Karlsruhe Institute of Technology

Wave phenomena
analysis and numerics

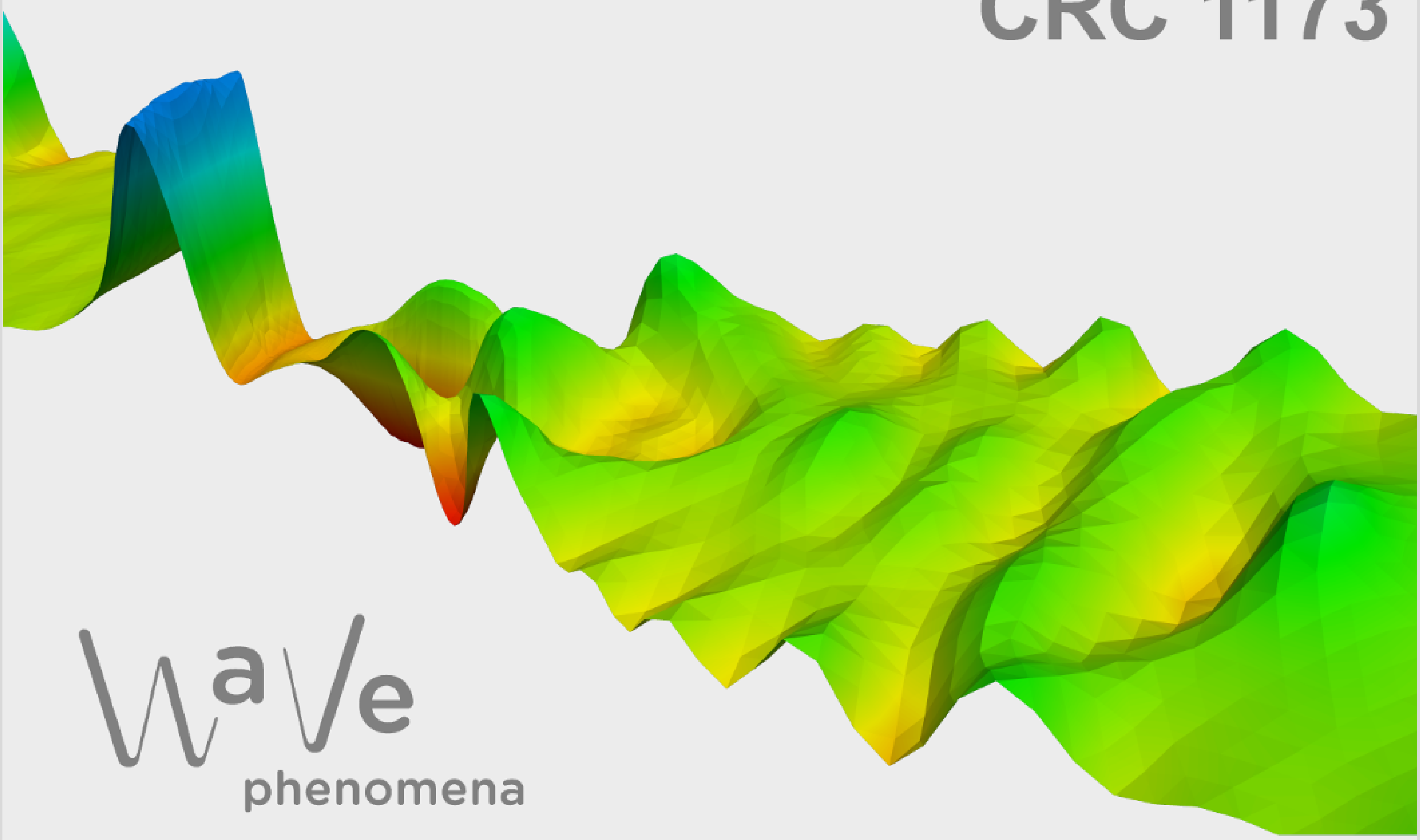
Variational Gaussian approximation for the magnetic Schrödinger equation

Selina Burkhard, Marlis Hochbruck,
Benjamin Dörich, Caroline Lasser

CRC Preprint 2023/4, January 2023

KARLSRUHE INSTITUTE OF TECHNOLOGY

CRC 1173



Wave phenomena

Participating universities

Universität Stuttgart

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

TU WIEN

Funded by

DFG

ISSN 2365-662X

VARIATIONAL GAUSSIAN APPROXIMATION FOR THE MAGNETIC SCHRÖDINGER EQUATION

SELINA BURKHARD, BENJAMIN DÖRICH, MARLIS HOCHBRUCK, AND CAROLINE LASSER

Abstract. In the present paper we consider the semiclassical magnetic Schrödinger equation, which describes the dynamics of particles under the influence of a magnetic field. The solution of the Schrödinger equation is approximated by Gaussian wave packets via the time-dependent variational formulation by Dirac and Frenkel. For the numerical approximation we derive ordinary differential equations for the parameters of the variational solution. Moreover, we prove L^2-error bounds and observable error bounds for the approximating Gaussian wave packet.

1. Introduction

In the present paper we study the semiclassical magnetic Schrödinger equation

$$\mathrm{i}\varepsilon\partial_t\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0, \quad t \in \mathbb{R}, \tag{1.1a}$$

on $\mathbb{R}^d$ with magnetic Hamiltonian

$$H(t) = \frac{1}{2}\big(\mathrm{i}\varepsilon\nabla_x + A(t,x)\big)^2 + V(t,x), \tag{1.1b}$$

and initial value $\psi_0 \in L^2(\mathbb{R}^d)$ with semiclassical parameter $0 < \varepsilon \ll 1$. Here, A is a magnetic vector potential, and V is the electric potential. This equation arises in the modeling of the quantum dynamics of nuclei in a molecule subject to external magnetic fields. From a numerical point of view, solving this time-dependent partial differential equation raises three major problems. First, it is a high-dimensional problem, since the space dimension is typically given by $d = 3N$, where N is the number of nuclear particles in the system. Further, the computational domain $\mathbb{R}^d$ is naturally unbounded, and thus most numerical methods require truncation before discretization. For the method of lines (first discretize space, then time), high dimension combined with an unbounded domain leads to inadequately if not unattractably large systems that have to be integrated in time. Another challenge is given by the high oscillations induced by the small semiclassical parameter ε. For standard time integration schemes severe stepsize restrictions have to be imposed and leave these methods impracticable.

