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Comments on eikonal and sudden approximations†

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Abstract. An approximation scheme is presented which leads systematically from the exact Møller (or scattering) operator to the eikonal approximation and then to the sudden approximation. In terms of the Møller (or scattering) operator, the eikonal approximation is local in position space and is parametrised by the average incoming free momentum. Carrying the procedure a step further decouples the internal and translational motions to produce the sudden approximation. Distorted as well as straight-line approximations are considered. To do so, distorted scattering conditions are presented which define distorted Møller, transition and scattering operators. Some properties of these operators are discussed. Relations with the usual Møller, transition and scattering operators are presented. Finally, an eikonal approximation to the Møller super-operator is presented which does not depend explicitly upon the form of the dynamics that is used. Quantally, the eikonal Møller super-operator is equivalent to the eikonal Møller operator and, in the limit of small $\hbar$, reduces to the classical eikonal Møller super-operator. This classical Møller super-operator gives a particle picture for the eikonal approximation in contrast to the traditional wave picture.

1. Introduction

Exponential approximations abound in the literature of scattering theory. Two particular examples are the eikonal and sudden approximations. The purpose of this paper is twofold; first, to present a systematic approximation scheme which links these two approximations and, second, to relate the eikonal approximation to a classical particle picture approximation (in contrast to the traditional wave picture).

To relate the eikonal and sudden approximations systematically it is convenient to review some formal scattering results and to define distorted collision operators. This is done in § 2. In particular, scattering wavefunctions $\Psi(t)$ are usually defined (Newton 1966, Levine 1969, Child 1974) by equating them in norm to the free wavefunctions $\phi(t)$ in the distant past or future:

$$\|\Psi(t)-\phi(t)\| \xrightarrow[t\to\mp\infty]{} 0. \tag{1.1}$$

These conditions define Møller operators from which transition and scattering operators are obtained. Distorted operators (Levine 1969, Child 1974), also, have occasionally been considered. Here, formal distorted scattering conditions are presented which *define* these distorted operators. From these formal definitions, some properties of the distorted operators are obtained together with their relationship to the usual operators. Time integral representations are used rather than the usual energy

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parametrisation. An advantage of this is that it avoids the formal necessity of introducing convergence factors.

The scattering condition, equation (1.1), is not a unique prescription because any reference scattering wavefunction, $\phi_0(t)$, can be used in place of $\phi(t)$. Such a reference wavefunction requires a distorted scattering condition, namely

$$\|\Psi(t) - P_c(H_0)\phi_0(t)\| \xrightarrow[t\to\mp\infty]{} 0. \tag{1.2}$$

Here, $P_c(H_0)$ is the projection onto the continuum eigenstates of the reference Hamiltonian H_0. The inclusion of this projection ensures that the reference wavefunction $\phi_0(t)$ is indeed a scattering wavefunction, for, in general, H_0 may have bound states. Equation (1.2) defines distorted Møller operators from which distorted transition and distorted scattering operators can be obtained.

Scattering information, such as the cross section, can be extracted directly from the distorted operators and the (known) reference scattering wavefunction $\phi_0(t)$. On the other hand, the reference scattering wavefunction can be related to the free wavefunctions by reference operators. In this way, the usual operators can be connected with products of distorted and reference operators.

Two standard procedures for obtaining the eikonal approximation exist. In one of these (see, for example, Schiff 1968), the position representation of the wavefunction is written approximately as the exponential of a function involving a path integral of the potential. In the other procedure (see, for example, Joachain and Quigg 1974), the wavefunction is written in terms of the free Green function. A high-energy approximation to this Green function then leads to the eikonal wavefunction.

Rather than using one of these procedures, a different technique for obtaining the eikonal approximation is presented in § 3. It has the advantage of being readily related to the sudden approximation without need of expansions in any basis set. The procedure begins with the Møller (or scattering) operator written in terms of the motion group for the interaction picture wavefunction. This group involves a nonlocal potential that depends upon time through a straight-line trajectory. This potential is localised in position space by partially randomising the initial conditions of the trajectory (Turner and Dahler 1980). The eikonal Møller (or scattering) operators produced in this way are, themselves, local in position space. Furthermore, these operators depend parametrically on the average of the incident free momentum which occurs also in the associated eikonal wavefunction.

In § 2 a formal prescription has been given for defining distorted collision operators. Then, in § 3, it is shown how one can proceed from the distorted Møller (or scattering) operator to the corresponding classical trajectory distorted eikonal approximation. The usual Møller operator is the product of the distorted Møller operator and a reference Møller operator; a similar result holds for the scattering operator. Making eikonal approximations to both the distorted and reference operators defines a double eikonal approximation for the usual collisional operators. This double eikonal approximation is compared with the distorted eikonal approximation of McCann and Flannery (1975).

For comparison with the sudden approximation (Pack 1972, Stallcop 1974, Kramer and Bernstein 1964), an internal degree of freedom is introduced in § 4. This leads to the multichannel eikonal approximations of McCann and Flannery (1975) for both rectilinear and curved trajectories. Although local in translational position space, the eikonal approximations still couple the translational and internal motions. These motions can be decoupled by completely randomising the initial conditions of the trajectories involved in the potentials (Turner and Dahler 1980). When this randomisation is performed, the sudden approximations result. In the standard derivations of the sudden approximation (see, for example, Stallcop 1974, Goldflam *et al* 1977), this decoupling of the internal and translational motions is made in one fell swoop. Here, it is shown that by resolving the decoupling into two successive steps, one obtains the eikonal approximation for the intermediate stage.

The eikonal approximation was first introduced in geometric optics as an approximation to the classical wave equation (for a review, see, for example, Goldstein 1950, Born and Wolf 1959). This wave concept was then applied (Molière 1947, Schiff 1956, Glauber 1959) as an approximation to the continuum wavefunctions in the quantum description of particle scattering events. Here, in § 5, the eikonal approximation is applied to the scattering density operator through the Møller super-operator, a scheme which is equivalent to the usual eikonal wavefunction approximation. In the limit of small h, the classical eikonal Møller super-operator is obtained. It provides a classical (phase-point to phase-point) particle picture of the eikonal approximation.

Through the use of observables and statistical states (Turner 1978) scattering information such as generalised cross sections can be expressed in a formalism that is valid for both classical and quantum mechanics. This has the advantage that the effects of approximation schemes on both mechanics can be compared easily. Such a scheme is the eikonal approximation. Statistical scattering states (density operators and distribution functions) are related to free incoming statistical states by the Møller super-operator (Snider and Sanctuary 1971, Miles and Dahler 1970). Following the method used in § 3 to obtain the eikonal Møller operator, the eikonal Møller super-operator is obtained. This definition is independent of the mechanics which is used in the formal description. Of course, explicit evaluations using this approximation will be different in each mechanics. In particular, the quantal eikonal Møller super-operator is presented in a phase-space representation. The phase-space representation used is the Weyl (1927) correspondence (Wigner (1932) equivalence representation). Using the relation between the Møller super-operator and the Møller operator which has been established previously by Jauch *et al* (1968) and Turner (1977), this eikonal Møller super-operator is shown to be equivalent to the eikonal Møller operator. The classical limit of this eikonal Møller super-operator is presented. Finally, the phase-space representation of the classical eikonal Møller super-operator is obtained directly from the general definition. It is equal to the classical limit of the quantal eikonal Møller super-operator as dictated by the correspondence principle. This classical eikonal Møller super-operator gives a phase-point to phase-point particle description of the eikonal approximation.

2. Distorted operators

2.1. Standard operators

Binary collisions are considered. The Hamiltonian, H, is written as the sum of the kinetic energy K and a potential V. Associated with the Hamiltonian H is the wavefunction $\Psi(t)$ which satisfies the Schrödinger equation

$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = H|\Psi(t)\rangle. \tag{2.1}$$

In order to identify $\Psi(t)$ as a scattering wavefunction (see, for example, Newton 1966, Levine 1969), its norm is set equal in the distant past to that of the *incoming* free wavefunction,

$$|\phi_{\rm in}(t)\rangle = \exp[-{\rm i}K(t-t')/\hbar]|\phi_{\rm in}(t')\rangle. \tag{2.2}$$

The scattering condition, equation (1.1), becomes

$$\|\Psi(t)-\phi_{\rm in}(t)\| \xrightarrow[t\to-\infty]{} 0. \tag{2.3}$$

This prior condition defines the Møller operator $\Omega^{(+)}$,

$$\Omega^{(+)} = \lim_{t\to-\infty} \exp({\rm i}Ht/\hbar)\exp(-{\rm i}Kt/\hbar) = 1-({\rm i}/\hbar)\int_{-\infty}^{0} {\rm d}s\, \exp({\rm i}Hs/\hbar)V\exp(-{\rm i}Ks/\hbar), \tag{2.4}$$

where the last form is the time integral of a Lippmann–Schwinger equation. Making use of the identity

$$\exp({\rm i}Hs/\hbar) = \exp({\rm i}Ks/\hbar) + ({\rm i}/\hbar)\int_0^s {\rm d}t\, \exp({\rm i}Kt/\hbar)V\exp(-{\rm i}H(t-s)/\hbar), \tag{2.5}$$

equation (2.4) becomes

$$\Omega^{(+)} = 1-({\rm i}/\hbar)\int_{-\infty}^{0} {\rm d}s\, \exp({\rm i}Ks/\hbar)t_{\rm op}\exp(-{\rm i}Ks/\hbar) \tag{2.6}$$

where $t_{\rm op} = V\Omega^{(+)}$ is the transition operator. Furthermore, the scattering state wavefunction $\Psi(t)$ is given by

$$|\Psi(t)\rangle = \Omega^{(+)}|\phi_{\rm in}(t)\rangle, \tag{2.7}$$

in terms of the Møller operator $\Omega^{(+)}$ and the incoming free wavefunction, $\phi_{\rm in}(t)$.

The Møller operator $\Omega^{(+)}$ connects the incoming free wavefunction $\phi_{\rm in}(t)$, equation (2.2), with the complete wavefunction $\Psi(t)$ at all times t. For times in the distant future, the particles will be described by an *outgoing* free wavefunction $\phi_{\rm out}(t)$, provided that no capture states are available (a capture state is one which is free in the distant past, but bound in the distant future). For purposes of defining a scattering operator, Hamiltonians with capture states (see, for example, Taylor 1972) are excluded from the following discussion.

