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The semiclassical limit of quantum dynamics II: Scattering Theory

by

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ABSTRACT. — We study the $\hbar \rightarrow 0$ limit of the quantum scattering determined by the Hamiltonian $H(\hbar) = -\frac{\hbar^2}{2m}\Delta + V$ on $L^2(\mathbb{R}^n)$ for short range potentials V . We obtain classically determined asymptotic behavior of the quantum scattering operator applied to certain states of compact support. Our main result is the extension of a theorem of Yajima to the position representation. The techniques involve convolution with Gaussian states. The error terms are shown to have L^2 norms of order $\hbar^{1/2-\varepsilon}$ for arbitrarily small positive ε .

RÉSUMÉ. — Dans cet article nous étudions la limite $\hbar \rightarrow 0$ de la diffusion quantique de l'opérateur $H(\hbar) = -\hbar^2/2m\Delta + V$ sur $L^2(\mathbb{R}^n)$ où V est un potentiel à courte portée. Nous obtenons le comportement asymptotique de l'opérateur d'onde appliqué à certains états à support compact. Notre résultat principal est une extension d'un résultat de Yajima à la représentation de position. La méthode employée consiste à faire une convolution avec un état Gaussien. Les termes de correction ont une norme L^2 qui tend vers zéro plus vite que $\hbar^{1/2-\varepsilon}$ pour tout nombre positif ε .

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1. INTRODUCTION

In this paper we study the relation between the classical and quantum descriptions of potential scattering in the semiclassical limit. We prove a theorem on the small \hbar asymptotics of the quantum scattering operator $\mathcal{A}(\hbar)$ applied to states of the form $\psi_-(x) = e^{iS_-(x)/\hbar}f(x)$ where S_- is real-valued and f is of compact support. The rigorous scattering theory in similar contexts has been studied by Yajima ([Y1], [Y2]) and Hagedorn ([Ha1]) and the semiclassical limit of the scattering cross section and scattering amplitudes have also received some rigorous attention ([ES], [SY], [Y3]). Our theorem can be viewed as the extension of the theorem of Yajima ([Y1]) to the more natural position representation, a result apparently unobtainable by Yajima's Fourier integral operator techniques. Hagedorn's results are concerned with incoming states of a certain Gaussian form and are basic to our technique. Our proof mimicks the proof of our previous result on the semiclassical time evolution ([R]).

We now introduce enough notation and definitions to allow us to state our main result. For technical reasons we must restrict our attention to dimension $n \geq 3$.

ASSUMPTION 1.1. — Suppose $V \in C^{l+2}(\mathbb{R}^n, \mathbb{R})$ for some integer $l \geq 1 + \frac{n}{2}$ and assume there exist constants C_α and $\nu > 0$ such that

$$\left| \left(\frac{\partial}{\partial x} \right)^\alpha V(x) \right| \leq C_\alpha (1 + |x|)^{-1 - |\alpha| - \nu}$$

for all multi-indices α with $|\alpha| \leq l + 2$.

For such potentials the quantum Hamiltonian $H(\hbar) = -\frac{\hbar^2}{2m}\Delta + V$ is self-adjoint on the self-adjoint domain of the free Hamiltonian $H_0(\hbar) = -\frac{\hbar^2}{2m}\Delta$ ([RS1]). It is well known ([RS2]) that for potentials satisfying Assumption 1.1 the wave operators

$$\Omega^\pm(\hbar) = s\text{-}\lim_{t \rightarrow \mp\infty} e^{itH(\hbar)/\hbar} e^{-itH_0(\hbar)/\hbar}$$

exist and are asymptotically complete ($\text{Ran}(\Omega^+(\hbar)) = \text{Ran}(\Omega^-(\hbar)) =$ the absolutely continuous spectral subspace of $L^2(\mathbb{R}^n)$ with respect to $H(\hbar)$) for each $\hbar > 0$. Moreover, the quantum mechanical scattering matrix $\mathcal{A}(\hbar) = \Omega^-(\hbar)^* \Omega^+(\hbar)$ is a unitary operator on $L^2(\mathbb{R}^n)$.

The problem of the classical scattering has been studied in some detail and the following facts can be found in or are consequences of facts found in [Ha1], [Hu], [Sie], [Sim] and [RS2]: There exists a set $\varepsilon_0 \subset \mathbb{R}^{2n}$ of

Lebesgue measure zero such that for any $(a_-, \eta_-) \in \mathbb{R}^{2n} \setminus \varepsilon_0$ there is a unique solution $(a(a_-, \eta_-, t), \eta(a_-, \eta_-, t))$ of the system

$$\frac{\partial}{\partial t} a(t) = \frac{1}{m} \eta(t) \tag{1.1 a}$$

$$\frac{\partial}{\partial t} \eta(t) = -\nabla V(a(t)) \tag{1.1 b}$$

and a unique vector $(a_+(a_-, \eta_-), \eta_+(a_-, \eta_-)) \in \mathbb{R}^{2n}$ with $\eta_+(a_-, \eta_-) \neq 0$ such that

$$\lim_{t \rightarrow -\infty} \left| a(a_-, \eta_-, t) - a_- - \frac{t}{m} \eta_- \right| = 0$$

$$\lim_{t \rightarrow -\infty} |\eta(a_-, \eta_-, t) - \eta_-| = 0$$

and

$$\lim_{t \rightarrow \infty} \left| a(a_-, \eta_-, t) - a_+(a_-, \eta_-) - \frac{t}{m} \eta_+(a_-, \eta_-) \right| = 0$$

$$\lim_{t \rightarrow \infty} |\eta(a_-, \eta_-, t) - \eta_+(a_-, \eta_-)| = 0.$$

The classical scattering matrix s_{cl} defined on $\mathbb{R}^{2n} \setminus \varepsilon_0$ by

$$s_{cl}(a_-, \eta_-) = (a_+(a_-, \eta_-), \eta_+(a_-, \eta_-))$$

is a class C^2 measure preserving map. We now state our main result.