We consider the case that the initial value ψ_0 is strongly localized and given by a Gaussian wave packet,

$$\psi_0(x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\big(\frac{1}{2}(x-q)^T\mathcal{C}(x-q) + (x-q)^Tp + \zeta\big)\Big),$$

Key words and phrases. magnetic Schrödinger equation, semiclassical analysis, variational approximation, observables.

Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) – Project-ID 2587So 4477 – SFB 1173.

where $q, p \in \mathbb{R}^d$ are the packet's position and momentum center, $\mathcal{C} \in \mathbb{C}^{d\times d}$ is the width matrix of the envelope, and $\zeta \in \mathbb{C}$ a phase and weight parameter. For $A = 0$ it is well established that it is possible to reasonably approximate the solution by a Gaussian wave packet with parameters that are evolved according to ordinary differential equations. First studies in this direction are due to K. Hepp [22] and G. Hagedorn [14] from the perspective of mathematical physics, and E. Heller [20, 21] as well as R. Coalson, M. Karplus [7] with already an eye on numerical computation. The evolution equations for the parameters of all Gaussian wave packet approximations can be classified in two categories:

Variational: The variational approach relies on the time-dependent Dirac–Frenkel principle for deriving the parameter equations of motion. By the variational construction, the Gaussian wave packet automatically inherits several conservation properties of the exact solution.

Semiclassical: The semiclassical approach expands the wave packet ansatz with respect to sthe semiclassical parameter ε and derives ε independent parameter equations by matching terms with the same order.

Both types of ordinary differential equations have the advantageous property, that their solutions are non-oscillatory. Both approximations have the same convergence order with respect to the semiclassical parameter ε in L^2-norm, and both reproduce the exact solution for Schrödinger operators with linear magnetic potential A and quadratic electric potential V. For a further discussion, we refer to [6, Chapter 10.2] for a monograph that covers the semiclassical construction and [26, Chapter II.4] or [25, Chapter 3] for a short book and a review presenting the variational case. Our main contribution in this paper is to first show that for the magnetic Schrödinger equation the variational approximation is still given by a system of ordinary differential equations for the parameters defining the Gaussian wave packet. Second, we prove rigorous error bounds for this approximation in terms of the semiclassical parameter ε. The presented results generalize the bounds established in [25, 26] to non-vanishing magnetic potentials A and further allow for time-dependencies in both the electric and the magnetic potential. This includes convergence in the L^2-norm with order $\mathcal{O}(\sqrt{\varepsilon})$ as well as for expectation values of observables, which resemble certain measurable physical quantities of the wave function, with order $\mathcal{O}(\varepsilon)$. Let us point out that the design and the analysis of time integrators for the magnetic variational equations of motion are currently under investigation.

Further wave packet results for $A = 0$. Hagedorn wave packets [14–16] are a multivariate anisotropic generalization of the Hermite functions. They are Gaussian wave packets with a polynomial prefactor, such that a family of them constitutes an orthonormal basis of $L^2(\mathbb{R}^d)$. In [1, 9, 11], time splitting integrators for Hagedorn wave packet approximations are proposed, that combine parameter propagation by ordinary differential equations with a Galerkin step. A spawning method for several families of Hagedorn wave packets is introduced in [29]. For variational Gaussian wave packets, a time splitting integrator, which is robust in the semiclassical parameter ε, is proposed in [10]. Recently in [28], the convergence of the expectation value of position and momentum is studied for a Gaussian wave packet, whose parameters evolve non-variationally but with an ε correction to the usual semiclassical construction. Due to the modification, the convergence rate is improved to $\mathcal{O}(\varepsilon^{3/2})$.

Related wave packet results for $A \neq 0$. The most general result for the semiclassical wave packet approach is given in [30, Theorem 21] of the monograph by D. Robert and M. Combescure. There, the propagation of Gaussian and Hagedorn wave packets is covered for a general class of time-dependent Hamiltonian operators $H(t)$, that includes the magnetic Schrödinger operator. The error analysis is with respect to the L^2-norm, but not for observables. The semiclassical construction there also receives corrections, such it can be accurate to order $\mathcal{O}(\varepsilon^{k/2})$ for any $k \geq 1$. An extension of the Hagedorn Galerkin method [9] to the case of magnetic Schrödinger equations is studied in [32], including an error analysis with respect to the L^2-norm. However, no error bounds for the observables are investigated there. For linear magnetic potentials of a particular structure, in [12] a problem adapted splitting method for Hagedorn wave packets is derived but without error analysis. A slightly different approach, called the Gaussian wave packet transform, is proposed for the magnetic Schrödinger equation in [33]. There, the ordinary differential equations for the Gaussian parameters are the semiclassical ones except for an additional term for the scalar parameter ζ.

Outline of the paper. The rest of the paper is structured as follows. For our error analysis we introduce the analytical framework and the variational Gaussian wave packet ansatz in Section 2. We present our main results in Section 3 including the equations for the parameters, the conservation of different quantities, the convergence in the L^2-norm and the convergence of the observables. The proofs of the corresponding results are given in Sections 4 to 7. A technical computation regarding the symbols for the observables is postponed to Appendix A.

Notation. Throughout the paper, we denote by $L^p(\mathbb{R}^d)$ the classical Lebesgue spaces, and by $\mathcal{S}(\mathbb{R}^d)$ the Schwartz space of rapidly decreasing functions. Further, we make use of the multiindex notation and let for $\alpha = (\alpha_1, \ldots, \alpha_d) \in \mathbb{N}_0^d$, $x \in \mathbb{R}^d$, $f \in \mathcal{S}(\mathbb{R}^d)$

$$|\alpha| \coloneqq \alpha_1 + \ldots + \alpha_d, \qquad x^\alpha \coloneqq x_1^{\alpha_1} \ldots x_d^{\alpha_d}, \qquad \partial^\alpha f \coloneqq \partial_1^{\alpha_1} \ldots \partial_d^{\alpha_d} f.$$

For a function $W\colon \mathbb{R}^d \to \mathbb{R}^L$, $L \geq 1$, we define the average

$$\langle W \rangle_u \coloneqq \langle u | W u \rangle \coloneqq \int_{\mathbb{R}^d} W(x) |u(x)|^2 \, \mathrm{d}x,$$

if the integral exists.