The outgoing free wavefunction $\phi_{\rm out}(t)$ provides an alternative means of characterising $\Psi(t)$ as a scattering wavefunction. In particular, the norm of the wavefunction $\Psi(t)$ is required to equal that of $\phi_{\rm out}(t)$ in the distant *future*, i.e.

$$\|\Psi(t)-\phi_{\rm out}(t)\| \xrightarrow[t\to\infty]{} 0, \tag{2.8}$$

in contrast to equation (2.3). This condition defines the post Møller operator $\Omega^{(-)}$:

$$\begin{aligned}\Omega^{(-)} &\equiv \lim_{t\to+\infty} \exp({\rm i}Ht/\hbar)\exp(-{\rm i}Kt/\hbar) = 1+({\rm i}/\hbar)\int_0^{\infty} {\rm d}s\, \exp({\rm i}Hs/\hbar)V\exp(-{\rm i}Ks/\hbar)\\ &= 1+({\rm i}/\hbar)\int_0^{\infty} {\rm d}s\, \exp({\rm i}Ks/\hbar)V\Omega^{(-)}\exp(-{\rm i}Ks/\hbar).\end{aligned} \tag{2.9}$$

The last two forms of equation (2.9) are the time integral representations of the usual Lippmann–Schwinger equations (see, for example, Levine 1969). Thus the scattered wavefunction, $\Psi(t)$, can be written in terms of the Møller operator $\Omega^{(-)}$ and the outgoing free wavefunction $\phi_{\rm out}(t)$; in particular,

$$|\Psi(t)\rangle = \Omega^{(-)}|\phi_{\rm out}(t)\rangle. \tag{2.10}$$

Møller operators are partial isometries (see, for example, Newton 1966), as exemplified by their properties,

$$\Omega^{(\pm)\dagger}\Omega^{(\pm)} = 1 \qquad \Omega^{(\pm)}\Omega^{(\pm)\dagger} = P_{\rm c}(H), \tag{2.11}$$

where $P_{\rm c}(H)$ is a projection onto the continuum eigenstates of H.

Combining equations (2.10) and (2.7) while using the partial isometries of the Møller operators, the free outgoing and free incoming wavefunctions are connected through the scattering operator

$$S \equiv \Omega^{(-)\dagger}\Omega^{(+)} \tag{2.12}$$

by the equation

$$|\phi_{\rm out}(t)\rangle = S|\phi_{\rm in}(t)\rangle. \tag{2.13}$$

Using the isometry of the Møller operators, the scattering operator is found to be unitary (see, for example, Levine 1966). The scattering operator can also be written in terms of the transition operator when the integral forms of the Møller operators are used. In particular, it becomes

$$\begin{aligned} S = \Omega^{(-)\dagger}\Omega^{(+)} &= \left(1 - ({\rm i}/\hbar)\int_0^\infty {\rm d}s\, \exp({\rm i}Ks/\hbar)\, V \exp(-{\rm i}Hs/\hbar)\right)\Omega^{(+)} \\ &= \Omega^{(+)} - ({\rm i}/\hbar)\int_0^\infty {\rm d}s\, \exp({\rm i}Ks/\hbar)\, V\Omega^{(+)} \exp(-{\rm i}Ks/\hbar) \\ &= 1 - ({\rm i}/\hbar)\int_{-\infty}^\infty {\rm d}s\, \exp({\rm i}Ks/\hbar) t_{\rm op} \exp(-{\rm i}Ks/\hbar), \end{aligned} \tag{2.14}$$

where use has been made of the intertwining relation (see appendix 1).

So far the dynamics has been presented in the Schrödinger picture. An alternative procedure is to use an interaction picture. To define the interaction picture, the potential, V, is written as the sum of a reference potential, V_0, and a potential V_1. The reference Hamiltonian is defined as the sum $H_0 = K + V_0$ while the complete Hamiltonian becomes $H = H_0 + V_1$. The interaction picture wavefunction is then defined by

$$|\psi(t)\rangle = \exp({\rm i}H_0 t/\hbar)|\Psi(t)\rangle \tag{2.15}$$

and satisfies the wave equation

$${\rm i}\hbar \frac{\rm d}{{\rm d}t}|\psi(t)\rangle = V_1^{H_0}(t)|\psi(t)\rangle. \tag{2.16}$$

The motion of this interaction picture wavefunction is generated by the time-dependent potential

$$V_1^{H_0}(t) = \exp({\rm i}H_0 t/\hbar)\, V_1 \exp(-{\rm i}H_0 t/\hbar) = \exp({\rm i}\mathscr{L}_0 t)\, V_1 \tag{2.17}$$

where $\mathscr{L}_0$ is the reference Liouville or von Neumann super-operator ($\hbar^{-1}$ multiplied by the commutator with H_0).

Formal solutions of wave equations with time-dependent Hamiltonians can be written with the aid of the Dyson (1949) chronological operator T. Thus, the solution of equation (2.16) becomes

$$|\psi(t)\rangle = G_{H_0}^{V_1}(t, t')|\psi(t')\rangle \tag{2.18}$$

where the group $G_{H_0}^{V_1}(t, t')$ can be written as a time-ordered exponential,

$$G_{H_0}^{V_1}(t, t') = T \exp\left(-(\mathrm{i}/\hbar)\int_{t'}^{t} \mathrm{d}s\, V_1^{H_0}(s)\right). \tag{2.19}$$

Here, the superscript refers to the potential in the exponential while the subscript refers to the Hamiltonian associated with its motion.

Equation (2.18) is a formal solution for the interaction picture wavefunction. By inverting equation (2.15), it also provides a formal solution of the Schrödinger picture wavefunction $\Psi(t)$,

$$\begin{aligned}|\Psi(t)\rangle &= \exp(-\mathrm{i}H_0 t/\hbar)|\psi(t)\rangle = \exp(-\mathrm{i}H_0 t/\hbar)G_{H_0}^{V_1}(t, t')\exp(\mathrm{i}H_0 t'/\hbar)|\Psi(t')\rangle \\ &\equiv U_{H_0}^{V_1}(t, t')|\Psi(t')\rangle.\end{aligned} \tag{2.20}$$

The last line of equation (2.20) defines the group $U_{H_0}^{V_1}(t, t')$. Making use of equation (2.19), this group can be written as

$$U_{H_0}^{V_1}(t, t') = G_{H_0}^{V_1}(0, t'-t)\exp[\mathrm{i}H_0(t'-t)/\hbar]. \tag{2.21}$$

Using the group $U_K^V(t, t')$ instead of the exponential of the Hamiltonian in the prior and post scattering conditions, equations (2.3) and (2.8), the Møller operators, can be written as

$$\begin{aligned}\Omega^{(\pm)} &= \lim_{t\to\mp\infty} U_K^V(t, t')^{-1}\exp[-\mathrm{i}K(t-t')/\hbar] = \lim_{t\to\mp\infty} U_K^V(t', t)\exp[-\mathrm{i}K(t-t')/\hbar] \\ &= \lim_{t\to\mp\infty} G_K^V(0, t-t') = G_K^V(0, \mp\infty),\end{aligned} \tag{2.22}$$

where the group properties of $U_K^V(t, t')$ and equation (2.21) have been used. In terms of the time-ordered exponentials, these operators are (see, for example, Child 1974)

$$\Omega^{(\pm)} = T \exp\left((-\mathrm{i}/\hbar)\int_{\mp\infty}^{0} \mathrm{d}s\, V^K(s)\right) \tag{2.23}$$

where the time-dependent potential is defined by

$$\begin{aligned}V^K(s) &= \exp(\mathrm{i}\mathscr{K}s)\, V \\ &= \exp(\mathrm{i}Ks/\hbar)\, V \exp(-\mathrm{i}Ks/\hbar)\end{aligned} \tag{2.24}$$

and where $\mathscr{K}$ is the kinetic (or drift) Liouville or von Neumann super-operator ($\hbar^{-1}$ multiplied by the commutator with K). In § 3, a local (in position space) approximation to this operator is shown to be equivalent to the eikonal approximation. In terms of the group $G_K^V(t, t')$, the scattering operator is (see, for example, Child 1974)

$$S = \Omega^{(-)\dagger}\Omega^{(+)} = G_K^V(0, \infty)^\dagger G_K^V(0, -\infty) = G_K^V(\infty, 0)G_K^V(0, -\infty) = G_K^V(\infty, -\infty). \tag{2.25}$$

2.2. Distorted operators

In the standard approach the scattering condition, equation (1.1), is the crucial step. It allows the scattering wavefunction $\Psi(t)$ to be uniquely determined from a given free wavefunction $\phi(t)$. However, this is not the only initial (post) condition that can be used. In the following, the distorted initial (post) condition, equation (1.2), is used instead. Thus, rather than being set equal in norm to a free wavefunction, the norm of the wavefunction $\Psi(t)$ is equated asymptotically with that of a reference wavefunction, $\phi_0(t)$ whose time evolution is given by

$$|\phi_0(t)\rangle = \exp[-\mathrm{i}H_0(t-t')/\hbar]|\phi_0(t')\rangle. \tag{2.26}$$

The distorted scattering conditions then define prior and post *distorted* Møller operators

$$\Omega_{\mathrm{D}}^{(\pm)} \equiv \lim_{t\to\mp\infty} \exp(\mathrm{i}Ht/\hbar)\exp(-\mathrm{i}H_0t/\hbar)P_{\mathrm{c}}(H_0) \equiv \bar{\Omega}_{\mathrm{D}}^{(\pm)}P_{\mathrm{c}}(H_0)$$

$$= \left(1-(\mathrm{i}/\hbar)\int_{\mp\infty}^{0} \mathrm{d}s\, \exp(\mathrm{i}Hs/\hbar)V_1\exp(-\mathrm{i}H_0s/\hbar)\right)P_{\mathrm{c}}(H_0), \tag{2.27}$$

which are to be compared with the usual Møller operators, $\Omega^{(\pm)}$ (cf equations (2.4) and (2.9)). Making use of an identity similar to equation (2.5), namely

$$\exp(\mathrm{i}Hs/\hbar) = \exp(+\mathrm{i}H_0s/\hbar) + (\mathrm{i}/\hbar)\int_0^s \mathrm{d}t\, \exp(\mathrm{i}H_0t/\hbar)V_1\exp[-\mathrm{i}H(t-s)/\hbar], \tag{2.28}$$

the distorted Møller operator $\Omega_{\mathrm{D}}^{(+)}$ becomes

$$\Omega_{\mathrm{D}}^{(+)} = P_{\mathrm{c}}(H_0) - (\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s\, \exp(\mathrm{i}H_0s/\hbar)t_{\mathrm{D}}\exp(-\mathrm{i}H_0s/\hbar) \tag{2.29}$$

where the distorted transition operator (Levine 1969) is defined by

$$t_{\mathrm{D}} = V_1\Omega_{\mathrm{D}}^{(+)} = V_1\Omega_{\mathrm{D}}^{(+)}P_{\mathrm{c}}(H_0). \tag{2.30}$$