THÉORÈME 1.2. — Suppose that the space dimension n is greater than 2 and assume V satisfies Assumption 1.1. Let $S_- \in C^3(\mathbb{R}^n, \mathbb{R})$ and let \mathcal{A} be a closed subset of \mathbb{R}^n containing the set $\{x \in \mathbb{R}^n : (x, \nabla S_-(x)) \in \varepsilon_0\}$. Suppose $f \in C_0^1(\mathbb{R}^n, \mathbb{C})$ is such that $\text{supp}(f)$ is contained in $\mathbb{R}^n \setminus \mathcal{A}$ and let $\lambda \in (0, 1/2)$. Define $Q_+ : \mathbb{R}^n \setminus \mathcal{A} \mapsto \mathbb{R}^n$ by $Q_+(q_-) = a_+(q_-, \nabla S_-(q_-))$ and assume $\det \left[\frac{\partial Q_+}{\partial q_-}(x) \right] \neq 0$ for $x \in \text{supp}(f)$. Then there exist $\delta > 0$ and a constant C independent of \hbar such that

$$\left\| s(\hbar)(e^{iS_-/\hbar} f) - \sum_j e^{i(\mu_j + S_+(x_j)/\hbar)} \cdot \left| \det \left[\frac{\partial Q_+}{\partial q_-}(x_j) \right] \right|^{-1/2} f(x_j) \right\|_2 \leq C \hbar^\lambda$$

for all $\hbar \leq \delta$. The dependence on x of the term involving the summation is implicit. For fixed x the summation is over all x_j such that $Q_+(x_j) = x$ and is finite. $S_+(x_j)$ is given by

$$S_+(x_j) = S_-(x_j) - 2 \int_{-\infty}^{\infty} V(a(x_j, \nabla S_-(x_j), \tau)) d\tau$$

and μ_j is an integer multiple of $\frac{\pi}{2}$ defined explicitly in the proof.

Remarks. — 1. The norm appearing above is of course the norm of $L^2(\mathbb{R}^n, d^n x)$.

2. Yajima ([Y1]) has shown a similar theorem using Fourier integral operator techniques as developed by Hörmander and Asada and Fujiwara. Not only do we feel that our methods are much less complicated, but Yajima's approach is restricted to the momentum representation while our methods are applicable even in mixed representations.

2. NOTATION AND DEFINITIONS

Throughout this paper n denotes the space dimension. $L^2(\mathbb{R}^n)$ is the Hilbert space of square integrable, complex valued functions on \mathbb{R}^n with the usual inner product $\langle \cdot, \cdot \rangle$ and norm $\| \cdot \|_2$. The quantum mechanical Hamiltonian $H(\hbar)$ is the operator $-\frac{\hbar^2}{2m} \Delta + V$ on $L^2(\mathbb{R}^n)$. Here, Δ is the n -dimensional Laplacian operator

$$\Delta = \left(\frac{\partial}{\partial x_1} \right)^2 + \dots + \left(\frac{\partial}{\partial x_n} \right)^2,$$

\hbar is a small positive parameter (a dimensionless multiple of Planck's constant), m is a positive constant, and V is a real valued function on \mathbb{R}^n viewed here as a multiplication operator on $L^2(\mathbb{R}^n)$. A multi-index α is an ordered n -tuple $(\alpha_1, \alpha_2, \dots, \alpha_n)$ of nonnegative integers, and we use the standard notation for the order $|\alpha|$ and the factorial $\alpha!$ of α . For

$x = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$ the symbol x^α is defined by $x^\alpha = \prod_{i=1}^n x_i^{\alpha_i}$. D^α stands for the partial differential operator

$$D^\alpha = \left(\frac{\partial}{\partial x} \right)^\alpha = \frac{\partial^{|\alpha|}}{(\partial x_1)^{\alpha_1} (\partial x_2)^{\alpha_2} \dots (\partial x_n)^{\alpha_n}}.$$

For $x \in \mathbb{R}^n$ or \mathbb{C}^n , $|x|$ denotes the Euclidean norm of x . We denote the usual inner product on \mathbb{R}^n or \mathbb{C}^n by $\langle u, v \rangle = \sum_{i=1}^n \bar{u}_i v_i$ and let $\{e_i\}_{i=1}^n$ be

the standard basis for \mathbb{R}^n or \mathbb{C}^n . For sufficiently smooth functions f , $\frac{\partial f}{\partial x}$ is the matrix $\left(\frac{\partial f_i}{\partial x_j} \right)$. We will write $f^{(1)}$ to denote the gradient of f and $f^{(2)}$ to denote the Hessian matrix $\left(\frac{\partial^2 f}{\partial x_i \partial x_j} \right)$. We will not explicitly distinguish row and column vectors in \mathbb{R}^n or \mathbb{C}^n in our computations. The symbol $\mathbb{1}$

will stand for the $n \times n$ identity matrix. For an $n \times n$ complex matrix A we will use the symbol $\|A\|$ for the norm of the matrix $A = (a_{ij})$ which

we choose to be given by $\|A\| = \sup_{1 \leq i \leq n} \left(\sum_{j=1}^n |a_{ij}|^2 \right)^{1/2}$. We will use $|A|$

to denote the matrix $(AA^*)^{1/2}$ where A^* is the adjoint (complex conjugate transpose) of A . \mathcal{U}_A will denote the unique unitary matrix guaranteed by the polar decomposition theorem such that $A = |A| \mathcal{U}_A$, $|A| = (AA^*)^{1/2}$.

Following Hagedorn ([Ha3]) we define generalized Hermite polynomials on \mathbb{R}^n recursively as follows: We set $\mathcal{H}_0(x) = 1$ and $\mathcal{H}_1(v; x) = 2 \langle v, x \rangle$ where v is an arbitrary non-zero vector in \mathbb{C}^n . For v_1, \dots, v_m arbitrary non-zero vectors in \mathbb{C}^n we set

$$\begin{aligned} \tilde{\mathcal{H}}_m(v_1, \dots, v_m; x) &= 2 \langle v_m, x \rangle \tilde{\mathcal{H}}_{m-1}(v_1, \dots, v_{m-1}; x) \\ &\quad - 2 \sum_{i=1}^{m-1} \langle v_m, \bar{v}_i \rangle \tilde{\mathcal{H}}_{m-2}(v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_{m-1}; x). \end{aligned}$$

The polynomials \mathcal{H}_m are independent of the ordering of the vectors v_1, \dots, v_m . Given a complex invertible $n \times n$ matrix A and a multi-index α we define the polynomial

$$\mathcal{H}_\alpha(A; x) = \tilde{\mathcal{H}}_{|\alpha|}(\mathcal{U}_A e_1, \dots, \mathcal{U}_A e_1, \mathcal{U}_A e_2, \dots, \mathcal{U}_A e_n; x)$$

where the vector $\mathcal{U}_A e_i$ appears α_i times in the list of variables of $\tilde{\mathcal{H}}_{|\alpha|}$.

