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► To cite this version:

Clotilde Fermanian Kammerer, Caroline Lasser, Didier Robert. Adiabatic and non-adiabatic evolution of wave packets and applications to initial value representations. *Partial Differential Equations, Spectral Theory, and Mathematical Physics. The Ari Laptev Anniversary*, 2021. ⟨hal-02985675⟩

HAL Id: hal-02985675

<https://hal.science/hal-02985675v1>

Submitted on 2 Nov 2020

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Adiabatic and non-adiabatic evolution of wave packets and applications to initial value representations

Clotilde Fermanian Kammerer Caroline Lasser
Didier Robert

To Ari Laptev for his 70th birthday

Abstract

We review some recent results obtained for the time evolution of wave packets for systems of equations of pseudo-differential type, including Schrödinger ones, and discuss their application to the approximation of the associated unitary propagator. We start with scalar equations, propagation of coherent states, and applications to the Herman–Kluk approximation. Then we discuss the extension of these results to systems with eigenvalues of constant multiplicity or with smooth crossings.

1 Introduction

We consider semi-classical systems of the form

$$i\varepsilon\partial_t\psi^\varepsilon(t) = \widehat{H(t)}\psi^\varepsilon(t), \quad \psi^\varepsilon|_{t=t_0} = \psi_0^\varepsilon \quad (1.1)$$

where (ψ_0^ε) is a bounded family in $L^2(\mathbb{R}^d, \mathbb{C}^N)$, $\|\psi_0^\varepsilon\|_{L^2(\mathbb{R}^d, \mathbb{C}^N)} = 1$ and $\widehat{H}(t)$ is the ε -Weyl quantization of a smooth Hermitian symbol $H(t, x, \xi)$ satisfying suitable growth assumptions. We are interested in approximate realizations of the unitary propagator associated with this equation relying on the use of continuous superpositions of Gaussian wave packets. Before explaining these ideas in more detail (in particular the definition of the quantization that the reader will find below), let us first emphasize different types of systems that we have in mind.

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The simplest case is the one where $H(t)$ is independent of (x, ξ) , which implies that the operator $\widehat{H}(t)$ coincides with the matrix $H(t)$. In this case it is known that for $N \geq 2$ new phenomena appear by comparison with the scalar case $N = 1$. When the eigenvalues of $H(t)$ are not crossing, the adiabatic theorem says that if ψ_0^ε is an eigenfunction of $H(t_0)$, then at every time $\psi^\varepsilon(t)$ has an asymptotic expansion for $\varepsilon \rightarrow 0$, and the leading term is an eigenfunction of $H(t)$. The first complete proof was given by Friedrichs ([9] after first results by Born-Fock [2] and Kato [17]). In [9, Part III], Friedrichs considered a non-adiabatic situation where $H(t)$ is a 2×2 Hermitian matrix with two analytic eigenvalues $h_\pm(t)$ such that $h_+(t) \neq h_-(t)$ for $t \neq 0$ and

$$(h_+ - h_-)(0) = 0, \quad \frac{d}{dt}(h_+ - h_-)(0) \neq 0.$$

In this spirit, we here consider a toy model for space dependent Hamiltonians of the following form: We choose $d = 1$, $N = 2$, $\theta \in \mathbb{R}_+$, $k \in \mathbb{R}^*$, and

$$\widehat{H}_{k,\theta} = \frac{\varepsilon}{i} \frac{d}{dx} \mathbb{I}_{\mathbb{C}^2} + kx \begin{pmatrix} 0 & e^{i\theta x} \\ e^{-i\theta x} & 0 \end{pmatrix}. \quad (1.2)$$

Its semiclassical symbol $H_{k,\theta}(x, \xi) = \xi + kx \begin{pmatrix} 0 & e^{i\theta x} \\ e^{-i\theta x} & 0 \end{pmatrix}$ has the eigenvalues and associated eigenvectors (the latter depending only in x)

$$h_\pm(x, \xi) = \xi \pm kx, \quad \vec{V}_\pm(x) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta x} \\ \pm 1 \end{pmatrix} \quad (1.3)$$

So for $k \neq 0$ we have a crossing at $x = 0$ that we call *smooth crossing* because there exists smooth eigenvalues and eigenprojectors. We shall use this toy-model all along this article. Notice that one can prove that the operator $\widehat{H}_{k,\theta}$ is essentially self-adjoint in $L^2(\mathbb{R}, \mathbb{C}^2)$ by using a commutator criterion with the standard harmonic oscillator (see [22, Appendix A]). As we shall see later, the solutions of the Schrödinger equation for $\widehat{H}_{k,\theta}$ can be computed by solving an ODE asymptotically as $\varepsilon \rightarrow 0$, see (5.4), and by using non-adiabatic asymptotic results from Friedrichs [9] and Hagedorn [11].

More generally, of major interest because of their applications to molecular dynamics, are the Schrödinger Hamiltonians with matrix-valued potential considered by Hagedorn in his monograph [12, Chapter 5],

$$\widehat{H}_S = -\frac{\varepsilon^2}{2} \Delta_x \mathbb{I}_{\mathbb{C}^N} + V(x), \quad V \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}^{N \times N}), \quad (1.4)$$

or the models arising in solid state physics in the context of Bloch band decompositions studied by Watson and Weinstein in [29].

$$\widehat{H}_A = A(-i\varepsilon \nabla_x) + W(x) \mathbb{I}_{\mathbb{C}^2}, \quad A \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}^{N \times N}), \quad W \in \mathcal{C}^\infty(\mathbb{R}^d, \mathbb{C}). \quad (1.5)$$

The notation \widehat{H} refers to the Weyl quantization that we shall use extensively in this article. For $a \in \mathcal{C}^\infty(\mathbb{R}^{2d}, \mathbb{C}^{N \times N})$ with adequate control on the growth of derivatives, the operator \widehat{a} is defined by its action on functions $f \in \mathcal{S}(\mathbb{R}^d, \mathbb{C}^N)$:

$$\text{op}_\varepsilon^w(a)f(x) := \widehat{a}f(x) := (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^d} a\left(\frac{x+y}{2}, \xi\right) e^{\frac{i}{\varepsilon}\xi \cdot (x-y)} f(y) dy d\xi.$$

It turns out that the propagator $\mathcal{U}_H^\varepsilon(t, t_0)$ associated with \widehat{H} is well defined according to [22, Theorem 5.15] provided that the map $(t, z) \mapsto H(t, z)$ is in $\mathcal{C}^\infty(\mathbb{R} \times \mathbb{R}^{2d}, \mathbb{C}^{N \times N})$ valued in the set of self-adjoint matrices and that it has subquadratic growth, i.e.

$$\forall \alpha \in \mathbb{N}^{2d}, |\alpha| \geq 2, \exists C_\alpha > 0, \sup_{(t,z) \in \mathbb{R} \times \mathbb{R}^{2d}} \|\partial^\alpha H(t, z)\|_{\mathbb{C}^{N \times N}} \leq C_\alpha. \quad (1.6)$$

Using the commutator methods of [22], we could extend main of our results to a more general setting. However, the assumptions (1.6) are enough to guarantee the existence of solutions to equation (1.1) in $L^2(\mathbb{R}^d, \mathbb{C}^N)$. One of our objectives here is to describe different Gaussian-based approximations of the semi-group $\mathcal{U}_H^\varepsilon(t, t_0)$ in the limit $\varepsilon \rightarrow 0$.

Let g_z^ε denote the Gaussian wave packet centered in $z = (q, p) \in \mathbb{R}^{2d}$ with standard deviation $\sqrt{\varepsilon}$:

$$g_z^\varepsilon(x) = (\pi\varepsilon)^{-d/4} \exp\left(-\frac{1}{2\varepsilon}|x-q|^2 + \frac{i}{\varepsilon}p \cdot (x-q)\right). \quad (1.7)$$

The family of wave packets $(g_z^\varepsilon)_{z \in \mathbb{R}^{2d}}$ forms a continuous frame and provides for all square integrable functions $f \in L^2(\mathbb{R}^d)$ the reconstruction formula

$$f(x) = (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle g_z^\varepsilon, f \rangle g_z^\varepsilon(x) dz. \quad (1.8)$$

The leading idea is then to write the unitary propagation of general, square integrable initial data $\psi_0^\varepsilon \in L^2(\mathbb{R}^d)$ as

$$\mathcal{U}_H^\varepsilon(t, t_0)\psi_0^\varepsilon = (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi_0^\varepsilon \rangle \mathcal{U}_H^\varepsilon(t, t_0)g_z^\varepsilon dz, \quad (1.9)$$

and to take advantage of the specific properties of the propagation of Gaussian states to obtain an integral representation that allows in particular for an efficient numerical realization of the propagator.

Such a program has been completely accomplished in the scalar case ($N = 1$). It appeared first in the 80's in theoretical chemistry [14, 16, 18] and has led to the so-called Herman–Kluk approximation. The mathematical proof of the convergence of this approximation is more recent [26, 24]. Here, we revisit these results in Section 2 and Section 5, and discuss some extensions to the case of systems ($N \geq 1$), first for the gapped situation in Section 3 and then for smooth crossings in Section 4.