Similarly, the post distorted Møller operator $\Omega_{\mathrm{D}}^{(-)}$ satisfies the integral relationship

$$\Omega_{\mathrm{D}}^{(-)} = P_{\mathrm{c}}(H_0) + (\mathrm{i}/\hbar)\int_0^{\infty} \mathrm{d}s\, \exp(\mathrm{i}H_0s/\hbar)V_1\Omega_{\mathrm{D}}^{(-)}\exp(-\mathrm{i}H_0s/\hbar). \tag{2.31}$$

Equations (2.27), (2.29) and (2.31) are the time integral forms of the distorted Lippmann–Schwinger equations. In terms of the interaction picture group, $G_{H_0}^{V_1}(t, t')$, these distorted Møller operators become

$$\Omega_{\mathrm{D}}^{(\pm)} = G_{H_0}^{V_1}(0, \mp\infty)P_{\mathrm{c}}(H_0) \equiv \bar{\Omega}_{\mathrm{D}}^{(+)}P_{\mathrm{c}}(H_0). \tag{2.32}$$

The scattered wavefunction $\Psi(t)$ can be written in terms of the prior distorted Møller operator $\Omega_{\mathrm{D}}^{(+)}$ and the *incoming* reference wavefunction $\phi_0^{\mathrm{in}}(t)$,

$$|\Psi(t)\rangle = \Omega_{\mathrm{D}}^{(+)}|\phi_0^{\mathrm{in}}(t)\rangle, \tag{2.33}$$

or it can be written in terms of the post distorted Møller operator $\Omega_{\mathrm{D}}^{(-)}$ and the *outgoing* reference wavefunction $\phi_0^{\mathrm{out}}(t)$,

$$|\Psi(t)\rangle = \Omega_{\mathrm{D}}^{(-)}|\phi_0^{\mathrm{out}}(t)\rangle. \tag{2.34}$$

These distorted Møller operators are partial isometries if the Hamiltonian H_0 supports no bound states. In general, though, the products of these distorted operators and their adjoints are

$$\Omega_{\mathrm{D}}^{(\pm)\dagger}\Omega_{\mathrm{D}}^{(\pm)} = P_{\mathrm{c}}(H_0) \qquad \Omega_{\mathrm{D}}^{(\pm)}\Omega_{\mathrm{D}}^{(\pm)\dagger} = P_{\mathrm{c}}(H). \tag{2.35}$$

By combining equations (2.33) and (2.34) and using equation (2.35), the outgoing reference wavefunction can be written as

$$P_c(H_0)|\phi_0^{\text{out}}(t)\rangle = \Omega_D^{(-)\dagger}\Omega_D^{(+)}|\phi_0^{\text{in}}(t)\rangle \equiv S_D|\phi_0^{\text{in}}(t)\rangle, \tag{2.36}$$

in terms of the distorted scattering operator (Child 1974),

$$S_D \equiv \Omega_D^{(-)\dagger}\Omega_D^{(+)}, \tag{2.37}$$

and the incoming reference wavefunction $\phi_0^{\text{in}}(t)$. The projection $P_c(H_0)$ ensures $\phi_0^{\text{out}}(t)$ is a scattering (continuum) wavefunction. Using equation (2.32), the distorted scattering operator can be written in terms of the interaction picture group $G_{H_0}^{V_1}(t, t')$ as

$$S_D = P_c(H_0)G_{H_0}^{V_1}(\infty, -\infty)P_c(H_0) \equiv P_c(H_0)\bar{S}_D P_c(H_0), \tag{2.38}$$

a result which is comparable to equation (2.25) for the scattering operator S.

The use of a procedure similar to that employed in the derivation of equation (2.14) permits the distorted scattering operator S_D to be written in terms of the distorted transition operator t_D defined by equation (2.30):

$$S_D = \Omega_D^{(-)\dagger}\Omega_D^{(+)} = P_c(H_0)\left(1 - (\mathrm{i}/\hbar)\int_{-\infty}^{\infty} \mathrm{d}s\, \exp(\mathrm{i}H_0 s/\hbar) t_D \exp(-\mathrm{i}H_0 s/\hbar)\right)P_c(H_0). \tag{2.39}$$

The unitary condition for the scattering operator S is paralleled by the condition

$$S_D^\dagger S_D = S_D S_D^\dagger = P_c(H_0) \tag{2.40}$$

for the distorted scattering operator. If the Hamiltonian H_0 supports no bound states, then the distorted scattering operator is unitary.

The distorted Møller operators were defined by the distorted scattering conditions, equation (1.2). The wavefunction $\Psi(t)$ was then related to the incoming and outgoing reference wavefunctions $\phi_0^{\text{in}}(t)$ and $\phi_0^{\text{out}}(t)$, equations (2.33) and (2.34) respectively. These reference scattering wavefunctions can themselves be related to the incoming and outgoing free wavefunctions $\phi_{\text{in}}(t)$ and $\phi_{\text{out}}(t)$ through reference Møller operators $\Omega_0^{(+)}$ and $\Omega_0^{(-)}$. In particular, the incoming reference wavefunction $\phi_0^{\text{in}}(t)$ becomes

$$|\phi_0^{\text{in}}(t)\rangle = \Omega_0^{(+)}|\phi_{\text{in}}(t)\rangle, \tag{2.41}$$

while the outgoing wavefunction is

$$|\phi_0^{\text{out}}(t)\rangle = \Omega_0^{(-)}|\phi_{\text{out}}(t)\rangle. \tag{2.42}$$

From these equations it follows that

$$|\Psi(t)\rangle = \Omega_D^{(+)}\Omega_0^{(+)}|\phi_{\text{in}}(t)\rangle \tag{2.43}$$

and

$$|\Psi(t)\rangle = \Omega_D^{(-)}\Omega_0^{(-)}|\phi_{\text{out}}(t)\rangle. \tag{2.44}$$

A comparison of equations (2.7) and (2.43) reveals that the Møller operator $\Omega^{(+)}$ is the product of the distorted Møller operator $\Omega_D^{(+)}$ and the reference Møller operator $\Omega_0^{(+)}$:

$$\Omega^{(+)} = \Omega_D^{(+)}\Omega_0^{(+)} \equiv \bar{\Omega}_D^{(+)}\Omega_0. \tag{2.45}$$

An algebraic proof of this relation is given in appendix 2. In a similar manner, the post

Møller operator $\Omega^{(-)}$ can be written as the product

$$\Omega^{(-)}=\Omega_D^{(-)}\Omega_0^{(-)}\equiv\bar{\Omega}_D^{(-)}\Omega_0. \tag{2.46}$$

In terms of the interaction picture groups, these Møller operators become

$$\Omega^{(+)}=G_{H_0'}^{V_1}(0,-\infty)G_K^{V_0}(0,-\infty) \tag{2.47}$$

and

$$\Omega^{(-)}=G_{H_0'}^{V_1}(0,\infty)G_K^{V_0}(0,\infty). \tag{2.48}$$

The scattering operator S defined by equation (2.12) becomes

$$S=\Omega^{(-)\dagger}\Omega^{(+)}=\Omega_0^{(-)\dagger}\Omega_D^{(-)\dagger}\Omega_D^{(+)}\Omega_0^{(+)}=\Omega_0^{(-)\dagger}S_D\Omega_0^{(+)} \tag{2.49}$$

in terms of the reference Møller operators and the distorted scattering operator S_D. Levine (1969) has obtained a similar result. In terms of the interaction picture groups, equation (2.49) becomes

$$S=G_K^{V_0}(\infty,0)G_{H_0'}^{V_1}(\infty,-\infty)G_K^{V_0}(0,-\infty). \tag{2.50}$$

The scattering operator S was written in terms of the transition operator in equation (2.14). Now, using equation (2.39), it can be written in terms of the distorted transition operator t_D as

$$S=S_0-(\mathrm{i}/\hbar)\int_{-\infty}^{\infty}\mathrm{d}s\,\exp(\mathrm{i}Ks/\hbar)\Omega_0^{(-)\dagger}t_D\Omega_0^{(+)}\exp(-\mathrm{i}Ks/\hbar) \tag{2.51}$$

where the reference scattering operator S_0 is $S_0=\Omega_0^{(-)\dagger}\Omega_0^{(+)}$.

3. Eikonal approximations

3.1. Straight-line trajectory

The Møller operator $\Omega^{(+)}$ has been written in terms of the motion group $G_K^V(t,t')$ (see equation (2.22)). Turner and Dahler (1980) have shown that, in terms of a rectilinear trajectory, the time-dependent potential $V^K(s)$, equation (2.24), can be written *exactly* in the form

$$V^K(s)=h^{-3}\int \mathrm{d}\boldsymbol{X}\,\mathrm{d}\boldsymbol{Y}\,\mathrm{d}\boldsymbol{P}\exp[-\mathrm{i}\boldsymbol{P}.(\boldsymbol{X}-\boldsymbol{Y})/\hbar]|\boldsymbol{Y}\rangle V[\tfrac{1}{2}(\boldsymbol{X}+\boldsymbol{Y})+\boldsymbol{P}s/\mu]\langle\boldsymbol{X}|. \tag{3.1}$$

Here μ is the reduced mass. Furthermore, the scattering operator is related to the interaction picture motion group by equation (2.25).

Rather than using the exact form of the potential $V^K(s)$, equation (3.1), in the Møller or scattering operators, a local (in position space) approximation can be introduced. To localise $V^K(s)$ the momentum $\boldsymbol{P}$ in the rectilinear trajectory $[\tfrac{1}{2}(\boldsymbol{X}+\boldsymbol{Y})+\boldsymbol{P}s/\mu]$ is replaced by a constant momentum $\boldsymbol{P}''$ (Turner and Dahler 1980). The resulting localised potential is

$$V^{K,L}(s|\boldsymbol{P}'')=\int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle V(\boldsymbol{X}+\boldsymbol{P}''s/\mu)\langle\boldsymbol{X}|. \tag{3.2}$$

Using $V^{K,L}(s|\boldsymbol{P}'')$ in lieu of $V^K(s)$ in equation (2.22) defines the Møller operator

$$\begin{aligned}\Omega^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}} &\equiv T\exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\, V^{K,L}(s|\boldsymbol{P}'')\Big)\\ &= \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle T\exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\, V(\boldsymbol{X}+\boldsymbol{P}''s/\mu)\Big)\langle\boldsymbol{X}|\\ &= \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle \exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\, V(\boldsymbol{X}+\boldsymbol{P}''s/\mu)\Big)\langle\boldsymbol{X}|. \end{aligned}\tag{3.3}$$

Because the potential $V^{K,L}(s|\boldsymbol{P}'')$ is local in position, so also is the exponential occurring in $\Omega^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}}$. Here, as illustrated by the second line of equation (3.3), one encounters the time-ordered exponential of a function which is, of course, the usual exponential. Consequently, the last of the expressions in equation (3.3) is the *exact* form of the Møller operator associated with the localised potential $V^{K,L}(s|\boldsymbol{P}'')$. This operator is local in position space and is parametrised by a momentum $\boldsymbol{P}''$. The corresponding local eikonal scattering operator is

$$S(\boldsymbol{P}'')^{\mathrm{EA}} = \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle \exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{\infty}\mathrm{d}s\, V(\boldsymbol{X}+\boldsymbol{P}''s/\mu)\Big)\langle\boldsymbol{X}|. \tag{3.4}$$

A scattering wavefunction $\Psi(t)$ associated with the Hamiltonian H is given by equation (2.7) in terms of the Møller operator $\Omega^{(+)}$ and the incoming free wavefunction $\phi_{\mathrm{in}}(t)$. This incoming free wavefunction is parametrised by the average momentum, $\boldsymbol{P}'$, of the free system. A corresponding eikonal wavefunction is defined by the expression

$$|\Psi(t)^{\mathrm{EA}}_{\boldsymbol{P}'}\rangle \equiv \Omega^{(+)}(\boldsymbol{P}')^{\mathrm{EA}}|\phi_{\mathrm{in},\boldsymbol{P}'}(t)\rangle \tag{3.5}$$

where the momentum which parametrises the eikonal Møller operator is identified with the average momentum associated with the incident free motion.