We will find it useful to consider complex $n \times n$ matrices A and B satisfying the following conditions:

$$A \text{ and } B \text{ are invertible} \tag{2.1a}$$

$$BA^{-1} \text{ is symmetric} \tag{2.1b}$$

$$\text{Re}(BA^{-1}) \text{ is strictly positive definite} \tag{2.1c}$$

$$(\text{Re}(BA^{-1}))^{-1} = AA^* \tag{2.1d}$$

(Here, symmetric means (real symmetric) + i (real symmetric)).

For complex $n \times n$ matrices A and B satisfying conditions (2.1), vectors a and $\eta \in \mathbb{R}^n$, multi-indices α , and positive \hbar we define

$$\begin{aligned} \phi_\alpha(A, B, \hbar, a, \eta, x) &= (\pi \hbar)^{-n/4} (2^{|\alpha|} \alpha!)^{-1/2} [\det(A)]^{-1/2} \\ &\quad \cdot \mathcal{H}_\alpha(A; \hbar^{-1/2} |A|^{-1}(x - a)) \\ &\quad \cdot \exp \left\{ -\frac{1}{2\hbar} \langle (x - a), BA^{-1}(x - a) \rangle + \frac{i}{\hbar} \langle \eta, (x - a) \rangle \right\}. \end{aligned}$$

The branch of the square root of $\det(A)$ will be specified in the context in which the functions ϕ_α are used. Whenever we write $\phi_\alpha(A, B, \hbar, a, \eta, x)$ we are assuming that the matrices A and B satisfy conditions (2.1). For

fixed A, B, \hbar, a , and η the functions $\phi_a(A, B, \hbar, a, \eta, x)$ form an orthonormal basis of $L^2(\mathbb{R}^n)$. For a proof of this fact and other properties of these functions, see [Ha3]. Using Lemma 2.2 of [Ha3] we obtain

$$e^{-i\mathbf{H}_0(\hbar)/\hbar} \phi_a(A, B, \hbar, a, \eta, x) = e^{it\langle \eta, \eta \rangle / 2m\hbar} \phi_a\left(A + i\frac{t}{m}B, B, a + \frac{t}{m}\eta, \eta, x\right). \quad (2.2)$$

3. PROOF OF THE THEOREM

In this section we prove the technical details required for the proof of Theorem 1.2. We do not actually prove the theorem but argue by analogy to the proof of Theorem 1.2 of [R] once we have proved the technicalities. We first sketch the idea of our proof.

For the purpose of explaining the idea behind the proof we restrict ourselves to the case in which Q_+ is a diffeomorphism on some open ball $\mathcal{N} \supset \text{supp}(f)$. In this case the summation appearing in the statement of the theorem contains only one term. The general case is obtained by introducing a smooth partition of unity on $\text{supp}(f)$ and patching local diffeomorphisms. For brevity, we write $F(\hbar, x) = G(\hbar, x) + O(\hbar^\lambda)$ to mean that there exist positive constants δ and C independent of \hbar such that $\hbar < \delta$ implies $\|F(\hbar, \cdot) - G(\hbar, \cdot)\|_2 \leq C\hbar^\lambda$. By Lemma 3.1 of [R] we have

$$\begin{aligned} \psi_-(x) &= (2\pi\hbar)^{-n/2} \int_{\mathcal{N}} (\det [\mathbb{1} + S^{(2)}(a_-)])^{1/2} \psi_-(a_-) \\ &\quad \times \exp\left\{-\frac{1}{2\hbar}|x - a_-|^2 + \frac{i}{\hbar}\langle S^{(1)}(a_-), (x - a_-)\rangle\right\} d^n a_- + O(\hbar^\lambda). \end{aligned}$$

We then apply the scattering operator to ψ_- and pass it through the integral sign. We require a lemma contained in [H1], [H2] and [H3] on the semiclassical behavior of Gaussian states such as the exponential term in the integrand. This lemma allows us to approximate $\mathcal{A}(\hbar)\psi_-$ by a rather involved integral expression of the form

$$\begin{aligned} \mathcal{A}(\hbar)\psi_-(x) &= (2\pi\hbar)^{-n/2} \int_{\mathcal{N}} (\det [\mathbb{1} + S^{(2)}(a_-)])^{1/2} f(a_-) \\ &\quad \times \mathcal{H}(a_-, \hbar, x) \exp\left\{-\frac{1}{2\hbar}\langle (x - Q_+(a_-)), T(a_-)(x - Q_+(a_-))\rangle\right. \\ &\quad \left.+ \frac{i}{\hbar}[S(a_-) + \langle P_+(a_-), (x - Q_+(a_-))\rangle]\right\} d^n a_- + O(\hbar^\lambda) \end{aligned}$$

where $\mathcal{H}(a_-, \hbar, x)$ is a polynomial in x with coefficients depending on a_- and \hbar , $P_+(a_-) = \eta_+(a_-)$, $S^{(1)}(a_-)$, $S(a_-)$ is a real valued function related to the classical action associated with the trajectory $(a_-, S^{(1)}(a_-), t)$,

$\eta(a_-, S_-^{(1)}(a_-, t))$ and $T(a_-)$ is a complex $n \times n$ matrix valued function with rather nice properties. We then change variables from a_- to $Q_+ = Q_+(a_-)$ to obtain an integral which has a convolution structure. An estimate much like the first of the estimates in this sketch along with certain properties of the function T then yields the desired result. We now provide the details needed for the proof.