2 Propagation of Gaussian states and the Herman–Kluk approximation for scalar equations

In this section, $N = 1$ and the equation (1.1) is associated with a scalar Hamiltonian $H(t) = h(t)$ of subsquadratic growth (1.6). In that case, the approximate propagation of Gaussian states is described by classical quantities, leading to a simple Herman–Kluk approximation. We set

$$J = \begin{pmatrix} 0 & \mathbb{I}_{\mathbb{R}^d} \\ -\mathbb{I}_{\mathbb{R}^d} & 0 \end{pmatrix}$$

and for $z_0 \in \mathbb{R}^{2d}$ we consider the classical Hamiltonian trajectory $z(t) = (q(t), p(t))$ defined by the ordinary differential equation

$$\dot{z}(t) = J\partial_z h(t, z(t)), \quad z(t_0) = z_0.$$

The associated flow map is then denoted by

$$\Phi_h^{t, t_0}(z_0) = z(t) = (q(t), p(t)), \quad (2.1)$$

and the blocks of its Jacobian matrix $F(t, t_0, z_0) = \partial_z \Phi_h^{t, t_0}(z_0)$ by

$$F(t, t_0, z_0) = \begin{pmatrix} A(t, t_0, z_0) & B(t, t_0, z_0) \\ C(t, t_0, z_0) & D(t, t_0, z_0) \end{pmatrix}.$$

We note that the Jacobian satisfies the linearized flow equation

$$\partial_t F(t, t_0, z_0) = J \text{Hess}_z h(t, z(t)) F(t, t_0, z_0), \quad F(t_0, t_0, z_0) = \mathbb{I}_{\mathbb{R}^{2d}}. \quad (2.2)$$

Thus, F is a smooth in t, t_0, z with any derivative in z bounded. We will also use the action integral

$$\partial_t S(t, t_0, z_0) = p(t) \cdot \dot{q}(t) - h(t, z(t)), \quad S(t_0, t_0, z_0) = 0. \quad (2.3)$$

Then, the Herman–Kluk approximation (also called *frozen Gaussian approximation* in the literature) of the unitary propagator $\mathcal{U}_h^\varepsilon(t, t_0)$ writes as follows.

Theorem 2.1 ([26, 24]). *Assuming (1.6), the evolution through the scalar equation with $N = 1$ and $H = h|_{\mathbb{C}}$ in (1.1) satisfies for every $J \geq 0$,*

$$\mathcal{U}_h^\varepsilon(t, t_0) = \mathcal{I}_h^{\varepsilon, J}(t, t_0) + O(\varepsilon^{J+1})$$

in the norm of bounded operators on $L^2(\mathbb{R}^d)$, where the Herman–Kluk propagator is defined for all $\psi \in L^2(\mathbb{R}^d)$,

$$\mathcal{I}_h^{\varepsilon, J}(t, t_0)\psi = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle u^{\varepsilon, J}(t, t_0, z) e^{\frac{i}{\varepsilon} S(t, t_0, z)} g_{\Phi_h^{t, t_0}(z)}^\varepsilon dz, \quad (2.4)$$

with

$$u^{\varepsilon,J}(t, t_0, z) = \sum_{0 \leq j \leq J} \varepsilon^j u_j(t, t_0, z),$$

where every u_j is smooth in t, t_0, z , with any derivative in z bounded. The function u_0 is the Herman–Kluk prefactor,

$$u_0(t, t_0, z) = 2^{-d/2} \det^{1/2} (A(t, t_0, z) + D(t, t_0, z) + i(C(t, t_0, z) - B(t, t_0, z))), \quad (2.5)$$

which has the branch of the square root determined by continuity in time.

Let us remark that the Gaussian wave packets in (2.4) all have the same covariance matrix $\Gamma = \mathbb{I}_{\mathbb{C}^{2d}}$, that is, in the terminology put forward by E. Heller [13], the Gaussians are frozen. The first statement of the form (2.4) at leading order ($J = 0$) is due to M. Herman and E. Kluk (1984)[14]. Then, W.H. Miller (2002) [23] noticed that (2.4) can be deduced from the Van Vleck approximation of the propagator (hence related with a Feynman integral). In more recent work [26, 24], (2.4) was established using Fourier-Integral operator techniques. Here we shall comment in more details on a proof based on the propagation of Gaussian wave packets, via a thawed Gaussian approximation (see Section 5). This proof has the advantage that it can be used in the case of systems of Schrödinger equations, which were not treated in the preceding references.

A Gaussian wave packet is a wave packet with profile function belonging to the class of Gaussian states with variance taken in the Siegel set $\mathfrak{S}^+(d)$ of $d \times d$ complex-valued symmetric matrices with positive imaginary part,

$$\mathfrak{S}^+(d) = \left\{ \Gamma \in \mathbb{C}^{d \times d}, \Gamma = \Gamma^\tau, \Im \Gamma > 0 \right\}.$$

With $\Gamma \in \mathfrak{S}^+(d)$ and $z \in \mathbb{R}$, we associate the Gaussian state

$$g_z^{\Gamma, \varepsilon}(x) = c_\Gamma (\pi \varepsilon)^{-d/4} \exp \left(\frac{i}{\varepsilon} p \cdot (x - q) + \frac{i}{2\varepsilon} \Gamma (x - q) \cdot (x - q) \right),$$

where $c_\Gamma = \det^{1/4}(\Im \Gamma)$ is a positive normalization constant in $L^2(\mathbb{R}^d)$. We note that the standardized Gaussian defined in (1.7) satisfies $g_z^\varepsilon = g_z^{\text{Id}, \varepsilon}$.

We shall use the notation $\text{WP}_z^\varepsilon(\varphi)$ to denote the bounded family in $L^2(\mathbb{R}^d)$ associated with $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and $z = (q, p) \in \mathbb{R}^{2d}$ by

$$\text{WP}_z^\varepsilon(\varphi)(x) = \varepsilon^{-d/4} e^{\frac{i}{\varepsilon} p \cdot (x - q)} \varphi \left(\frac{x - q}{\sqrt{\varepsilon}} \right). \quad (2.6)$$

With wave packet notation, the above Gaussian states satisfy $g_z^{\Gamma, \varepsilon} = \text{WP}_z^\varepsilon(g_0^{\Gamma, 1})$.

Theorem 2.2 ([4, 25]). *Assuming (1.6) with $N = 1$ and $H = h\mathbb{I}_{\mathbb{C}}$, there exists a family of time-dependent Schwartz functions $(\varphi_j(t))_{j \in \mathbf{N}}$ such that for all $N_0 \in \mathbf{N}$, in $L^2(\mathbb{R}^d)$,*

$$\mathcal{W}_h^\varepsilon(t, t_0) g_{z_0}^{\Gamma_0, \varepsilon} = e^{iS(t, t_0, z_0)} \left(g_{\Phi^{t, t_0}(z_0)}^{\Gamma(t, t_0, z_0), \varepsilon} + \sum_{j=1}^{N_0} \varepsilon^{j/2} \mathbf{WP}_{\Phi^{t, t_0}(z_0)}^\varepsilon(\varphi_j(t)) \right) + \mathcal{O}(\varepsilon^{(N_0+1)/2}) \quad (2.7)$$

with

$$\Gamma(t, t_0, z_0) = (C(t, t_0, z_0) + D(t, t_0, z_0)\Gamma_0)(A(t, t_0, z_0) + B(t, t_0, z_0)\Gamma_0)^{-1} \quad (2.8)$$

and $c_{\Gamma(t, t_0, z_0)} = c_{\Gamma_0} \det^{-1/2}(A(t, t_0, z_0) + B(t, t_0, z_0)\Gamma_0)$, where the complex square root is continuous in time.

Note that we have $\Gamma(t_0, t_0, z_0) = \Gamma_0$ in the statement above. Actually, explicit information is obtained on the profiles $(\varphi_j(t))_{j \in \mathbf{N}}$, in particular about $\varphi_1(t)$ (see [4, Section 4.1.2] or Proposition 2.3 in [7]). As we shall see in Section 5, this result can be a starting point for proving the Herman–Kluk approximation of Theorem 2.1.

The result above also holds for general wave packets as in (2.6) with profiles that are not necessarily Gaussians (see [4, Section 4.1.2]). Moreover, also the norm can be generalized to

$$\|f\|_{\Sigma_k^\varepsilon} = \sup_{|\alpha|+|\beta| \leq k} \|x^\alpha (\varepsilon \partial_x)^\beta f\|_{L^2}, \quad k \in \mathbf{N}.$$

Example 2.3. Both Theorem 2.1 and 2.2 are exact when the Hamiltonian h is quadratic. For the Hamiltonians $h_\pm(z) = p \pm kq$ associated with the toy model (see (1.3)), the classical flow is linear

$$\Phi_{h_\pm}^{t, t_0}(z_0) =: (q_\pm(t), p_\pm(t)) = z_0 + (t - t_0)(1, \mp k), \quad z_0 = (q_0, p_0),$$

the width of the Gaussian is constant, $\Gamma_\pm(t, t_0, z_0) = \Gamma_0$, and the actions only depend on q_0 and are given by $S_\pm(t, t_0, q_0) = \mp k q_0 (t - t_0) \mp \frac{k}{2} (t - t_0)^2$.

3 Herman–Kluk formula in the adiabatic setting

We need adaptations for generalizing the scalar ideas to systems. The first one replaces the scalar Herman–Kluk prefactor $u_0(t, t_0, z_0)$ by a vector-valued one $\tilde{U}(t, t_0, z_0)$ that is expanded in a basis of eigenvectors of $H(t, z)$, taken along the classical trajectory $\Phi_h^{t, t_0}(z)$ of the corresponding eigenvalue (denoted here by $h(t, z)$). This is done by parallel transport, and it is sufficient for an order ε approximation as long as the system is gapped.