In the special case that the incoming free momentum is known exactly, that is, $|\phi_{\mathrm{in},\boldsymbol{P}'}(t)\rangle = |P'\rangle$, then the eikonal wavefunction (see, for example, Schiff 1968) becomes

$$\begin{aligned}|\Psi(t)^{\mathrm{EA}}_{\boldsymbol{P}'}\rangle &= h^{-3/2}\int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle \exp\Big[(\mathrm{i}/\hbar)\Big(\boldsymbol{X}\cdot\boldsymbol{P}' - \int_{-\infty}^{0}\mathrm{d}s\, V(\boldsymbol{X}+\boldsymbol{P}'s/\mu)\Big)\Big]\\ &= h^{-3/2}\int_{-\infty}^{\infty}\mathrm{d}z\int \mathrm{d}^2\boldsymbol{B}|z,\boldsymbol{B}\rangle \exp\Big[(\mathrm{i}/\hbar)\Big(zP' - (\mu/P')\int_{-\infty}^{z}\mathrm{d}z'\, V(\boldsymbol{B}+z'\hat{\boldsymbol{P}}')\Big)\Big]\end{aligned}\tag{3.6}$$

where the position $\boldsymbol{X}$ has been written as $\boldsymbol{B}+z\hat{\boldsymbol{P}}'(\boldsymbol{B}\cdot\hat{\boldsymbol{P}}'=0)$. Similar results are obtained for the outgoing free wavefunction $\phi_{\mathrm{out}}(t)$.

From the viewpoint of the collisional operators the eikonal approximation is local in position space and is parametrised by the average incoming free momentum. Furthermore, this approximation involves the use of rectilinear trajectories. In § 3.2, the generalisation to distorted (classical) trajectories is made by means of the formal distorted operators given in § 2.2. A comparison with the distorted eikonal approximation of McCann and Flannery (1975) is also made.

3.2. *Distorted trajectory*

In § 3.1, the Hamiltonian H was written as the sum of a kinetic energy K and a potential energy V. Now, the potential energy is split into a reference potential V_0 and the remainder V_1. Associated with this form of the Hamiltonian is the distorted Møller operator, equation (2.32), and the distorted scattering operator, equation (2.38). These operators involve the time-dependent potential $V_1^{H_0}(t)$, equation (2.17). Turner and Dahler (1980) have obtained the operator

$$V_1(s)^{\mathrm{CTA}} = h^{-3}\int \mathrm{d}\boldsymbol{X}\int \mathrm{d}\boldsymbol{Y}\,\mathrm{d}\boldsymbol{P}\exp[-\mathrm{i}(\boldsymbol{X}-\boldsymbol{Y})\,.\,\boldsymbol{P}/\hbar]|\boldsymbol{Y}\rangle V_1[\boldsymbol{R}_0(s|\tfrac{1}{2}(\boldsymbol{X}+\boldsymbol{Y}),\boldsymbol{P})]\langle\boldsymbol{X}|, \tag{3.7}$$

which is the correspondence principle analogue of the classical observable $\exp(\mathrm{i}\mathscr{L}_{0,\mathrm{CM}}s)V_1$. Here $\boldsymbol{R}_0(s|\frac{1}{2}(\boldsymbol{X}+\boldsymbol{Y}),\boldsymbol{P})$ is a classical trajectory in configuration space which satisfies the initial condition $(\frac{1}{2}(\boldsymbol{X}+\boldsymbol{Y}),\boldsymbol{P})$ and is generated by the classical reference Liouville super-operator $\mathscr{L}_{0,\mathrm{CM}}$ (Poisson bracket with the reference Hamiltonian H_0). The operator $V_1(s)^{\mathrm{CTA}}$ is the classical trajectory limit of $V_1^{H_0}(s)$. It is a nonlocal operator which depends upon time through the *uniquely* determined classical position trajectory $\boldsymbol{R}_0(s|\frac{1}{2}(\boldsymbol{X}+\boldsymbol{Y}),\boldsymbol{P})$.

As with the straight-line situation (cf equation (3.1)), it is possible to localise the operator $V_1(s)^{\mathrm{CTA}}$ by randomising the initial momentum $\boldsymbol{P}$. The distorted analogue of the localised potential $V^{K,L}(s|\boldsymbol{P}'')$ is then

$$V_1(s|\boldsymbol{P}'')^{\mathrm{CTA,L}} = \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle V_1[\boldsymbol{R}_0(s|\boldsymbol{X},\boldsymbol{P}'')]\langle\boldsymbol{X}|. \tag{3.8}$$

Using the local potential $V_1(s|\boldsymbol{P}'')^{\mathrm{CTA,L}}$ in equation (2.32), the (classical trajectory) eikonal distorted Møller operator becomes

$$\begin{aligned}\Omega_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}} &= \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle\exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\,V_1[\boldsymbol{R}_0(s|\boldsymbol{X},\boldsymbol{P}'')]\Big)\langle\boldsymbol{X}|P_{\mathrm{c}}(H_0)\\ &\equiv \tilde{\Omega}_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}}P_{\mathrm{c}}(H_0).\end{aligned} \tag{3.9}$$

Also, the (classical trajectory) eikonal distorted scattering operator is

$$\begin{aligned}S_{\mathrm{D}}(\boldsymbol{P}'')^{\mathrm{EA}} &= \int \mathrm{d}\boldsymbol{X}\,P_{\mathrm{c}}(H_0)|\boldsymbol{X}\rangle\exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{\infty}\mathrm{d}s\,V_1[\boldsymbol{R}_0(s|\boldsymbol{X},\boldsymbol{P}'')]\Big)\langle\boldsymbol{X}|P_{\mathrm{c}}(H_0)\\ &\equiv P_{\mathrm{c}}(H_0)\tilde{S}_{\mathrm{D}}(\boldsymbol{P}'')^{\mathrm{EA}}P_{\mathrm{c}}(H_0).\end{aligned} \tag{3.10}$$

Scattering wavefunctions $\Psi(t)$ are related to the distorted Møller operator and the incoming reference wavefunction $\phi_0^{\mathrm{in}}(t)$ by equation (2.33). As with the free incoming wavefunction $\phi_{\mathrm{in}}(t)$, there is an average momentum $\boldsymbol{P}'$ associated with the initial reference wavefunction $\phi_0^{\mathrm{in}}(t')$. However, unlike the free situation, the average reference momentum is not a constant in time. For purposes of defining a distorted eikonal wavefunction the momentum $\boldsymbol{P}''$ which parametrises $\Omega_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}}$ is taken to be the given initial $(t=t')$ average reference momentum $\boldsymbol{P}'$. The distorted eikonal wavefunction is then

$$\begin{aligned}|\Psi(t)_{\boldsymbol{P}'}^{\mathrm{DEA}}\rangle &= \Omega_{\mathrm{D}}^{(+)}(\boldsymbol{P}')^{\mathrm{EA}}|\phi_{0,\boldsymbol{P}'}^{\mathrm{in}}(t)\rangle\\ &= \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle\exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\,V_1[\boldsymbol{R}_0(s|\boldsymbol{X},\boldsymbol{P}')]\Big)\phi_{0,\boldsymbol{P}'}^{\mathrm{in}}(\boldsymbol{X}|t)\end{aligned} \tag{3.11}$$

where the incoming reference wavefunction has been assumed to be a scattering state. A similar result links the outgoing reference eikonal wavefunction, the distorted eikonal scattering operator and the incoming reference wavefunction.

Rather than dealing explicitly with the reference wavefunctions, a return to the free incoming and outgoing wavefunctions can be made through the reference Møller operators $\Omega_0^{(+)}$ and $\Omega_0^{(-)}$. In particular, the Møller operator $\Omega^{(+)}$ is given by the product of the distorted Møller operator and the reference Møller operator, equation (2.45). A double eikonal approximation to the Møller operator $\Omega^{(+)}$ is now defined by using eikonal approximations to both operators in equation (2.45). The result of this is the operator

$$\Omega^{(+)}(\boldsymbol{P}'')^{\mathrm{DEA}} \equiv \bar{\Omega}_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}}\Omega_0^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}}$$
$$= \int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle \exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s[V_1[\boldsymbol{R}_0(s|\boldsymbol{X}, \boldsymbol{P}'')] + V_0(\boldsymbol{X}+\boldsymbol{P}''s/\mu)]\Big)\langle\boldsymbol{X}|, \tag{3.12}$$

where only one constant momentum $\boldsymbol{P}''$ has been used to parametrise the eikonal Møller operators. It is, of course, possible to parametrise each operator with a different value of the momentum. As with the eikonal Møller operator, equation (3.3), the double eikonal Møller operator is local in position.

