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2006 J. Phys. A: Math. Gen. 39 163

(http://iopscience.iop.org/0305-4470/39/1/012)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **39** (2006) 163–183 doi:10.1088/0305-4470/39/1/012

The flux-across-surfaces theorem under conditions on the scattering state

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Received 15 September 2005, in final form 27 October 2005
Published 7 December 2005
Online at stacks.iop.org/JPhysA/39/163

Abstract
The flux-across-surfaces theorem (FAST) describes the outgoing asymptotics of the quantum flux density of a scattering state. The FAST has been proven for potential scattering under conditions on the outgoing asymptote ψ_{out} (and of course under suitable conditions on the scattering potential). In this paper, we prove the FAST under conditions on the scattering state itself. In the proof, we will also establish new mapping properties of the wave operators.

PACS number: 03.65.NK

1. Introduction

The flux-across-surfaces theorem (FAST) is basic to the empirical content of scattering theory. The FAST describes the relation between the integrated quantum flux density of a scattering state over a (detector) surface and a (detection) time interval and the momentum distribution of the corresponding outgoing asymptote ψ_{out}. In this paper, we deal with the simplest case of one-particle potential scattering. We remark that the extension of the FAST to many-particle scattering theory is problematical, see [14].

With the quantum flux density (* denotes the complex conjugate)

$$\boldsymbol{j}^{\psi} = \text{Im}(\psi^* \nabla \psi)$$

and without spelling out the conditions under which it can be proven, the FAST reads

$$\lim_{R\to\infty} \int_T^{\infty} \int_{R\Sigma} \boldsymbol{j}^{\psi}(\boldsymbol{x}, t) \cdot \mathrm{d}\boldsymbol{\sigma}\, \mathrm{d}t = \lim_{R\to\infty} \int_T^{\infty} \int_{R\Sigma} |\boldsymbol{j}^{\psi}(\boldsymbol{x}, t) \cdot \mathrm{d}\boldsymbol{\sigma}|\, \mathrm{d}t = \int_{C_\Sigma} |\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2\, \mathrm{d}^3 k, \tag{1}$$

where $\Sigma \subset S^2$ is a subset of the unit sphere, $R\Sigma := \{\boldsymbol{x} \in \mathbb{R}^3 : \boldsymbol{x} = R\boldsymbol{\omega}, \boldsymbol{\omega} \in \Sigma\}$ is the spherical surface covering the solid angle Σ and $C_\Sigma := \{\boldsymbol{k} \in \mathbb{R}^3 : \boldsymbol{e}_k \in \Sigma\}$ is the cone given by Σ. Furthermore $\hat{}$ denotes the Fourier transform and ψ_{out} the outgoing asymptote to the corresponding scattering state $\psi = \Omega_+\psi_{\text{out}}$ with the wave operator Ω_+.

The left-hand side is interpreted and also shown to be the crossing probability of the particle crossing the surface $R\Sigma$ [5–8, 12, 20]. From the crossing probability one derives the scattering cross section [11, 12]. The right-hand side of (1) relates the crossing probability to the S-matrix. Technically, the FAST (1) has been proven requiring conditions on ψ_{out}. But it is clear that when all is said and done one needs the conditions on the scattering state for which the FAST holds. In particular, the microscopic derivation of the cross section needs the FAST under conditions on the scattering state [11]. In the present paper, we establish the FAST (1) under conditions on the scattering state.

The FAST has been put into a mathematically rigorous setting by Combes, Newton and Shtokhammer in 1975 [7]. In 1996, the FAST was proven by Daumer *et al* [8] for the Schrödinger case without a potential. One year later Amrein, Pearson and Zuleta proved the FAST for short- and long-range potentials using methods in the context of Kato's H-smoothness, requiring an energy cut-off on the outgoing asymptote [3, 4]. (More precisely, supp $\widehat{\psi}_{\text{out}}$ is compact.) This at first sight innocently looking requirement seems however to be an important hindrance towards the physically relevant formulation of the FAST with conditions on the scattering state itself. We shall discuss this in somewhat more detail later. In 1999, Teufel, Dürr and Berndl gave a proof based on eigenfunction expansions without an energy cut-off, but still requiring smoothness properties of the outgoing asymptote for potentials falling off faster than x^{-4} [25]. Panati and Teta gave a proof for the special case of point interactions under conditions on the scattering state [21] with similar methods as in [25]. In 2003, Nagao [19] proved a weaker result, namely leaving out the second equality in equation (1). This proof works for short-range potentials falling off faster than the dimension of the space (= 3) and requires only conditions on the scattering state. By leaving out the second equality in (1), the result does not establish the connection to empirical data of a typical scattering experiment, as it does not establish the probabilistic meaning of the quantum flux as a crossing probability or in technical terms it does not establish that the flux points asymptotically outwards. In the same year, Dürr and Pickl [13] proved the FAST for a Dirac particle under conditions on the scattering state alone using eigenfunction expansions.

We provide now a proof for the Schrödinger case combining the techniques of the proofs in [13, 25] to establish the FAST under conditions on the scattering state and for potentials falling off faster than x^{-4}. The idea is to prove the FAST under almost optimal conditions on ψ_{out}, which can be translated to reasonable and easily checkable conditions on the scattering state. It is clearly essential that there is no energy cut-off on ψ_{out}, because it is highly unclear whether there are any reasonable conditions on the scattering state ensuring a cut-off on ψ_{out} (cf (2)). Having formulated the task to prove the FAST under conditions on the outgoing asymptote which can be transferred to conditions on the scattering state we like to remark that there are no suitable assertions in the literature which allow us to transfer conditions on ψ to ψ_{out} in the context of the proof of the FAST[3]. We shall elaborate this further considering eigenfunction expansions. We recall the generalized Fourier transform (see lemma 1), which maps the scattering state ψ to the ordinary Fourier transform $\widehat{\psi}_{\text{out}}$ of ψ_{out}:

$$\widehat{\psi}_{\text{out}}(\boldsymbol{k}) = (2\pi)^{-\frac{3}{2}} \int \varphi_+^*(\boldsymbol{x}, \boldsymbol{k})\psi(\boldsymbol{x})\,\mathrm{d}^3x, \tag{2}$$

where $\varphi_+^*(\boldsymbol{x}, \boldsymbol{k})$ are the generalized eigenfunctions. In lemma 2, we collect the properties of the eigenfunctions which are—concerning smoothness and boundedness—in general very

[3] For mapping properties between ψ and ψ_{out}, which are not applicable in our case, see e.g. [27].

poor: the generalized eigenfunctions are solutions of the Lippmann–Schwinger equations:

$$\varphi_{\pm}(\boldsymbol{x},\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} - \frac{1}{2\pi}\int \frac{\mathrm{e}^{\mp \mathrm{i}k|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|} V(\boldsymbol{x}')\varphi_{\pm}(\boldsymbol{x}',\boldsymbol{k})\,\mathrm{d}^3x', \tag{3}$$

in which we note the appearance of the absolute value k of $\boldsymbol{k}$ in the spherical wave part. Derivatives of k of higher order than 1 behave singular for $k \to 0$. Therefore, we expect in general that the derivatives of the generalized eigenfunctions (of higher order than 1) are unbounded for small k.[4] In view of (2) this singular behaviour is typically inherited by ψ_{out} and it is hard to see how 'extreme' conditions on ψ_{out} like ψ_{out} in Schwartz space or $\widehat{\psi}_{\text{out}}$ compactly supported can be satisfied by reasonable scattering potentials or states. This caveat applies to the above-cited works on the FAST except [13, 19, 21]. Our task is thus to read from (2) proper conditions on ψ_{out} which can be formulated in terms of the scattering state and then to prove the FAST under these conditions.

The paper is organized as follows: in section 2, we recall the mathematical basics of scattering theory including recent results and fix notations; in section 3, we formulate and prove the FAST under weaker conditions on the asymptote than in [25]. The conditions will be transformed by the mapping lemma 3 to sufficient conditions on the scattering state. The most complete statement is corollary 1. Technically, the FAST is proven by stationary phase methods, which turns out—due to our necessarily weak conditions—to be a rather involved modification of standard results, e.g., theorem 7.7.5 in [15]. The proof of the modified assertion is done in the appendix.

2. The mathematical framework of potential scattering

We list those results of scattering theory (e.g., [2, 10, 16, 18, 22–25]) which are essential for the proof of the FAST in section 3.

We use the usual description of a nonrelativistic spinless system by the Hamiltonian H (we use natural units $\hbar = m = 1$):

$$H := -\tfrac{1}{2}\Delta + V(\boldsymbol{x}) =: H_0 + V(\boldsymbol{x}),$$

with the real-valued potential $V \in (V)_n$, defined as follows:

Definition 1. *V is in $(V)_n$, $n = 2, 3, 4, \ldots,$ if*

(i) $V \in L^2(\mathbb{R}^3)$,

(ii) V is locally Hölder continuous except at a finite number of singularities,

(iii) there exist positive numbers ϵ, C_0, R_0 such that

$$|V(\boldsymbol{x})| \leqslant C_0\langle x\rangle^{-n-\epsilon} \qquad \textit{for} \quad |\boldsymbol{x}| \geqslant R_0,$$

where $\langle\cdot\rangle := (1+(\cdot)^2)^{\frac{1}{2}}$.

Under these conditions (see, e.g., [18]), H is self-adjoint on the domain $\mathrm{D}(H) = \mathrm{D}(H_0) = \{f \in L^2(\mathbb{R}^3) : \int |k^2\widehat{f}(\boldsymbol{k})|^2\,\mathrm{d}^3k < \infty\}$, where $\widehat{f} := \mathcal{F}f$ is the Fourier transform:

$$\widehat{f}(\boldsymbol{k}) := (2\pi)^{-\frac{3}{2}}\int \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} f(\boldsymbol{x})\,\mathrm{d}^3x. \tag{4}$$

[4] For a point interaction, the generalized eigenfunctions can be explicitly computed [1], p 39. They have exactly this singular behaviour.

Let $U(t) = \mathrm{e}^{-\mathrm{i}Ht}$. Since H is self-adjoint on the domain D(H), $U(t)$ is a strongly continuous one-parameter unitary group on $L^2(\mathbb{R}^3)$. Let $\phi \in \mathrm{D}(H)$. Then, $\phi_t \equiv U(t)\phi \in \mathrm{D}(H)$ and satisfies the Schrödinger equation:

$$\mathrm{i}\frac{\partial}{\partial t}\phi_t(\boldsymbol{x}) = H\phi_t.$$

We define the wave operators $\Omega_\pm$ with the range $\mathrm{Ran}(\Omega_\pm)$ in the usual way:

$$\Omega_\pm : L^2(\mathbb{R}^3) \to \mathrm{Ran}(\Omega_\pm), \qquad \Omega_\pm := \text{s-}\lim_{t\to\pm\infty} \mathrm{e}^{\mathrm{i}Ht}\mathrm{e}^{-\mathrm{i}H_0 t},$$

where s- lim denotes the limit in the L^2-sense. Ikebe [16] proved that for a potential $V \in (V)_2$ the wave operators exist and have the range (this property is called asymptotic completeness):

$$\mathrm{Ran}(\Omega_\pm) = \mathcal{H}_{\mathrm{cont}}(H) = \mathcal{H}_{\mathrm{a.c.}}(H),$$

where $\mathcal{H}_{\mathrm{cont}}(H)$ and $\mathcal{H}_{\mathrm{a.c.}}(H)$ denote the subspaces of $L^2(\mathbb{R}^3)$ consisting of states, which belong to the continuous and the absolutely continuous part of the spectrum of H. Then, we have for every $\psi \in \mathcal{H}_{\mathrm{a.c.}}(H)$ asymptotes $\psi_{\mathrm{in}}, \psi_{\mathrm{out}} \in L^2(\mathbb{R}^3)$ with

$$\Omega_-\psi_{\mathrm{in}} = \psi = \Omega_+\psi_{\mathrm{out}}. \tag{5}$$

On $\mathrm{D}(H_0)$ the wave operators satisfy the so-called intertwining property

$$H\Omega_\pm = \Omega_\pm H_0.$$

On $\mathcal{H}_{\mathrm{a.c.}}(H) \cap \mathrm{D}(H)$, we have then

$$H_0\Omega_\pm^{-1} = \Omega_\pm^{-1}H. \tag{6}$$

We will need the time evolution of a state $\psi \in \mathcal{H}_{\mathrm{a.c.}}(H)$ with the Hamiltonian H. Its diagonalization on $\mathcal{H}_{\mathrm{a.c.}}(H)$ is given by the eigenfunctions $\varphi_\pm$:

$$\left(-\frac{1}{2}\Delta + V(\boldsymbol{x})\right)\varphi_\pm(\boldsymbol{x},\boldsymbol{k}) = \frac{k^2}{2}\varphi_\pm(\boldsymbol{x},\boldsymbol{k}). \tag{7}$$

Applying $\left(-\frac{1}{2}\Delta - \frac{k^2}{2} \mp \mathrm{i}0\right)^{-1}$ in (7) one obtains the Lippmann–Schwinger equation. We recall the main parts of a result on this due to Ikebe in [16] which is collected in the present form in [25].