3.1 Parallel transport

The following construction generalizes [3, Proposition 1.9], which was inspired by the work of G. Hagedorn, see [12, Proposition 3.1]. The details are given in [7]. In the sequel, we denote the complementary orthogonal projector by $\Pi^\perp(t, z) = \mathbb{I}_{\mathbb{C}^N} - \Pi(t, z)$ and assume that

$$H(t, z) = h(t, z)\Pi(t, z) + h^\perp(t, z)\Pi^\perp(t, z) \quad (3.1)$$

with the second eigenvalue given by $h^\perp(t, z) = \text{tr}(H(t, z)) - h(t, z)$. We introduce the auxiliary matrices

$$\Omega(t, z) = -\frac{1}{2}(h(t, z) - h^\perp(t, z))\Pi(t, z)\{\Pi, \Pi\}(t, z)\Pi(t, z),$$

$$K(t, z) = \Pi^\perp(t, z)(\partial_t \Pi(t, z) + \{h, \Pi\}(t, z))\Pi(t, z),$$

$$\Theta(t, z) = i\Omega(t, z) + i(K - K^*)(t, z),$$

that are smooth and satisfy some algebraic properties. In particular, Ω is skew-symmetric and Θ is self-adjoint: $\Omega = -\Omega^*$ and $\Theta = \Theta^*$.

Proposition 3.1 ([7]). *Let $H(t, z)$ be a smooth Hamiltonian that satisfies (1.6) and has a smooth spectral decomposition (3.1). We assume that both eigenvalues are of subquadratic growth as well. We consider $\vec{V}_0 \in \mathcal{C}_0^\infty(\mathbb{R}^{2d}, \mathbb{C}^N)$ and $z_0 \in \mathbb{R}^{2d}$ such that there exists a neighborhood U of z_0 such that for all $z \in U$*

$$\vec{V}_0(z) = \Pi(t_0, z)\vec{V}_0(z) \quad \text{and} \quad \|\vec{V}_0(z)\|_{\mathbb{C}^N} = 1.$$

Then, there exists a smooth normalized vector-valued function $\vec{V}(t, t_0)$ satisfying

$$\vec{V}(t, t_0, z) = \Pi(t, z)\vec{V}(t, t_0, z) \quad \text{for all } z \in \Phi_h^{t, t_0}(U),$$

such that for all $t \in \mathbb{R}$ and $z \in \Phi_h^{t, t_0}(U)$,

$$\partial_t \vec{V}(t, t_0, z) + \{h, \vec{V}\}(t, t_0, z) = -i\Theta(t, z)\vec{V}(t, t_0, z), \quad \vec{V}(t_0, t_0, z) = \vec{V}_0(z). \quad (3.2)$$

We note that the results of this Proposition are valid as long as smooth eigenprojectors and eigenvalues do exist. It does not require an explicit adiabatic situation and we will use that observation in Section 4. In the case of Schrödinger systems, one refers to (3.2) as parallel transport because the vectors $\partial_t \vec{V}(t) + \{h, \vec{V}\}(t)$ belong to the range of $\Pi^\perp(t)$ at any time of the evolution.

Example 3.2. For the toy model $H_{k, \theta}(x, \xi)$, the auxiliary matrices are

$$\Omega_\pm = 0, \quad K_\pm = \frac{i\theta}{4} \begin{pmatrix} 1 & \pm e^{i\theta x} \\ \mp e^{-i\theta x} & -1 \end{pmatrix}, \quad \Theta_\pm = \frac{\theta}{2} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Initiating the parallel transport equation by the eigenvectors given in (1.3), we obtain

$$\vec{V}_\pm(t, t_0, q) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta/2(t-t_0)} e^{i\theta(q-t+t_0)} \\ \pm e^{-i\theta/2(t-t_0)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-\frac{i}{2}\theta(t-t_0)} e^{i\theta q} \\ \pm e^{-\frac{i}{2}\theta(t-t_0)} \end{pmatrix}.$$

Note that they do not depend on p .

3.2 Herman-Kluk approximation in an adiabatic setting

In the context of the preceding section, and in presence of an eigenvalue gap,

$$\exists \delta > 0 : \text{dist}(h(t, z), h^\perp(t, z)) \geq \delta \text{ for all } (t, z),$$

it is well-known that one has *adiabatic decoupling*: If the initial data are scalar multiples of an eigenvector associated with the eigenvalue, then the solution keeps this property to leading order in ε . For an approximation to higher order in ε , one has to consider perturbations of the eigenprojector, the so-called *superadiabatic projectors* (see [1, 27] and the new edition of [4] that should appear soon). Adiabatic theory implies a Herman–Kluk approximation of the propagator that we state next.

Theorem 3.3. [7] *In the situation of Proposition 3.1, we assume the existence of an eigenvalue gap for the eigenvalue h of H and consider initial data of the form*

$$\psi_0^\varepsilon = \widehat{V}_0 v_0^\varepsilon + O(\varepsilon) \text{ in } L^2(\mathbb{R}^d),$$

where \widehat{V}_0 is a smooth eigenvector and $(v_0^\varepsilon)_{\varepsilon>0}$ a family of functions uniformly bounded in $L^2(\mathbb{R}^d, \mathbb{C})$. Then, in $L^2(\mathbb{R}^d)$,

$$\mathcal{W}_H^\varepsilon(t, t_0) \psi_0^\varepsilon = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \vec{U}(t, t_0, z) e^{\frac{i}{\varepsilon} S(t, t_0, z)} g_{\Phi_h^{t, t_0}(z)}^\varepsilon dz + O(\varepsilon)$$

$$\text{with } \vec{U}(t, t_0, z) = u_0(t, t_0, z) \vec{V}(t, t_0, \Phi_h^{t, t_0}(z))$$

where $u_0(t, t_0, z)$ is given by (2.5) and the eigenvector $\vec{V}(t, t_0, z)$ by (3.2).

We describe in Section 5 a proof of this result that crucially uses the approximate evolution of a Gaussian state, that is [25, Section 3],

$$\mathcal{W}_H^\varepsilon(t, t_0) (\widehat{V}_0 g_z^{\Gamma, \varepsilon}) = e^{\frac{i}{\varepsilon} S(t, t_0, z)} \widehat{\vec{V}}(t, t_0) g_{\Phi_h^{t, t_0}(z)}^{\Gamma(t, t_0, z), \varepsilon} \left(1 + \sqrt{\varepsilon} \vec{a}(t) \cdot \frac{(x - q(t))}{\sqrt{\varepsilon}} \right) + O(\varepsilon) \quad (3.3)$$

with $\vec{a}(t) = \vec{a}(t, t_0, z)$ a smooth and bounded map. Note that using superadiabatic projectors [25], one can push the asymptotics further and exhibit $O(\varepsilon)$ contributions that will have components on the other mode. Here again, a formula similar to (3.3) can be proved for general wave packets [4].

3.3 Algorithmic realization of the propagator

Numerical realizations of the Herman–Kluk approximation have been first developed in [15] and are still in practical use in theoretical chemistry [30]. Below, we follow the more recent account given in [19, 20]. We stay with the assumptions of Theorem 3.3 and consider initial data associated with the (gapped) mode h .

Step 1: Initial sampling. Choose a set of numerical quadrature points

$$z_1 = (q_1, p_1), \dots, z_N = (q_N, p_N)$$

with associated weights $w_1, \dots, w_N > 0$, and evaluate the initial transform $\langle g_z^\varepsilon, v_0^\varepsilon \rangle$ in these points. This provides an approximation to the initial data,

$$\psi_0^\varepsilon(x) \sim (2\pi\varepsilon)^{-d} \sum_{1 \leq j \leq N} \langle g_{z_j}^\varepsilon, v_0^\varepsilon \rangle \vec{V}_0(z_j) g_{z_j}^\varepsilon(x) w_j,$$

which is of order ε in $L^2(\mathbb{R}^d)$, as long as the chosen quadrature rule is sufficiently accurate.

Step 2: Transport. For each of the points z_j , $j = 1, \dots, N$, compute

- (1) the classical trajectories $z_j(t)$ defined by (2.1),
- (2) the eigenvectors $\vec{V}(t, t_0, z_j(t))$ along the flow by use of equation (??),
- (3) the Jacobian matrices $F(t, t_0, z_j)$ using equation (2.2),
- (4) the action integrals $S(t, t_0, z_j)$ using equation (2.3),
- (5) the Herman-Kluk prefactor $u_0(t, t_0, z_j)$ using the Jacobians and equation (2.5).

If the time-discretization is symplectic and sufficiently accurate, then the overall accuracy of order ε is not harmed, see [19, Theorem 2].

Step 3: Conclusion. At the end of these thwo steps, we are left with the Hermann-Kluk quadrature formula:

$$\psi^\varepsilon(t, x) \sim (2\pi\varepsilon)^{-d} \sum_{1 \leq j \leq N} \langle g_{z_j}^\varepsilon, v_0^\varepsilon \rangle \vec{U}(t, t_0, z) e^{\frac{i}{\varepsilon} S(t, t_0, z_j)} g_{z_j(t)}^\varepsilon w_j.$$

Of course, the algorithm generalizes to initial data which has several components on separated eigenspaces. In higher dimensional applications, often Monte-Carlo quadrature is used. Then, the initial transform could be written as

$$(2\pi\varepsilon)^{-d} \langle g_z^\varepsilon, v_0^\varepsilon \rangle dz = r_0^\varepsilon(z) \mu_0^\varepsilon(dz),$$

$$\text{where } \mu_0^\varepsilon(dz) = \left(\int |\langle g_z^\varepsilon, v_0^\varepsilon \rangle| dz \right)^{-1} |\langle g_z^\varepsilon, v_0^\varepsilon \rangle| dz$$

is a probability measure and $r_0^\varepsilon(z)$ a complex-valued function of $L^1(\mathbb{R}^{2d}, d\mu_0^\varepsilon)$ according to the Radon–Nikodym Theorem. The quadrature nodes z_1, \dots, z_N are then chosen independently and identically distributed according to the measure μ_0^ε , while the weights are all the same, $w_j = 1/N$ for all j .