The double eikonal wavefunction

$$|\Psi(t)_{\boldsymbol{P}'}^{\mathrm{DDEA}}\rangle = \Omega^{(+)}(\boldsymbol{P}')^{\mathrm{DEA}}|\phi_{\mathrm{in},\boldsymbol{P}'}(t)\rangle \tag{3.13}$$

is obtained by using equation (3.12) in equation (2.7). If the free incoming wavefunction $|\phi_{\mathrm{in},\boldsymbol{P}'}(t)\rangle$ is given by $|\boldsymbol{P}'\rangle$, then the double eikonal wavefunction becomes

$$|\Psi(t)_{\boldsymbol{P}'}^{\mathrm{DDEA}}\rangle = h^{-3/2}\int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle \exp\Big[(\mathrm{i}/\hbar)\Big(\boldsymbol{X}\cdot\boldsymbol{P}' - \int_{-\infty}^{0} \mathrm{d}s\, V_1[\boldsymbol{R}_0(s|\boldsymbol{X}, \boldsymbol{P}')]$$
$$- \int_{-\infty}^{0} \mathrm{d}s\, V_0(\boldsymbol{X}+\boldsymbol{P}'s/\mu)\Big)\Big], \tag{3.14}$$

cf equation (3.6). In contrast to this double eikonal approximation, the distorted eikonal approximation of McCann and Flannery (1975) is defined by

$$\Omega^{(+)}(\boldsymbol{P}'')^{\mathrm{MF}} = \bar{\Omega}_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}}. \tag{3.15}$$

It corresponds to dropping the reference potential term in equation (3.14) or, equivalently, to replacing the incoming reference wavefunction $\phi_{0,\boldsymbol{P}'}^{\mathrm{in}}(t)$ with the incoming free wavefunction $\phi_{\mathrm{in},\boldsymbol{P}'}(t)$ in equation (3.11).

In the following section an internal degree of freedom is introduced to give the multichannel eikonal approximations of McCann and Flannery (1975). The approximation scheme is completed by decoupling the internal and translational motions. This decoupling is accomplished by completely randomising the initial conditions of the trajectories. The resulting decoupled approximations define the class of sudden approximations.

4. Multichannel eikonal and sudden approximations

An internal degree of freedom is now added to the system. The Hamiltonian H becomes the sum of the isolated internal Hamiltonian H_{int}, the reference Hamiltonian H_0 and the potential V_1. For convenience, H_0 and H_{int} are assumed to commute so that the potential V_1 is responsible for the coupling between the translational and internal motions. Thus, V_1 is an operator on both the translational and internal motions. The group $G_{V_1}^{H_0}(t, t')$ is replaced by the group $G_{U_1}^{H_0}(t, t')$ which involves the potential

$$U_1^{H_0}(s; s) = \exp(\mathrm{i}\mathscr{L}_{\mathrm{int}}s)\, V_1^{H_0}(s) = \exp(\mathrm{i}H_{\mathrm{int}}s/\hbar)\, V_1^{H_0}(s) \exp(-\mathrm{i}H_{\mathrm{int}}s/\hbar) \tag{4.1}$$

where $\mathscr{L}_{\mathrm{int}}$ is the isolated internal Liouville or von Neumann super-operator ($\hbar^{-1}$ multiplied by the commutator with H_{int}). Reference operators such as $\Omega_0^{(+)}$ act only on the translational motion.

4.1. *Straight-line approximations*

When the reference potential V_0 is zero, the Møller operator $\Omega^{(+)}$ becomes

$$\Omega^{(+)} = T \exp\left(-(\mathrm{i}/\hbar) \int_{-\infty}^{0} \mathrm{d}s\, U_1^K(s; s)\right), \tag{4.2}$$

while the multichannel eikonal Møller operator equivalent to the results of McCann and Flannery (1975) becomes

$$\Omega^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}} = T \int \mathrm{d}\boldsymbol{X} |\boldsymbol{X}\rangle \exp\left(-(\mathrm{i}/\hbar) \int_{-\infty}^{0} \mathrm{d}s\, U_1(\boldsymbol{X} + \boldsymbol{P}''s/\mu; s)\right)\langle \boldsymbol{X}|. \tag{4.3}$$

Equation (4.3) was obtained from equation (3.1) by replacing $V_1(\boldsymbol{X} + \boldsymbol{P}''s/\mu)$ with $U_1(\boldsymbol{X} + \boldsymbol{P}''s/\mu; s) = \exp(\mathrm{i}\mathscr{L}_{\mathrm{int}}s)\, V_1(\boldsymbol{X} + \boldsymbol{P}''s/\mu)$. Unlike the translational situation, summarised by equations (3.3) and (3.4), $U_1(\boldsymbol{X} + \boldsymbol{P}''s/\mu; s)$ is an operator on internal states and, thus, the time-ordered exponential is not equal to the time-disordered exponential. The multichannel eikonal approximation, equation (4.3), is a local (in position space) translational operator and, in general, a nonlocal internal operator. In a similar manner, the multichannel eikonal scattering operator is

$$S(\boldsymbol{P}'')^{\mathrm{EA}} = T \int \mathrm{d}\boldsymbol{X} |\boldsymbol{X}\rangle \exp\left(-(\mathrm{i}/\hbar) \int_{-\infty}^{\infty} \mathrm{d}s\, U_1(\boldsymbol{X} + \boldsymbol{P}''s/\mu; s)\right)\langle \boldsymbol{X}|. \tag{4.4}$$

To borrow the terminology of the sudden approximation theory (see, for example, Pack 1972), infinite and first-order multichannel eikonal approximations can be defined depending upon the treatment of the internal motion.

The translational and internal spaces are, of course, decoupled in the incoming free wavefunction. A further approximation to the eikonal Møller (or scattering) operator which decouples the interacting motion can be made. This decoupling is obtained by randomising the position $\boldsymbol{X}$ in the trajectory $(\boldsymbol{X} + \boldsymbol{P}''s/\mu)$ (Turner and Dahler 1980). A reasonable and standard choice (see, for example, Levine 1969) for this position is the initial impact parameter $\boldsymbol{B}$. Making this substitution, the multichannel eikonal Møller operator reduces to

$$\begin{aligned} \Omega^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}} &\simeq T \int \mathrm{d}\boldsymbol{X} |\boldsymbol{X}\rangle\langle \boldsymbol{X}| \exp\left(-(\mathrm{i}/\hbar) \int_{-\infty}^{0} \mathrm{d}s\, U_1(\boldsymbol{B} + \boldsymbol{P}''s/\mu; s)\right) \\ &\equiv 1_{\mathrm{tr}}\Omega^{(+)}(\boldsymbol{B}, \boldsymbol{P}'')^{\mathrm{SA}}, \end{aligned} \tag{4.5}$$

which is the product between the unit operator on the translational space, 1_{tr}, and the general *sudden* Møller operator

$$\Omega^{(+)}(\boldsymbol{B}, \boldsymbol{P}'')^{\mathrm{SA}} = T \exp\left((-\mathrm{i}/\hbar) \int_{-\infty}^{0} \mathrm{d}s\, U_1(\boldsymbol{B} + \boldsymbol{P}''s/\mu; s)\right). \tag{4.6}$$

In a similar manner, the multichannel eikonal scattering operator reduces to

$$S(\boldsymbol{P}'')^{\mathrm{EA}} \simeq 1_{\mathrm{tr}}\, S(\boldsymbol{B}, \boldsymbol{P}'')^{\mathrm{SA}}, \tag{4.7}$$

in terms of the general *sudden* scattering operator (see, for example, Stallcop 1974)

$$S(\boldsymbol{B}, \boldsymbol{P}'')^{\mathrm{SA}} = T \exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{\infty} \mathrm{d}s\, U_1(\boldsymbol{B}+\boldsymbol{P}''s/\mu\,;\, s)\Big). \tag{4.8}$$

Generally, sudden approximations are either defined as the time-disordered exponentials (first-order Magnus approximations) or they are defined according to the treatment of the internal motion. Here, it is noted that the crucial step is the decoupling of the internal and translational motions irrespective of the time ordering or the treatment of the internal states.

These sudden operators act on the internal space only and are parametrised by a given but not unique straight-line translational trajectory. In the standard derivation of the sudden operators the randomisation of the initial conditions of the trajectory is done in one step. Here, it has been seen that a two-step procedure of randomisation gives the eikonal operators as intermediates between the exact and sudden cases.

Since the eikonal operators reduce to products of translational and internal operators in the sudden limit, the resulting wavefunctions become tensor products of the translational and internal wavefunctions. In particular, the sudden scattering wavefunction is

$$|\Psi(t)^{\mathrm{SA}}\rangle = |\phi_{\mathrm{in},\boldsymbol{P}'}(t)\rangle \otimes \Omega^{(+)}(\boldsymbol{B}, \boldsymbol{P}')^{\mathrm{SA}} |\phi^{\mathrm{in}}_{\mathrm{int}}(t)\rangle. \tag{4.9}$$

Similar results are obtained for the sudden outgoing free wavefunction. In the straight-line trajectory case the sudden approximation treats the translational motion as if it were free motion. The internal motion is then parametrised by a straight-line trajectory.

4.2. *Distorted approximations*

Distorted multichannel eikonal Møller and scattering operators can be obtained in a manner similar to the straight-line results. Thus, in terms of the classical reference (configuration space) trajectory $\boldsymbol{R}_0(s|\boldsymbol{X}, \boldsymbol{P}'')$, these operators can be written as

$$\Omega_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}} = T\int \mathrm{d}\boldsymbol{X}|\boldsymbol{X}\rangle \exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s\, U_1(\boldsymbol{R}_0(s|\boldsymbol{X}, \boldsymbol{P}'');\, s)\Big)\langle \boldsymbol{X}|P_{\mathrm{c}}(H_0) \tag{4.10}$$

and

$$S_{\mathrm{D}}(\boldsymbol{P}'')^{\mathrm{EA}} = T\int \mathrm{d}\boldsymbol{X}\, P_{\mathrm{c}}(H_0)|\boldsymbol{X}\rangle \exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{\infty} \mathrm{d}s\, U_1(\boldsymbol{R}_0(s|\boldsymbol{X}, \boldsymbol{P}'');\, s)\Big)\langle \boldsymbol{X}|P_{\mathrm{c}}(H_0) \tag{4.11}$$

respectively. Double multichannel eikonal and distorted multichannel eikonal (McCann and Flannery 1975) approximations follow from these in a straightforward manner.