Lemma 1. *Let $V \in (V)_2$. Then for any $\boldsymbol{k} \in \mathbb{R}^3\backslash\{0\}$ there are unique solutions $\varphi_\pm(\cdot,\boldsymbol{k}) : \mathbb{R}^3 \to \mathbb{C}$ of the Lippmann–Schwinger equations*

$$\varphi_\pm(\boldsymbol{x},\boldsymbol{k}) = \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} - \frac{1}{2\pi}\int \frac{\mathrm{e}^{\mp\mathrm{i}k|\boldsymbol{x}-\boldsymbol{x}'|}}{|\boldsymbol{x}-\boldsymbol{x}'|}V(\boldsymbol{x}')\varphi_\pm(\boldsymbol{x}',\boldsymbol{k})\,\mathrm{d}^3x', \tag{8}$$

with the boundary conditions $\lim_{|\boldsymbol{x}|\to\infty}(\varphi_\pm(\boldsymbol{x},\boldsymbol{k}) - \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}) = 0$, which are also classical solutions of the stationary Schrödinger equation (7), such that

(i) For any $f \in L^2(\mathbb{R}^3)$, the generalized Fourier transforms[5]

$$(\mathcal{F}_\pm f)(\boldsymbol{k}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\mathrm{l.i.m.}\int \varphi_\pm^*(\boldsymbol{x},\boldsymbol{k})f(\boldsymbol{x})\,\mathrm{d}^3x$$

exist in $L^2(\mathbb{R}^3)$.

(ii) $\mathrm{Ran}(\mathcal{F}_\pm) = L^2(\mathbb{R}^3)$ and $\mathcal{F}_\pm : \mathcal{H}_{\mathrm{a.c.}}(H) \to L^2(\mathbb{R}^3)$ are unitary and the inverse of $\mathcal{F}_\pm$ is given by

$$\left(\mathcal{F}_\pm^{-1}f\right)(\boldsymbol{x}) = \frac{1}{(2\pi)^{\frac{3}{2}}}\mathrm{l.i.m.}\int \varphi_\pm(\boldsymbol{x},\boldsymbol{k})f(\boldsymbol{k})\,\mathrm{d}^3k.$$

[5] l.i.m. $\int$ denotes s- $\lim_{R\to\infty}\int_{x\leqslant R}$.

(iii) *For any* $f \in L^2(\mathbb{R}^3)$, *the relation* $\Omega_\pm f = \mathcal{F}_\pm^{-1}\mathcal{F} f$ *hold, where* $\mathcal{F}$ *is the ordinary Fourier transform given by (4).*

(iv) *For any* $f \in \mathrm{D}(H) \cap \mathcal{H}_{\mathrm{a.c.}}(H)$, *we have*

$$Hf(\boldsymbol{x}) = \left(\mathcal{F}_\pm^{-1}\frac{k^2}{2}\mathcal{F}_\pm f\right)(\boldsymbol{x}),$$

and therefore for any $f \in \mathcal{H}_{\mathrm{a.c.}}(H)$

$$\mathrm{e}^{-\mathrm{i}Ht} f(\boldsymbol{x}) = \left(\mathcal{F}_\pm^{-1}\mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t}\mathcal{F}_\pm f\right)(\boldsymbol{x}).$$

In order to apply stationary phase methods we will need estimates on the derivatives of the generalized eigenfunctions:

Lemma 2. *Let the potential satisfy the condition* $(V)_n$ *for some* $n \geqslant 3$. *Then,*

(i) $\varphi_\pm(\boldsymbol{x},\cdot) \in C^{n-2}(\mathbb{R}^3\backslash\{0\})$ *for all* $\boldsymbol{x} \in \mathbb{R}^3$ *and the partial derivatives*[6] $\partial_{\boldsymbol{k}}^\alpha \varphi_\pm(\boldsymbol{x},\boldsymbol{k})$, $|\alpha| \leqslant n-2$ *are continuous with respect to* $\boldsymbol{x}$ *and* $\boldsymbol{k}$.

If, in addition, zero is neither an eigenvalue nor a resonance of H, then

(ii) $\sup_{\boldsymbol{x}\in\mathbb{R}^3,\boldsymbol{k}\in\mathbb{R}^3} |\varphi_\pm(\boldsymbol{x},\boldsymbol{k})| < \infty$

and for any α *with* $|\alpha| \leqslant n-2$ *there is a* $c_\alpha < \infty$ *such that*

(iii) $\sup_{\boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}} \left|\kappa^{|\alpha|-1}\partial_{\boldsymbol{k}}^\alpha\varphi_\pm(\boldsymbol{x},\boldsymbol{k})\right| < c_\alpha\langle x\rangle^{|\alpha|}$ *with* $\kappa := \frac{k}{\langle k\rangle}$.

Similarly, for any $l \in \{1,\ldots,n-2\}$ *there is a* $c_l < \infty$ *such that*

(iv) $\sup_{\boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}} \left|\frac{\partial^l}{\partial k^l}\varphi_\pm(\boldsymbol{x},\boldsymbol{k})\right| < c_l\langle x\rangle^l$.

Remark 1. Zero is a resonance of H if there exists a solution f of $Hf = 0$ such that $\langle x\rangle^{-\gamma} f \in L^2(\mathbb{R}^3)$ for any $\gamma > \frac{1}{2}$ but not for $\gamma = 0$.[7] The appearance of a zero eigenvalue or resonance can be regarded as an exceptional event: for a Hamiltonian $H = H_0 + cV$, $c \in \mathbb{R}$, this can only happen in a discrete subset of $\mathbb{R}$, see [1], p 20 and [17], p 589.

Remark 2. Lemma 2, except the assertion (iii), was proved in [25], theorem 3.1. Assertion (iii) repairs a false statement in theorem 3.1 which did not include the necessary $\kappa^{|\alpha|-1}$ factor, which we have in (iii). For $|\alpha| = 1$ which was the important case in that paper there is however no difference. For completeness we comment on the proof of this corrected version in the appendix. We note that the problem which we address here comes from the appearance of the absolute value of $\boldsymbol{k}$ in the Lippmann–Schwinger equation (8), see also the introduction. In fact, lemma 2(iii) is to our knowledge the best one can say about the derivatives of the generalized eigenfunctions w.r.t. the coordinates. Note that the higher derivatives ($|\alpha| \geqslant 2$) become unbounded for small k. In [9], it is claimed that the derivatives stay bounded for small k, see proposition 3.8 therein. The proof of this proposition apparently disregard the behaviour of the coordinate derivatives of k.

3. The flux-across-surfaces theorem

The FAST (1) is a relation between a scattering state and its corresponding asymptote. As already emphasized, it is important to establish the FAST with conditions only on the scattering state (and the potential V). Since $\psi = \Omega_+\psi_{\mathrm{out}}$, we get by the well-known expansion lemma 1(ii)–(iv): $\psi(\boldsymbol{x},t) = \mathcal{F}_+^{-1}\mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})$ and we can express the flux in (1) by its

[6] We use the usual multi-index notation: $\alpha = (\alpha_1,\alpha_2,\alpha_3), \alpha_i \in \mathbb{N}_0, |\alpha| := \alpha_1+\alpha_2+\alpha_3$ and $\partial_{\boldsymbol{k}}^\alpha f(\boldsymbol{k}) := \partial_{k_1}^{\alpha_1}\partial_{k_2}^{\alpha_2}\partial_{k_3}^{\alpha_3} f(\boldsymbol{k})$.

[7] There are various definitions, see e.g. [27], p 552; [1], p 20 and [17], p 584.

asymptote $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$. Therefore, we will proceed in the following way: we will first prove a FAST under conditions on $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$ and then we will translate these conditions to the corresponding scattering state. The connection between a scattering state and its corresponding asymptote is given by the expansion lemma 1(ii) and (iii), cf (2).[8] That means, as already emphasized in the introduction, that the properties of $\widehat{\psi}_{\text{out}}$ are via (2) inherited by the properties of the generalized eigenfunctions, which are in general very poor, see lemma 2, especially (iii). More precisely, we will see later in the mapping lemma 3 that the decay properties (i.e., for large k) of $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$ and its derivatives depend mostly on the differentiability of $\psi(\boldsymbol{x})$, while the properties of $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$ and its derivatives for small k are closely related to the corresponding properties of the generalized eigenfunctions $\varphi_+^*(\boldsymbol{x},\boldsymbol{k})$. Therefore, we now define a class of asymptotes, $\mathcal{G}^+$, for which we can prove the FAST and which has the same poor properties for small k as the generalized eigenfunctions in lemma 2. The exponents which determine the decay for large k are optimized to get a large class and are of technical interest. The class $\mathcal{G}^+$ of the suitable asymptotes is defined as follows: (in the following definition we have the Fourier transform of $\psi_{\text{out}} = \Omega_+^{-1}\psi$ (cf (5)) in mind)

Definition 2. *A function $f : \mathbb{R}^3\backslash\{0\} \to \mathbb{C}$ is in $\mathcal{G}^+$ if there is a constant $C \in \mathbb{R}_+$ with*

$$|f(\boldsymbol{k})| \leqslant C\langle k\rangle^{-15},$$

$$\left|\partial_{\boldsymbol{k}}^{\alpha} f(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-6}, \qquad |\alpha| = 1,$$

$$\left|\kappa\, \partial_{\boldsymbol{k}}^{\alpha} f(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-5}, \qquad |\alpha| = 2, \qquad \kappa = \frac{k}{\langle k\rangle}$$

$$\left|\frac{\partial^2}{\partial k^2} f(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-3}.$$

With that class we can formulate a FAST under conditions on $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$.

Theorem 1. *Let the potential satisfy the condition $(V)_4$ and let zero be neither a resonance nor an eigenvalue of H. Let $\widehat{\psi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+$. Then, $\psi(\boldsymbol{x},t) = \mathrm{e}^{-\mathrm{i}Ht}\Omega_+\psi_{\text{out}}(\boldsymbol{x})$ is continuously differentiable except at the singularities of V and for any measurable $\Sigma \subset S^2$ and any $T \in \mathbb{R}$:*

$$\lim_{R\to\infty}\int_T^\infty \int_{R\Sigma} \boldsymbol{j}^{\psi}(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}t = \lim_{R\to\infty}\int_T^\infty \int_{R\Sigma} |\boldsymbol{j}^{\psi}(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}|\,\mathrm{d}t = \int_{C_\Sigma} |\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2\,\mathrm{d}^3k, \tag{9}$$

where $R\Sigma := \{\boldsymbol{x} \in \mathbb{R}^3 : \boldsymbol{x} = R\boldsymbol{\omega}, \boldsymbol{\omega} \in \Sigma\}$ and $C_\Sigma := \{\boldsymbol{k} \in \mathbb{R}^3 : \boldsymbol{e}_k \in \Sigma\}$.

The crucial condition in theorem 1 is $\widehat{\psi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+$. We introduce now the class $\mathcal{G}$ of scattering states for which we can prove that the corresponding asymptotes are in $\mathcal{G}^+$.

Definition 3. *$f : \mathbb{R}^3 \to \mathbb{C}$ is in $\mathcal{G}^0$ if*[9]

$$f \in \mathcal{H}_{\text{a.c.}}(H) \cap C^8(H),$$

$$\langle x\rangle^2 H^n f \in L^2(\mathbb{R}^3), \qquad n \in \{0,1,2,\ldots,8\},$$

$$\langle x\rangle^4 H^n f \in L^2(\mathbb{R}^3), \qquad n \in \{0,1,2,3\}.$$

Then, $\mathcal{G} := \bigcup_{t\in\mathbb{R}} \mathrm{e}^{-\mathrm{i}Ht}\mathcal{G}^0$.