4 What about smooth crossings ?

For simplicity we assume here that the Hermitian matrix $H(t, z)$ is 2×2 ($N = 2$) (the same results are also proved for two eigenvalues with arbitrary multiplicity [7]). We

assume that it has smooth eigenvalues $h_1(t, z)$ and $h_2(t, z)$ and smooth eigenprojectors $\Pi_1(t, z)$ and $\Pi_2(t, z)$. To ensure control on the derivatives of the eigenprojectors, we suppose a non crossing assumption at infinity: there exist $c_0, n_0, r_0 > 0$ such that

$$|h_1(t, z) - h_2(t, z)| \geq c_0 \langle z \rangle^{-n_0} \text{ for all } (t, z) \text{ with } |z| \geq r_0,$$

where we denote $\langle z \rangle = (1 + |z|^2)^{1/2}$. We assume the following form of the matrix:

Assumption (SC). There exist scalar functions $v, f \in \mathcal{C}^\infty(\mathbb{R}^{2d+1}, \mathbb{R})$ and a vector-valued function $u \in \mathcal{C}^\infty(\mathbb{R}^{2d+1}, \mathbb{R}^3)$ with $|u(t, z)| = 1$ for all (t, z) such that

$$H(t, z) = v(t, z)\text{Id} + f(t, z) \begin{pmatrix} u_1(t, z) & u_2(t, z) + iu_3(t, z) \\ u_2(t, z) - iu_3(t, z) & -u_1(t, z) \end{pmatrix}.$$

Besides, the crossing is *generic* in Υ in the sense that

$$(\partial_t f + \{v, f\})(t^b, z^b) \neq 0, \quad \forall (t^b, z^b) \in \Upsilon.$$

In that case, the crossing set Υ is a submanifold of codimension one, and all the classical trajectories that reach Υ are transverse to it.

Example 4.1. For the toy model (1.2), $u(x) = (0, \cos(\theta x), \sin(\theta x))$, $v(\xi) = \xi$ and $f(\xi) = k\xi$. Hence we have Assumption (SC) : $\Upsilon = \{x = 0\}$ and $\{v, f\} = k \neq 0$.

In contrast to the previous adiabatic situation, initial data associated with one eigenspace generates a component on the other eigenspace, that is larger than the adiabatic $O(\varepsilon)$, namely $O(\sqrt{\varepsilon})$.

Starting at time t_0 with a Gaussian wave packet, that is associated with the eigenvalue h_1 and localized far from the crossing set Υ , an approximation of the form (3.3) holds as long as the trajectory does not reach Υ . The apparition of a $\sqrt{\varepsilon}$ contribution on the other mode then occurs exactly on Υ . One can interpret this phenomenon in terms of *hops*: starting at time t_0 from some point $z_0 \notin \Upsilon$ for which the Hamiltonian trajectory $z_1(t, t_0) = \Phi_1^{t, t_0}(z_0)$ passes through the crossing at time $t = t^b(z_0)$ and point $z^b = z_1(t^b, t_0)$, we generate a new trajectory $\Phi_2^{t, t^b}(z^b)$ associated with the mode h_2 . This results in the construction of a *hopping trajectory* that hops from one mode to the other one at time t^b .

Such an interpretation is crucial for describing the dynamics of systems with eigenvalue crossings. It has been introduced around the 70s in the chemical literature for avoided and conical crossings of eigenvalues and has been widely used since then (see [28]). The first mathematical results on the subject are more recent and analyse the propagation of Wigner functions through singular crossings (see [5, 6]).

We now aim at a precise description of these new contributions in the case of smooth crossing, first for initial data that are Gaussian wave packets, then we lift this result to a Herman–Kluk formula for smooth crossings in the case of the toy model.

4.1 Wave packet propagation

Let us now give a precise statement for the propagation of wave packets through a smooth crossing. We start with initial data of the form

$$\psi_0^\varepsilon = \widehat{V}_0 v_0^\varepsilon, \quad v_0^\varepsilon = g_{z_0}^{\Gamma_0, \varepsilon}$$

with $H(t_0, z)\widehat{V}_0(z) = h_1(t_0, z)\widehat{V}_0(z)$ in a neighborhood of z_0 . We use Proposition 3.1 to construct two families of time-dependent eigenvectors: $(\widehat{V}_1(t, z))_{t \geq t_0}$ is associated with the eigenvalue $h_1(t, z)$ and initial data at time t_0 given by $\widehat{V}_1(t_0, z) = \widehat{V}_0(z)$, while $(\widehat{V}_2(t, z))_{t \geq t^b}$ is constructed for $t \geq t^b$ (the crossing time introduced in the previous paragraph) for the eigenvalue $h_2(t, z)$ with initial data at time $t^b = t^b(z_0)$ satisfying

$$\widehat{V}_2(t^b, z) = -\gamma(t^b, z)^{-1} \Pi_2 (\partial_t \Pi_2 + \{v, \Pi_2\}) \widehat{V}_1(t^b, z)$$

$$\text{with } \gamma(t^b, z) = \|(\partial_t \Pi_2 + \{v, \Pi_2\}) \widehat{V}_1(t^b, z)\|_{\mathbb{C}^N}.$$

We next introduce a family of transformations, which describes the non-adiabatic effects for a wave packet that passes the crossing. For parameters $(\mu, \alpha, \beta) \in \mathbb{R} \times \mathbb{R}^{2d}$ and $\varphi \in \mathcal{S}(\mathbb{R}^d)$, we set

$$\mathcal{T}_{\mu, \alpha, \beta} \varphi(y) = \int_{-\infty}^{+\infty} e^{i(\mu - \alpha \cdot \beta / 2)s^2} e^{is\beta \cdot y} \varphi(y - s\alpha) ds.$$

This operator maps $\mathcal{S}(\mathbb{R}^d)$ into itself if and only if $\mu \neq 0$. Moreover, for $\mu \neq 0$, it is a metaplectic transformation of the Hilbert space $L^2(\mathbb{R}^d)$, multiplied by a complex number. In particular, for any Gaussian function g^Γ , the function $\mathcal{T}_{\mu, \alpha, \beta} g^\Gamma$ is a Gaussian:

$$\mathcal{T}_{\mu, \alpha, \beta} g^\Gamma = c_{\mu, \alpha, \beta, \Gamma} g^{\Gamma_{\mu, \alpha, \beta, \Gamma}},$$

where $\Gamma_{\mu, \alpha, \beta, \Gamma} \in \mathfrak{S}^+(d)$ and $c_{\mu, \alpha, \beta, \Gamma} \in \mathbb{C}$ can be computed explicitly (see [7, Appendix E]).

Combining the parallel transport for the eigenvector and the metaplectic transformation for the non-adiabatic transitions, we obtain the following result.

Theorem 4.2 (Propagation through a smooth crossing). *Let Assumption (SC) on the Hamiltonian matrix $H(t)$ hold and that the crossing is generic. Assume that the initial data $(\psi_0^\varepsilon)_{\varepsilon > 0}$ are wave packets as above. Let $T > 0$ be such that the interval $[t_0, t^b]$ is strictly included in the interval $[t_0, t_0 + T]$. Then, for all $k \in \mathbf{N}$ there exists a constant $C > 0$ such that for all $t \in [t_0, t^b] \cup (t^b, t_0 + T]$ and for all $\varepsilon \leq |t - t^b|^{9/2}$,*

$$\left\| \psi^\varepsilon(t) - \widehat{V}_1(t) v_1^\varepsilon(t) - \sqrt{\varepsilon} \mathbf{1}_{t > t^b} \widehat{V}_2(t) v_2^\varepsilon(t) \right\|_{L^2(\mathbb{R}^d)} \leq C \varepsilon^m,$$

with an exponent $m \geq 5/9$. The components of the approximate solution are

$$v_1^\varepsilon(t) = \mathcal{U}_{h_1}^\varepsilon(t, t_0) g_{z_0}^{\Gamma_0, \varepsilon} \quad \text{and} \quad v_2^\varepsilon(t) = \mathcal{U}_{h_2}^\varepsilon(t, t^b) v_2^\varepsilon(t^b)$$

$$\text{with } v_2^\varepsilon(t^b) = \gamma^b e^{iS^b/\varepsilon} \mathbf{WP}_{z^b}^\varepsilon(\mathcal{T}^b \varphi_0(t^b)),$$

where $\varphi_0(t) = g_0^{\Gamma_1(t, t_0, z), 1}$ is the leading order profile of the coherent state $v_1^\varepsilon(t)$ given by Theorem 2.2, and

$$\gamma^b = \gamma(t^b, z^b) = \|(\{v, \Pi_2\} + \partial_t \Pi_2) \vec{V}_1(t^b, z^b)\|_{\mathbb{C}^N}.$$

The transition operator $\mathcal{T}^b = \mathcal{T}_{\mu^b, \alpha^b, \beta^b}$ is defined by the parameters

$$\mu^b = \frac{1}{2}(\partial_t f + \{v, f\})(t^b, z^b) \text{ and } (\alpha^b, \beta^b) = Jd_z f(t^b, z^b).$$

The constant $C = C(T, k, z_0, \Gamma_0) > 0$ is ε -independent but depends on the Hamiltonian $H(t, z)$, the final time T , and on the initial wave packet's center z_0 and width Γ_0 .