2. General setting

We first discuss the analytic framework for our analysis and introduce the Gaussian wave packets. We further call some results on the wellposedness from the literature. For the vector potential we choose the Coulomb gauge, i.e. $\operatorname{div} A = 0$. In order to shorten notation, we rewrite the Hamiltonian in (1.1b) as

$$H(t) = -\frac{\varepsilon^2}{2}\Delta + \mathrm{i}\varepsilon A(t) \cdot \nabla + \widetilde{V}(t), \qquad \widetilde{V} \coloneqq \frac{1}{2}|A|^2 + V. \tag{2.1}$$

Throughout this paper we make the following smoothness assumption on the potentials.

Assumption 2.1. *The scalar potential $V\colon \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}$ and the vector valued potential $A = (A_j)_{j=1,\ldots,d}\colon \mathbb{R} \times \mathbb{R}^d \to \mathbb{R}^d$ are infinitely often differentiable and in addition*

(a) *V is subquadratic, i.e. $\nabla^k V$ is bounded for all $k \geq 2$, and*
(b) *A is sublinear, i.e. $\nabla^k A$ is bounded for all $k \geq 1$.*

If this assumption is satisfied, then it can be shown that the initial value problem (1.1a) is well posed for initial values in a polynomially weighted scaled Sobolev space defined as follows, cf. [30, Def. 1].

Definition 2.2. Let $l, m \in \mathbb{N}_0$ and $\varepsilon \in (0, \infty)$ and let φ be a sufficiently regular function such that

$$|\varphi|_{\alpha,\beta;\varepsilon} \coloneqq \left\| \varepsilon^{|\beta|} x^\alpha \partial^\beta \varphi \right\|_{L^2} < \infty \tag{2.2}$$

for all multiindeces $\alpha, \beta \in \mathbb{N}_0^d$ with $|\alpha| \leq l, |\beta| \leq m$. Further, we define the space

$$\Sigma_{l,m}^\varepsilon \coloneqq \left\{ \varphi \in L^2(\mathbb{R}^d) \;\middle|\; |\varphi|_{\alpha,\beta;\varepsilon} < \infty \;\forall\, |\alpha| \leq l, |\beta| \leq m \right\}$$

and equip it with the norm

$$\|\varphi\|_{l,m;\varepsilon} \coloneqq \sum_{|\alpha|\leq l,\, |\beta|\leq m} |\varphi|_{\alpha,\beta;\varepsilon} < \infty.$$

Note that the space $\Sigma_{l,m}^\varepsilon$ is in fact independent of ε since the norms for different values of ε are equivalent. However, the following wellposedness result shows that the seminorm (2.2) of the solution of (1.1a) can be bounded in terms of the initial data with a constant being independent of ε.

Theorem 2.3 ([30, Prop. 123])**.** *Let Assumption 2.1 hold and let $t \in \mathbb{R}$.*

(a) *There exists a unitary evolution family $(U(t,s))_{t,s\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$ such that for all $\psi_0 \in L^2(\mathbb{R}^d)$ the solution ψ of (1.1a) is given by*
$$\psi(t) = U(t,0)\psi_0. \tag{2.3}$$
(b) *Let $\psi_0 \in \Sigma_{l,m}^\varepsilon$ for some $l, m \in \mathbb{N}_0$ and let ψ be the solution of (1.1a). Then we have*
$$\|\psi(t)\|_{l,m;\varepsilon} \leq C_{l,m} \mathrm{e}^{C_{l,m} t} \|\psi_0\|_{l,m;\varepsilon},$$
where $C_{T,\alpha,\beta}$ is independent of ε.

In the case of time-independent potentials the evolution family $(U(t,s))_{t,s\in[0,T]}$ reduces to the unitary group $(e^{-it/\varepsilon H})_{t\in\mathbb{R}}$ on $L^2(\mathbb{R}^d)$ which commutes with the Hamiltonian.

Following [25, Chapter 3], we approximate the solution ψ of (1.1a) in the manifold $\mathcal{M}$ of Gaussian wave packets given by

$$\begin{aligned} \mathcal{M} = \Big\{ g \in L^2(\mathbb{R}^d) \;\Big|\; g(x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon} \big(\frac{1}{2} (x-q)^T \mathcal{C} (x-q) + (x-q)^T p + \zeta \big) \Big), \\ q,\, p \in \mathbb{R}^d,\, \mathcal{C} = \mathcal{C}^T \in \mathbb{C}^{d\times d},\, \operatorname{Im} \mathcal{C} \text{ positive definite}, \zeta \in \mathbb{C} \Big\}. \end{aligned} \tag{2.4}$$

The approximating Gaussian wave packet is characterized by the Dirac–Frenkel variational formulation, cf. [25, 26]: seek $u(t) \in \mathcal{M}$ such that for all $t \in [0,T]$ it holds

$$\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}, \big\langle \mathrm{i}\varepsilon \partial_t u(t) - H(t)u(t) | v \big\rangle = 0 \quad \text{for all} \quad v \in \mathcal{T}_{u(t)}\mathcal{M},$$

with initial value $u(0) = u_0 \in \mathcal{M}$. Using the projection $P_u : L^2(\mathbb{R}^d) \to \mathcal{T}_u\mathcal{M}$ we can equivalently write

$$\mathrm{i}\varepsilon \partial_t u(t) = P_{u(t)}\big(H(t)u(t)\big), \quad u(0) = u_0 \in \mathcal{M}. \tag{2.5}$$

Remark 2.4. In the time-independent and non-magnetic case, one can also treat initial values $\psi_0 \notin \mathcal{M}$ using thawed and frozen Gaussians, see [25, Ch. 5]. The extension to the case (1.1b), however, is beyond the scope of the present work.

For the manifold $\mathcal{M}$ defined in (2.4) the tangent space $\mathcal{T}_u\mathcal{M}$ takes the following simple form.

Lemma 2.5 ([25, Lemma 3.1]). *For $u \in \mathcal{M}$ we have*

$$\mathcal{T}_u\mathcal{M} = \{\varphi u \,|\, \varphi \text{ } d\text{-variate complex polynomial of degree at most } 2\}\,.$$

The approximation by Gaussian wave packets seems appropriate due to the following exactness result, which is a consequence of Lemma 2.5 together with (2.5) and Theorem 2.3.