As with the straight-line cases, these eikonal operators can be reduced to products of translational and internal operators by randomising the position $\boldsymbol{X}$ in the reference trajectory $\boldsymbol{R}_0(s|\boldsymbol{X}, \boldsymbol{P}'')$. The multichannel eikonal distorted Møller operator reduces to

$$\Omega_{\mathrm{D}}^{(+)}(\boldsymbol{P}'')^{\mathrm{EA}} \approx \Omega_{\mathrm{D}}^{(+)}(\boldsymbol{B}, \boldsymbol{P}'')^{\mathrm{SA}} P_{\mathrm{c}}(H_0), \tag{4.12}$$

while the multichannel eikonal distorted scattering operator becomes

$$S_D(\boldsymbol{P}'')^{EA} \approx S_D(\boldsymbol{B}, \boldsymbol{P}'')^{SA} P_c(H_0). \tag{4.13}$$

This factorisation is possible because the reference Hamiltonian was assumed to be a translational operator only. The sudden distorted Møller operator is

$$\Omega_D^{(+)}(\boldsymbol{B}, \boldsymbol{P}'')^{SA} = T \exp\left(-(\mathrm{i}/\hbar) \int_{-\infty}^{0} \mathrm{d}s\, U_1(\boldsymbol{R}_0(s|\boldsymbol{B}, \boldsymbol{P}''); s)\right), \tag{4.14}$$

while the usual sudden distorted scattering operator (see, for example, Levine 1969) is

$$S(\boldsymbol{B}, \boldsymbol{P}'')^{SA} = T \exp\left(-(\mathrm{i}/\hbar) \int_{-\infty}^{\infty} \mathrm{d}s\, U_1(\boldsymbol{R}_0(s|\boldsymbol{B}, \boldsymbol{P}''); s)\right). \tag{4.15}$$

The distorted sudden wavefunction

$$|\Psi(t)^{DSA}\rangle = |\phi_{0,\boldsymbol{P}'}^{in}(t)\rangle \otimes \Omega_D^{(+)}(\boldsymbol{B}, \boldsymbol{P}'')^{SA} |\phi_{int}^{in}(t)\rangle \tag{4.16}$$

is then the tensor product of the incoming *reference* wavefunction and the distorted internal wavefunction $\Omega_D^{(+)}(\boldsymbol{B}, \boldsymbol{P}'')^{SA}|\phi_{int}^{in}(t)\rangle$. The distorted sudden approximation treats the translational motion as if it were the reference motion while it parametrises the internal motion with a reference classical trajectory.

5. Eikonal super-operator approximations

5.1. General formalism

Let us return to the relative motion of two colliding structureless particles. The interacting statistical state $S(t)$ and the free incoming statistical state $s_{in}(t|\boldsymbol{p}'')$ are connected with one another by the relationship

$$S(t) = \Omega_L s_{in}(t|\boldsymbol{p}'') \tag{5.1}$$

which involves the Møller super-operator (Snider and Sanctuary 1971, Miles and Dahler 1970)

$$\Omega_L \equiv \lim_{t\to-\infty} \exp(\mathrm{i}\mathscr{L}t) \exp(-\mathrm{i}\mathscr{K}t). \tag{5.2}$$

Quantally, the statistical state $S(t)$ is the density operator $\rho(t)$. For free motion, the statistical state (density operator) $s_{in}(t|\boldsymbol{p}'')$ has motion generated by the kinetic Liouville or von Neumann super-operator $\mathscr{K}_Q$. It is parametrised by the constant average momentum $\boldsymbol{p}''$. The difference between $\mathscr{L}_Q$ and $\mathscr{K}_Q$ is the potential super-operator $\mathscr{V}_Q$. Classically the statistical state $S(t)$ is a distribution function. For convenience the classical operators on phase-space functions are termed super-operators since their quantal counterparts are super-operators. The classical free distribution function $s_{in}(t|\boldsymbol{p}'')$ has motion generated by the Liouville super-operator $\mathscr{K}_{CM}$ and is also parametrised by a fixed value of the momentum $\boldsymbol{p}''$. Again, the difference between $\mathscr{L}_{CM}$ and $\mathscr{K}_{CM}$ is the classical potential super-operator $\mathscr{V}_{CM}$.

As with the Møller operator, the Møller super-operator can be written in terms of the interaction picture group $\mathscr{G}_K^V(t, t')$, namely

$$\Omega_L = \mathscr{G}_K^V(0, -\infty) = T \exp\left(-\mathrm{i} \int_{-\infty}^{0} \mathrm{d}s\, \mathscr{V}(s)\right). \tag{5.3}$$

Here, the time-dependent potential super-operator is

$$\mathscr{V}(s) = \exp(\mathrm{i}\mathscr{H}s)\mathscr{V}\exp(-\mathrm{i}\mathscr{H}s). \tag{5.4}$$

This formulation is valid for both mechanics and is used to define the eikonal Møller super-operator. In § 3, the eikonal Møller operator was obtained by randomising the initial momentum in the straight-line trajectory associated with the group $G_K^V(t, t')$. Thus, the eikonal Møller super-operator is defined as

$$\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}} \equiv T\exp\left(-\mathrm{i}\int_{-\infty}^{0} \mathrm{d}s\, \mathscr{V}(s|\boldsymbol{p}'')\right). \tag{5.5}$$

Here the initial momentum of the straight-line trajectory associated with $\mathscr{V}(s)$ is randomised to define $\mathscr{V}(s|\boldsymbol{p}'')$. Explicit forms of these super-operators are now given for both mechanics. In particular, in § 5.2 the eikonal Møller super-operator is shown to be equivalent to the eikonal Møller operator.

Finally, the eikonal statistical state is defined as

$$S(t)^{\mathrm{EA}} \equiv \Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}} s_{\mathrm{in}}(t|\boldsymbol{p}'') \tag{5.6}$$

where the momentum $\boldsymbol{p}''$ which parametrises $\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}}$ is taken to be the average momentum of the incoming free statistical state.

5.2. *Quantal eikonal Møller super-operator*

The eikonal Møller super-operator was defined abstractly by equation (5.5). To evaluate this approximation explicitly a representation is required. Here, the Weyl (1927) correspondence (Wigner (1932) equivalence representation) is used to define a phase-space representation. In terms of the operator

$$\begin{aligned}\Delta(\boldsymbol{r}, p) &= \int \mathrm{d}\boldsymbol{R}\, \exp(-\mathrm{i}\boldsymbol{R}\cdot p/\hbar)|\boldsymbol{r} - \tfrac{1}{2}\boldsymbol{R}\rangle\langle \boldsymbol{r} + \tfrac{1}{2}\boldsymbol{R}| \\ &= \int \mathrm{d}\boldsymbol{P}\, \exp(\mathrm{i}\boldsymbol{P}\cdot \boldsymbol{r}/\hbar)|\boldsymbol{p} - \tfrac{1}{2}\boldsymbol{P}\rangle\langle \boldsymbol{p} + \tfrac{1}{2}\boldsymbol{P}|\end{aligned} \tag{5.7}$$

defined by Leaf (1968), the statistical state (density operator) $S(t)$ is represented by the Wigner function

$$\begin{aligned}F(\boldsymbol{r}, \boldsymbol{p}|t) &= {}_{\mathscr{O}}\langle\!\langle \boldsymbol{r}, \boldsymbol{p}|S(t)\rangle\!\rangle_{\mathscr{S}} \\ &= h^{-3}\,\mathrm{Tr}\,\Delta(\boldsymbol{r}, \boldsymbol{p})\rho(t)\end{aligned} \tag{5.8}$$

where $|\boldsymbol{r}, \boldsymbol{p}\rangle\!\rangle_{\mathscr{O}}$ $(= h^{-3}\Delta(\boldsymbol{r}, \boldsymbol{p}))$ is an ideal observable-space element (see, for example, Turner 1978). An observable $A(t)$ is represented by

$$a(\boldsymbol{r}, \boldsymbol{p}|t) = {}_{\mathscr{S}}\langle\!\langle \boldsymbol{r}, \boldsymbol{p}|A(t)\rangle\!\rangle_{\mathscr{O}} = \mathrm{Tr}\,\Delta(\boldsymbol{r}, \boldsymbol{p})A(t) \tag{5.9}$$

where $|\boldsymbol{r}, \boldsymbol{p}\rangle\!\rangle_{\mathscr{S}}$ $(= \Delta(\boldsymbol{r}, \boldsymbol{p}))$ is an ideal statistical-state space element. These ideal elements are complete, bi-orthonormal and define a representation, namely the Weyl correspondence.

In this phase-space representation super-operators become kernels of integral equations. For example, the von Neumann equation for the density operator

$$\mathrm{d}\rho(t)/\mathrm{d}t = -\mathrm{i}\mathscr{L}_{\mathrm{Q}}\rho(t) \tag{5.10}$$

is represented in phase space by the integro-differential equation

$$\frac{\mathrm{d}}{\mathrm{d}t}F(\boldsymbol{r},\boldsymbol{p}|t) = -\mathrm{i}\int \mathrm{d}\boldsymbol{r}'\,\mathrm{d}\boldsymbol{p}'\,{}_{\mathscr{C}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\mathscr{L}_{\mathrm{Q}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathscr{S}} F(\boldsymbol{r}',\boldsymbol{p}'|t) \tag{5.11}$$

where the phase-space representation of the super-operator $\mathscr{L}_{\mathrm{Q}}$ is

$${}_{\mathscr{C}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\mathscr{L}_{\mathrm{Q}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathscr{S}} = h^{-3}\,\mathrm{Tr}\,\Delta(\boldsymbol{r},\boldsymbol{p})\mathscr{L}_{\mathrm{Q}}\Delta(\boldsymbol{r}',\boldsymbol{p}'). \tag{5.12}$$

To obtain the phase-space representation of the quantal eikonal Møller super-operator the representation of the Liouville potential super-operator

$$\mathscr{V}_{\mathrm{Q}}(s) \equiv \exp(\mathrm{i}\mathscr{H}_{\mathrm{Q}}s)\mathscr{V}_{\mathrm{Q}}\exp(-\mathrm{i}\mathscr{H}_{\mathrm{Q}}s) = \hbar^{-1}[V(s),\ \ ]_{-} \tag{5.13}$$

is required so that the corresponding eikonal super-operator $\mathscr{V}_{\mathrm{Q}}(s|\boldsymbol{p}'')$ can be defined. In particular, the phase-space representation of $\mathscr{V}_{\mathrm{Q}}(s)$ is

$$\begin{aligned}{}_{\mathscr{C}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\mathscr{V}_{\mathrm{Q}}(s)|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathscr{S}} &= {}_{\mathscr{C}}\langle\!\langle \boldsymbol{r}+\boldsymbol{p}s/\mu,\boldsymbol{p}|\mathscr{V}_{\mathrm{Q}}|\boldsymbol{r}'+\boldsymbol{p}'s/\mu,\boldsymbol{p}'\rangle\!\rangle_{\mathscr{S}} \\ &= \pi(2/h)^4\delta(\boldsymbol{r}+\boldsymbol{p}s/\mu-\boldsymbol{r}'-\boldsymbol{p}'s/\mu)\int \mathrm{d}\boldsymbol{R}\,\exp[2\mathrm{i}\boldsymbol{R}\cdot(\boldsymbol{p}'-\boldsymbol{p})/\hbar] \\ &\quad\times(V(\boldsymbol{r}+\boldsymbol{R}+\boldsymbol{p}s/\mu)-V(\boldsymbol{r}-\boldsymbol{R}+\boldsymbol{p}s/\mu))\end{aligned} \tag{5.14}$$

in terms of the straight-line trajectories $\boldsymbol{r}+\boldsymbol{p}s/\mu$ and $\boldsymbol{r}'+\boldsymbol{p}'s/\mu$. The super-operator $\mathscr{V}_{\mathrm{Q}}(s|\boldsymbol{p}'')$ is then defined by replacing the momenta $\boldsymbol{p}$ and $\boldsymbol{p}'$ in these trajectories with the fixed momentum $\boldsymbol{p}''$, namely

$$\begin{aligned}&{}_{\mathscr{C}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\mathscr{V}_{\mathrm{Q}}(s|\boldsymbol{p}'')|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathscr{S}} \\ &\quad\equiv \pi(2/h)^4\delta(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}\boldsymbol{R}\,\exp[2\mathrm{i}\boldsymbol{R}\cdot(\boldsymbol{p}'-\boldsymbol{p})/\hbar] \\ &\quad\times(V(\boldsymbol{r}+\boldsymbol{p}''s/\mu+\boldsymbol{R})-V(\boldsymbol{r}+\boldsymbol{p}''s/\mu-\boldsymbol{R})).\end{aligned} \tag{5.15}$$