Note that by the transversality assumption we have $\mu^b \neq 0$, which guarantees that $\mathcal{T}^b \varphi_0(t^b)$ is Schwartz class. The coefficient γ^b quantitatively describes the distortion of the eigenprojector $\Pi_1(t)$ during its evolution along the flow generated by $h_1(t)$. If the matrix $H(t, z)$ is diagonal (or diagonalizes in a fixed orthonormal basis that is (t, z) -independent), then $\gamma^b = 0$: the equations are decoupled (or can be decoupled), and one can then apply the result for a system of two independent equations with a scalar Hamiltonian and, of course, there is no interaction of order $\sqrt{\varepsilon}$ between the modes.

The previous theorem extends to more general wave packets as defined in (2.6) and also holds with respect to Σ_k^ε -norms for $k \in \mathbf{N}$ (see [7, Theorem 3.8]). As mentioned alongside the proof [7], the argument contains the germs for a full asymptotic expansion in powers of $\sqrt{\varepsilon}$ (with $\log \varepsilon$ corrections).

Example 4.3. Notice that for the toy model $H_{k, \theta}$, we have at any point of $\Upsilon = \{x = 0\}$,

$$\mu^b = \frac{k}{2}, \quad \alpha^b = 0, \quad \beta^b = -k, \quad \gamma^b = \frac{|\theta|}{2},$$

and $\mathcal{T}^b \varphi(y) = \sqrt{\frac{2\pi}{ik}} e^{\frac{k}{2i} y^2} \varphi(y)$ for all $\varphi \in \mathcal{S}(\mathbb{R})$ and all $y \in \mathbb{R}$. Besides, if $t_0 \leq 0$, the trajectories of the minus mode that reach Υ are those arising from points $z = (q, p)$ with $q < 0$. One then has $t^b = t_0 - q$, $p^b = p - kq$ and the trajectory on the plus mode issued from $z^b = (0, p^b)$ is

$$\Phi_+^{t, t^b}(0, p^b) = (t - t^b, p^b - k(t - t^b)) = (t - t_0 + q, p - 2kq - k(t - t_0)).$$

4.2 Towards a Herman–Kluk approximation

The preceding result implies that the leading order of the propagation is still driven by the modes in which the initial data had been taken and we have an Herman–Kluk formula similar to the one obtained in the adiabatic regime, however, with a remainder

which is worse. One can conjecture that a more accurate Herman–Kluk approximation holds in a weaker sense (see [8]). We define the operator $\mathcal{J}_{sc}^\varepsilon(t)$ by its actions on functions of the form

$$\psi_0^\varepsilon = \widehat{V}_0 v_0^\varepsilon + O(\sqrt{\varepsilon}) \text{ in } L^2(\mathbb{R}^d)$$

with $v_0^\varepsilon \in L^2(\mathbb{R}^d)$ as

$$\begin{aligned} \mathcal{J}_{sc}^\varepsilon(t) \psi_0^\varepsilon(x) &= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \vec{U}_1(t, t_0, z) e^{\frac{i}{\varepsilon} S_1(t, t_0, z)} g_{\Phi_{h_1}^{t, t_0}(z)}^\varepsilon dz + \sqrt{\varepsilon} (2\pi\varepsilon)^{-d} \\ &\times \int_{\mathbb{R}^{2d}} \mathbf{1}_{t > t^b(z)} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \vec{U}_2(t, t^b(z), z) e^{\frac{i}{\varepsilon} S_1(t^b(z), t_0, z) + \frac{i}{\varepsilon} S_2(t, t^b(z), \mathfrak{z}^b(z))} g_{\Phi_{h_2}^{t, t^b(z)}(\mathfrak{z}^b)}^\varepsilon dz \end{aligned}$$

with $\mathfrak{z}^b(z) = \Phi_{h_1}^{t^b(z), t_0}(z)$ and with some adequate formula (taking into account the transfer coefficients $\gamma^b(z)$) for the prefactor $\vec{U}_2(t, t^b(z), z) = v_2(t, t^b(z), z) \vec{V}_2(t, t^b(z), \mathfrak{z}^b(z))$.

The conjecture is, that if Assumptions (SC) are satisfied, then, for all $\chi \in \mathcal{C}_0^\infty(\mathbb{R})$, in $L^2(\mathbb{R}^d)$, one has

$$\int_{\mathbb{R}} \chi(t) (\mathcal{J}_{sc}^\varepsilon(t) \psi_0^\varepsilon - \mathcal{U}_H^\varepsilon(t, t_0) \psi_0^\varepsilon) dt = o(\sqrt{\varepsilon}) \quad (4.1)$$

Estimates that are ‘‘averaged in time’’ have been previously obtained for systems (see [10, 5, 6] for example). They correspond to an observation period that is a short, but non negligible, time interval.

An approximation as (4.1) can be easily proved for the toy-model (1.2) (see Section 5.5) below. The proof in the general case is work in progress [8]. It involves more refined estimates than those of Theorem 3.3, that we present in the next section.

The authors believe that the technics used for treating the apparition of a new contribution when trajectories reach a hypersurface (the crossing one in this special case) will be useful for developing Herman–Kluk approximations for avoided crossings and conical ones, using the hopping trajectories of [6] and [5] respectively. However, we point out, that conical crossings pose the additional difficulty that Gaussians states do not remain Gaussian, even at leading order, as emphasized in [12].

5 A sketchy proof for Herman–Kluk approximations

We consider here the scalar and the adiabatic case and we discuss the proof of Theorems 2.1 and 3.3.

5.1 The proof strategy

As mentioned in the introduction, the underlying idea for constructing Gaussian based approximations for unitary propagators is to start from equation (1.9). Let us develop a proof strategy based on this idea.

Step 1. For each $z \in \mathbb{R}^{2d}$, we build a thawed wave packet approximation $\psi_{\text{th},z}^\varepsilon(t)$ to the Schrödinger system (1.1) with initial data

$$\psi_{|t=t_0}^\varepsilon = \psi_0^\varepsilon = \begin{cases} g_z^\varepsilon & \text{for } N = 1, \\ \widehat{V}_0 g_z^\varepsilon & \text{for } N > 1. \end{cases}$$

We prove that $\psi_{\text{th},z}^\varepsilon(t)$ satisfies an evolution equation of the form

$$i\varepsilon \partial_t \psi_{\text{th},z}^\varepsilon(t) = \widehat{H}(t) \psi_{\text{th},z}^\varepsilon(t) + \varepsilon^2 R_z^\varepsilon(t), \quad \psi_{\text{th},z}^\varepsilon(t_0) = \psi_0^\varepsilon \quad (5.1)$$

with source term $R_z^\varepsilon(t)$.

Step 2. For the thawed Gaussian propagation of general initial data

$$\psi_{|t=t_0}^\varepsilon = \psi_0^\varepsilon = \begin{cases} v_0^\varepsilon & \text{for } N = 1, \\ \widehat{V}_0 v_0^\varepsilon & \text{for } N > 1, \end{cases}$$

with $v_0^\varepsilon \in L^2(\mathbb{R}^d, \mathbb{C})$ we consider

$$\mathcal{I}_{\text{th}}^\varepsilon(t, t_0) \psi_0^\varepsilon = (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \psi_{\text{th},z}^\varepsilon(t) dz.$$

The error $e_{\text{th}}^\varepsilon(t) = \mathcal{U}_H^\varepsilon(t, t_0) \psi_0^\varepsilon - \mathcal{I}_{\text{th}}^\varepsilon(t, t_0) \psi_0^\varepsilon$ satisfies the evolution equation

$$i\varepsilon \partial_t e_{\text{th}}^\varepsilon(t) = \widehat{H}(t) e_{\text{th}}^\varepsilon(t) + \varepsilon^2 \Sigma_{\text{th}}^\varepsilon(t), \quad e_{\text{th}}^\varepsilon(t_0) = 0$$

with source term

$$\Sigma_{\text{th}}^\varepsilon(t) = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi_0^\varepsilon \rangle R_z^\varepsilon(t) dz.$$

Since $\widehat{H}(t)$ is self-adjoint, the usual energy argument provides

$$\|e_{\text{th}}^\varepsilon(t)\| \leq \varepsilon \int_{t_0}^t \|\Sigma_{\text{th}}^\varepsilon(s)\| ds.$$

Step 3. For analysing the source term $\Sigma_{\text{th}}^\varepsilon(t)$, we consider the integral operator

$$\psi \mapsto (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle R_z^\varepsilon(t) dz$$

and its Bargmann kernel

$$k_{\mathcal{B}}(t; X, Y) = (2\pi\varepsilon)^{-2d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, g_Y^\varepsilon \rangle \langle g_X^\varepsilon, R_z^\varepsilon(t) \rangle dz, \quad X, Y \in \mathbb{R}^{2d}.$$

We aim at establishing constants $C_1(t), C_2(t) > 0$, that do not depend on the semiclassical parameter ε , such that

$$\sup_X \int_{\mathbb{R}^{2d}} |k_{\mathcal{B}}(t; X, Y)| dY \leq C_1(t), \quad \sup_Y \int_{\mathbb{R}^{2d}} |k_{\mathcal{B}}(t; X, Y)| dX \leq C_2(t), \quad (5.2)$$

since then, by the Schur test,

$$\|\Sigma_{\text{th}}^\varepsilon(t)\| \leq \sqrt{C_1(t)C_2(t)} \|\psi_0^\varepsilon\|.$$

Step 4. For systems, that is, for $N > 1$, we use the additional observation that

$$\begin{aligned} \mathcal{J}_{\text{th}}^\varepsilon(t, t_0) \psi_0^\varepsilon &= (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \vec{V}(t, t_0, \Phi_h^{t, t_0}(z)) e^{i\varepsilon S(t, t_0, z)} g_{\Phi_h^{t, t_0}(z)}^{\Gamma(t, t_0, z), \varepsilon} dz + O(\varepsilon). \end{aligned}$$

Step 5. We turn the thawed propagation in a frozen one, in proving that

$$\mathcal{J}_{\text{th}}^\varepsilon(t, t_0) = \mathcal{J}_{\text{fr}}^\varepsilon(t, t_0) + O(\varepsilon)$$

in the norm of bounded operators on $L^2(\mathbb{R}^d)$, where the frozen propagator is defined by the Herman–Kluk formula

$$\mathcal{J}_{\text{fr}}^\varepsilon(t, t_0) \psi_0^\varepsilon = (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle g_z^\varepsilon, v_0^\varepsilon \rangle \vec{U}(t, t_0, z) e^{i\varepsilon S(t, t_0, z)} g_{\Phi_h^{t, t_0}(z)}^\varepsilon dz$$

with

$$\vec{U}(t, t_0, z) = \begin{cases} u_0(t, t_0, z) & \text{for } N = 1, \\ u_0(t, t_0, z) \vec{V}(t, t_0, \Phi_h^{t, t_0}(z)) & \text{for } N > 1. \end{cases}$$

Once the previous steps have been carried out, we have proven the basic $J = 0$ version of the scalar Herman–Kluk formula of Theorem 2.1 and its generalization to the adiabatic situation given in Theorem 3.3.