Proposition 2.6 ([25, Prop. 3.2]). *Let $V(t,\cdot)$ be quadratic and $A(t,\cdot)$ be linear in space for all $t \in [0,T]$. If $\psi_0 \in \mathcal{M}$, then the variational approximation u defined by (2.5) is exact, i.e., $u(t) = \psi(t)$, where ψ denotes the solution of (1.1a).*

In the next section we derive a system of ordinary differential equations to determine parameters of the variational solution $u \in \mathcal{M}$ and present error bounds for the variational approximation.

3. Main results

In the remaining paper we consider (1.1a) and (2.5) for initial data satisfying

$$\psi_0 = u_0 \in \mathcal{M} \quad \text{and} \quad \|u_0\|_{L^2} = 1. \tag{3.1}$$

Our first step is to derive equations of motions for the parameters defining the variational solution u. Then we show that in the limit $\varepsilon \to 0$, these equations tend to classical equations of motions. Moreover, we study geometric properties of the solution and the variational approximation. Finally, we state error bounds for the solution in the L^2-norm and for averages of observables. Our work generalizes the results in [25] in the sense that we treat time-dependent, magnetic Hamiltonians. For the sake of readability, we postpone the proofs to Sections 4 to 7.

3.1. Semiclassical equations of motion.

In order to write equations of motion for the parameters of a Gaussian wave packet $u \in \mathcal{M}$ we use the short notation

$$\begin{aligned} \mathcal{C}_{\mathrm{R}} &= \operatorname{Re}\mathcal{C}, & \mathcal{C}_{\mathrm{I}} &= \operatorname{Im}\mathcal{C}, \\ v &= (v_j)_{j=1}^d \in \mathbb{C}^d, & A &= (A_j)_{j=1}^d, \\ J_A &= \big(\partial_j A_k\big)_{j,k=1}^d, & (D^2_{A,v})_{k,l} &= \textstyle\sum_{j=1}^d \partial_l\partial_k A_j v_j. \end{aligned}$$

We start by deriving two equivalent sets of equations for $0 < \varepsilon \ll 1$. In the following section, we discuss the limit $\varepsilon \to 0$ and show that the two sets lead to different formulations of classical equations of motion for charged particles in a magnetic field.

Theorem 3.1. *Let u_0 satisfy (3.1) and be given by its parameters $q_0, p_0, \mathcal{C}_0, \zeta_0$ defined in (2.4). Then, the parameters of the solution $u \in \mathcal{M}$ of (2.5) satisfy*

$$\dot q = p - \langle A\rangle_u, \tag{3.2a}$$

$$\dot p = \frac{\varepsilon}{2}\left\langle \nabla \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\right)\right\rangle_u + \langle J_A\rangle_u^T p - \langle \nabla \widetilde V\rangle_u, \tag{3.2b}$$

$$\begin{aligned}\dot{\mathcal{C}} = &-\mathcal{C}^2 + \langle D^2_{A,p}\rangle_u + \langle J_A\rangle_u^T \mathcal{C} + \mathcal{C}\langle J_A\rangle_u - \langle \nabla^2 \widetilde V\rangle_u. \\ &+ \frac{\varepsilon}{2}\left\langle \nabla^2 \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\right)\right\rangle_u,\end{aligned} \tag{3.2c}$$

$$\begin{aligned}\dot\zeta = &\frac12 |p|^2 + \frac{\varepsilon}{2}\left\langle \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\right)\right\rangle_u + \frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C}) \\ &- \frac{\varepsilon}{4}\mathrm{tr}\Big(\mathcal{C}_\mathrm{I}^{-1}\big(\frac{\varepsilon}{2}\left\langle \nabla^2 \mathrm{tr}\left(J_A^T \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\right)\right\rangle_u + \langle J_A\rangle_u^T \mathcal{C}_\mathrm{R} + \mathcal{C}_\mathrm{R}\langle J_A\rangle_u + \langle D^2_{A,p}\rangle_u\big)\Big) \\ &- \langle \widetilde V\rangle_u + \frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_\mathrm{I}^{-1}\langle \nabla^2 \widetilde V\rangle_u\big),\end{aligned} \tag{3.2d}$$

with initial data $(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0)$.

The proof of Theorem 3.1 is given in Section 4.

Remark 3.2. In order to solve (3.2) numerically, one might adapt the Boris algorithm originally proposed in [2] and recently analyzed in [17, 18]. This algorithm is constructed for the classical equations of motion for charged particle systems. Details or an efficient numerical algorithm are ongoing work which will be presented elsewhere.

An alternative approach presented in [25] makes use of a factorization of the width matrix $\mathcal{C}$ due to Hagedorn. For the magnetic Schrödinger equation, it leads to differential equations for the factors of $\mathcal{C}$ instead of (3.2c). By [25, Lemma 3.16], we can write

$$\mathcal{C} = PQ^{-1} \quad \text{and} \quad \mathrm{Im}\,\mathcal{C} = (QQ^*)^{-1}, \tag{3.3}$$

with complex, invertible, and symplectic matrices P and Q. The latter means that for

$$Y := \begin{pmatrix}\mathrm{Re}\,Q & \mathrm{Im}\,Q \\ \mathrm{Re}\,P & \mathrm{Im}\,P\end{pmatrix} \qquad \text{and} \qquad J := \begin{pmatrix} 0 & -\mathrm{Id} \\ \mathrm{Id} & 0\end{pmatrix} \in \mathbb{R}^{2d\times 2d} \tag{3.4}$$

it holds $Y^T J Y = J$, or equivalently

$$Q^T P - P^T Q = 0, \tag{3.5a}$$

$$Q^* P - P^* Q = 2\mathrm{i}\,\mathrm{Id}. \tag{3.5b}$$

In fact, if Q and P are complex matrices satisfying (3.5), then Q and P are invertible and the matrix $\mathcal{C} = PQ^{-1}$ is symmetric with positive definite imaginary part $(QQ^*)^{-1}$. This allows us to write the Gaussian wave packet (2.4) as

$$u(\cdot, x) = \exp\Big(\frac{\mathrm{i}}{\varepsilon}\Big(\frac12 (x-q)^T PQ^{-1}(x-q) + p^T(x-q) + \zeta\Big)\Big) \tag{3.6}$$

and to derive equations of motion for the parameters (q, p, Q, P, ζ).