The classical scattering theory for potentials satisfying Assumption 1.1 is quite complete and the following facts are known ([Ha1], [Hu], [RS2], [Sie], [Sim]). There exists a subset $\varepsilon_0 \subset \mathbb{R}^{2n}$ of Lebesgue measure zero such that given $(a_-, \eta_-) \in \mathbb{R}^{2n} \setminus \varepsilon_0$ there is a unique solution

$$[a(a_-, \eta_-, t), \eta(a_-, \eta_-, t), A(a_-, \eta_-, t), B(a_-, \eta_-, t), S(a_-, \eta_-, t)]$$

of the system

$$\frac{\partial}{\partial t} a(t) = \frac{1}{m} \eta(t)$$

$$\frac{\partial}{\partial t} \eta(t) = -V^{(1)}(a(t))$$

$$\frac{\partial}{\partial t} A(t) = \frac{i}{m} B(t)$$

$$\frac{\partial}{\partial t} B(t) = iV^{(2)}(a(t))A(t)$$

$$\frac{\partial t}{\partial t} S(t) = \frac{1}{2m} |\eta(t)|^2 - V(a(t))$$

such that

$$\lim_{t \rightarrow -\infty} \left| a(a_-, \eta_-, t) - a_- - \frac{t}{m} \eta_- \right| = 0 \quad (3.1a)$$

$$\lim_{t \rightarrow -\infty} |\eta(a_-, \eta_-, t) - \eta_-| = 0 \quad (3.1b)$$

$$\lim_{t \rightarrow -\infty} \left\| A(a_-, \eta_-, t) - \mathbb{1} - i \frac{t}{m} \mathbb{1} \right\| = 0 \quad (3.1c)$$

$$\lim_{t \rightarrow -\infty} \|B(a_-, \eta_-, t) - \mathbb{1}\| = 0 \quad (3.1d)$$

$$\lim_{t \rightarrow -\infty} \left| S(a_-, \eta_-, t) - S_-(a_-) - \frac{t}{2m} |\eta_-|^2 \right| = 0. \quad (3.1e)$$

We note that $\{(a, \eta) \in \mathbb{R}^{2n} : \eta = 0\} \subset \varepsilon_0$. We denote the closure of ε_0 by ε .

The matrices $A(a_-, \eta_-, t)$ and $B(a_-, \eta_-, t)$ satisfy conditions (2.1) for all $t \in \mathbb{R}$. Moreover, there exist complex $n \times n$ matrices $A_+(a_-, \eta_-)$ and

$B_+(a_-, \eta_-)$, vectors $a_+(a_-, \eta_-)$ and $\eta_+(a_-, \eta_-)$ in \mathbb{R}^n with $\eta_+(a_-, \eta_-) \neq 0$, and a real number $S_+(a_-, \eta_-)$ such that

$$\lim_{t \rightarrow \infty} \left| a(a_-, \eta_-, t) - a_+(a_-, \eta_-) - \frac{t}{m} \eta_+(a_-, \eta_-) \right| = 0 \quad (3.2a)$$

$$\lim_{t \rightarrow \infty} |\eta(a_-, \eta_-, t) - \eta_+(a_-, \eta_-)| = 0 \quad (3.2b)$$

$$\lim_{t \rightarrow \infty} \left\| A(a_-, \eta_-, t) - A_+(a_-, \eta_-) - i \frac{t}{m} B_+(a_-, \eta_-) \right\| = 0 \quad (3.2c)$$

$$\lim_{t \rightarrow \infty} \| B(a_-, \eta_-, t) - B_+(a_-, \eta_-) \| = 0 \quad (3.2d)$$

$$\lim_{t \rightarrow \infty} \left| S(a_-, \eta_-, t) - S_+(a_-, \eta_-) - \frac{t}{2m} |\eta_+(a_-, \eta_-)|^2 \right| = 0. \quad (3.2e)$$

The functions a , a_+ , η , and η_+ are of class C^1 in $a_-, \eta_- \in \mathbb{R}^n \setminus \varepsilon$ and satisfy

$$a(a_-, \eta_-, t) = a_- + \frac{t}{m} \eta_- - \frac{1}{m} \int_{-\infty}^t ds \int_{-\infty}^s V^{(1)}(a(a_-, \eta_-, r)) dr \quad (3.3a)$$

$$\eta(a_-, \eta_-, t) = \eta_- - \int_{-\infty}^t V^{(1)}(a(a_-, \eta_-, s)) ds \quad (3.3b)$$

$$\frac{\partial a}{\partial a_-}(a_-, \eta_-, t) = \mathbb{1} - \frac{1}{m} \int_{-\infty}^t ds \int_{-\infty}^s V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, r) dr \quad (3.4a)$$

$$\frac{\partial a}{\partial \eta_-}(a_-, \eta_-, t) = \frac{t}{m} \mathbb{1} - \frac{1}{m} \int_{-\infty}^t ds \int_{-\infty}^s V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, r) dr \quad (3.4b)$$

$$\frac{\partial \eta}{\partial a_-}(a_-, \eta_-, t) = - \int_{-\infty}^t V^{(2)}(a(a_-, \eta_-, s)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, s) ds \quad (3.4c)$$

$$\frac{\partial \eta}{\partial \eta_-}(a_-, \eta_-, t) = \mathbb{1} - \int_{-\infty}^t V^{(2)}(a(a_-, \eta_-, s)) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, s) ds \quad (3.4d)$$

$$a_+(a_-, \eta_-) = a_- - \frac{1}{m} \int_{-\infty}^0 ds \int_{-\infty}^s V^{(1)}(a(a_-, \eta_-, r)) dr + \frac{1}{m} \int_0^{\infty} ds \int_s^{\infty} V^{(1)}(a(a_-, \eta_-, r)) dr \quad (3.5a)$$

$$\eta_+(a_-, \eta_-) = \eta_- - \int_{-\infty}^{\infty} V^{(1)}(a(a_-, \eta_-, s)) ds \quad (3.5b)$$

$$\begin{aligned} \frac{\partial a_+}{\partial a_-}(a_-, \eta_-) &= \mathbb{1} - \frac{1}{m} \int_{-\infty}^0 ds \int_{-\infty}^s V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, r) dr \\ &\quad + \frac{1}{m} \int_0^{\infty} ds \int_s^{\infty} V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, r) dr \end{aligned} \quad (3.6a)$$

$$\begin{aligned} \frac{\partial a_+}{\partial \eta_-}(a_-, \eta_-) = & -\frac{1}{m} \int_{-\infty}^0 ds \int_{-\infty}^s V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, r) dr \\ & + \frac{1}{m} \int_0^\infty ds \int_s^\infty V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, r) dr \end{aligned} \quad (3.6b)$$

$$\frac{\partial \eta_+}{\partial a_-}(a_-, \eta_-) = - \int_{-\infty}^\infty V^{(2)}(a(a_-, \eta_-, s)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, s) ds \quad (3.6c)$$

$$\frac{\partial \eta_+}{\partial \eta_-}(a_-, \eta_-) = \mathbb{1} - \int_{-\infty}^\infty V^{(2)}(a(a_-, \eta_-, s)) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, s) ds. \quad (3.6d)$$