This super-operator is local in position but nonlocal in momentum. Thus, the phase-space representation of the quantal eikonal Møller super-operator, equation (5.5), is

$$\begin{aligned}&{}_{\mathscr{C}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\Omega_{\mathrm{L}}(\boldsymbol{p}'')_{\mathrm{Q}}^{\mathrm{EA}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathscr{S}} \\ &\quad= h^{-3}\delta(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}\boldsymbol{R}\,\exp[-\mathrm{i}\boldsymbol{R}\cdot(\boldsymbol{p}-\boldsymbol{p}')/\hbar] \\ &\quad\times\exp\left(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s(V(\boldsymbol{r}+\boldsymbol{p}''s/\mu+\tfrac{1}{2}\boldsymbol{R})-V(\boldsymbol{r}+\boldsymbol{p}''s/\mu-\tfrac{1}{2}\boldsymbol{R}))\right).\end{aligned} \tag{5.16}$$

It is local in position. The equivalence of this quantal eikonal Møller super-operator with the eikonal Møller operator can be obtained by using the relation (Jauch *et al* 1968, Turner 1977)

$$\Omega_{\mathrm{L,Q}}\rho = \Omega^{(+)}\rho\,\Omega^{(+)\dagger} \tag{5.17}$$

between the Møller super-operator and the Møller operator. Associated with the eikonal Møller operator, equation (3.3), is the Møller super-operator

$$\Omega'_{\mathrm{L,Q}}\rho_{\boldsymbol{p}''} = \Omega^{(+)}(\boldsymbol{p}'')^{\mathrm{EA}}\rho_{\boldsymbol{p}''}\Omega^{(+)}(\boldsymbol{p}'')^{\mathrm{EA}\dagger} \tag{5.18}$$

whose phase-space representation is

$$
\begin{aligned}
{}_{\mathcal{O}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\Omega'_{\mathrm{L,Q}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathcal{S}}
&= h^{-3}\,\mathrm{Tr}\,\Delta(\boldsymbol{r},\boldsymbol{p})\Omega^{(+)}(\boldsymbol{p}'')^{\mathrm{EA}}\Delta(\boldsymbol{r}',\boldsymbol{p}')\Omega^{(+)}(\boldsymbol{p}'')^{\mathrm{EA}\dagger}\\
&= h^{-3}\delta(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}\boldsymbol{R}\,\exp[-\mathrm{i}\boldsymbol{R}\,.\,(\boldsymbol{p}-\boldsymbol{p}')/\hbar]\\
&\quad\times\exp\Big(-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\big(V(\boldsymbol{r}+\boldsymbol{p}''s/\mu+\tfrac{1}{2}\boldsymbol{R})-V(\boldsymbol{r}+\boldsymbol{p}''s/\mu-\tfrac{1}{2}\boldsymbol{R})\big)\Big)\\
&= {}_{\mathcal{O}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}}_{\mathrm{Q}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathcal{S}},
\end{aligned}
\tag{5.19}
$$

a result which demonstrates the equivalence of $\Omega^{(+)}(\boldsymbol{p}'')^{\mathrm{EA}}$ and $\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}}_{\mathrm{Q}}$.

Equation (5.16) is the super-operator equivalent of the usual eikonal approximation of quantum scattering theory. Here, the eikonal approximation has been written in a form that readily admits a classical limit. In particular, writing $\hbar\boldsymbol{z}$ for $\boldsymbol{R}$, the quantal eikonal Møller super-operator becomes

$$
\begin{aligned}
{}_{\mathcal{O}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}}_{\mathrm{Q}}|\boldsymbol{r}'\boldsymbol{p}'\rangle\!\rangle_{\mathcal{S}}
&= (2\pi)^{-3}\delta(\boldsymbol{r}-\boldsymbol{r}')\int \mathrm{d}\boldsymbol{z}\,\exp[-\mathrm{i}\boldsymbol{z}\,.\,(\boldsymbol{p}-\boldsymbol{p}')]\\
&\quad\times\exp\Big((-\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\big(V(\boldsymbol{r}+\boldsymbol{p}''s/\mu+\hbar\boldsymbol{z}/2)-V(\boldsymbol{r}+\boldsymbol{p}''s/\mu-\hbar\boldsymbol{z}/2)\big)\Big),
\end{aligned}
\tag{5.20}
$$

where Planck's constant appears only in the potentials. Expanding the potentials in Taylor series about the trajectory gives

$$
\hbar^{-1}\big(V(\boldsymbol{r}+\boldsymbol{p}''s/\mu+\hbar\boldsymbol{z}/2)-V(\boldsymbol{r}+\boldsymbol{p}''s/\mu-\hbar\boldsymbol{z}/2)\big)=-\boldsymbol{z}\,.\,\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}''s/\mu)+\mathrm{O}(\hbar)
\tag{5.21}
$$

where $\boldsymbol{F}(\boldsymbol{r})$ is the force $-\partial V(\boldsymbol{r})/\partial\boldsymbol{r}$. The classical limit of the quantal eikonal Møller super-operator is then

$$
{}_{\mathcal{O}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}}_{\mathrm{Q}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathcal{S}}\underset{\hbar\to 0}{\approx}\delta(\boldsymbol{r}-\boldsymbol{r}')\delta\Big(\boldsymbol{p}-\boldsymbol{p}'-\int_{-\infty}^{0}\mathrm{d}s\,\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}''s/\mu)\Big).
\tag{5.22}
$$

It is local in position but the momentum is displaced by a time integral of the force evaluated with a straight-line trajectory. In the following section it is shown that this classical approximation is equivalent to the classical result obtained from direct use of the classical super-operator in equation (5.5).

5.3. Classical eikonal Møller super-operator

The classical eikonal Møller super-operator was obtained in the last section as the small-h limit of the quantal super-operator. It can also be obtained directly from equation (5.5) using the classical phase-space representation. In particular, the phase-space representation of $\mathcal{V}_{\mathrm{CM}}(s)$ is given by

$$
{}_{\mathcal{O}}\langle\!\langle \boldsymbol{r},\boldsymbol{p}|\mathcal{V}_{\mathrm{CM}}(s)|\boldsymbol{r}',\boldsymbol{p}'\rangle\!\rangle_{\mathcal{S}}=-\mathrm{i}\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}s/\mu)\,.\,\frac{\partial}{\partial\boldsymbol{p}}\delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{r}-\boldsymbol{r}')
\tag{5.23}
$$

in terms of the force $\boldsymbol{F}$. This super-operator also contains the trajectory $\boldsymbol{r}+\boldsymbol{p}s/\mu$. As with the quantal case, the super-operator $\mathscr{V}_{\mathrm{CM}}(s|\boldsymbol{p}'')$ is defined by replacing the momentum $\boldsymbol{p}$ in the trajectory with the constant momentum $\boldsymbol{p}''$, namely

$$_{\mathscr{C}}\langle\langle \boldsymbol{r},\boldsymbol{p}|\mathscr{V}_{\mathrm{CM}}(s|\boldsymbol{p}'')|\boldsymbol{r}',\boldsymbol{p}'\rangle\rangle_{\mathscr{S}} = -\mathrm{i}\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}''s/\mu)\cdot\frac{\partial}{\partial \boldsymbol{p}}\delta(\boldsymbol{p}-\boldsymbol{p}')\delta(\boldsymbol{r}-\boldsymbol{r}'). \quad (5.24)$$

It is the classical limit of $\mathscr{V}_{\mathrm{Q}}(s|\boldsymbol{p}'')$. Using equation (5.24), the classical eikonal Møller super-operator, equation (5.5), becomes

$$\begin{aligned} _{\mathscr{C}}\langle\langle \boldsymbol{r},\boldsymbol{p}|\Omega_{\mathrm{L}}(\boldsymbol{p}'')^{\mathrm{EA}}_{\mathrm{CM}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\rangle_{\mathscr{S}} &= {}_{\mathscr{C}}\left\langle\!\!\left\langle \boldsymbol{r},\boldsymbol{p}\left|\exp\left(-\mathrm{i}\int_{-\infty}^{0}\mathrm{d}s\,\mathscr{V}_{\mathrm{CM}}(s|\boldsymbol{p}^{\circ})\right)\right|\boldsymbol{r}',\boldsymbol{p}'\right\rangle\!\!\right\rangle_{\mathscr{S}} \\ &= \exp\left(-\int_{-\infty}^{0}\mathrm{d}s\,\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}''s/\mu)\cdot\frac{\partial}{\partial\boldsymbol{p}}\right)\delta(\boldsymbol{r}-\boldsymbol{r}')\delta(\boldsymbol{p}-\boldsymbol{p}') \\ &= \delta(\boldsymbol{r}-\boldsymbol{r}')\delta\left(\boldsymbol{p}-\boldsymbol{p}'-\int_{-\infty}^{0}\mathrm{d}s\,\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}''s/\mu)\right) \end{aligned} \quad (5.25)$$

where the exponential has been identified as the Taylor series.