8 Because of lemma 2 (ii) we can use the generalized Fourier transform without the l.i.m. whenever $\psi \in L^1(\mathbb{R}^3)$.

9 $C^8(H) := \bigcap_{n=1}^{8} \mathrm{D}(H^n)$.

That means $\mathcal{G}$ is a subset of $\mathcal{H}_{\text{a.c.}}(H)$ and is invariant under finite time shifts, i.e. if $f \in \mathcal{G}$ then $\mathrm{e}^{-\mathrm{i}Ht} f \in \mathcal{G}, \forall t \in \mathbb{R}$. Furthermore, $\mathcal{G}$ is dense in $\mathcal{H}_{\text{a.c.}}(H)$ which can be seen, e.g., by the results used in [4], p 5368: let $\mathcal{D}_4 := \{g(H)\langle x\rangle^{-4}\psi | g \in C_0^\infty(]0,\infty[), \psi \in L^2(\mathbb{R}^3)\}$. Since our potentials have no positive eigenvalues (cf section 2) we have $\mathcal{D}_4 \subseteq \mathcal{H}_{\text{a.c.}}(H)$. It is easy to check that $\mathcal{D}_4$ is dense in $\mathcal{H}_{\text{a.c.}}(H)$. Moreover (cf [4]) we have that $\mathcal{D}_4 \subseteq \mathrm{D}(H) \cap \mathrm{D}(\langle x\rangle^4)$. Again by [4] $H\mathcal{D}_4 \subseteq \mathcal{D}_4$ which implies that $\mathcal{D}_4 \subseteq \mathcal{G}$. Hence, $\mathcal{G}$ is dense in $\mathcal{H}_{\text{a.c.}}(H)$. Note that the condition $\psi \in \mathcal{G}$ can be formulated also more explicitly (cf remark 3). We wish to remark that the condition $\psi \in C^8(H)$ seems to be natural: wave functions in thermal equilibrium are typically in $C^\infty(H)$, see [26].

With definition 3, we can state now the important mapping lemma:

Lemma 3. *Let $V \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H. Then,*

$$\psi(\boldsymbol{x}) \in \mathcal{G} \quad \Rightarrow \quad \widehat{\Omega_+\psi}(\boldsymbol{k}) = \widehat{\psi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+.$$

The proof is adapted from [13] and can be found in the appendix. The lemma also holds for Ω_+ replaced by Ω_- and ψ_{out} by ψ_{in}.[10]

Theorem 1 and lemma 3 give the following corollary, the FAST under conditions on the scattering state.

Corollary 1. *Let $V \in (V)_4$ and let zero be neither a resonance nor an eigenvalue of H. Let $\psi \in \mathcal{G}$. Then, for any measurable $\Sigma \subset S^2$ and any $T \in \mathbb{R}$:*

$$\lim_{R\to\infty} \int_T^\infty \int_{R\Sigma} \boldsymbol{j}^\psi(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\, \mathrm{d}t = \lim_{R\to\infty} \int_T^\infty \int_{R\Sigma} |\boldsymbol{j}^\psi(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\,|\, \mathrm{d}t = \int_{C_\Sigma} |\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2\, \mathrm{d}^3k.$$

Remark 3. Instead of the condition $\psi \in \mathcal{G}$ one can also give of course the condition on ψ and V more explicitly. In the following, we will give two examples for ψ and V such that $\psi \in \mathcal{G}^0$. The set of wavefunctions $\mathcal{G}$ for which the FAST holds is then—according to definition 3—given by the set

$$\mathcal{G} = \bigcup_{t\in\mathbb{R}} \mathrm{e}^{-\mathrm{i}Ht}\mathcal{G}^0.$$

Let $H^{m,s}$ the weighted Sobolev space

$$H^{m,s} := \{f \in L^2(\mathbb{R}^3) \mid (1+x^2)^{\frac{s}{2}}(1-\Delta)^{\frac{m}{2}} f \in L^2(\mathbb{R}^3)\}.$$

Then one can find, for example, the following conditions for which $\psi \in \mathcal{G}^0$:

(i) $V \in (V)_2, V \in C^{14}(\mathbb{R}^3\backslash\mathcal{E})$, where $\mathcal{E}$ denotes the set of singularities of V and $\psi \in \mathcal{H}_{\text{a.c.}}(H) \cap C_0^{16}(\mathbb{R}^3\backslash\mathcal{E})$.

(ii) $V \in (V)_2, V \in H^{14,2} \cap H^{4,4}$ and $\psi \in \mathcal{H}_{\text{a.c.}}(H) \cap H^{16,2} \cap H^{6,4}$.

Clearly both sets for ψ are dense in $\mathcal{H}_{\text{a.c.}}(H)$.

Proof of theorem 1. We will prove the flux-across-surfaces theorem (9) for some $T > 0$. This is sufficient since ($\widetilde{T} \leqslant 0, T > 0$)

$$\lim_{R\to\infty} \int_{\widetilde{T}}^\infty \int_{R\Sigma} \boldsymbol{j}^\psi(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\, \mathrm{d}t = \lim_{R\to\infty} \int_T^\infty \int_{R\Sigma} \boldsymbol{j}^{\widetilde{\psi}}(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\, \mathrm{d}t, \tag{10}$$

[10] It would be interesting to have similar mapping properties for $\Omega_\pm^{-1}$.

with (in the second line we use lemma 1(ii)–(iv), again without the l.i.m., because of lemma 2(ii) and $\widehat{\psi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+ \subset L^1(\mathbb{R}^3)$)

$$\widetilde{\psi}(\boldsymbol{x},t) = \psi(\boldsymbol{x}, t+\widetilde{T}-T) = (2\pi)^{-\frac{3}{2}} \int \mathrm{e}^{-\mathrm{i}\frac{k^2 t}{2}}\, \mathrm{e}^{\mathrm{i}\frac{k^2(T-\widetilde{T})}{2}}\, \widehat{\psi}_{\text{out}}(\boldsymbol{k})\varphi_+(\boldsymbol{x},\boldsymbol{k})\,\mathrm{d}^3k$$

$$=: (2\pi)^{-\frac{3}{2}} \int \mathrm{e}^{-\mathrm{i}\frac{k^2 t}{2}}\, \widehat{\chi}_{\text{out}}(\boldsymbol{k})\varphi_+(\boldsymbol{x},\boldsymbol{k})\,\mathrm{d}^3k. \tag{11}$$

It is easy to check that $\widehat{\chi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+$, if $\widehat{\psi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+$, which means that $\mathcal{G}^+$ is invariant under finite time shifts. Hence, with (10) and (11) we get

$$\lim_{R\to\infty} \int_{\widetilde{T}}^{\infty} \int_{R\Sigma} \boldsymbol{j}^{\psi}(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}t = \lim_{R\to\infty} \int_{T}^{\infty} \int_{R\Sigma} \boldsymbol{j}^{\widetilde{\psi}}(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}\,\mathrm{d}t$$

$$= \int_{C_\Sigma} |\widehat{\chi}_{\text{out}}(\boldsymbol{k})|^2\,\mathrm{d}^3k = \int_{C_\Sigma} |\widehat{\psi}_{\text{out}}(\boldsymbol{k})|^2\,\mathrm{d}^3k.$$

Of course, this argument is also valid for the integration over $|\boldsymbol{j}^{\psi}(\boldsymbol{x},t)\cdot \mathrm{d}\boldsymbol{\sigma}|$.

Let $T > 0$ be fixed. Using lemma 1(ii)–(iv) and (8), we get

$$\psi(\boldsymbol{x},t) = (2\pi)^{-\frac{3}{2}} \int \mathrm{e}^{-\mathrm{i}\frac{k^2 t}{2}}\, \widehat{\psi}_{\text{out}}(\boldsymbol{k})\varphi_+(\boldsymbol{x},\boldsymbol{k})\,\mathrm{d}^3k$$

$$=: (2\pi)^{-\frac{3}{2}} \int \mathrm{e}^{-\mathrm{i}\frac{k^2 t}{2}}\, \widehat{\psi}_{\text{out}}(\boldsymbol{k})\,\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,\mathrm{d}^3k + (2\pi)^{-\frac{3}{2}} \int \mathrm{e}^{-\mathrm{i}\frac{k^2 t}{2}}\, \widehat{\psi}_{\text{out}}(\boldsymbol{k})\eta(\boldsymbol{x},\boldsymbol{k})\,\mathrm{d}^3k$$

$$=: \alpha(\boldsymbol{x},t) + \beta(\boldsymbol{x},t). \tag{12}$$

The flux generated by this wavefunction is

$$\boldsymbol{j}^{\psi}(\boldsymbol{x},t) = \operatorname{Im}(\alpha^*\nabla\alpha + \alpha^*\nabla\beta + \beta^*\nabla\alpha + \beta^*\nabla\beta), \tag{13}$$

where α is obviously continuously differentiable and for the differentiability of β see [25], (20) and (28)–(30). In [8] and [25], the function $\alpha(\boldsymbol{x},t)$ is estimated using the formula

$$\alpha(\boldsymbol{x},t) = (2\pi \mathrm{i} t) \int \mathrm{e}^{\mathrm{i}\frac{|\boldsymbol{x}-\boldsymbol{y}|^2}{2t}}\, \psi_{\text{out}}(\boldsymbol{y})\,\mathrm{d}^3y \tag{14}$$

and conditions on $\psi_{\text{out}}(\boldsymbol{x})$. According to lemma 3 we can control $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$, but not $\psi_{\text{out}}(\boldsymbol{x})$. Hence, we have to estimate $\alpha(\boldsymbol{x},t)$ directly in terms of $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$. This will be done by using stationary phase methods. First, we will calculate $\boldsymbol{j}_0^{\psi} = \operatorname{Im}(\alpha^*\nabla\alpha)$ by using lemma 4, which is formulated for a special class of wavefunctions $\widehat{\mathcal{K}} \supset \mathcal{G}^+$. This set has similar weak conditions as the set $\mathcal{G}^+$ due to the necessarily poor properties of $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$ (see the discussion before definition 3). Again we give here optimized decay properties, which are, however, not that strong as in the case of $\mathcal{G}^+$. □

Definition 4. *A function $f : \mathbb{R}^3\backslash\{0\} \to \mathbb{C}$ is in $\widehat{\mathcal{K}}$ if there is a constant $C \in \mathbb{R}_+$ with*

$$|f(\boldsymbol{k})| \leqslant C\langle k\rangle^{-4}, \qquad \left|\partial_{\boldsymbol{k}}^{\alpha} f(\boldsymbol{k})\right| \leqslant C, \qquad |\alpha| = 1,$$

$$\left|\kappa\,\partial_{\boldsymbol{k}}^{\alpha} f(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-1}, \qquad |\alpha| = 2,$$

$$\left|\frac{\partial}{\partial k} f(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-1}, \qquad \left|\frac{\partial^2}{\partial k^2} f(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-2}.$$

With that class of wavefunctions we can formulate

Lemma 4. *Let $\chi(\boldsymbol{k})$ be in $\widehat{\mathcal{K}}$. Then there exists a constant $L \in \mathbb{R}_+$ so that for all $\boldsymbol{x} \in \mathbb{R}^3$ and $t \in \mathbb{R}, t \neq 0$:*

$$\left| \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,\chi(\boldsymbol{k})\,\mathrm{d}^3k - \left(\frac{2\pi}{\mathrm{i}t}\right)^{\frac{3}{2}} \mathrm{e}^{\mathrm{i}\frac{x^2}{2t}}\,\chi(\boldsymbol{k}_{\mathrm{s}}) \right| < \frac{L}{t^2}, \tag{15}$$

where $\boldsymbol{k}_{\mathrm{s}} = \frac{\boldsymbol{x}}{t}$.

The proof of the lemma can be found in the appendix.

