag{A11}$$

We use induction on the length of I. For $I = (i_1)$ the statement is trivial. For $I = (i_1 \ldots i_N)$, $N \geqslant 2$, the left-hand side equals

$$1 + \sum_{\substack{I_1 \circ \cdots \circ I_\kappa = I \\ \kappa \geqslant 2}} (-1)^\kappa = 1 - \sum_{I_\kappa} \sum_{I_1 \circ \cdots \circ I_{\kappa-1} = I \setminus I_\kappa} (-1)^{\kappa-2} = 1 - 1 = 0$$

by induction hypothesis.

To prove Eq. (2.34) we use Eqs. (2.31) and (A.11) to calculate

$$\begin{aligned} Q_{\mathscr{T}}([I]J) &= \sum_{I_1 \circ \cdots \circ I_\kappa = I} Q_{\mathscr{T}}(I_1 \ldots I_\kappa J) \\ &= \sum_{I_1 \circ \cdots \circ I_{\kappa-1} = I} (-1)^{\kappa-1} \{ Q_{\mathscr{T}}(I_1 \ldots I_\kappa) + Q_{\mathscr{T}}(J) \\ &\qquad + \hat{\mathscr{T}}^*(I_1 \ldots I_\kappa)\mathscr{T}^*(J) \\ &\qquad + \mathscr{T}(J)\hat{\mathscr{T}}(I_1 \ldots I_\kappa)\} \\ &= Q_{\mathscr{T}}[I] + \delta_{1|I|} Q_{\mathscr{T}}(J) + \hat{\mathscr{T}}^*[I]\mathscr{T}^*(J) + \mathscr{T}(J)\hat{\mathscr{T}}[I] \end{aligned} \tag{A12}$$

From Eq. (A.7) we then have, with $I = (i_1 \ldots i_N)$,

$$\begin{aligned} Q_{\mathscr{T}}(I) = {} & Q_{\mathscr{T}}[i_1 \ldots i_{N-1}] + \cdots + Q_{\mathscr{T}}[i_1] + Q_{\mathscr{T}}(i_2 \ldots i_N) \\ & + \{\mathscr{T}(i_N)\mathscr{T}[i_1 \ldots i_{N-1}] + \cdots \\ & + \mathscr{T}(i_1 \ldots i_N)\hat{\mathscr{T}}[i_1]\} + \{\cdots\}^* \end{aligned} \tag{A13}$$

By Eq. (2.10) the curly bracket becomes

$$\{\cdots\} = \sum_{\substack{I_1 \circ \cdots \circ I_{\kappa+1} = I \\ |I_{\kappa+1}| > 0;\ \kappa \geqslant 2}} \mathscr{T}[I_\kappa]\mathscr{S}[I_{\kappa-1}] \ldots \mathscr{S}[I_2]\hat{\mathscr{T}}[I_1] \tag{A14}$$

where, for $\kappa \geqslant 2$, the $\mathscr{S}$ factors are omitted. Straightforward induction on the length of I now yields Eq. (2.34). The proof for $Q_{\mathscr{D}}$ is identical.

For completeness' sake we mention that one derives with the same method

$$\hat{\mathscr{T}}(I) = \sum_{\substack{I_0 \circ \cdots \circ I_\kappa = I \\ |I_0| \geqslant 0}} \mathscr{S}[I_1] \ldots \mathscr{S}[I_{\kappa-1}] \hat{\mathscr{T}}[I_\kappa] \tag{A15}$$

where, as indicated, I_0 may be empty and where, for $\kappa = 1$, the $\mathscr{S}$ factors are omitted.

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