Theorem 3.3. *Let u_0 satisfy (3.1) and be given by the parameters $q_0, p_0, \mathcal{C}_0, \zeta_0$. Then the Gaussian wave packet (3.6) with parameters (q, p, Q, P, ζ) solving*

$$\dot Q = P - \langle J_A\rangle_u Q,$$

$$\dot P = \langle J_A\rangle_u^T P + \frac{\varepsilon}{2}\left\langle \nabla^2 \mathrm{tr}\left(J_A \mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\right)\right\rangle_u Q + \left\langle D^2_{A,p}\right\rangle_u Q - \left\langle \nabla^2 \widetilde V\right\rangle_u Q,$$

and (3.2a), (3.2b), *and* (3.2d) *is the variational solution* (2.5) *with initial data*

$$(q(0), p(0), \mathcal{C}(0), \zeta(0)) = (q_0, p_0, \mathcal{C}_0, \zeta_0).$$

If the initial matrices Q_0 *and* P_0 *are symplectic, then* $Q(t)$ *and* $P(t)$ *are symplectic for all times* $t \geq 0$.

In [24], the same equations (3.7) are derived using a different approach and the authors show that the flow of (3.7) is symplectic. The proof of Theorem 3.3 is given in Section 4.

3.2. **Equations of motion in the limit** $\varepsilon \to 0$**.** The classical, time-dependent Hamiltonian function for charged particles in a magnetic field is given by

$$h(t, q, p) = \frac{1}{2}|p|^2 - A(t, q) \cdot p + \frac{1}{2}|A(t, q)|^2 + V(t, q), \tag{3.8}$$

cf. [13, 19]. The Hamiltonian function (3.8) induces the non-autonomous classical Hamiltonian system

$$\begin{aligned} \begin{pmatrix} \dot{q}(t) \\ \dot{p}(t) \end{pmatrix} &= J^{-1}\nabla h(t, q(t), p(t)) \\ &= \begin{pmatrix} p(t) - A(t, q(t)) \\ J_A^T(t, q(t))p(t) - \frac{1}{2}\nabla|A(t, q(t))|^2 - \nabla V(t, q(t)) \end{pmatrix} \end{aligned} \tag{3.9}$$

with initial data $q(s) = q_s, p(s) = p_s$ and with J defined in (3.4). We denote by

$$\Phi^{t,s} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}, \ (q_s, p_s) \mapsto (q_s(t), p_s(t))$$

the classical flow, which maps initial values at time s to the solution of (3.9) at time t and abbreviate $\Phi^{t,0} := \Phi^t$.

The bound in [25, Lemma 3.15] states that $\langle \cdot \rangle_u$ tend to point evaluations at q as $\varepsilon \to 0$, i.e., $\langle A \rangle_u \to A(q)$. Hence, we observe that the magnetic equations of motion (3.2a) and (3.2b) tend to classical equations (3.9) as $\varepsilon \to 0$ and (3.2d) to

$$\dot{\zeta} = \frac{1}{2}|p|^2 - \widetilde{V}(\cdot, q).$$

In order link the set of equations (3.7) to classical mechanics, we consider the linearization of (3.8) along the position and momentum parameters (q, p), i.e.,

$$\begin{aligned} \begin{pmatrix} \dot{Q} \\ \dot{P} \end{pmatrix} &= J^{-1}\nabla^2 h(\cdot, p, q) \begin{pmatrix} Q \\ P \end{pmatrix} \\ &= \begin{pmatrix} P - J_A(\cdot, q)Q \\ \left(D^2_{A(\cdot,q),p} - \nabla^2\widetilde{V}(\cdot, q)\right) Q + J_A(\cdot, q)^T P \end{pmatrix}. \end{aligned} \tag{3.10}$$

By the same reasoning, we observe that the equations (3.7) tend to the linearized equations classical equations (3.10) as $\varepsilon \to 0$.

3.3. **Averages.** A further remarkable property of Gaussian wave packets is the conservation of several physical quantities. In the following, we recall the definitions of the linear and angular momentum for quantum dynamical systems.

Let $x = (x_1, \ldots, x_N)$, where $x_k \in \mathbb{R}^3$, $k = 1, \ldots, N$ and $d = 3N$, be position variables. We recall the follwoing definition given in [25, Chapter 3].

Definition 3.4. (a) The quantum mechanical total linear momentum operator is given by

$$\mathcal{P} := -\mathrm{i}\varepsilon \sum_{k=1}^{N} \nabla_{x_k}.$$

(b) The quantum mechanical total angular momentum operator is given by

$$\mathcal{L} := \sum_{k=1}^{N} x_k \times (-\mathrm{i}\varepsilon \nabla_{x_k}) = -\mathrm{i}\varepsilon \sum_{k=1}^{N} \begin{pmatrix} x_{k_2}\partial_{k_3} - x_{k_3}\partial_{k_2} \\ x_{k_3}\partial_{k_1} - x_{k_1}\partial_{k_3} \\ x_{k_1}\partial_{k_2} - x_{k_2}\partial_{k_1} \end{pmatrix}.$$

Next, we state sufficient conditions on the potentials A and V, which lead to the conservation of averages of the observables from Definition 3.4.

Definition 3.5. We call a potential $W = (W_j)_{j=1,\dots,d} : (\mathbb{R}^3)^N \to \mathbb{R}^d$

(a) translation invariant, if

$$W_j(x_1, \dots, x_N) = W_j(x_1 + r, \dots, x_N + r),$$

for all $r \in \mathbb{R}^3$ and $j = 1, \dots, d$,

(b) rotation invariant if for all orthogonal matrices $R \in \mathbb{R}^{3\times 3}$ with $\det R = 1$ it holds

$$W_j(x_1, \dots, x_N) = W_j(Rx_1, \dots, Rx_N),$$

where $j = 1, \dots, d$.

In the next lemma we provide a representation for the energy and state conservation properties of the momenta.

Lemma 3.6. *The following assertions hold.*

(a) We have $\|\psi(t)\|_{L^2} = \|u(t)\|_{L^2} = \|u_0\|_{L^2}$ *for all* $0 \le t \le T$.