Applying that lemma on $\alpha(\boldsymbol{x},t)$ in (12) we get, with an appropriately chosen constant L,

$$\left|\alpha(\boldsymbol{x},t)-\left(\frac{1}{\mathrm{i}t}\right)^{\frac{3}{2}}\mathrm{e}^{\mathrm{i}\frac{x^2}{2t}}\widehat{\psi}_{\mathrm{out}}\left(\frac{\boldsymbol{x}}{t}\right)\right|<\frac{L}{t^2} \tag{16}$$

and analogously

$$\left|\nabla\alpha(\boldsymbol{x},t)-\mathrm{i}\left(\frac{1}{\mathrm{i}t}\right)^{\frac{3}{2}}\mathrm{e}^{\mathrm{i}\frac{x^2}{2t}}\left(\frac{\boldsymbol{x}}{t}\right)\widehat{\psi}_{\mathrm{out}}\left(\frac{\boldsymbol{x}}{t}\right)\right|<\frac{L}{t^2}, \tag{17}$$

which gives for the flux $\boldsymbol{j}_0^{\psi}=\mathrm{Im}(\alpha^*\nabla\alpha)$

$$\left|\boldsymbol{j}_0^{\psi}(\boldsymbol{x},t)-\left(\frac{1}{t}\right)^{3}\left(\frac{\boldsymbol{x}}{t}\right)\left|\widehat{\psi}_{\mathrm{out}}\left(\frac{\boldsymbol{x}}{t}\right)\right|^2\right|<\frac{L}{t^{\frac{7}{2}}}. \tag{18}$$

We begin with the first term $\boldsymbol{j}_0^{\psi}$ in (13) for times $t>R^{\frac{5}{6}}$ (we choose R big enough, so that $R^{\frac{5}{6}}>T$)

$$\int_{R^{\frac{5}{6}}}^{\infty}\int_{\Sigma}\boldsymbol{j}_0^{\psi}(R\boldsymbol{n},t)\cdot\boldsymbol{n}R^2\,\mathrm{d}\Omega\,\mathrm{d}t. \tag{19}$$

Inserting the asymptotic expression (18) for the flux $\boldsymbol{j}_0^{\psi}$ we get instead of (19)

$$\int_{R^{\frac{5}{6}}}^{\infty}\int_{\Sigma}\left|\widehat{\psi}_{\mathrm{out}}\left(\frac{R\boldsymbol{n}}{t}\right)\right|^2\frac{R^3}{t^4}\,\mathrm{d}\Omega\,\mathrm{d}t=\int_0^{R^{\frac{1}{6}}}\int_{\Sigma}|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})|^2k^2\,\mathrm{d}\Omega\,\mathrm{d}k, \tag{20}$$

where we substituted $\boldsymbol{k}:=\frac{R\boldsymbol{n}}{t}$. Equation (20) gives in the limit already the right result:

$$\lim_{R\to\infty}\int_0^{R^{\frac{1}{6}}}\int_{\Sigma}|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})|^2k^2\,\mathrm{d}\Omega\,\mathrm{d}k=\int_{C_\Sigma}|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})|^2\,\mathrm{d}^3k. \tag{21}$$

From (18)–(20) it is clear that the modulus of $\boldsymbol{j}_0^{\psi}$ also gives the right result. Hence, by justifying the use of the asymptotic expression for $\boldsymbol{j}_0^{\psi}$, showing that the integral (19) is negligible for times smaller than $R^{\frac{5}{6}}$ (and large R) and by proving the smallness of the contributions of the three other terms in (13) we get theorem 1.

Using (18) we can estimate the error between (19) and (20):

$$L\int_{R^{\frac{5}{6}}}^{\infty}\int_{\Sigma}R^2t^{-\frac{7}{2}}\,\mathrm{d}\Omega\,\mathrm{d}t=\frac{8\pi L}{5}R^{-\frac{1}{12}}, \tag{22}$$

which tends to zero for large R.

We evaluate now the flux integral for times smaller than $R^{\frac{5}{6}}$:

$$\int_{T}^{R^{\frac{5}{6}}}\int_{\Sigma}\boldsymbol{j}_0^{\psi}(\boldsymbol{n}R,t)\cdot\boldsymbol{n}R^2\,\mathrm{d}\Omega\,\mathrm{d}t. \tag{23}$$

Substituting $t\to Rt$, we get

$$\left|\int_{\frac{T}{R}}^{R^{-\frac{1}{6}}}\int_{\Sigma}\boldsymbol{j}_0^{\psi}(R\boldsymbol{n},tR)\cdot\boldsymbol{n}R^3\,\mathrm{d}\Omega\,\mathrm{d}t\right|\leqslant\int_{\frac{T}{R}}^{R^{-\frac{1}{6}}}\int_{\Sigma}|\alpha(R\boldsymbol{n},tR)||\nabla_{\boldsymbol{x}}\alpha(\boldsymbol{x},tR)|_{\boldsymbol{x}=R\boldsymbol{n}}R^3\,\mathrm{d}\Omega\,\mathrm{d}t. \tag{24}$$

We estimate α and $\nabla\alpha$ separately. We start with α:

$$\alpha(R\boldsymbol{n},tR)=(2\pi)^{-\frac{3}{2}}\int\exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R-\boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\,\mathrm{d}^3k. \tag{25}$$

The exponent of the e-function has the stationary point at $k_{\text{stat}} = \frac{1}{t}$. Since $t \in \left[\frac{T}{R}, R^{-\frac{1}{6}}\right]$, $k_{\text{stat}} \in \left[R^{\frac{1}{6}}, \frac{R}{T}\right[$. Big momenta should be negligible, hence we divide the integration over $\boldsymbol{k}$ in small momenta up to $k < R^{\frac{1}{6}}$ and larger ones. This will be done by the following functions:

$$f_1(\boldsymbol{k}) = \begin{cases} 1, & \text{for} \quad k < \frac{1}{2}R^{\frac{1}{6}}, \\ \cos^2\left(\left(k - \frac{1}{2}R^{\frac{1}{6}}\right)\frac{\pi}{2}\right), & \text{for} \quad \frac{1}{2}R^{\frac{1}{6}} \leqslant k \leqslant \frac{1}{2}R^{\frac{1}{6}} + 1, \\ 0, & \text{otherwise}, \end{cases} \tag{26}$$

$$f_2(\boldsymbol{k}) = \begin{cases} 0, & \text{for} \quad k < \frac{1}{2}R^{\frac{1}{6}}, \\ \sin^2\left(\left(k - \frac{1}{2}R^{\frac{1}{6}}\right)\frac{\pi}{2}\right), & \text{for} \quad \frac{1}{2}R^{\frac{1}{6}} \leqslant k \leqslant \frac{1}{2}R^{\frac{1}{6}} + 1, \\ 1, & \text{otherwise}. \end{cases} \tag{27}$$

We have then $f_1(\boldsymbol{k}) + f_2(\boldsymbol{k}) \equiv 1$ and get for (25)

$$\begin{aligned} \alpha(R\boldsymbol{n}, tR) = (2\pi)^{-\frac{3}{2}} &\int \exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k})\,\mathrm{d}^3k \\ &+ (2\pi)^{-\frac{3}{2}}\int \exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_2(\boldsymbol{k})\,\mathrm{d}^3k =: I_1 + I_2. \end{aligned} \tag{28}$$

We choose now R large enough (such that $\frac{1}{2}R^{\frac{1}{6}} > 1$), which means that the first integral in (28) has no stationary point anymore. We will do two integration by parts:

$$\begin{aligned} I_1 &= (2\pi)^{-\frac{3}{2}}\int \exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k})\,\mathrm{d}^3k \\ &= (2\pi)^{-\frac{3}{2}}\int\left(\nabla_{\boldsymbol{k}}\exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\right)\cdot\frac{-\mathrm{i}(Rt\boldsymbol{k} - R\boldsymbol{n})}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k})\,\mathrm{d}^3k \\ &= -(2\pi)^{-\frac{3}{2}}\int \exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\left(\nabla_{\boldsymbol{k}}\cdot\left(\frac{-\mathrm{i}(Rt\boldsymbol{k} - R\boldsymbol{n})}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k})\right)\right)\mathrm{d}^3k \\ &=: (2\pi)^{-\frac{3}{2}}\int \exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)(\nabla_{\boldsymbol{k}}\cdot\boldsymbol{g}(\boldsymbol{k}))\,\mathrm{d}^3k \\ &= (2\pi)^{-\frac{3}{2}}\int \exp\left(-\mathrm{i}t\left(\frac{k^2}{2}R - \boldsymbol{k}\frac{R\boldsymbol{n}}{t}\right)\right)\left(\nabla_{\boldsymbol{k}}\cdot\left(\frac{-\mathrm{i}(Rt\boldsymbol{k} - R\boldsymbol{n})}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}(\nabla_{\boldsymbol{k}}\cdot\boldsymbol{g}(\boldsymbol{k}))\right)\right)\mathrm{d}^3k. \end{aligned} \tag{29}$$

The gradient can be written as

$$\nabla_{\boldsymbol{k}}\cdot\left(\frac{-\mathrm{i}(Rt\boldsymbol{k} - R\boldsymbol{n})}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}(\nabla_{\boldsymbol{k}}\cdot\boldsymbol{g}(\boldsymbol{k}))\right) = \sum_{i,j=1}^{3}\partial_{k_j}\left(\frac{-\mathrm{i}(Rt\boldsymbol{k}_j - R\boldsymbol{n}_j)}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}\left(\partial_{k_i}\boldsymbol{g}_i(\boldsymbol{k})\right)\right). \tag{30}$$

A straightforward calculation yields for the right-hand side of (30) (we consider one summand)

$$\begin{aligned} \left|\partial_{k_j}\left(\frac{-\mathrm{i}(Rt\boldsymbol{k}_j - R\boldsymbol{n}_j)}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}\left(\partial_{k_i}\boldsymbol{g}_i(\boldsymbol{k})\right)\right)\right| &\leqslant C_1\frac{R^2t^2|\widehat{\psi}_{\text{out}}(\boldsymbol{k})||f_1(\boldsymbol{k})|}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^4} + C_2\frac{Rt\left|\partial_{k_i}(\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k}))\right|}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^3} \\ &+ C_3\frac{Rt\left|\partial_{k_j}(\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k}))\right|}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^3} + C_4\frac{\left|\partial_{k_i}\partial_{k_j}(\widehat{\psi}_{\text{out}}(\boldsymbol{k}) f_1(\boldsymbol{k}))\right|}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}, \end{aligned} \tag{31}$$

with constants $C_k > 0$, $k = 1, 2, 3, 4$. Since $0 \leqslant k < \frac{1}{2}R^{\frac{1}{6}} + 1$ and $0 < t \leqslant R^{-\frac{1}{6}}$, we have

$$|Rt\boldsymbol{k} - R\boldsymbol{n}| \geqslant \tfrac{1}{2}R - R^{\frac{5}{6}} \geqslant \tfrac{1}{3}R, \tag{32}$$

if R is large enough. Using (32) and the definition of $f_1(\boldsymbol{k})$ we find, with an appropriately chosen constant $M > 0$, instead of (31)

$$\begin{aligned}\left|\partial_{k_j}\left(\frac{-\mathrm{i}(Rt\boldsymbol{k}_j - R\boldsymbol{n}_j)}{|Rt\boldsymbol{k} - R\boldsymbol{n}|^2}\left(\partial_{k_i}\boldsymbol{g}_i(\boldsymbol{k})\right)\right)\right| &\leqslant \frac{Mt^2}{R^2}|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})| \\ &+ \frac{Mt}{R^2}\left(|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})| + \left|\partial_{k_i}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| + \left|\partial_{k_j}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right|\right) \\ &+ \frac{M}{R^2}\left(\left|\partial_{k_j}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| + \left|\partial_{k_i}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| + \left|\partial_{k_i}\partial_{k_j}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right|\right) \\ &+ \frac{M}{R^2}\left(|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})|\left|\partial_{k_i}\partial_{k_j} f_1(\boldsymbol{k})\right|\right). \qquad (33)\end{aligned}$$