The matrices $A_+(a_-, \eta_-)$ and $B_+(a_-, \eta_-)$ satisfy conditions (2.1) and the following relations hold:

$$A(a_-, \eta_-, t) = \frac{\partial a}{\partial a_-}(a_-, \eta_-, t) + i \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, t) \quad (3.7a)$$

$$B(a_-, \eta_-, t) = \frac{\partial \eta}{\partial \eta_-}(a_-, \eta_-, t) - i \frac{\partial \eta}{\partial a_-}(a_-, \eta_-, t) \quad (3.7b)$$

$$A_+(a_-, \eta_-) = \frac{\partial a_+}{\partial a_-}(a_-, \eta_-) + i \frac{\partial a_+}{\partial \eta_-}(a_-, \eta_-) \quad (3.7c)$$

$$B_+(a_-, \eta_-) = \frac{\partial \eta_+}{\partial \eta_-}(a_-, \eta_-) - i \frac{\partial \eta_+}{\partial a_-}(a_-, \eta_-). \quad (3.7d)$$

$S(a_-, \eta_-, t)$ and $S_+(a_-, \eta_-)$ are given by

$$S(a_-, \eta_-, t) = S_-(a_-) + \frac{t}{2m} |\eta_-|^2 - 2 \int_{-\infty}^t V(a(a_-, \eta_-, s)) ds \quad (3.8a)$$

$$S_+(a_-, \eta_-) = S_-(a_-) - 2 \int_{-\infty}^\infty V(a(a_-, \eta_-, s)) ds. \quad (3.8b)$$

Our next three propositions are concerned with the smoothness and large $|t|$ asymptotics of the functions discussed above.

PROPOSITION 3.1. — The functions $a, \eta, A, B, a_+, \eta_+, A_+$ and B_+ are of class C^2 in the variables $(a_-, \eta_-) \in \mathbb{R}^{2n} \setminus \varepsilon$, and the classical scattering matrix $\mathcal{J}_{\text{cl}} : \mathbb{R}^{2n} \setminus \varepsilon \mapsto \mathbb{R}^{2n}$ defined by $\mathcal{J}_{\text{cl}}(a_-, \eta_-) = (a_+(a_-, \eta_-), \eta_+(a_-, \eta_-))$ is a measure preserving class C^2 transformation.

Proof. — We omit the proof of this proposition noting that the arguments of Section XI.2 of [RS2] can easily be extended to this case. ■

PROPOSITION 3.2. — Let \mathcal{K} be a compact subset of $\mathbb{R}^{2n} \setminus \varepsilon$ and let ν be

as in Assumption 1.1. Then there exist positive constants C and T depending only on \mathcal{K} such that $|t| \geq T$ implies

$$\begin{aligned} \left| a(a_-, \eta_-, t) - a_{\pm}(a_-, \eta_-) - \frac{t}{m} \eta_{\pm}(a_-, \eta_-) \right| &\leq C |t|^{-\nu} \\ \left| \eta(a_-, \eta_-, t) - \eta_{\pm}(a_-, \eta_-) \right| &\leq C |t|^{-1-\nu} \\ \left\| A(a_-, \eta_-, t) - A_{\pm}(a_-, \eta_-) - i \frac{t}{m} B_{\pm}(a_-, \eta_-) \right\| &\leq C |t|^{-\nu} \\ \left\| B(a_-, \eta_-, t) - B_{\pm}(a_-, \eta_-) \right\| &\leq C |t|^{-1-\nu} \\ \left| S(a_-, \eta_-, t) - S_{\pm}(a_-, \eta_-) - \frac{t^2}{2m} |\eta_{\pm}(a_-, \eta_-)|^2 \right| &\leq C |t|^{-\nu} \\ \left\| \frac{\partial}{\partial a_-} (a(a_-, \eta_-, t) - a_{\pm}(a_-, \eta_-) - \frac{t}{m} \eta_{\pm}(a_-, \eta_-)) \right\| &\leq C |t|^{-\nu} \\ \left\| \frac{\partial}{\partial a_-} (\eta(a_-, \eta_-, t) - \eta_{\pm}(a_-, \eta_-)) \right\| &\leq C |t|^{-1-\nu} \\ \left\| \frac{\partial}{\partial \eta_-} (a(a_-, \eta_-, t) - a_{\pm}(a_-, \eta_-) - \frac{t}{m} \eta_{\pm}(a_-, \eta_-)) \right\| &\leq C |t|^{-\nu} \\ \left\| \frac{\partial}{\partial \eta_-} (\eta(a_-, \eta_-, t) - \eta_{\pm}(a_-, \eta_-)) \right\| &\leq C |t|^{-1-\nu} \end{aligned}$$

for all $(a_-, \eta_-) \in \mathcal{K}$. For brevity we have denoted $a_-(a_-, \eta_-) = a_-$, $\eta_-(a_-, \eta_-) = \eta_-$, $A_-(a_-, \eta_-) = \mathbb{1}$, $B_-(a_-, \eta_-) = \mathbb{1}$, $S_-(a_-, \eta_-) = S_-(a_-)$ and the inequalities above are understood to hold with \pm replaced by $-$ for $t \leq -T$ and $+$ for $t \geq T$.