(b) If the potentials A *and* V *are both time-independent, then*

$$\langle H\rangle_{\psi(t)} = \langle H\rangle_{\psi_0} \quad \text{and} \quad \langle H\rangle_{u(t)} = \langle H\rangle_{u_0}.$$

(c) For $\varphi = \psi, u$ *the energy* $\langle H\rangle_\varphi$ *is given by*

$$\langle H(t)\rangle_{\varphi(t)} = \langle H(0)\rangle_{\varphi(0)} + \int_0^t \left\langle \mathrm{i}\varepsilon\partial_s A(s)\cdot\nabla\right\rangle_{\varphi(s)} + \left\langle \partial_s \widetilde{V}(s)\right\rangle_{\varphi(s)} \mathrm{d}s.$$

(d) For $\mathcal{P}$ *and* $\mathcal{L}$ *from Definition 3.4 we have:*

(i) If V *and* $A = (A_j)_{j=1}^d$ *given in Assumption 2.1 are invariant under translations*

$$\langle \mathcal{P}\rangle_{\psi(t)} = \langle \mathcal{P}\rangle_{\psi_0} \quad \text{and} \quad \langle \mathcal{P}\rangle_{u(t)} = \langle \mathcal{P}\rangle_{u_0}.$$

(ii) If $\widetilde{V}$ *defined in (2.1) is invariant under rotations and* $A(\cdot, x) = \alpha(\cdot)x$ *for some* $\alpha(\cdot) \in \mathbb{R}$*, then*

$$\langle \mathcal{L}\rangle_{\psi(t)} = \langle \mathcal{L}\rangle_{\psi_0} \quad \text{and} \quad \langle \mathcal{L}\rangle_{u(t)} = \langle \mathcal{L}\rangle_{u_0}.$$

The proof of Lemma 3.6 is given in Section 6.

3.4. **L^2-error bound.** In this section, we present the approximation property of the Gaussian wave packet with respect to to the L^2-norm. Since our error bounds depend on parameters characterizing the Gaussian wave packet in (2.4), we first consider the boundedness of these parameters up to a time T specified by ODE-theory.

Lemma 3.7. *There exists a time $T > 0$, such that the set of equations (3.2) is well posed on $[0, T]$ independently of ε. Furthermore, the solution parameters are bounded independently of ε, i.e.*

$$|\nu| \leq c_{\nu_0}, \qquad \textit{for all} \;\; \nu \in \{q, p, \mathcal{C}, \zeta\},$$

uniformly on $[0, T]$, where c_{ν_0} depends on the initial values and on the potentials V, A.

We note that by Theorem 3.3 the matrix $\mathcal{C}_{\mathrm{I}}$ is invertible for all $t \in [0, T]$. To formulate the following results, we denote by $\rho > 0$ the lower bound on the smallest eigenvalue of $\mathcal{C}_{\mathrm{I}}$ on $[0, T]$. For a discussion of relevant time scales on which ρ is sufficiently large compared to ε, called the Ehrenfest time, we refer to [25, Sec. 3.6]. With this, we can state our approximation result.

Theorem 3.8. *Let ψ, u be the solution of (1.1a) and (2.5), respectively, and let u_0 satisfy (3.1). Then the error bound*

$$\|\psi(t) - u(t)\|_{L^2} \leq tc\sqrt{\varepsilon}, \qquad t \in [0, T],$$

holds with a constant c which depends on ρ, the bounds on the parameters from Lemma 3.7 and on the potentials, but is independent of ε and t.

We provide the details and the proof of the theorem in Section 5.

3.5. **Observable error bound.** In classical mechanics physical states are described by the position and momentum parameters $q, p \in \mathbb{R}^d$. Observables are functions depending smoothly on $(q, p) \in \mathbb{R}^{d \times d}$, see, for example, [19, 31]. Classical mechanics can be linked to quantum mechanics via Weyl quantization, which asigns a classical observable to a quantum mechanical one using semiclassical Fourier transformation, cf. [8, Thm. 4.14] or [19, 27]. Formally, for $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and an observable $\boldsymbol{a}$, we define

$$\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})\varphi(x) \coloneqq \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big) \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} \varphi(q) \,\mathrm{d}(q, p). \tag{3.11}$$

The Weyl quantization of the projections to the first or second component of the classical variables are

$$\mathrm{op}_{\mathrm{Weyl}}(p)\varphi = \mathrm{i}\varepsilon\nabla\varphi \quad \text{ and } \quad \mathrm{op}_{\mathrm{Weyl}}(q)\varphi = x\varphi.$$

Relevant quantum mechanical observables are, e.g., unbounded multiplication operators or derivatives with respect to the space variable x. To cover these, we consider observables stemming from polynomially bounded classical observables, cf. [8]. In this case, we also incorporate suitable seminorms from Definition 2.2, see also [30]. The class of admissible symbols is defined in the following.

Definition 3.9. (a) For $\omega \in \mathbb{R}^d$ we set

$$\langle\omega\rangle \coloneqq \sqrt{1 + |\omega|^2},$$

and for $l, m \in \mathbb{N}_0$ we define the class of polynomially bounded classical symbols as

$$S(l,m) := \left\{ \boldsymbol{a} \in C^\infty(\mathbb{R}^d \times \mathbb{R}^d) \;\middle|\; \begin{array}{l} \forall \alpha \in \mathbb{N}_0^{2d} \; \exists C_\alpha > 0 \text{ such that} \\ |\partial^\alpha \boldsymbol{a}(q,p)| \le C_\alpha \langle q\rangle^l \langle p\rangle^m \; \forall q,p \in \mathbb{R}^d \end{array} \right\}.$$

(b) We denote the set of bounded symbols by $S^0 := S(0,0)$.