Using $\left|\partial_{\boldsymbol{k}}^{\alpha}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-4}, |\alpha| \leqslant 1$, we get by (29) and (33) an appropriate constant $M' > 0$ with

$$\begin{aligned}|I_1| \leqslant \frac{M'(t+1)^2}{R^2} &+ \frac{M(t+1)^2}{R^2}\int \left|\partial_{k_i}\partial_{k_j}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right|k^2\,\mathrm{d}k\,\mathrm{d}\Omega \\ &+ \frac{MC(t+1)^2}{R^2}\int \langle k\rangle^{-4}\left|\partial_{k_i}\partial_{k_j} f_1(\boldsymbol{k})\right|k^2\,\mathrm{d}k\,\mathrm{d}\Omega. \qquad (34)\end{aligned}$$

To integrate the second derivatives we use $\left|\kappa\partial_{\boldsymbol{k}}^{\alpha}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-4}, |\alpha| = 2$ and $k\left|\partial_{k_i}\partial_{k_j} f_1(\boldsymbol{k})\right| \leqslant C\langle k\rangle$. Hence, with an appropriately chosen constant C', we arrive at

$$|I_1| \leqslant \frac{C'(t+1)^2}{R^2}. \qquad (35)$$

We estimate now I_2. Since $\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k}) \in \mathcal{G}^+$, we have

$$|I_2| \leqslant (2\pi)^{-\frac{3}{2}}C\int_{k>\frac{1}{2}R^{\frac{1}{6}}}\langle k\rangle^{-15}\,\mathrm{d}^3k \leqslant C''R^{-2}, \qquad (36)$$

with an appropriately chosen constant $C'' > 0$. Hence, we find

$$|\alpha(R\boldsymbol{n}, tR)| = |I_1 + I_2| \leqslant (C' + C'')(1+t)^2R^{-2} =: C'(1+t)^2R^{-2}. \qquad (37)$$

In a similar way, we can estimate $\nabla\alpha$ by

$$|\nabla_{\boldsymbol{x}}\alpha(\boldsymbol{x}, tR)|_{\boldsymbol{x}=R\boldsymbol{n}} \leqslant C'(1+t)R^{-1}. \qquad (38)$$

To get this estimate we split again the analogous integral to (25) into small and big momenta. The first part will be estimated by one partial integration using $\left|\partial_{\boldsymbol{k}}^{\alpha}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-5}, |\alpha| \leqslant 1$ and $\left|\kappa\partial_{\boldsymbol{k}}^{\alpha}\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-5}, |\alpha| = 2$, the second part (which is analogous to (36)) by using $|\widehat{\psi}_{\mathrm{out}}(\boldsymbol{k})| \leqslant C\langle k\rangle^{-10}$. Inserting (37) and (38) into (24), we get

$$\int_{\frac{T}{R}}^{R^{-\frac{1}{6}}}\int_{\Sigma}|\alpha(R\boldsymbol{n}, tR)||\nabla_{\boldsymbol{x}}\alpha(\boldsymbol{x}, tR)|_{\boldsymbol{x}=R\boldsymbol{n}}R^3\,\mathrm{d}\Omega\,\mathrm{d}t \leqslant 4\pi C'^2\int_0^{R^{-\frac{1}{6}}}(1+t)^3\mathrm{d}t, \qquad (39)$$

which tends to zero for $R \to \infty$.

It remains to show that the three other terms in (13) are negligible. In [25] (equations (15) and (16)), the function $\beta(\boldsymbol{x}, t)$ is estimated for some $R_0 > 0$ by

$$\sup_{\boldsymbol{x}\in\Sigma_R} |\beta(\boldsymbol{x}, t)| \leqslant c\frac{1}{R(t+R)}, \qquad \forall R > 0, \tag{40}$$

$$\sup_{\boldsymbol{x}\in\Sigma_R} |\nabla\beta(\boldsymbol{x}, t)| \leqslant c\frac{1}{R(t+R)}, \qquad \forall R > R_0, \tag{41}$$

for $t \geqslant T$. The constant c depends on T, $\widehat{\psi}_{\text{out}}(\boldsymbol{k})$ and $\frac{\partial}{\partial k}\widehat{\psi}_{\text{out}}(\boldsymbol{k})$, and is finite for $\widehat{\psi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+$ (cf (20)–(28) in [25]). It is also shown that the last term in (13) is negligible (cf p 10 in [25]). In [25], there are also estimates on the $\alpha(\boldsymbol{x}, t)$ terms, but not under the conditions which we must require. We start with the second term in (13):

$$\left|\int_T^\infty\int_\Sigma \text{Im}(\alpha^*\nabla\beta)R^2\boldsymbol{n}\,\text{d}\Omega\,\text{d}t\right| \leqslant \int_T^\infty\int_\Sigma |\alpha||\nabla\beta|R^2\,\text{d}\Omega\,\text{d}t$$
$$\leqslant \int_0^\infty\int_\Sigma |\alpha|\frac{c}{R(t+R)}R^2\,\text{d}\Omega\,\text{d}t. \tag{42}$$

We divide again the time integration into two parts:

$$\int_0^\infty\int_\Sigma |\alpha|\frac{c}{R(t+R)}R^2\,\text{d}\Omega\,\text{d}t = \int_0^{R^{\frac{5}{6}}}\int_\Sigma |\alpha|\frac{c}{R(t+R)}R^2\,\text{d}\Omega\,\text{d}t$$
$$+ \int_{R^{\frac{5}{6}}}^\infty\int_\Sigma |\alpha|\frac{c}{R(t+R)}R^2\,\text{d}\Omega\,\text{d}t. \tag{43}$$

Hence, with (37) the first part is

$$\int_0^{R^{\frac{5}{6}}}\int_\Sigma |\alpha(R\boldsymbol{n}, t)|\,\frac{c}{R(t+R)}R^2\,\text{d}\Omega\,\text{d}t = \int_0^{R^{-\frac{1}{6}}}\int_\Sigma |\alpha(R\boldsymbol{n}, tR)|\,\frac{c}{R^2(1+t)}R^3\,\text{d}\Omega\,\text{d}t$$
$$\leqslant \int_0^{R^{-\frac{1}{6}}}\int_\Sigma \frac{C'c(1+t)}{R}\,\text{d}\Omega\,\text{d}t, \tag{44}$$

which tends to zero for $R \to \infty$.

It remains the second term in (43). Applying the asymptotic expression (16) for α, we get

$$\int_{R^{\frac{5}{6}}}^\infty\int_\Sigma |\alpha(R\boldsymbol{n}, t)|\,\frac{cR^2}{R(t+R)}\,\text{d}\Omega\,\text{d}t \leqslant \int_{R^{\frac{5}{6}}}^\infty\int_\Sigma \left(\frac{1}{t}\right)^{\frac{3}{2}}\left|\widehat{\psi}_{\text{out}}\left(\frac{R\boldsymbol{n}}{t}\right)\right|\frac{cR^2}{R(t+R)}\,\text{d}\Omega\,\text{d}t$$
$$+ \int_{R^{\frac{5}{6}}}^\infty\int_\Sigma \frac{L}{t^2}\frac{cR^2}{R(t+R)}\,\text{d}\Omega\,\text{d}t$$
$$\leqslant \frac{4\pi c}{\sqrt{R}}\int_0^{R^{\frac{1}{6}}} |\widehat{\psi}_{\text{out}}(\boldsymbol{k})|\frac{1}{\sqrt{k}}\text{d}k + 4\pi cLR^{-\frac{5}{6}}, \tag{45}$$

where we substituted $\boldsymbol{k} := \frac{R\boldsymbol{n}}{t}$. Since $\widehat{\psi}_{\text{out}} \in \mathcal{G}^+$ the bound in (45) is finite and tends to zero for $R \to \infty$. The third term in (13) can be treated analogously to (42)–(45).

Appendix

Proof of lemma 2. Lemma 2 is proven—following the idea of Ikebe [16]—in [25]. The latter however contains a mistake concerning the assertion (iii), which overlooked the need for the smoothing factor $\kappa = \frac{k}{1+k}$, which puts the higher derivatives of the generalized eigenfunctions into the 'right' Banach space. The need for this smoothing factor arises from the derivative of k which appears in the spherical wave part in (8), see also the remarks in the introduction. Observing that the proof goes through verbatim. Our statement (iv) also follows from the proof in [25], replacing coordinate derivatives by the derivatives after k. In this case, we note that there is no need for any smoothing factor. □

Proof of lemma 3. Let $\psi \in \mathcal{G}$. Then there is a $\chi \in \mathcal{G}^0$ and a $t \in \mathbb{R}$ with

$$\psi = \mathrm{e}^{-\mathrm{i}Ht}\chi.$$

Using the intertwining property (6), we get

$$\psi_{\mathrm{out}} = \Omega_+^{-1}\psi = \Omega_+^{-1}\,\mathrm{e}^{-\mathrm{i}Ht}\chi = \mathrm{e}^{-\mathrm{i}H_0t}\Omega_+^{-1}\chi = \mathrm{e}^{-\mathrm{i}H_0t}\chi_{\mathrm{out}}. \tag{A.1}$$

Since $\mathcal{G}^+$ is invariant under multiplication by $\mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t}$ it suffices to show that $\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})$ is in $\mathcal{G}^+$. Let $\chi \in \mathcal{G}^0$. Since $\langle x\rangle^2 H^n\chi(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$, $0 \leqslant n \leqslant 8$ and $\langle x\rangle^4 H^n\chi(\boldsymbol{x}) \in L^2(\mathbb{R}^3)$, $0 \leqslant n \leqslant 3$, we have

$$\begin{aligned} &H^n\chi(\boldsymbol{x}) \in L_1(\mathbb{R}^3)\cap L^2(\mathbb{R}^3), && 0\leqslant n\leqslant 8,\\ &\langle x\rangle^j H^n\chi(\boldsymbol{x}) \in L_1(\mathbb{R}^3)\cap L^2(\mathbb{R}^3), && 0\leqslant n\leqslant 3, \quad j=\{1,2\}. \end{aligned} \tag{A.2}$$

Using the intertwining property (6) and lemma 1(ii) and (iii) (cf (2) and footnote 5), we have

$$\begin{aligned} \frac{k^2}{2}\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k}) &= \widehat{H_0\chi}_{\mathrm{out}}(\boldsymbol{k}) = \mathcal{F}\big(H_0\Omega_+^{-1}\chi\big)(\boldsymbol{k}) = \mathcal{F}\big(\Omega_+^{-1}H\chi\big)(\boldsymbol{k})\\ &= (2\pi)^{-\frac{3}{2}}\int \varphi_+^*(\boldsymbol{x},\boldsymbol{k})(H\chi)(\boldsymbol{x})\,\mathrm{d}^3x. \end{aligned} \tag{A.3}$$

Applying H_0 n times on $\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})$ $(0\leqslant n\leqslant 8)$, we get

$$\frac{k^{2n}}{2^n}\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k}) = (2\pi)^{-\frac{3}{2}}\int \varphi_+^*(\boldsymbol{x},\boldsymbol{k})(H^n\chi)(\boldsymbol{x})\,\mathrm{d}^3x. \tag{A.4}$$

Since the generalized eigenfunctions are bounded (lemma 2(ii)) and $H^n\chi \in L_1(\mathbb{R}^3)$, $0\leqslant n\leqslant 8$, we have with an appropriate constant C

$$|\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})| \leqslant C\langle k\rangle^{-16} \leqslant C\langle k\rangle^{-15}. \tag{A.5}$$

Because of lemma 2(iii) and (A.2) we can differentiate $\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})$ w.r.t. the coordinates and get an appropriate constant C with

$$\big|\partial_{k_i}\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})\big| = \left|(2\pi)^{-\frac{3}{2}}\int \big(\partial_{k_i}\varphi_+^*(\boldsymbol{x},\boldsymbol{k})\big)\chi(\boldsymbol{x})\,\mathrm{d}^3x\right| \leqslant C, \qquad \forall \boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}. \tag{A.6}$$

Applying H_0 three times in (A.3) and differentiating w.r.t. k_i, we get similarly to (A.6)

$$k^6\partial_{k_i}\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k}) = 8(2\pi)^{-\frac{3}{2}}\int \big(\partial_{k_i}\varphi_+^*(\boldsymbol{x},\boldsymbol{k})\big)(H^3\chi)(\boldsymbol{x})\,\mathrm{d}^3x - 6k^5\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})\frac{k_i}{k}. \tag{A.7}$$

Again the right-hand side is bounded because of lemma 2(iii), (A.2) and (A.5). Hence, we get together with (A.6)

$$\big|\partial_{k_i}\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})\big| \leqslant C\langle k\rangle^{-6}, \qquad \forall \boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}. \tag{A.8}$$