This classical eikonal Møller super-operator can be compared with the exact classical Møller super-operator,

$$\begin{aligned} &_{\mathscr{C}}\langle\langle \boldsymbol{r},\boldsymbol{p}|\Omega_{\mathrm{L,CM}}|\boldsymbol{r}',\boldsymbol{p}'\rangle\rangle_{\mathscr{S}} \\ &\quad = \delta\left(\boldsymbol{r}-\boldsymbol{r}'-\mu^{-1}\int_{-\infty}^{0}\mathrm{d}s(\boldsymbol{p}(-\infty|\boldsymbol{r},\boldsymbol{p})-\boldsymbol{p}(s|\boldsymbol{r},\boldsymbol{p}))\right) \\ &\quad\quad \times\delta\left(\boldsymbol{p}-\boldsymbol{p}'-\int_{-\infty}^{0}\mathrm{d}s\,\boldsymbol{F}(\boldsymbol{r}(s|\boldsymbol{r},\boldsymbol{p}))\right). \end{aligned} \quad (5.26)$$

Here, $\boldsymbol{p}(s|\boldsymbol{r},\boldsymbol{p})$ and $\boldsymbol{r}(s|\boldsymbol{r},\boldsymbol{p})$ are classical trajectories (solutions of Hamilton's equations) with initial conditions $\boldsymbol{p}(0|\boldsymbol{r},\boldsymbol{p})=\boldsymbol{p}$ and $\boldsymbol{r}(0|\boldsymbol{r},\boldsymbol{p})=\boldsymbol{r}$. Physically, starting with the phase-point $(\boldsymbol{r},\boldsymbol{p})$, the motion is traced backwards along the interacting path until it is asymptotically free and then forward along a straight-line path (with momentum $\boldsymbol{p}(-\infty|\boldsymbol{r},\boldsymbol{p})$) for an equal time period until it ends at the phase-point $(\boldsymbol{r}',\boldsymbol{p}')$.

The eikonal approximation to the Møller super-operator, equation (5.25), can be obtained from the exact Møller super-operator, equation (5.26), by replacing the trajectories $\boldsymbol{r}(s|\boldsymbol{r},\boldsymbol{p})$ and $\boldsymbol{p}(s|\boldsymbol{r},\boldsymbol{p})$ with the parametrised straight-line trajectories $\boldsymbol{r}+\boldsymbol{p}''s/\mu$ and $\boldsymbol{p}''$. In this case, the position and the momentum in the Møller super-operator are treated differently. Starting at $\boldsymbol{r}$, the position is traced backward along a straight line into the distant past and then forward along the *same* straight-line path for the same time to end up at the same starting position, $\boldsymbol{r}'=\boldsymbol{r}$. Thus, the eikonal approximation treats the position as being unaffected by the presence of the scattering event. This also holds for the quantal case. On the other hand, the momentum is treated differently. Starting at $\boldsymbol{p}$, the momentum is traced backward along a curved trajectory (due to the force evaluated with the straight-line trajectory $\boldsymbol{r}+\boldsymbol{p}''s/\mu$) to the distant past and then forward with the constant momentum $\boldsymbol{p}-\int_{-\infty}^{0}\mathrm{d}s\,\boldsymbol{F}(\boldsymbol{r}+\boldsymbol{p}''s/\mu)$ to $\boldsymbol{p}'$. It is through the momentum dependence that the classical and quantal eikonal approximations differ.

6. Discussion

Distorted scattering conditions, equations (1.2), have been used to formally define previously identified (see, for example, Levine 1969, Child 1974) distorted Møller operators and, thus, distorted transition and distorted scattering operators. These operators have been written in their time-integral representations (rather than the energy-parametrised Lippmann–Schwinger forms) and have been related to the interaction picture motion group.

Some properties of the distorted operators have been discussed. For example, the distorted scattering operator S_D is, in general, not unitary (see equation (2.40)). This is a direct consequence of the fact that the distorted Møller operators are not, in general, partial isometries (see equations (2.35)). The usual Møller, transition and scattering operators have been written as products of distorted and reference operators.

A systematic approximation scheme starting with the Møller and scattering operators (written in terms of the interaction picture motion group) and leading to the eikonal and sudden approximations has been presented. In the first stage of the approximation scheme, i.e. the eikonal approximation, the collisional operators have been localised in position space. This localisation was accomplished by randomising the initial momentum of the trajectory involved in the interaction picture motion group. In the second stage of this scheme, the initial position of the trajectory was randomised. The resulting sudden operators involved decoupled translational and internal motions. Distorted as well as straight-line approximations have been considered.

The standard eikonal approximation of binary (relative) quantum collision theory has been related to the density operator approach. It has been found that the eikonal Møller super-operator is equivalent to the eikonal Møller operator and, thus, that the eikonal density operator is equivalent to the eikonal wavefunction. The classical limit of the eikonal Møller super-operator produces a phase-point to phase-point particle picture of the eikonal approximation. Straight-line eikonal approximations have been considered. Following the formal definitions of the distorted Møller operators, distorted Møller super-operators can be defined. Distorted classical and quantal eikonal Møller super-operators then follow in manner similar to the straight-line approximations presented here.

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Appendix 1

To obtain equation (2.14), which relates the scattering operator to the transition operator, the intertwining relation (Newton 1966)

$$\exp(\mathrm{i}Ht/\hbar)\Omega^{(+)} = \Omega^{(+)} \exp(\mathrm{i}Kt/\hbar) \tag{A.1}$$

was used. Here a time-integral proof of this relation is presented. Using equation (2.4) the left-hand side of equation (A.1) becomes

$$\exp(\mathrm{i}Ht/\hbar)\Omega^{(+)} = \exp(\mathrm{i}Ht/\hbar) + (-\mathrm{i}/\hbar)\int_{-\infty}^{t} \mathrm{d}s' \exp(\mathrm{i}Hs'/\hbar)\, V \exp[-\mathrm{i}K(s'-t)/\hbar]. \quad (A.2)$$

A change of variable has been performed in the second term. Making use of an identity similar to equation (2.5), namely

$$\exp(\mathrm{i}Ht/\hbar) = \exp(\mathrm{i}Kt/\hbar) - (\mathrm{i}/\hbar)\int_{t}^{0} \mathrm{d}s' \exp(\mathrm{i}Hs'/\hbar)\, V \exp[-\mathrm{i}K(s'-t)/\hbar], \quad (A.3)$$

equation (A.2) becomes

$$\begin{aligned}\exp(\mathrm{i}Ht/\hbar)\Omega^{(+)} &= \left(1 - (\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s \exp(\mathrm{i}Hs/\hbar)\, V \exp(-\mathrm{i}Ks/\hbar)\right) \exp(\mathrm{i}Kt/\hbar) \\ &= \Omega^{(+)} \exp(\mathrm{i}Kt/\hbar), \end{aligned} \quad (A.4)$$

which is equation (A.1).

Appendix 2

The Møller operator $\Omega^{(+)}$ was written in equation (2.45) as the product of the distorted Møller operator $\Omega_{\mathrm{D}}^{(+)}$ and the reference Møller operator $\Omega_0^{(+)}$. An algebraic proof of this relation is now given. Using equation (2.27) the right-hand side of equation (2.45) can be written as

$$\begin{aligned}\Omega_{\mathrm{D}}^{(+)}\Omega_0^{(+)} &= \left(1 - (\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s \exp(\mathrm{i}Hs/\hbar)\, V_1 \exp(-\mathrm{i}H_0 s/\hbar)\right) P_{\mathrm{c}}(H_0)\Omega_0^{(+)} \\ &= \Omega_0^{(+)} - (\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s \exp(\mathrm{i}Hs/\hbar)\, V_1 \Omega_0^{(+)} \exp(-\mathrm{i}Ks/\hbar) \end{aligned} \quad (A.5)$$

where the intertwining relations

$$P_{\mathrm{c}}(H_0)\Omega_0^{(+)} = \Omega_0^{(+)} P_{\mathrm{c}}(K) = \Omega_0^{(+)} \quad (A.6)$$

and

$$\exp(-\mathrm{i}H_0 s/\hbar)\Omega_0^{(+)} = \Omega_0^{(+)} \exp(-\mathrm{i}Ks/\hbar) \quad (A.7)$$

have been used. Also, the projection onto the continuum of the kinetic energy operator K has been recognised as the unit operator. Now, using the integral form

$$\Omega_0^{(+)} = 1 - (\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s' \exp(\mathrm{i}H_0 s'/\hbar)\, V_0 \exp(-\mathrm{i}Ks'/\hbar) \quad (A.8)$$

of the reference Møller operator $\Omega_0^{(+)}$, equation (A.5) can be written as

$$\begin{aligned}\Omega_{\mathrm{D}}^{(+)}\Omega_0^{(+)} &= \Omega_0^{(+)} - (\mathrm{i}/\hbar)\int_{-\infty}^{0} \mathrm{d}s \exp(\mathrm{i}Hs/\hbar)\, V_1 \exp(-\mathrm{i}Ks/\hbar) \\ &\quad + (\mathrm{i}/\hbar)^2 \int_{-\infty}^{0} \mathrm{d}s \int_{-\infty}^{0} \mathrm{d}s' \exp(\mathrm{i}Hs/\hbar)\, V_1 \exp(\mathrm{i}H_0 s'/\hbar)\, V_0 \\ &\quad \times \exp[-\mathrm{i}K(s'+s)/\hbar]. \end{aligned} \quad (A.9)$$

The time s' in the last term of equation (A.9) is now defined as $t'-s$ and the order of integration is changed. This term becomes

$$-(\mathrm{i}/\hbar)^2\int_{-\infty}^{0}\mathrm{d}t'\left(\int_0^{t'}\mathrm{d}s\,\exp(\mathrm{i}Hs/\hbar)V_1\exp(-\mathrm{i}H_0s/\hbar)\right)\exp(+\mathrm{i}H_0t'/\hbar)V_0\exp(-\mathrm{i}Kt'/\hbar)$$

$$=-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}t'[\exp(\mathrm{i}Ht'/\hbar)\exp(-\mathrm{i}H_0t'/\hbar)-1]$$
$$\times\exp(\mathrm{i}H_0t'/\hbar)V_0\exp(-\mathrm{i}Kt'/\hbar)$$
$$=-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}t'\exp(\mathrm{i}Ht'/\hbar)V_0\exp(-\mathrm{i}Kt'/\hbar)+(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}t'$$
$$\times\exp(\mathrm{i}H_0t'/\hbar)V_0\exp(-\mathrm{i}Kt'/\hbar)$$
$$=-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}t'\exp(\mathrm{i}Ht'/\hbar)V_0\exp(-\mathrm{i}Kt'/\hbar)+1-\Omega_0^{(+)}. \qquad (A.10)$$

Using equation (A.10) in equation (A.9), the right-hand side of equation (2.45) becomes

$$\Omega_D^{(+)}\Omega_0^{(+)}=1-(\mathrm{i}/\hbar)\int_{-\infty}^{0}\mathrm{d}s\,\exp(\mathrm{i}Hs/\hbar)V\exp(-\mathrm{i}Ks/\hbar)\equiv\Omega^{(+)}, \qquad (A.11)$$

which is the desired relation.

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