Further examples of physically relevant observables stemming from classical symbols are

$$\mathrm{op}_{\mathrm{Weyl}}(|p|^2)\psi(x) = -\varepsilon^2 \Delta\psi(x)$$

and

$$\mathrm{op}_{\mathrm{Weyl}}(A(q)\cdot p)\psi(x) = -(A(x)\cdot \mathrm{i}\varepsilon\nabla)\psi(x).$$

In order to state our approximation result for observables, let us consider for any $z \in \mathbb{R}^{2d}$ the ordinary differential equation

$$\dot{\tilde{z}}(t) = -J\nabla_z h(t, \tilde{z}(t)), \tag{3.12a}$$

$$\tilde{z}(s) = z, \tag{3.12b}$$

which is a reformulation of (3.9). Since $h(t)$ is subquadratic, this ordinary differential equation has a globally Lipschitz continuous right-hand side, and the Picard–Lindelöf theorem provides a unique global solution

$$\mathbb{R} \to \mathbb{R}^{2d}, \quad t \mapsto \tilde{z}(t) = \Phi^{t,s}(z).$$

The Jacobian of $\Phi^{t,s}(z)$ is a symplectic matrix and thus invertible. Hence, by the inverse function theorem, the mapping $\Phi^{t,s} : \mathbb{R}^{2d} \to \mathbb{R}^{2d}$ is a diffeomorphism. In addition, the map $(\Phi^{t,s})^{-1}$ inherits the regularity of $\Phi^{t,s}$. More details and the proof will be given in Section 7.

Theorem 3.10. *Let ψ, u be the solution of (1.1a) and (2.5), respectively, and let u_0 satisfy (3.1). Moreover, let $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})$ be an observable stemming from a classical observable $\boldsymbol{a}$. Further, assume that for $j, m, l, k \in \mathbb{N}_0$*

(a) $\boldsymbol{a} \circ (\Phi^{t,s})^{-1} \in S(j,m)$,

(b) $A \in S(k,0)$, *and* $V \in S(l,0)$.

Then for $n := \max\{2k+3, l+3, k+4\}$ we have the error bound

$$\left| \langle \psi(t) | \mathbf{A}\psi(t) \rangle - \langle u(t) | \mathbf{A}u(t) \rangle \right| \le tc\varepsilon \|u(t)\|_{M(m,d),n+j;\varepsilon},$$

where c depends on the parameters, on the potentials, and on $\boldsymbol{a}$, but is independent of ε and t. The index $M(m,d)$ only depends on m and d.

Note that the convergence in the observables is of order $\mathcal{O}(\varepsilon)$ while the convergence in the L^2-norm presented in Theorem 3.8 is of order $\mathcal{O}(\sqrt{\varepsilon})$. This is in alignment with the results obtained in [25]. The rest of the paper is devoted to the proofs of the results presented in this section.

4. Equations of motions: proof of Theorems 3.1 and 3.3

In this section we derive equations of motion for the parameters $(q, p, \mathcal{C}, \zeta)$ as well as for the factorization matrices Q and P. To do so, we compute both sides of (2.5) and compare the coefficients.

Proof of Theorem 3.1. In order to use the projection formula derived in [25, Prop. 3.14] for (2.5), we observe that derivatives with respect to x of a Gaussian wave packet turn into scalar functions of x times u. In particular, we have

$$\begin{aligned}
&\mathrm{i}\varepsilon A\cdot\nabla u = -A\cdot\big(\mathcal{C}(x-q)+p\big)u,\\
&-\frac{\varepsilon^2}{2}\Delta u = \Big(\frac{1}{2}(x-q)^T\mathcal{C}^2(x-q)+p^T\mathcal{C}(x-q)+\frac{1}{2}|p|^2-\frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C})\Big)u,
\end{aligned}$$

and for the time derivative it holds that

$$\mathrm{i}\varepsilon\partial_t u(\cdot,x) = \Big(-\frac{1}{2}(x-q)^T\dot{\mathcal{C}}(x-q)+\dot{q}^T\mathcal{C}(x-q)-\dot{p}^T(x-q)+p^T\dot{q}-\dot{\zeta}\Big)u.$$

Motivated by the classical magnetic Hamiltonian system (3.9), we eliminate one degree of freedom by setting $\dot{q}=p-\langle A\rangle_u$, see [13, 19]. Incorporating the above formulas, we compare the coefficients in x on both sides of (2.5) and arrive at equations of motions of the form

$$\begin{aligned}
\dot{q} &= p-\langle A\rangle_u,\\
\dot{p} &= \big\langle J_A^T\mathcal{C}_\mathrm{R}(x-q)\big\rangle_u+\big\langle J_A\big\rangle_u^T p-\big\langle\nabla\widetilde{V}\big\rangle_u,\\
\dot{\mathcal{C}} &= -\mathcal{C}^2+\big\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\big\rangle_u+\big\langle D^2_{A,p}\big\rangle_u+\big\langle J_A\big\rangle_u^T\mathcal{C}+\mathcal{C}\big\langle J_A\big\rangle_u-\big\langle\nabla^2\widetilde{V}\big\rangle_u,\\
\dot{\zeta} &= \frac{1}{2}|p|^2+\big\langle A^T\mathcal{C}_\mathrm{R}(x-q)\big\rangle_u+\frac{\mathrm{i}\varepsilon}{2}\mathrm{tr}(\mathcal{C})\\
&\quad-\frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_\mathrm{I}^{-1}\big(\big\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\big\rangle_u+\langle J_A\rangle_u^T\mathcal{C}_\mathrm{R}+\mathcal{C}_\mathrm{R}\langle J_A\rangle_u+\langle D^2_{A,p}\rangle_u\big)\big)\\
&\quad-\langle\widetilde{V}\rangle_u+\frac{\varepsilon}{4}\mathrm{tr}\big(\mathcal{C}_\mathrm{I}^{-1}\big\langle\nabla^2\widetilde{V}\big\rangle_u\big).
\end{aligned}$$

It remains to extract the additional power of ε from the terms that contain the difference $x-q$. From

$$|u(x)|^2 = \exp\Big(-\frac{1}{\varepsilon}(x-q)^T\mathcal{C}_\mathrm{I}(x-q)-\frac{2}{\varepsilon}\mathrm{Im}\,\zeta\Big)$$

we obtain the derivative

$$\nabla|u(x)|^2 = -\frac{2}{\varepsilon}\mathcal{C}_\mathrm{I}(x-q)|u(x)|^2, \tag{4.1}$$

and apply integration by parts to obtain

$$\begin{aligned}
\big\langle A^T\mathcal{C}_\mathrm{R}(x-q)\big\rangle_u &= \big\langle A^T\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{I}(x-q)\big\rangle_u\\
&= \int_{\mathbb{R}^d}A^T\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{I}(x-q)|u(x)|^2\mathrm{d}x\\
&= \frac{\varepsilon}{2}\big\langle\mathrm{tr}\,\big(J_A^T\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\big)\big\rangle_u.
\end{aligned}$$