To control a second derivative with respect to the coordinates we have to multiply by the factor κ, since then the derivatives of the generalized eigenfunctions $\varphi_\pm$ are bounded by $c\langle x\rangle^2$, see lemma 2(iii). Hence, by (A.2)

$$\big|\kappa\,\partial_{k_j}\partial_{k_i}\widehat{\chi}_{\mathrm{out}}(\boldsymbol{k})\big| = \left|8(2\pi)^{-\frac{3}{2}}\int \big(\kappa\,\partial_{k_j}\partial_{k_i}\varphi_+^*(\boldsymbol{x},\boldsymbol{k})\big)\,\chi(\boldsymbol{x})\,\mathrm{d}^3x\right| \leqslant C, \qquad \forall \boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}. \tag{A.9}$$

Using (A.7), we get

$$k^6\kappa\,\partial_{k_j}\partial_{k_i}\widehat{\chi}_{\text{out}}(\boldsymbol{k}) = 8(2\pi)^{-\frac{3}{2}}\int\left(\kappa\,\partial_{k_j}\partial_{k_i}\varphi_+^*(\boldsymbol{x},\boldsymbol{k})\right)(H^3\chi)(\boldsymbol{x})\,\mathrm{d}^3x - 30k^4\frac{k_j}{k}\frac{k_i}{k}\kappa\widehat{\chi}_{\text{out}}(\boldsymbol{k})$$
$$- 6k^5\frac{k_i}{k}\kappa\,\partial_{k_j}\widehat{\chi}_{\text{out}}(\boldsymbol{k}) - 6k^5\widehat{\chi}_{\text{out}}(\boldsymbol{k})\kappa\frac{k\delta_{ij}k - k_ik_j}{k^3} - 6k^5\frac{k_j}{k}\kappa\,\partial_{k_i}\widehat{\chi}_{\text{out}}(\boldsymbol{k}), \quad (A.10)$$

where the right-hand side is bounded because of lemma 2(iii), (A.2), (A.4) and (A.8). Hence,

$$\left|\kappa\,\partial_{\boldsymbol{k}}^{\alpha}\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-6} \leqslant C\langle k\rangle^{-5}, \qquad |\alpha| = 2, \quad \forall\boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}. \quad (A.11)$$

Equation (A.8) also implies

$$|\partial_k\widehat{\chi}_{\text{out}}(\boldsymbol{k})| \leqslant C\langle k\rangle^{-6}, \qquad \forall\boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}. \quad (A.12)$$

Applying H_0 two times in (A.3) and differentiating two times w.r.t. k, we get by lemma 2(iv), (A.2), (A.5) and (A.12) analogously to (A.11):

$$\left|\partial_k^2\widehat{\chi}_{\text{out}}(\boldsymbol{k})\right| \leqslant C\langle k\rangle^{-4} \leqslant C\langle k\rangle^{-3}, \qquad \forall\boldsymbol{k}\in\mathbb{R}^3\backslash\{0\}, \quad (A.13)$$

which means that $\widehat{\chi}_{\text{out}}(\boldsymbol{k}) \in \mathcal{G}^+$. □

Proof of Lemma 4. At first sight lemma 4 looks like a standard stationary phase result, e.g., theorem 7.7.5 in [15]. But in our case we have (by necessity) very weak conditions on the function $\chi(\boldsymbol{k})$, since we need to use the lemma for $\chi(\boldsymbol{k}) = \widehat{\psi}_{\text{out}}(\boldsymbol{k})$. Especially, the second derivative of $\chi(\boldsymbol{k})$ w.r.t. the coordinates becomes unbounded for $k \to 0$. Furthermore, the stationary point $\boldsymbol{k}_{\text{s}}$ is moving with $\boldsymbol{x}$ and t.

First, we extract the leading order term of the integral (15)

$$\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\chi(\boldsymbol{k})\,\mathrm{d}^3k = \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\left(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_{\text{s}}) + \chi(\boldsymbol{k}_{\text{s}})\right)\mathrm{d}^3k$$
$$= \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\chi(\boldsymbol{k}_{\text{s}})\,\mathrm{d}^3k + \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\left(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_{\text{s}})\right)\mathrm{d}^3k. \quad (A.14)$$

The leading order term can be easily calculated:

$$\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\chi(\boldsymbol{k}_{\text{s}})\,\mathrm{d}^3k = \left(\frac{2\pi}{\mathrm{i}t}\right)^{\frac{3}{2}}\mathrm{e}^{\mathrm{i}\frac{x^2}{2t}}\chi(\boldsymbol{k}_{\text{s}}). \quad (A.15)$$

We will now calculate the error between the left-hand side of (A.14) and the leading order term (A.15):

$$\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\left(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_{\text{s}})\right)\mathrm{d}^3k. \quad (A.16)$$

The following splitting of the integration area turns out to be convenient (cf. figure 1 below):

$$A_1 := \left\{\boldsymbol{k}\in\mathbb{R}^3 : \widetilde{k} = |\boldsymbol{k} - \boldsymbol{k}_{\text{s}}| < \frac{k_{\text{s}}}{2}\right\},$$
$$A_2 := \left\{\boldsymbol{k}\in\mathbb{R}^3 : k < 2k_{\text{s}} \wedge |\boldsymbol{k} - \boldsymbol{k}_{\text{s}}| \geqslant \frac{k_{\text{s}}}{2}\right\}, \quad (A.17)$$
$$A_3 := \left\{\boldsymbol{k}\in\mathbb{R}^3 : k \geqslant \frac{3}{2}k_{\text{s}}\right\}.$$

The areas A_2 and A_3 have a small overlap. This is due to the use of suitable mollifiers. In A_1 and A_2 we shall perform two partial integrations w.r.t. the coordinates, in A_3 we shall perform the derivatives w.r.t. k. Our proof will assume $\boldsymbol{x} \neq 0$. The case $\boldsymbol{x} = 0$ must be handled separately, but is much easier than the proof we give. It can be done by two partial integrations w.r.t. k similarly to our procedure which handles the area A_3 (A.17).

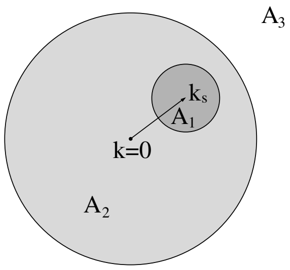

Figure 1. Sketch of the three integration areas in the $\boldsymbol{k}$-frame.

We first divide the integration area into $A_1 \cup A_2$ and A_3 by using the mollifier $\rho(\boldsymbol{k})$:

$$\rho(\boldsymbol{k}) = \begin{cases} 1, & \text{for} \quad k < \frac{3}{2}k_s, \\ e \exp\left(-\frac{1}{1 - \frac{(k-\frac{3}{2}k_s)^2}{(\frac{k_s}{2})^2}} \right), & \text{for} \quad \frac{3}{2}k_s \leqslant k < 2k_s, \\ 0, & \text{for} \quad k \geqslant 2k_s. \end{cases} \tag{A.18}$$

The mollifier has the following properties:

$\operatorname{supp} \rho = A_1 \cup A_2, \qquad |\rho(\boldsymbol{k})| \leqslant 1, \qquad |1 - \rho(\boldsymbol{k})| \leqslant 1,$

There is an $M > 0$ such that

$$\begin{aligned} &|\partial_k \rho(\boldsymbol{k})|, && \left|\partial_{\boldsymbol{k}}^\alpha \rho(\boldsymbol{k})\right| \leqslant \frac{M}{k_s}, && |\alpha| = 1, && \text{and} \\ &|\partial_k^2 \rho(\boldsymbol{k})|, && |\partial_{\boldsymbol{k}}^\alpha \rho(\boldsymbol{k})| \leqslant \frac{M}{k_s^2}, && |\alpha| = 2. \end{aligned} \tag{A.19}$$

Using ρ, we can write for (A.16):

$$\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} (\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_s)) \, \mathrm{d}^3k = \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \rho(\boldsymbol{k}) \, (\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_s)) \, \mathrm{d}^3k$$
$$+ \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} (1 - \rho(\boldsymbol{k})) \, (\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_s)) \, \mathrm{d}^3k =: I_{12} + I_3. \tag{A.20}$$

We start with the estimation of I_{12}. We define

$$f(\boldsymbol{k}) := \rho(\boldsymbol{k}) \, (\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_s)), \qquad \widetilde{\boldsymbol{k}} := \boldsymbol{k} - \boldsymbol{k}_s \tag{A.21}$$

and get with two partial integration w.r.t. to $\boldsymbol{k}$

$$\begin{aligned} |I_{12}| &= \left| \int \mathrm{e}^{-\mathrm{i}t(\frac{k^2}{2} - \boldsymbol{k}\cdot\boldsymbol{k}_s)} f(\boldsymbol{k}) \, \mathrm{d}^3k \right| \\ &= \frac{1}{t} \left| \int \left(\nabla_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \right) \cdot \frac{\widetilde{\boldsymbol{k}}}{\widetilde{k}^2} f(\boldsymbol{k}) \, \mathrm{d}^3k \right| \\ &= \frac{1}{t} \left| \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \left(\frac{\widetilde{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{k}} f(\boldsymbol{k}) - f(\boldsymbol{k})}{\widetilde{k}^2} \right) \mathrm{d}^3k \right| \\ &= \frac{1}{t^2} \left| \int \left(\nabla_{\boldsymbol{k}} \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} \right) \cdot \frac{\widetilde{\boldsymbol{k}}}{\widetilde{k}^2} \left(\frac{\widetilde{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{k}} f(\boldsymbol{k}) - f(\boldsymbol{k})}{\widetilde{k}^2} \right) \mathrm{d}^3k \right| \end{aligned}$$

$$= \frac{1}{t^2}\left|\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\left(\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}+\frac{1}{\widetilde{k}^4}\sum_{|\alpha_1|+|\alpha_2|=2}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}f(\boldsymbol{k})\right)\mathrm{d}^3k\right|$$

$$\leqslant \frac{1}{t^2}\int\left|\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}\right|\mathrm{d}^3k+\frac{1}{t^2}\int\left|\frac{1}{\widetilde{k}^4}\sum_{|\alpha_1|+|\alpha_2|=2}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}f(\boldsymbol{k})\right|\mathrm{d}^3k. \quad \text{(A.22)}$$

Because of the definition of ρ, the integration area in (A.22) is $A_1 \cup A_2$ (cf (A.17) and (A.18)). We will divide this area into A_1 and A_2. Hence, I_{12} is estimated by

$$|I_{12}| \leqslant \frac{1}{t^2}\int_{A_1}\left|\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}\right|\mathrm{d}^3k+\frac{1}{t^2}\int_{A_1}\left|\frac{1}{\widetilde{k}^4}\sum_{|\alpha_1|+|\alpha_2|=2}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}f(\boldsymbol{k})\right|\mathrm{d}^3k$$

$$+\frac{1}{t^2}\int_{A_2}\left|\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}\right|\mathrm{d}^3k+\frac{1}{t^2}\int_{A_2}\left|\frac{1}{\widetilde{k}^4}\sum_{|\alpha_1|+|\alpha_2|=2}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}f(\boldsymbol{k})\right|\mathrm{d}^3k$$

$$=: I_1+\frac{1}{t^2}\int_{A_2}\left|\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}\right|\mathrm{d}^3k+\frac{1}{t^2}\int_{A_2}\left|\frac{1}{\widetilde{k}^4}\sum_{|\alpha_1|+|\alpha_2|=2}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}f(\boldsymbol{k})\right|\mathrm{d}^3k$$

$$=: I_1+I_2. \quad \text{(A.23)}$$

We first estimate I_1. With (A.17) and (A.18), we see that for $\boldsymbol{k}\in A_1$, $\rho(\boldsymbol{k})\equiv 1$ and thus we have for (A.21): $f(\boldsymbol{k})=\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_{\mathrm{s}})$. Using Taylors formula and then substituting $\boldsymbol{k}$ by $\widetilde{\boldsymbol{k}}$ (cf (A.21)), we get for the first term I_1^1 of I_1

$$I_1^1 = \frac{1}{t^2}\int_{A_1}\left|\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}\right|\mathrm{d}^3k$$