5.2 The thawed remainder

We first consider scalar wave packet propagation as described in Theorem 2.2 with an accuracy of order ε , that is, for $N_0 = 1$. The corresponding thawed Gaussian wave packet $\psi_{\text{th}, z}^\varepsilon(t)$ that is defined by the right hand side of (2.7) satisfies an evolution equation of the form (5.1) with a source term

$$R_z^\varepsilon(t) = e^{i\varepsilon S(t, t_0, z)} \text{op}_\varepsilon^w(L_z(t, t_0)) g_{\Phi_h^{t, t_0}(z)}^{\Gamma(t, t_0, z), \varepsilon},$$

where $w \mapsto L_z(t, t_0, w)$ is a smooth function, that is polynomially bounded. It depends on the remainder of Taylor expansions of $h(t, \cdot)$ around the point $\Phi_h^{t, t_0}(z)$, see [4, Section 4.3.1]. For adiabatic propagation by systems with eigenvalue gaps, as presented in Theorem 3.3, we work with

$$\psi_{\text{th}, z}^\varepsilon(t) = e^{i\varepsilon S(t, t_0, z)} \widehat{\vec{V}(t, t_0)} \left(1 + \sqrt{\varepsilon} \vec{a}(t, t_0, z) \cdot \frac{x - q(t, t_0, z)}{\sqrt{\varepsilon}} \right) g_{\Phi_h^{t, t_0}(z)}^{\Gamma(t, t_0, z), \varepsilon},$$

where the vector $\vec{a}(t, t_0, z; x)$ can be constructed explicitly. This wave packet satisfies an evolution equation of the form (5.1) with source term

$$R_z^\varepsilon(t) = e^{i\varepsilon S(t, t_0, z)} \text{op}_\varepsilon^w(\vec{L}_z(t, t_0)) g_{\Phi_h^{t, t_0}(z)}^{\Gamma(t, t_0, z), \varepsilon},$$

where the vector-valued function $w \mapsto \vec{L}_z(t, t_0, w)$ contains remainder terms of Taylor expansions of $h(t, \cdot)$ around the classical trajectory. We note that $\vec{L}_z(t, t_0, \cdot)$ has contributions both in the range of $\vec{V}(t, t_0, \cdot)$ but also in the orthogonal complement.

5.3 The Schur estimate

We now analyse the Bargmann kernel of the source term $\Sigma_{\text{th}}^\varepsilon(t)$. Since

$$|\langle g_z^\varepsilon, g_Y^\varepsilon \rangle| = e^{-\frac{|Y-z|^2}{4\varepsilon}},$$

we have

$$|k_{\mathcal{B}}(t; X, Y)| \leq (2\pi\varepsilon)^{-2d} \int_{\mathbb{R}^{2d}} e^{-\frac{|Y-z|^2}{4\varepsilon}} |\langle g_X^\varepsilon, R_z^\varepsilon(t) \rangle| dz.$$

Hence, the crucial estimate that is required concerns the Bargmann transform of the remainder $R_z^\varepsilon(t)$. We write the remainder as

$$R_z^\varepsilon(t) = e^{\frac{i}{\varepsilon}S(t, t_0, z)} \text{op}_\varepsilon^w(L_z(t, t_0)) g_{\Phi_z}^{\Gamma_z, \varepsilon},$$

where $w \mapsto L_z(t, t_0, w)$ is a smooth function on phase space, that grows at most polynomially, and $\Gamma_z = \Gamma(t, t_0, z)$, $\Phi_z = \Phi^{t, t_0}(z)$ are short-hand notations for the classical quantities defined in (2.1) and (2.8), respectively. We express the Bargmann transform as a phase space integral

$$\langle g_X^\varepsilon, R_z^\varepsilon(t) \rangle = e^{\frac{i}{\varepsilon}S(t, t_0, z)} \int_{\mathbb{R}^{2d}} L_z(t, t_0, w) \text{Wig}(g_X^\varepsilon, g_{\Phi_z}^{\Gamma_z, \varepsilon})(w) dw$$

with respect to the cross-Wigner function of two Gaussian wave packets with different centers and different width. One can prove (see [20, Lemma 5.20]) that

$$\begin{aligned} & \text{Wig}(g_X^\varepsilon, g_{\Phi_z}^{\Gamma_z, \varepsilon})(w) \\ &= (\pi\varepsilon)^{-d} \gamma_{X, z} \exp\left(\frac{i}{\varepsilon}J(X - \Phi_z) \cdot w + \frac{i}{2\varepsilon}G_z(t)(w - m_{X, z}) \cdot (w - m_{X, z})\right), \end{aligned}$$

where $m_{X, z} = \frac{1}{2}(X + \Phi_z)$ is the mean of the two centres, while $\gamma_{X, z}$ is a complex number with $|\gamma_{X, z}| \leq 1$ and $G_z(t) \in \mathfrak{S}^+(2d)$. Repeated integration by parts, see [20, Proposition 5.21], yields an upper bound

$$|\langle g_X^\varepsilon, R_z^\varepsilon(t) \rangle| \leq c_z(t) \left\langle \frac{X - \Phi^{t, t_0}(z)}{\sqrt{\varepsilon}} \right\rangle^{-(d+1)},$$

where the constant $c_z(t) > 0$ depends on bounds of the function $L_z(t, t_0, w)$ and is inversely proportional to the smallest eigenvalue of $\mathfrak{I}G_z(t)$. A combination of arguments given in the proofs of [20, Lemma 5.18] and [24, Lemma 3.2], reveals that the spectrum of $\mathfrak{I}G_z(t)$ is bounded away from zero uniformly in z , which implies the existence of constant $c(t) > 0$ such that

$$|\langle g_X^\varepsilon, R_z^\varepsilon(t) \rangle| \leq c(t) \left\langle \frac{X - \Phi^{t, t_0}(z)}{\sqrt{\varepsilon}} \right\rangle^{-(d+1)}.$$

This gives us enough decay to deduce the existence of constants $C_1(t), C_2(t) > 0$ such that the Schur estimate (5.2) holds.

5.4 Passing from thawed to frozen approximation

Here we present a slight variant of [24, Proposition 4.1] for passing from a thawed to a frozen Gaussian approximation by a linear deformation argument.

Proposition 5.1. *Let $\vec{U}(t, t_0, z)$ be a smooth function with values in \mathbb{C}^N , $N \geq 1$, whose derivatives are at most of polynomial growth. Then,*

$$\begin{aligned} & (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle \vec{U}(t, t_0, z) e^{\frac{i}{\varepsilon} S(t, t_0, z)} g_{\Phi_h^{t, t_0}(z)}^{\Gamma(t, t_0, z), \varepsilon} dz \\ &= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle u_0(t, t_0, z) \vec{U}(t, t_0, z) e^{\frac{i}{\varepsilon} S(t, t_0, z)} g_{\Phi_h^{t, t_0}(z)}^\varepsilon dz + O(\varepsilon) \end{aligned}$$

uniformly for all $\psi \in L^2(\mathbb{R}^d, \mathbb{C})$ with norm one.

Proof. For notational simplicity, we omit the time-dependance in $S = S(t, t_0, z)$, $\Phi = \Phi_h^{t, t_0}(z)$, $\Gamma = \Gamma(t, t_0, z)$, and $\vec{U} = \vec{U}(t, t_0, z)$. We consider both operators, the thawed and the frozen one, as special members of a class of linear operators of the form

$$\mathcal{I}\psi = (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle (x - \Phi_q(z))^\alpha \vec{W}(z) e^{\frac{i}{\varepsilon} S(z)} g_{\Phi(z)}^{\mathcal{G}(z), \varepsilon} dz,$$

that are defined by two smooth functions $\mathcal{G} : \mathbb{R}^{2d} \rightarrow \mathfrak{S}^+(d)$ and $\vec{W} : \mathbb{R}^{2d} \rightarrow \mathbb{C}^N$. The Siegel half-space $\mathfrak{S}^+(d)$ is invariant under inversion in the sense that any $G \in \mathfrak{S}^+(d)$ is invertible with $-G^{-1} \in \mathfrak{S}^+(d)$. We require that the smallest eigenvalue of $\mathfrak{I}(\mathcal{G}(z))$ and $\mathfrak{I}(-\mathcal{G}^{-1}(z))$ are bounded away from zero uniformly in z . The monomial powers $(x - \Phi_q(z))^\alpha$ with $\alpha \in \mathbf{N}_0^d$ are included for technical reasons, that will become clear soon. These operators are bounded on $L^2(\mathbb{R}^d)$ and satisfy

$$\|\mathcal{I}\| \leq C \varepsilon^{\lceil |\alpha|/2 \rceil}, \quad (5.3)$$

where the constant $C > 0$ independent of ε , and $\lceil |\alpha|/2 \rceil$ denotes the smallest integer $\geq |\alpha|/2$, see [20, Proposition 5.12]. We linearly link the thawed matrix function $z \mapsto \Gamma(z)$ and the frozen $z \mapsto i\text{Id}$ by setting

$$\mathcal{G}(z, s) = (1 - s)\Gamma(z) + is\text{Id} \in \mathfrak{S}^+(d), \quad s \in [0, 1],$$

and consider the corresponding Gaussian function, that is only partially normalised,

$$\tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon}(x) = (\pi\varepsilon)^{-d/4} e^{\frac{i}{\varepsilon} \Phi_p(z) \cdot (x - \Phi_q(z)) + \frac{i}{2\varepsilon} \mathcal{G}(z, s) \cdot (x - \Phi_q(z)) \cdot (x - \Phi_q(z))}.$$

We now aim at constructing a smooth function $\vec{W}(z, s)$ with two properties.