Proof. — Theorem XI.2 (a) of [RS2] and its proof imply the existence of $T > 0$ such that

$$\left| a(a_-, \eta_-, t) - a_{\pm}(a_-, \eta_-) - \frac{t}{m} \eta_{\pm}(a_-, \eta_-) \right| \leq 1$$

if $|t| \geq T$ and $(a_-, \eta_-) \in \mathcal{K}$. We again emphasize that when we write inequalities containing both subscripts $+$ and $-$ we mean that the inequality holds with the $-$ subscript for large negative time and with the $+$ subscript for large positive time. A simple argument using the triangle inequality and compactness shows that there exists a constant C_1 such that $|a(a_-, \eta_-, t)| \geq C_1 |t|$ for all $|t| \geq T$ and $(a_-, \eta_-) \in \mathcal{K}$. Hence $|(D^{\alpha} V)(a(a_-, \eta_-, t))|$ is bounded from above by a constant multiple of $|t|^{-1-|\alpha|-\nu}$ uniformly in $(a_-, \eta_-) \in \mathcal{K}$ for all $|t| \geq T$. Equations (3.3a), (3.5a), and (3.5b) imply the existence of a constant C_2 such that

$$\left| a(a_-, \eta_-, t) - a_{\pm}(a_-, \eta_-) - \frac{t}{m} \eta_{\pm}(a_-, \eta_-) \right| \leq C_2 |t|^{-\nu}$$

uniformly in $(a_-, \eta_-) \in \mathcal{K}$ for all $|t| \geq T$. Equations (3.3b) and (3.5b) imply the existence of a constant C_3 such that

$$|\eta(a_-, \eta_-, t) - \eta_{\pm}(a_-, \eta_-)| \leq C_3 |t|^{-1-\nu}$$

uniformly in $(a_-, \eta_-) \in \mathcal{K}$ for all $|t| \geq T$. From conservation of energy, $|\eta_-| = |\eta_+(a_-, \eta_-)|$ and hence equations (3.8) imply the existence of a constant C_4 such that

$$\left| S(a_-, \eta_-, t) - S_{\pm}(a_-, \eta_-) - \frac{t^2}{2m} |\eta_{\pm}(a_-, \eta_-)|^2 \right| \leq C_4 |t|^{-\nu}$$

uniformly in $(a_-, \eta_-) \in \mathcal{K}$ for all $|t| \geq T$. The two inequalities concerning the matrices $A(a_-, \eta_-, t)$ and $B(a_-, \eta_-, t)$ follow from the last four and equations (3.7). We prove only one of the remaining inequalities involving the derivatives of $a(a_-, \eta_-, t)$ and $\eta(a_-, \eta_-, t)$ with respect to a_- and η_- , the others follow by similar arguments. Following an idea by Yajima (see the proof of Lemma 2.7 of [Y1]) we change the order of integration in (3.4a) to obtain

$$\frac{\partial a}{\partial a_-}(a_-, \eta_-, t) = \mathbb{1} - \frac{1}{m} \int_{-\infty}^t (t-r) V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, r) dr. \quad (3.4a')$$

By Gronwall's Lemma, $\left\| \frac{\partial a}{\partial a_-}(a_-, \eta_-, t) \right\|$ is bounded above by a constant for all $t \in \mathbb{R}$ and $(a_-, \eta_-) \in \mathcal{K}$. Hence, by (3.4a) or (3.4a') there exists a constant C_5 such that

$$\left\| \frac{\partial a}{\partial a_-}(a_-, \eta_-, t) - \mathbb{1} \right\| \leq C_5 |t|^{-\nu}$$

for all $t \leq -T$ and $(a_-, \eta_-) \in \mathcal{K}$. By equations (3.4a), (3.6a), (3.6c) and explicit computation

$$\begin{aligned} \frac{\partial}{\partial a_-}(a_-, \eta_-, t) - \frac{\partial a_+}{\partial a_-}(a_-, \eta_-) - \frac{t}{m} \frac{\partial \eta_+}{\partial a_-}(a_-, \eta_-) \\ = -\frac{1}{m} \int_t^{\infty} ds \int_s^{\infty} V^{(2)}(a(a_-, \eta_-, r)) \frac{\partial a}{\partial a_-}(a_-, \eta_-, r) dr \end{aligned}$$

and therefore there is a constant C'_5 such that

$$\left\| \frac{\partial a}{\partial a_-}(a_-, \eta_-, t) - \frac{\partial a_+}{\partial a_-}(a_-, \eta_-) - \frac{t}{m} \frac{\partial \eta_+}{\partial a_-}(a_-, \eta_-) \right\| \leq C'_5 |t|^{-\nu}$$

for all $t \geq T$ and $(a_-, \eta_-) \in \mathcal{K}$. ■

It is worth noting that the key ingredient in the proof of Proposition 3.2 is the existence of $T > 0$ such that $|a(a_-, \eta_-, t)|$ is bounded from below

by a constant multiple of $|t|$ and $|(D^\alpha V)(a(a_-, \eta_-, t))|$ is bounded from above by a constant multiple of $|t|^{-1-|\alpha|-v}$ uniformly in $(a_-, \eta_-) \in \mathcal{K}$ for all $|t| \geq T$.

PROPOSITION 3.3. — Let \mathcal{K} be a compact subset of $\mathbb{R}^{2n} \setminus \varepsilon$. Then the function $S_+(a_-, \eta_-)$ is of class C^1 in the variables $(a_-, \eta_-) \in \mathcal{K}$ and

$$\begin{aligned} \frac{\partial}{\partial a_-} S_+(a_-, \eta_-) &= S^{(1)}(a_-) + \eta_+(a_-, \eta_-) \frac{\partial a_+}{\partial a_-}(a_-, \eta_-) - \eta_- \\ \frac{\partial}{\partial \eta_-} S_+(a_-, \eta_-) &= \eta_+(a_-, \eta_-) \frac{\partial a_+}{\partial \eta_-}(a_-, \eta_-). \end{aligned}$$

Proof. — For $(a_-, \eta_-) \in \mathbb{R}^{2n} \setminus \varepsilon$ and $t, t_0 \in \mathbb{R}$ define

$$S'(a_-, \eta_-, t_0, t) = \int_{t_0}^t V(a(a_-, \eta_-, s)) ds.$$

By the conservation of energy, i. e.