$$= \frac{1}{t^2}\int_{A_1}\left|\frac{\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_{\mathrm{s}})-(\boldsymbol{k}-\boldsymbol{k}_{\mathrm{s}})\cdot\nabla_{\boldsymbol{k}}\chi(\boldsymbol{k})}{(\boldsymbol{k}-\boldsymbol{k}_{\mathrm{s}})^4}\right|\mathrm{d}^3k$$

$$= \frac{1}{t^2}\int_{A_1}\left|\frac{\sum_{|\alpha_1|+|\alpha_2|=2}(\boldsymbol{k}-\boldsymbol{k}_{\mathrm{s}})^{\alpha_1}(\boldsymbol{k}-\boldsymbol{k}_{\mathrm{s}})^{\alpha_2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}\chi(\boldsymbol{\xi})}{2(\boldsymbol{k}-\boldsymbol{k}_{\mathrm{s}})^4}\right|\mathrm{d}^3k$$

$$= \frac{1}{t^2}\int_{A_1}\left|\frac{\sum_{|\alpha_1|+|\alpha_2|=2}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}\chi(\boldsymbol{\xi})}{2\widetilde{k}^4}\right|\mathrm{d}^3\widetilde{k}, \quad \text{(A.24)}$$

where $\boldsymbol{\xi}$ is a vector between $\boldsymbol{k}_{\mathrm{s}}$ and $\boldsymbol{k}$. Hence, we have $\xi > \frac{k_{\mathrm{s}}}{2}$. Using definition 4, i.e. that $\partial_{k_i}\partial_{k_j}\chi(\boldsymbol{k}) \leqslant Ck^{-1}$, we get for (A.24)

$$I_1^1 \leqslant \frac{9C}{2t^2}\int_{A_1}\frac{1}{\widetilde{k}^2\xi}\mathrm{d}^3\widetilde{k} < \frac{36\pi C}{k_{\mathrm{s}}t^2}\int_{A_1}\mathrm{d}\widetilde{k} = \frac{18\pi C}{t^2}. \quad \text{(A.25)}$$

The second term of I_1 can be estimated analogously: instead of $\boldsymbol{\xi}$ we have $\boldsymbol{k}=\widetilde{\boldsymbol{k}}+\boldsymbol{k}_{\mathrm{s}}$ with $k>\frac{k_{\mathrm{s}}}{2}$. It follows that I_1 is of order t^{-2} uniform in $\boldsymbol{k}_{\mathrm{s}}$. The estimation of I_2 is very similar, but $\rho(\boldsymbol{k})\neq 1$ on A_2. We use the volume factor d^3k integrated over A_2. Hence, it suffices to show that the integrands of the two terms of I_2 are bounded by $\frac{L}{k_{\mathrm{s}}^3}$ or $\frac{L}{k_{\mathrm{s}}^2k}$ with some constant $L>0$ uniform in $\boldsymbol{k}_{\mathrm{s}}$. The first integrand is

$$\left|\frac{f(\boldsymbol{k})-\widetilde{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}f(\boldsymbol{k})}{\widetilde{k}^4}\right| \leqslant \left|\frac{\rho(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_{\mathrm{s}}))}{\widetilde{k}^4}\right|+\left|\frac{|\nabla_{\boldsymbol{k}}f(\boldsymbol{k})|}{\widetilde{k}^3}\right| \leqslant \left|\frac{\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_{\mathrm{s}})}{\widetilde{k}^4}\right|$$

$$+\sum_{i=1}^{3}\left|\frac{|\partial_{k_i}\chi(\boldsymbol{k})|}{\widetilde{k}^3}\right|+\sum_{i=1}^{3}\left|\frac{|(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_{\mathrm{s}}))\partial_{k_i}\rho(\boldsymbol{k})|}{\widetilde{k}^3}\right|. \quad \text{(A.26)}$$

By mean value theorem there exists a $\boldsymbol{\xi} \in (\boldsymbol{k}_\mathrm{s}, \boldsymbol{k})$ with

$$|\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s})| = |\nabla_{\boldsymbol{k}}\chi(\boldsymbol{\xi})||\boldsymbol{k} - \boldsymbol{k}_\mathrm{s}| \leqslant Ck + Ck_\mathrm{s}, \tag{A.27}$$

since $\chi(\boldsymbol{k}) \in \widehat{\mathcal{K}}$. Using (A.27), (A.19), $\boldsymbol{k} \in A_2$ (which means $k < 2k_\mathrm{s}, \widetilde{k} \geqslant \frac{k_\mathrm{s}}{2}$) as well as $\left|\partial_{k_i}\chi(\boldsymbol{k})\right| \leqslant C, i = \{1, 2, 3\}$, we obtain

$$\left|\frac{f(\boldsymbol{k}) - \widetilde{\boldsymbol{k}} \cdot \nabla_{\boldsymbol{k}} f(\boldsymbol{k})}{\widetilde{k}^4}\right| \leqslant \frac{32C}{k_\mathrm{s}^3} + \frac{16C}{k_\mathrm{s}^3} + \frac{24C}{k_\mathrm{s}^3} + \frac{48CM}{k_\mathrm{s}^3} + \frac{24CM}{k_\mathrm{s}^3}. \tag{A.28}$$

Similarly, we estimate the integrand of the second term of I_2 (A.23). We pick one summand ($|\alpha_1| + |\alpha_2| = 2$)

$$\begin{aligned}
\left|\frac{1}{\widetilde{k}^4}\widetilde{\boldsymbol{k}}^{\alpha_1}\widetilde{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2} f(\boldsymbol{k})\right| &\leqslant \left|\frac{1}{\widetilde{k}^2}\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2} f(\boldsymbol{k})\right| \\
&\leqslant \frac{4|\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s})|\left|\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}\rho(\boldsymbol{k})\right|}{k_\mathrm{s}^2} + \frac{4\left|\partial_{\boldsymbol{k}}^{\alpha_1}\rho(\boldsymbol{k})\right|\left|\partial_{\boldsymbol{k}}^{\alpha_2}\chi(\boldsymbol{k})\right|}{k_\mathrm{s}^2} \\
&\quad + \frac{4\left|\partial_{\boldsymbol{k}}^{\alpha_2}\rho(\boldsymbol{k})\right|\left|\partial_{\boldsymbol{k}}^{\alpha_1}\chi(\boldsymbol{k})\right|}{k_\mathrm{s}^2} + \frac{4\left|\partial_{\boldsymbol{k}}^{\alpha_1}\partial_{\boldsymbol{k}}^{\alpha_2}\chi(\boldsymbol{k})\right|}{k_\mathrm{s}^2} \\
&\leqslant \frac{8CM}{k_\mathrm{s}^3} + \frac{4CM}{k_\mathrm{s}^3} + \frac{8CM}{k_\mathrm{s}^3} + \frac{4C}{k_\mathrm{s}^2 k}.
\end{aligned} \tag{A.29}$$

It remains to estimate I_3 (A.20). We introduce a convergence factor $\rho_\epsilon(\boldsymbol{k})$:

$$\rho_\epsilon(\boldsymbol{k}) = \begin{cases} 1, & \text{for} \quad k < \dfrac{1}{\epsilon}, \\ \mathrm{e}^{-\left(k-\frac{1}{\epsilon}\right)^2}, & \text{for} \quad k \geqslant \dfrac{1}{\epsilon}, \end{cases} \tag{A.30}$$

with $0 < \epsilon < \min\left(\frac{1}{2k_\mathrm{s}}; 1\right)$. Then, we get for I_3 (A.20)

$$\begin{aligned}
I_3 &= \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho(\boldsymbol{k}))\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&= \int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho(\boldsymbol{k}))\,(1 - \rho_\epsilon(\boldsymbol{k}) + \rho_\epsilon(\boldsymbol{k}))\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&= \lim_{\epsilon\to 0}\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho(\boldsymbol{k}))\,(1 - \rho_\epsilon(\boldsymbol{k}) + \rho_\epsilon(\boldsymbol{k}))\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&= \lim_{\epsilon\to 0}\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho(\boldsymbol{k}))\,\rho_\epsilon(\boldsymbol{k})\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&\quad + \lim_{\epsilon\to 0}\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho(\boldsymbol{k}))\,(1 - \rho_\epsilon(\boldsymbol{k}))\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&= \lim_{\epsilon\to 0}\int \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho(\boldsymbol{k}))\,\rho_\epsilon(\boldsymbol{k})\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&\quad + \lim_{\epsilon\to 0}\int_{k=\frac{1}{\epsilon}}^{\infty} \mathrm{e}^{-\mathrm{i}\frac{k^2}{2}t + \mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}}\,(1 - \rho_\epsilon(\boldsymbol{k}))\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k,
\end{aligned} \tag{A.31}$$

since $1 - \rho \equiv 1$ on $\mathrm{supp}(1 - \rho_\epsilon)$ (cf (A.18) and (A.30)). The last term in the last line of (A.31) is zero (since $\chi(\boldsymbol{k}) \in \widehat{\mathcal{K}}$ and by a standard Riemann–Lebesgue argument) and we get for I_3

$$\begin{aligned}
I_3 &= \lim_{\epsilon\to 0}\int \mathrm{e}^{-\mathrm{i}t\left(\frac{k^2}{2} - \boldsymbol{k}\cdot\boldsymbol{k}_\mathrm{s}\right)}\,(1 - \rho(\boldsymbol{k}))\,\rho_\epsilon(\boldsymbol{k})\,(\chi(\boldsymbol{k}) - \chi(\boldsymbol{k}_\mathrm{s}))\,\mathrm{d}^3k \\
&=: \lim_{\epsilon\to 0}\int \mathrm{e}^{-\mathrm{i}t\left(\frac{k^2}{2} - \boldsymbol{k}\cdot\boldsymbol{k}_\mathrm{s}\right)} f_\epsilon(\boldsymbol{k}, \boldsymbol{k}_\mathrm{s}) k^2\,\mathrm{d}k\,\mathrm{d}\Omega.
\end{aligned} \tag{A.32}$$

We will perform now two partial integrations w.r.t. k:

$$
\begin{aligned}
|I_3| &= \left|\lim_{\epsilon\to0}\frac{1}{t}\int \mathrm{e}^{-\mathrm{i}t(\frac{k^2}{2}-\boldsymbol{k}\cdot\boldsymbol{k}_\mathrm{s})}\partial_k\left(\frac{k^2 f_\epsilon(\boldsymbol{k},\boldsymbol{k}_\mathrm{s})}{k-\boldsymbol{e}_k\cdot\boldsymbol{k}_\mathrm{s}}\right)\mathrm{d}k\,\mathrm{d}\Omega\right| \\
&= \left|\lim_{\epsilon\to0}\frac{1}{t^2}\int \mathrm{e}^{-\mathrm{i}t(\frac{k^2}{2}-\boldsymbol{k}\cdot\boldsymbol{k}_\mathrm{s})}\partial_k\left(\frac{1}{k-\boldsymbol{e}_k\cdot\boldsymbol{k}_\mathrm{s}}\partial_k\left(\frac{k^2 f_\epsilon(\boldsymbol{k},\boldsymbol{k}_\mathrm{s})}{k-\boldsymbol{e}_k\cdot\boldsymbol{k}_\mathrm{s}}\right)\right)\mathrm{d}k\,\mathrm{d}\Omega\right| \\
&\leqslant \frac{1}{t^2}\lim_{\epsilon\to0}\int\left|\partial_k\left(\frac{1}{k-\boldsymbol{e}_k\cdot\boldsymbol{k}_\mathrm{s}}\partial_k\left(\frac{k^2 f_\epsilon(\boldsymbol{k},\boldsymbol{k}_\mathrm{s})}{k-\boldsymbol{e}_k\cdot\boldsymbol{k}_\mathrm{s}}\right)\right)\right|\mathrm{d}k\,\mathrm{d}\Omega \\
&=: \frac{1}{t^2}\lim_{\epsilon\to0}\int_{k\geqslant\frac{3}{2}k_\mathrm{s}}|D|\,\mathrm{d}k\,\mathrm{d}\Omega \\
&\leqslant \frac{1}{t^2}\lim_{\epsilon\to0}\int_{\frac{3}{2}k_\mathrm{s}\leqslant k<2k_\mathrm{s}}|D|\,\mathrm{d}k\,\mathrm{d}\Omega+\frac{1}{t^2}\lim_{\epsilon\to0}\int_{2k_\mathrm{s}\leqslant k<\frac{1}{\epsilon}}|D|\,\mathrm{d}k\,\mathrm{d}\Omega+\frac{1}{t^2}\lim_{\epsilon\to0}\int_{k\geqslant\frac{1}{\epsilon}}|D|\,\mathrm{d}k\,\mathrm{d}\Omega \\
&=: I_3^1+I_3^2+I_3^3. \qquad \text{(A.33)}
\end{aligned}
$$