1. Firstly, we require that $\vec{W}(z, 0) = \det^{-1/2}(A(z) + iB(z))\vec{U}(z)$, ensuring that the deformation value $s = 0$ corresponds to the thawed approximation.

2. Secondly, we hope to achieve

$$\frac{\partial}{\partial s} (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle \vec{W}(z, s) e^{\frac{i}{\varepsilon} S(z)} \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon} dz = O(\varepsilon),$$

uniformly for all $\psi \in L^2(\mathbb{R}^d)$ of norm one.

Once this construction has been carried out, we will verify that the deformation yields the frozen approximation for $s = 1$, that is, $\vec{W}(z, 1) = u_0(z) \vec{U}(z)$. As a first step, we open the inner product involving the standard Gaussian g_z^ε and examine the multivariate exponential function

$$\overline{g_z^\varepsilon(y)} e^{\frac{i}{\varepsilon} S(z)} \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon}.$$

Using the derivative properties of the action $S(z)$, one obtains the identity

$$\begin{aligned} & (x - \Phi_q(z)) \overline{g_z^\varepsilon(y)} e^{\frac{i}{\varepsilon} S(z)} \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon} \\ &= \left(\frac{\varepsilon}{i} M_{\mathcal{G}(z, s)}^{-T}(z) (i\partial_q + \partial_p) - f(x, z, s) \right) \overline{g_z^\varepsilon(y)} e^{\frac{i}{\varepsilon} S(z)} \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon} \end{aligned}$$

where

$$M_{\mathcal{G}(z, s)}(z) = -i\mathcal{G}(z, s)A(z) - \mathcal{G}(z, s)B(z) + iC(z) + D(z)$$

is an invertible complex $d \times d$ and

$$f(x, z, s) = M_{\mathcal{G}(z, s)}^{-T}(z) \left(\frac{1}{2} \left((i\partial_{q_j} + \partial_{p_j}) \mathcal{G}(z, s) \right) (x - \Phi_q(z)) \cdot (x - \Phi_q(z)) \right)_{j=1}^d$$

is a vector-valued function, that is quadratic in $x - \Phi_q(z)$. Since $\frac{i}{2\varepsilon} (x - \Phi_q(z)) \cdot f(x, z, s)$ is cubic in $x - \Phi_q(z)$, we use (5.3) and recognize its contribution as a term of order ε . Thus, we have

$$\begin{aligned} & (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \langle g_z^\varepsilon, \psi \rangle \vec{W}(z, s) e^{\frac{i}{\varepsilon} S(z)} \partial_s \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon} dz \\ &= (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \vec{W}(z, s) L(z, s) (x - \Phi_q(z)) \cdot (i\partial_q + \partial_p) \langle g_z^\varepsilon, \psi \rangle e^{\frac{i}{\varepsilon} S(z)} \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon} dz + O(\varepsilon), \end{aligned}$$

with

$$L(z, s) = \frac{1}{2} M_{\mathcal{G}(z, s)}^{-1}(z) \partial_s \mathcal{G}(z, s).$$

We perform an integration by parts and arrive at

$$\begin{aligned} & - (2\pi\varepsilon)^{-d} \int_{\mathbb{R}^{2d}} \sum_{k=1}^d (i\partial_{q_k} + \partial_{p_k}) \left(\vec{W}(z, s) (L(z, s) (x - \Phi_q(z)))_k \right) \\ & \quad \times \langle g_z^\varepsilon, \psi \rangle e^{\frac{i}{\varepsilon} S(z)} \tilde{g}_{\Phi(z)}^{\mathcal{G}(z, s), \varepsilon} dz + O(\varepsilon). \end{aligned}$$

Computing the derivative we obtain several terms that are linear in $x - \Phi_q(z)$, and thus of order ε . The contributions we have to keep are

$$\begin{aligned} & -\vec{W}(z, s) \sum_{k, \ell=1}^d L(z, s)_{k\ell} (i\partial_{q_k} + \partial_{p_k})(x - \Phi_q(z))_{\ell} \\ & = \vec{W}(z, s) \sum_{k, \ell=1}^d L(z, s)_{k\ell} (iA(z) + B(z))_{\ell k} = \vec{W}(z, s) \operatorname{tr}(L(z, s)(iA(z) + B(z))). \end{aligned}$$

We observe that

$$L(z, s)(iA(z) + B(z)) = -\frac{1}{2} M_{\mathcal{G}(z, s)}^{-1}(z) \partial_s M_{\mathcal{G}(z, s)}(z).$$

This suggests that $\vec{W}(z, s)$ should solve the differential equation

$$\partial_s \vec{W}(z, s) - \frac{1}{2} \operatorname{tr} \left(M_{\mathcal{G}(z, s)}^{-1}(z) \partial_s M_{\mathcal{G}(z, s)}(z) \right) \vec{W}(z, s) = 0,$$

that is,

$$\vec{W}(z, s) = 2^{-d/2} \det^{1/2}(M_{\mathcal{G}(z, s)}(z)) \vec{U}(z),$$

by using Liouville's formula for the differentiation of determinants. Checking for the initial condition at $s = 0$, we observe that

$$\begin{aligned} M_{\mathcal{G}(z, 0)}(z) &= -i(\Gamma(z)(A(z) - iB(z)) - (C(z) - iD(z))) \\ &= -i \left(\Gamma(z) - \overline{\Gamma(z)} \right) (A(z) - iB(z)) \\ &= 2 \Im \Gamma(z) (A(z) - iB(z)) = 2 (A(z) + iB(z))^{-T} \end{aligned}$$

which implies $\vec{W}(z, 0) = \det^{-1/2}(A(z) + iB(z)) \vec{U}(z)$, indeed. \square

5.5 Herman-Kluk approximation for the toy model

The Schrödinger equation associated with (1.2) writes as a transport equation and, integrating along curves $s \mapsto (s, x + s)$ it reads

$$i\varepsilon \frac{d}{ds} \psi^\varepsilon(s, x + s) = k(x + s) V_\theta(x + s) \psi^\varepsilon(s, x + s) \quad (5.4)$$

with $V_\theta(x) = \begin{pmatrix} 0 & e^{i\theta x} \\ e^{-i\theta x} & 0 \end{pmatrix}$. The equation reduces to the system of ODEs

$$i\varepsilon \frac{d}{d\sigma} \eta^\varepsilon(\sigma) = k\sigma V_\theta(\sigma) \eta^\varepsilon(\sigma). \quad (5.5)$$

This problem was solved first in [9] then in a more general setting in [11] where an asymptotic expansion in power of $\varepsilon^{1/2}$ (with power of $\log \varepsilon$ corrections), at any order, is established for $\mathcal{R}_{k, \theta}^\varepsilon(\sigma, \sigma_0)$, the propagator (or resolvent matrix) of the linear differential equation (5.5); we shall use this result below. It is then possible to prove the Herman-Kluk approximation of the conjecture (4.1).

Proposition 5.2. Consider $t_0 < 0$ and an initial data of the form

$$\psi_0^\varepsilon = \vec{V}_- v_0^\varepsilon + O(\varepsilon) \text{ in } L^2(\mathbb{R}^d), \quad (5.6)$$

where \vec{V}_- is the smooth eigenvector for the minus mode (see (1.3)). Set

$$\begin{aligned} \mathcal{I}_{sc}^\varepsilon(v_0^\varepsilon) &= (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle v_0^\varepsilon, g_z^\varepsilon \rangle e^{\frac{i}{\varepsilon} S_-(t, t_0, q)} \vec{V}_-(t, t_0, q + t - t_0) g_{\Phi_-^{t, t_0}(z)}^\varepsilon dz \\ &\quad + \sqrt{\varepsilon} \kappa_- (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \mathbf{1}_{q>0} \mathbf{1}_{t>t^b(z)} \langle v_0^\varepsilon, g_z^\varepsilon \rangle e^{\frac{i}{\varepsilon} (S_-(t_0, t^b(z), q) + S_+(t, t^b(z), 0))} \\ &\quad \times \vec{V}_+(t, t^b(z), t - t^b(z)) g_{\Phi_+^{t, t^b(z)}(0, p^b(z))}^{\varepsilon, 1-ik} dz \end{aligned} \quad (5.7)$$

where $\kappa := \sqrt{\frac{2\pi}{ik}} \frac{\theta}{2}$ and for $z = (q, p)$, $t^b(z) = t_0 - q$, and $p^b(z) = p - kq$ have been computed in Example 4.3. Then, for all $\chi \in L^1(\mathbb{R})$, in $L^2(\mathbb{R}^d)$

$$\int_{\mathbb{R}} \chi(t) \left(\mathcal{I}_{sc}^\varepsilon(v_0^\varepsilon) - \mathcal{U}_{H_{k,\theta}}^\varepsilon(t, t_0) \psi_0^\varepsilon(x) \right) dt = o(\sqrt{\varepsilon}).$$

The scalar Herman-Kluk prefactor is 1 because the width of the Gaussians wave packet stays constant along the propagation (see Ex. 2.3). Note also (see Ex. 4.3)

$$\mathcal{F}^b g^1(y) = e^{-\frac{i}{2\varepsilon} k y^2} g^1 = g^{1, (1-ik/2)},$$

in the statement above, we have chosen not to freeze the Gaussian after crossing time. The value of the coefficient κ arises from Theorem 4.2 and Ex. 4.3.