$$\frac{1}{2m} |\eta_-|^2 = \frac{1}{2m} |\eta(a_-, \eta_-, t)|^2 + V((a(a_-, \eta_-, t))),$$

and some elementary manipulations involving differentiating under the integral sign and integrating by parts we obtain

$$\begin{aligned} \frac{\partial}{\partial a_-} S(a_-, \eta_-, t_0, t) \\ = -\frac{1}{2} \left[\eta(a_-, \eta_-, t) \frac{\partial a}{\partial a_-}(a_-, \eta_-, t) - \eta(a_-, \eta_-, t_0) \frac{\partial a}{\partial a_-}(a_-, \eta_-, t_0) \right] \end{aligned}$$

and

$$\begin{aligned} \frac{\partial}{\partial \eta_-} S'(a_-, \eta_-, t_0, t) \\ = -\frac{1}{2} \left[\eta(a_-, \eta_-, t) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, t) - \eta(a_-, \eta_-, t_0) \frac{\partial a}{\partial \eta_-}(a_-, \eta_-, t_0) - (t - t_0) \eta_- \right]. \end{aligned}$$

We remind the reader that we do not distinguish row and column vectors, clearly the vectors $\eta(a_-, \eta_-, t)$ and $\eta(a_-, \eta_-, t_0)$ appearing in the expressions above are row vectors. By Proposition 3.2,

$$\lim_{\substack{t \rightarrow \infty \\ t_0 \rightarrow -\infty}} \frac{\partial}{\partial a_-} S'(a_-, \eta_-, t_0, t) = -\frac{1}{2} \left[\eta_+(a_-, \eta_-) \frac{\partial a_+}{\partial a_-}(a_-, \eta_-) - \eta_- \right]$$

and

$$\lim_{\substack{t \rightarrow \infty \\ t_0 \rightarrow -\infty}} \frac{\partial}{\partial \eta_-} S'(a_-, \eta_-, t_0, t) = -\frac{1}{2} \eta_+(a_-, \eta_-) \frac{\partial a_+}{\partial \eta_-}(a_-, \eta_-)$$

where the limits are uniform on \mathcal{K} . The proposition follows from the fact that

$$S_+(a_-, \eta_-) = S_-(a_-) - 2 \lim_{\substack{t \rightarrow \infty \\ t_0 \rightarrow -\infty}} S'(a_-, \eta_-, t_0, t)$$

and standard theorems on the interchange of limits and derivatives (for example, Theorem 28.5 of [B] can be extended to be applied here). ■

Following the idea of Section 4 of [R], we would like to restrict the incoming asymptotes (a_-, η_-) to lie on a manifold $\{(q_-, p_-) : p_- = S^{(1)}(q_-)\}$. A complication arises in that we must avoid the set ε . Let

$$\mathcal{A} = \{q_- \in \mathbb{R}^n : (q_-, S^{(1)}(q_-)) \in \varepsilon\}.$$

We note that \mathcal{A} is closed by virtue of being the inverse image of the closed set ε under the continuous mapping $q_- \mapsto (q_-, S^{(1)}(q_-))$. We assume for the rest of the proof that $\text{supp}(f) \subset \mathbb{R}^n \setminus \mathcal{A}$. Define a C^2 mapping $Q_+ : \mathbb{R}^n \setminus \mathcal{A} \mapsto \mathbb{R}^n$ by

$$Q_+(q_-) = a_+(q_-, S^{(1)}(q_-))$$

and assume

$$\det \left[\frac{\partial Q_+}{\partial q_-}(x) \right] \neq 0$$

for all $x \in \text{supp}(f)$. As in [R], this gives rise to finitely many open balls $\mathcal{N}_k \subset \mathbb{R}^n \setminus \mathcal{A}$ covering $\text{supp}(f)$ such that $Q_{+,k} \equiv Q_+ \upharpoonright \mathcal{N}_k$ is a class C^2 diffeomorphism. We define, for $q \in Q_+[\mathcal{N}_k]$,

$$\begin{aligned} P_{+,k}(q) &= \eta_+(Q_{+,k}^{-1}(q), S^{(1)}(Q_{+,k}^{-1}(q))) \\ A_{+,k}(q) &= A_+(Q_{+,k}^{-1}(q), S^{(1)}(Q_{+,k}^{-1}(q))) \\ B_{+,k}(q) &= B_+(Q_{+,k}^{-1}(q), S^{(1)}(Q_{+,k}^{-1}(q))) \\ S_{+,k}(q) &= S_+(Q_{+,k}^{-1}(q), S^{(1)}(Q_{+,k}^{-1}(q))). \end{aligned}$$

By Proposition 3.3, for $q \in Q_+[\mathcal{N}_k]$ we have

$$P_{+,k}(q) = \frac{\partial}{\partial q} S_{+,k}(q) \tag{3.9}$$

and, since \mathcal{J}_{c_1} is measure-preserving, the argument of Proposition 4.1 of [R] shows

$$\begin{aligned} \det [B_{+,k}(q) + iS_{+,k}^{(2)}(q)A_{+,k}(q)] \\ = \det \left[\frac{\partial}{\partial q} Q_{+,k}^{-1}(q) \right] \cdot \det [1 + iS^{(2)}(Q_{+,k}^{-1}(q))]. \end{aligned} \tag{3.10}$$

We note that (3.9) implies that $S_{+,k}$ is of Class C^3 in $q \in Q_+[\mathcal{N}_k]$.

For $q \in Q_+[\mathcal{N}_k]$ we define the branch of the square root of $\det [A_{+,k}(q)]$

by first demanding that the branch of $\left(\det \left[\mathbb{1} + i \frac{t}{m} \mathbb{1} \right]\right)^{1/2}$ be determined by continuity from $t = 0$. We then determine

$$\left(\det \left[A(Q_{+,k}^{-1}(q), S_-^{(1)}(Q_{+,k}^{-1}(q))), t \right]\right)^{1/2}$$

by continuity in t and the requirement

$$\lim_{t \rightarrow -\infty} \left(\left(\det \left[A(Q_{+,k}^{-1}(q), S_-^{(1)}(Q_{+,k}^{-1}(q))), t \right]\right)^{1/2} - \left(\det \left[\mathbb{1} + i \frac{t}{m} \mathbb{1} \right]\right)^{1/2} \right) = 0.$$