We start with the estimation of I_3^1. Because of the integration area it suffices to show that D is of order k_s^{-1}. Since $\rho_\epsilon(\boldsymbol{k})\equiv1$ in this area, D is given by ($(\cdot)'$ denotes the derivative w.r.t. k)

$$
\begin{aligned}
|D| \leqslant{} & \left|\frac{k^2}{(k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s})^2}\right||((1-\rho(\boldsymbol{k}))(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))''| \\
&+\left|\left(\frac{k^2}{(k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s})^2}\right)'+\frac{1}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\left(\frac{k^2}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\right||((1-\rho(\boldsymbol{k}))(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))'| \\
&+\left|\left(\frac{k^2}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\right)''\frac{1}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}+\left(\frac{1}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\left(\frac{k^2}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\right| \\
&\cdot|(1-\rho(\boldsymbol{k}))(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))|\,. \qquad \text{(A.34)}
\end{aligned}
$$

We shall use (sometimes in a slightly modified version)

$$
\frac{k^2}{(k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s})^2}\leqslant\frac{k^2}{(k-k_\mathrm{s})^2}=\frac{(k-k_\mathrm{s}+k_\mathrm{s})^2}{(k-k_\mathrm{s})^2}\leqslant9,\qquad\text{for}\quad k\geqslant\frac{3}{2}k_\mathrm{s}. \qquad \text{(A.35)}
$$

Using (A.35) we get instead of (A.34)

$$
\begin{aligned}
|D| \leqslant{} & 9|((1-\rho(\boldsymbol{k}))(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))''|+\frac{39}{k-k_\mathrm{s}}|((1-\rho(\boldsymbol{k}))(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))'| \\
&+\frac{47}{(k-k_\mathrm{s})^2}|(1-\rho(\boldsymbol{k}))(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))|\,. \qquad \text{(A.36)}
\end{aligned}
$$

Using $\chi(\boldsymbol{k})\in\widehat{\mathcal{K}}$, i.e.,

$$
\begin{aligned}
&|(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))'|\leqslant C\langle k\rangle^{-1}\leqslant C, \\
&|(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))''|\leqslant C\langle k\rangle^{-2}\leqslant C\langle k\rangle^{-1}\leqslant C(1+k_\mathrm{s})^{-1},
\end{aligned} \qquad \text{(A.37)}
$$

since $k>k_\mathrm{s}$, (A.19), (A.27) and (A.35), we find

$$
|D|\leqslant\frac{818CM}{k_\mathrm{s}}+\frac{9C}{1+k_\mathrm{s}}. \qquad \text{(A.38)}
$$

It follows that I_3^1 is of order t^{-2} uniform in $\boldsymbol{k}_\mathrm{s}$. It remains to estimate I_3^2 and I_3^3. First, we consider 'large' k_s: let $2k_\mathrm{s}\geqslant1$. D on the integration area of I_3^2 (where $\frac{1}{\epsilon}>k\geqslant2k_\mathrm{s}$) is bounded by (we use again $|\chi'(\boldsymbol{k})|\leqslant C\langle k\rangle^{-1}$ and $|\chi''(\boldsymbol{k})|\leqslant C\langle k\rangle^{-2}$)

$$
|D|\leqslant\left|\frac{k^2}{(k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s})^2}\right||\chi''(\boldsymbol{k})|+\left|\left(\frac{k^2}{(k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s})^2}\right)'+\frac{1}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\left(\frac{k^2}{k-\boldsymbol{e}_{\boldsymbol{k}}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\right||\chi'(\boldsymbol{k})|
$$

$$+\left|\left(\frac{k^2}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}\right)''\frac{1}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}+\left(\frac{1}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\left(\frac{k^2}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\right||\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})|$$
$$\leqslant \frac{4C}{\langle k\rangle^2}+\frac{10C}{(k-k_\mathrm{s})\langle k\rangle}+\frac{52C}{(k-k_\mathrm{s})^2}, \tag{A.39}$$

where we used (A.35) (and analogous estimates) with $k \geqslant 2k_\mathrm{s}$. Inserting (A.39) into (A.32), we get

$$\left|I_3^2\right| = \frac{1}{t^2}\lim_{\epsilon\to 0}\int_{2k_\mathrm{s}\leqslant k<\frac{1}{\epsilon}}|D|\,\mathrm{d}k\,\mathrm{d}\Omega \leqslant \frac{1}{t^2}\lim_{\epsilon\to 0}\int_{2k_\mathrm{s}\leqslant k}|D|\,\mathrm{d}k\,\mathrm{d}\Omega = \frac{1}{t^2}\int_{2k_\mathrm{s}\leqslant k}|D|\,\mathrm{d}k\,\mathrm{d}\Omega, \tag{A.40}$$

which is integrable uniformly in $\boldsymbol{k}_\mathrm{s}$ for $2k_\mathrm{s} \geqslant 1$. Hence, I_3^2 is of order t^{-2} uniformly in $\boldsymbol{k}_\mathrm{s}$ for $2k_\mathrm{s} \geqslant 1$. Similarly, we can estimate I_3^3 since then we have for D

$$|D| \leqslant 4|(\rho_\epsilon(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))''| + \frac{10}{k-k_\mathrm{s}}|(\rho_\epsilon(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))'|$$
$$+\frac{26}{(k-k_\mathrm{s})^2}|\rho_\epsilon(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))|$$
$$\leqslant 4|(\rho_\epsilon(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))''| + 20|(\rho_\epsilon(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s})))'|$$
$$+104\,|\rho_\epsilon(\boldsymbol{k})(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))|\,. \tag{A.41}$$

The integration of (A.41) over the area $k \geqslant \frac{1}{\epsilon}$ yields a uniform bound in $\boldsymbol{k}_\mathrm{s}$ and ϵ for $2k_\mathrm{s} \geqslant 1$. It remains to estimate I_3^2 and I_3^3 for $2k_\mathrm{s} < 1$. I_3^3 can be estimated analogous to (A.41) since $k \geqslant \frac{1}{\epsilon} > 1$ and we have again

$$\frac{1}{k-k_\mathrm{s}} < \frac{1}{1-k_\mathrm{s}} < 2. \tag{A.42}$$

For I_3^2 we split the integration into

$$I_3^2 \leqslant \frac{1}{t^2}\lim_{\epsilon\to 0}\int_{2k_\mathrm{s}\leqslant k<1}|D|\,\mathrm{d}k\,\mathrm{d}\Omega + \frac{1}{t^2}\lim_{\epsilon\to 0}\int_{1\leqslant k<\frac{1}{\epsilon}}|D|\,\mathrm{d}k\,\mathrm{d}\Omega. \tag{A.43}$$

The second term on the right-hand side of (A.43) can be estimated analogous to I_3^2 for $2k_\mathrm{s} \geqslant 1$. Thus, remains the following integral:

$$\frac{1}{t^2}\lim_{\epsilon\to 0}\int_{2k_\mathrm{s}\leqslant k<1}|D|\,\mathrm{d}k\,\mathrm{d}\Omega. \tag{A.44}$$

The integrand is bounded by (we use again (A.35))

$$|D| \leqslant \left|\frac{k^2}{(k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s})^2}\right||\chi''(\boldsymbol{k})| + \left|\left(\frac{k^2}{(k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s})^2}\right)'\right||\chi'(\boldsymbol{k})|$$
$$+\left|\left(\left(\frac{k^2}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\frac{1}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))\right)'\right|$$
$$\leqslant 4C + \left|\left(\frac{k^2}{(k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s})^2}\right)'\right|C + \left|\left(\left(\frac{k^2}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}\right)'\frac{1}{k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s}}(\chi(\boldsymbol{k})-\chi(\boldsymbol{k}_\mathrm{s}))\right)'\right|$$
$$=: |D_1| + |D_2| + |D_3|. \tag{A.45}$$

We have to integrate D over a bounded interval. Hence, D_1 yields a uniform constant. The derivative in D_2 has at most two zeros in A_3. So we can divide the integration area into three subsets on which $\partial_k\left(\frac{k^2}{(k-\boldsymbol{e_k}\cdot\boldsymbol{k}_\mathrm{s})^2}\right)$ does not change the sign. Then, we can apply the fundamental theorem of calculus to conclude that the second term also yields a uniform constant, using (A.35). D_3 can be written as

$$
\begin{aligned}
|D_3| &= \left| \left(\left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (\chi(\boldsymbol{k}) - \chi(0) - k\chi'(0) + \chi(0) - \chi(\boldsymbol{k}_{\mathrm{s}}) + k\chi'(0)) \right)' \right| \\
&= \left| \left(\left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (\chi(\boldsymbol{k}) - \chi(0) - k\chi'(0) + k_{\mathrm{s}} g(\boldsymbol{k}_{\mathrm{s}}) + k\chi'(0)) \right)' \right| \\
&\leqslant \left| \left(\left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (\chi(\boldsymbol{k}) - \chi(0) - k\chi'(0)) \right)' \right| \\
&\quad + \left| \left(\left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (k_{\mathrm{s}} g(\boldsymbol{k}_{\mathrm{s}}) + k\chi'(0)) \right)' \right| \\
&=: \left| D_3^1 \right| + \left| D_3^2 \right|, \qquad \text{(A.46)}
\end{aligned}
$$

with appropriate bounded $g(\boldsymbol{k}_{\mathrm{s}})$: by Taylors formula and since $|\nabla_{\boldsymbol{k}} \chi(\boldsymbol{k})| \leqslant 3C$, we get

$$|g(\boldsymbol{k}_{\mathrm{s}})| \leqslant 3C. \qquad \text{(A.47)}$$

D_3^2 in (A.46) can be treated analogous to D_2 since the derivative has at most five zeros and

$$\left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (k_{\mathrm{s}} g(\boldsymbol{k}_{\mathrm{s}}) + k\chi'(0)) \right| \leqslant 40C. \qquad \text{(A.48)}$$

To get (A.48) we again use estimates like (A.35) with $k \geqslant 2k_{\mathrm{s}}$. Now we estimate D_3^1 in (A.46). Since the integration area is bounded it suffices to show that D_3^1 is uniformly bounded:

$$
\begin{aligned}
\left| D_3^1 \right| \leqslant{}& \left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)'' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (\chi(\boldsymbol{k}) - \chi(0) - k\chi'(0)) \right| \\
&+ \left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \left(\frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' (\chi(\boldsymbol{k}) - \chi(0) - k\chi'(0)) \right| \\
&+ \left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} (\chi'(\boldsymbol{k}) - \chi'(0)) \right|. \qquad \text{(A.49)}
\end{aligned}
$$

Using Taylors formula, we can linearize the $\chi(\boldsymbol{k})$-terms and get $(0 < \xi, \zeta < 1)$

$$
\begin{aligned}
\left| D_3^1 \right| \leqslant{}& \left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)'' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} k^2 \chi''(\xi \boldsymbol{k}) \right| + \left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \left(\frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' k^2 \chi''(\xi \boldsymbol{k}) \right| \\
&+ \left| \left(\frac{k^2}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} \right)' \frac{1}{k - \boldsymbol{e}_{\boldsymbol{k}} \cdot \boldsymbol{k}_{\mathrm{s}}} k \chi''(\zeta \boldsymbol{k}) \right|. \qquad \text{(A.50)}
\end{aligned}
$$

Using $|\chi''(\boldsymbol{k})| \leqslant C$ and (A.35) (again we also use similar estimates with $k \geqslant 2k_{\mathrm{s}}$), one gets

$$\left| D_3^1 \right| \leqslant 120C. \qquad \text{(A.51)}$$

Hence, I_3 is of order t^{-2} uniform in $\boldsymbol{k}_{\mathrm{s}}$. It follows lemma 4. □

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