The proof relies on the analysis of the propagator $\mathcal{R}_{k,\theta}^\varepsilon(\sigma, \sigma_0)$ as performed in [11] (see p. 280 therein). We denote by $Y_\pm(\sigma, \sigma_0)$ the time-dependent eigenprojectors of $V_\theta(\sigma)$ for the eigenvalues $E_\pm(\sigma) = \pm k\sigma$ (see Remark 3.2):

$$\vec{Y}_\pm(\sigma, \sigma_0) = \vec{V}_\pm(\sigma, \sigma_0, \sigma) = \vec{V}_\pm(\sigma + r, \sigma_0 + r, \sigma), \quad \forall r \in \mathbb{R}. \quad (5.8)$$

Then, the solutions $\eta(\sigma)$ with initial data at time $\sigma_0 < 0$ of the form $\eta(\sigma_0) = \eta_0 \vec{Y}_-(\sigma_0)$:

1. If $\sigma < 0$, then $\eta(\sigma) = e^{\frac{i}{\varepsilon} k \int_{\sigma_0}^\sigma \tau d\tau} \vec{Y}_-(\sigma, \sigma_0) \eta_0 + O(\varepsilon)$.

2. If $\sigma > 0$, then

$$\begin{aligned} \eta(\sigma) &= e^{\frac{i}{\varepsilon} k \int_{\sigma_0}^\sigma \tau d\tau} \vec{Y}_-(\sigma, \sigma_0) \eta_0 \\ &\quad - \sqrt{\varepsilon} (1-i) \sqrt{\pi} (-k)^{-1/2} h(0) e^{\frac{i}{\varepsilon} \lambda} e^{-\frac{i}{\varepsilon} k \int_0^\sigma \tau d\tau} \vec{Y}_+(\sigma, 0) \eta_0 + O(\varepsilon) \end{aligned}$$

with $h(0) = \left(\vec{Y}_+(\sigma, 0), \frac{d}{d\sigma} \vec{Y}_-(\sigma, 0) \right) \Big|_{\sigma=0} = -i\theta/2$ and $\lambda = k \int_{\sigma_0}^0 \tau d\tau$.

We observe that, with the notations of Ex. 4.3,

$$-(1-i)\sqrt{\pi}(-k)^{-1/2}h(0) = \sqrt{\frac{2\pi}{ik}} \frac{\theta}{2} = \sqrt{\frac{2\pi}{ik}} \gamma^b = \kappa.$$

Proof of Proposition 5.2. By (5.4),

$$\psi^\varepsilon(t, x) := \mathcal{W}_{H_{k,\theta}}^\varepsilon(t, t_0) \Psi_0^\varepsilon(x) = \mathcal{R}_{k,\theta}^\varepsilon(x, x-t+t_0) \Psi_0^\varepsilon(x-t+t_0),$$

and, in view of Friedrichs' description, we deduce

$$\begin{aligned} \psi^\varepsilon(t, x) = & e^{\frac{ik}{\varepsilon}x(t-t_0) - \frac{ik}{2\varepsilon}(t-t_0)^2} \vec{V}_-(t, t_0, x) v_0^\varepsilon(x-t+t_0) \\ & + \sqrt{\varepsilon} \kappa \mathbf{1}_{0 < x < t-t_0} e^{\frac{ik}{\varepsilon}x(t-t_0) - \frac{ik}{2\varepsilon}(t-t_0)^2 - \frac{i}{\varepsilon}x^2} v_0^\varepsilon(x-t+t_0) \vec{V}_+(x, 0, x) + o(\sqrt{\varepsilon}) \end{aligned}$$

where we have used

$$\vec{Y}_-(x, x-t+t_0) = \vec{V}_-(t, t_0, x), \quad \vec{Y}_+(\sigma, 0) = \vec{V}_+(x, 0, x) \quad \text{and} \quad \lambda = -\frac{k}{2}(x-t+t_0)^2.$$

Using (1.8), we write

$$v_0^\varepsilon(x-t+t_0) = (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle v_0^\varepsilon, g_z^\varepsilon \rangle g_z^\varepsilon(x-t+t_0) dz$$

and we observe that, in view of $S_-(t, t_0, z) = kq(t-t_0) + \frac{k}{2}(t-t_0)^2$, we have

$$g_z^\varepsilon(x-t+t_0) = e^{-\frac{ik}{\varepsilon}x(t-t_0) + \frac{i}{2\varepsilon}(t-t_0)^2} e^{\frac{i}{\varepsilon}S_-(t, t_0, z)} g_{\Phi_-^{t, t_0}(z)}^\varepsilon(x)$$

Similarly, using

$$\begin{aligned} S_+(t, t^b(z), q) &= -\frac{k}{2}(t-t_0+q)^2, \quad S_-(t^b, t_0, q) = \frac{3k}{2}q^2 \\ \text{and } \Phi_+^{t, t^b(z)}(0, p^b(z)) &= (t-t_0+q, p-2kq-k(t-t_0)), \end{aligned}$$

we obtain

$$\begin{aligned} g_z^\varepsilon(x-t+t_0) &= e^{\frac{i}{\varepsilon}k(x-t+t_0)(2q+(t-t_0))} g_{\Phi_+^{t, t^b(z)}(0, p^b(z))}^\varepsilon(x) \\ &= e^{\frac{i}{\varepsilon}S_-(t^b, t_0, q) + \frac{i}{\varepsilon}S_+(t, t^b, 0) + \frac{k}{i\varepsilon}(x-q-t+t_0)^2} g_{\Phi_+^{t, t^b(z)}(0, p^b(z))}^\varepsilon(x) \\ &= e^{\frac{i}{\varepsilon}S_-(t^b, t_0, q) + \frac{i}{\varepsilon}S_+(t, t^b, 0)} \mathbf{WP}_{\Phi_+^{t, t^b(z)}(0, p^b(z))}^\varepsilon(\mathcal{S}^b g^1) \end{aligned}$$

Putting these elements together, we are left with

$$\begin{aligned} \psi^\varepsilon(t, x) = & o(\sqrt{\varepsilon}) + (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle v_0^\varepsilon, g_z^\varepsilon \rangle e^{\frac{i}{\varepsilon}S_-(t, z)} \vec{V}_-(t, t_0, x) g_{\Phi_-^{t, t_0}(z)}^\varepsilon dz \\ & + \sqrt{\varepsilon} \kappa (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \mathbf{1}_{0 < x < t-t_0} \langle v_0^\varepsilon, g_z^\varepsilon \rangle e^{\frac{i}{\varepsilon}S_-(t^b, t_0, q) + \frac{i}{\varepsilon}S_+(t, t^b, 0)} \vec{V}_+(x, 0, x) g_{\Phi_+^{t, t^b}(z)}^\varepsilon dz. \end{aligned}$$

Using Taylor expansion and Lemma 5.3, we can transform the first part of the right-hand side of the preceding equation:

$$\begin{aligned} & (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle v_0^\varepsilon, g_z^\varepsilon \rangle e^{iS_-(t,z)} \vec{V}_-(t, t_0, x) g_{\Phi_-^{t,t_0}}^\varepsilon dz \\ &= (2\pi\varepsilon)^{-d} \int_{z \in \mathbb{R}^{2d}} \langle v_0^\varepsilon, g_z^\varepsilon \rangle e^{iS_-(t,z)} \vec{V}_-(t, t_0, q_-(t)) g_{\Phi_-^{t,t_0}}^\varepsilon dz + O(\varepsilon) \end{aligned}$$

in $L^2(\mathbb{R}^d)$, which allows to identify the first term of (5.7) since $q_-(t) = q + t - t_0$. In the second term, one can treat similarly the term $\vec{V}_+(x, 0, x)$ that turns into (using also (5.8))

$$\vec{V}(t - t_0 + q, 0, t - t_0 + q) = \vec{V}(t, t_0 - q, t - t_0 + q) = \vec{V}(t, t^b(z), t - t^b(z))$$

It remains to turn the discontinuous function $x \mapsto \mathbf{1}_{0 < x < t - t_0}$ into

$$\mathbf{1}_{0 < q_+(t) < t - t_0} = \mathbf{1}_{q < 0} \mathbf{1}_{t > t_0 - q} = \mathbf{1}_{q < 0} \mathbf{1}_{t > t^b(z)}.$$

One then takes advantage of the averaging in time to use the estimate of 5.3 despite the discontinuity. One regularizes the discontinuous function which will differ from its regularization on a set of small Lebesgue measure in the variable t . One can then use the preceding argument on the regularized term and gets rid of the correction ones by estimating them thanks to the estimate (5.3) and using the smallness of integrals on χ on sets of small Lebesgue measures. \square

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