Then, $\det [A_{+,k}(q)]^{1/2}$ is determined by continuity and the two requirements

$$\lim_{t \rightarrow 0} \left(\left(\det \left[A(Q_{+,k}^{-1}(q), S_-^{(1)}(Q_{+,k}^{-1}(q))), t \right]\right)^{1/2} - \left(\det \left[A(Q_{+,k}^{-1}(q), S_-^{(1)}(Q_{+,k}^{-1}(q))), t - i \frac{t}{m} B_{+,k}(q) \right]\right)^{1/2} \right) = 0$$

and

$$\lim_{t \rightarrow \infty} \left(\left(\det [A_{+,k}(q)]\right)^{1/2} - \left(\det \left[A(Q_{+,k}^{-1}(q), S_-^{(1)}(Q_{+,k}^{-1}(q))), t - i \frac{t}{m} B_{+,k}(q) \right]\right)^{1/2} \right) = 0.$$

We determine the branches of

$$\left(\det [B_{+,k}(q)A_{+,k}(q)^{-1} + iS_{+,k}^{(1)}(q)]\right)^{1/2}$$

and

$$\left(\det \left[\mathbb{1} + iS_-^{(2)}(Q_{+,k}^{-1}(q)) \right]\right)^{1/2}$$

by analytic continuation along $\xi \in [0, 1]$ of

$$\left(\det \left[\operatorname{Re} (B_{+,k}(q)A_{+,k}(q)^{-1}) + \xi i(S_{+,k}^{(2)}(q) + \operatorname{Im} (B_{+,k}(q)A_{+,k}(q)^{-1})) \right]\right)^{1/2}$$

and

$$\left(\det \left[\mathbb{1} + \xi iS_-^{(2)}(Q_{+,k}^{-1}(q)) \right]\right)^{1/2}$$

respectively, starting with positive values for $\xi = 0$. The branch of $\left(\det \left[\frac{\partial}{\partial q} Q_{+,k}^{-1}(q) \right]\right)^{1/2}$ is then determined by (3.10). As in [R], to each \mathcal{N}_k we can assign a unique (mod 4) index μ_k such that

$$\left(\det \left[\frac{\partial Q_+}{\partial q_-} (Q_{+,k}^{-1}(q)) \right]\right)^{1/2} = \left| \det \left[\frac{\partial Q_+}{\partial q_-} (Q_{+,k}^{-1}(q)) \right] \right|^{1/2} e^{i \frac{\pi}{2} \mu_k}$$

for all $q \in Q_+[\mathcal{N}_k]$. As in Section 4 of [R], we find that it is sufficient to consider a single ball \mathcal{N}_k and $C_0^1(\mathcal{N}_k, \mathbb{C})$ function f_k and prove the following analog of Lemma 4.3 of [R].

LEMMA 3.4. — Given $\lambda \in (0, 1/2)$, there exist positive constants δ and C independent of \hbar such that

$$\| \mathcal{A}(\hbar)(e^{iS_-/\hbar} f_k) - e^{i(S_+, \kappa/\hbar + \mu_k \pi/2)} \cdot \left| \det \left[\frac{\partial Q_+}{\partial q_-} (Q_{+,k}^{-1}(\cdot)) \right]^{-1/2} f_k(Q_{+,k}^{-1}(\cdot)) \chi_{Q_+[L, \kappa]} \right|_2 \| \leq C \hbar^\lambda$$

for all $\hbar \in (0, \delta)$.

Lemma 3.4 (and hence, Theorem 1.2) follows by mimicking the proof of Lemma 4.3 of [R] with the references to the work of Hagedorn replaced by the following proposition which represents a result contained in [Ha1], [Ha2], and [Ha3] though not explicitly stated there.

LEMMA 3.5. — Suppose V satisfies Assumption 1.1. Let $\mathcal{X} \subset \mathbb{R}^{2n} \setminus \varepsilon$ be compact and $\lambda \in (0, 1/2)$. Then there exist a positive number δ , functions $c_\alpha^+(a_-, \eta_-, \hbar)$, and a constant C independent of \hbar such that $\hbar \in (0, \delta]$ implies

$$\| \mathcal{A}(\hbar)(e^{iS_-(a_-)/\hbar} \phi_0(\mathbb{1}, \mathbb{1}, \hbar, a_-, \eta_-, \cdot)) - e^{iS_+(a_-, \eta_-)/\hbar} \sum_{|\alpha|=0}^{3(l-1)} c_\alpha^+(a_-, \eta_-, \hbar) \phi_\alpha(A_+(a_-, \eta_-), B_+(a_-, \eta_-), \hbar, a_+(a_-, \eta_-), \eta_+(a_-, \eta_-), \cdot) \|_2 \leq C \hbar^{\lambda l}$$

for all $(a_-, \eta_-) \in \mathcal{X}$. Moreover, the functions $c_\alpha^+(a_-, \eta_-, \hbar)$ are of class C^1 in $(a_-, \eta_-) \in \mathbb{R}^{2n} \setminus \varepsilon$ and the constant C can be chosen such that

$$|c_0^+(a_-, \eta_-, \hbar) - 1| \leq C \hbar^{1/2}$$

and $3(r-1) < |\alpha| \leq 3r \Rightarrow |c_\alpha^+(a_-, \eta_-, \hbar)| \leq C \hbar^{r/2}$

for all $(a_-, \eta_-) \in \mathcal{X}$, $r = 1, 2, \dots, l-1$.

To prove Lemma 3.5 we simply mimic the arguments used in the proofs of Theorem 1.2 of [Ha1] and Theorem 1.1 of [Ha3] using the uniform estimates of Proposition 3.2 to keep track of the dependence on t and t_0 . Standard contraction mapping and fixed point theorems (see, e. g., Section 4.9 of [LS] and Section XI.2 of [RS2]) guarantee the smoothness of the functions c_α^+ . We omit the details of this argument since all of the steps are the obvious analogues of the arguments of Hagedorn. The crucial estimate (the proof of which requires that $n \geq 3$) is the higher order extension of Lemma 3.2 of [Ha1].

Lemma 3.4 follows by using Lemma 3.5 and the argument of Lemma 4.3 of [R]. Theorem 1.2 then follows by the argument used to prove Theorem 1.2 of [R], using Lemma 3.4.

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