Similarly, we gain an order of ε for

$$\big(\big\langle J_A^T\mathcal{C}_\mathrm{R}(x-q)\big\rangle_u\big)_i = \big(\big\langle J_A^T\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\mathcal{C}_\mathrm{I}(x-q)\big\rangle_u\big)_i = \frac{\varepsilon}{2}\big\langle\partial_i\mathrm{tr}\,\big(J_A^T\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\big)\big\rangle_u,$$

as well as for

$$\begin{aligned}\left(\left\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\right\rangle_u\right)_{ij} &= \left(\left\langle D^2_{A,\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}\mathcal{C}_\mathrm{I}^{-1}(x-q)}\right\rangle_u\right)_{ij} \\ &= \Big\langle \sum_{k,l,m=1}^d \partial_i\partial_j A_k \mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_\mathrm{I}^{-1})_{lm} \sum_{n=1}^d \mathcal{C}_{\mathrm{I},mn}(x_n-q_n)\Big\rangle_u \\ &= \frac{\varepsilon}{2}\Big\langle \sum_{k,l,m=1}^d \partial_m\partial_i\partial_j A_k \mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_\mathrm{I}^{-1})_{lm}\Big\rangle_u.\end{aligned}$$

By the identity

$$\partial_{ij}\mathrm{tr}\left(J_A^T\mathcal{C}_\mathrm{R}\mathcal{C}_\mathrm{I}^{-1}\right) = \sum_{k,m,l=1}^d \partial_{ij}\partial_m A_k \mathcal{C}_{\mathrm{R},kl}(\mathcal{C}_\mathrm{I}^{-1})_{lm},$$

we conclude the equations of motion stated in (3.2). □

We now turn to the equations of motion for the Hagedorn factorization (3.3). The idea is to show that the product PQ^{-1} solves the same differential equation as $\mathcal{C}$ and conclude with the uniqueness of the variational solution u.

Proof of Theorem 3.3. We employ the differential identity

$$\partial_t(Q^{-1}) = -Q^{-1}\partial_t Q Q^{-1},$$

and use (3.7) to find that $\mathcal{C} = PQ^{-1}$ satisfies the differential equation with $\partial_t Q = \dot{Q}$

$$\begin{aligned}\dot{\mathcal{C}} &= P\partial_t(Q^{-1}) + \dot{P}Q^{-1} \\ &= -PQ^{-1}\dot{Q}Q^{-1} + \dot{P}Q^{-1} \\ &= -PQ^{-1}\left(P - \langle J_A\rangle_u Q\right)Q^{-1} \\ &\quad + \Big(\left\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\right\rangle_u Q + \left\langle D^2_{A,p}\right\rangle_u Q + \langle J_A\rangle_u^T P - \left\langle \nabla^2\widetilde{V}\right\rangle_u Q\Big)Q^{-1} \\ &= -\mathcal{C}^2 + \mathcal{C}\langle J_A\rangle_u + \left\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\right\rangle_u + \left\langle D^2_{A,p}\right\rangle_u + \langle J_A\rangle_u^T\mathcal{C} - \left\langle\nabla^2\widetilde{V}\right\rangle_u,\end{aligned}$$

which are the differential equations for $\mathcal{C}$ in (3.2c).

Concerning the symplectic relation in (3.5), we have

$$\partial_t(Q^TP - P^TQ) = \dot{Q}^TP + Q^T\dot{P} - \dot{P}^TQ - P^T\dot{Q},$$

and

$$\begin{aligned}\dot{Q}^TP &= P^TP - Q^T\langle J_A\rangle_u^T P \\ Q^T\dot{P} &= Q^T\left(\left\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\right\rangle_u + \left\langle D^2_{A,p}\right\rangle_u - \left\langle\nabla^2\widetilde{V}\right\rangle_u\right)Q + Q^T\langle J_A\rangle_u^T P \\ \dot{P}^TQ &= Q^T\left(\left\langle D^2_{A,\mathcal{C}_\mathrm{R}(x-q)}\right\rangle_u^T + \left\langle D^2_{A,p}\right\rangle_u^T - \left\langle\nabla^2\widetilde{V}\right\rangle_u^T\right)Q + P^T\langle J_A\rangle_u Q \\ P^T\dot{Q} &= P^TP - P^T\langle J_A\rangle_u Q.\end{aligned}$$

The same calculation holds for $\partial_t(Q^*P - P^*Q)$ with * replaced by ^{T}. Since p, q, A and V are real valued, we conclude

$$\partial_t(Q^*P - P^*Q) = \dot{Q}^*P + Q^*\dot{P} - \dot{P}^*Q - P^*\dot{Q} = 0,$$

which means that (3.5) holds true for all times. □

5. L^2-ERROR BOUND: PROOF OF LEMMA 3.7 AND THEOREM 3.8

This section is devoted to the wellposedness of the equations of motion (3.2) and the approximation quality of the variational solution in the L^2-norm.

We first state the following lemma which will be used frequently to obtain error bound with respect to ε. We recall that the lower bound on the eigenvalues of $\mathcal{C}_\mathrm{I}$ was denoted by $\rho > 0$.

Lemma 5.1 ([25, Lemma 3.8]). *For any $m \geq 0$ there exists a constant c_m such that for all $\varepsilon > 0$ it holds*

$$(\pi\varepsilon)^{-\frac{d}{4}} \det(\operatorname{Im}\mathcal{C})^{\frac{1}{4}} \Big(\int |x|^{2m} \exp\big(-\frac{1}{\varepsilon} x^T \mathcal{C}_\mathrm{I} x\big) \,\mathrm{d}x \Big)^{\frac{1}{2}} \leq c_m \Big(\frac{\varepsilon}{\rho}\Big)^{\frac{m}{2}},$$

where c_m is independent of ε and ρ.

We now prove the wellposedness result for (3.2) and show the boundedness of the parameters solving (3.2).

Proof of Lemma 3.7. We show that the right-hand side of (3.2) satisfies a local Lipschitz condition with Lipschitz constant independent of ε. To this end it is sufficient if the derivatives with respect to parameters $q, p, \mathcal{C}_\mathrm{R}, \mathcal{C}_\mathrm{I}, \zeta$ are bounded on a bounded domain.

The potentials in the averages of the equations of motion in (3.2) do not depend on ε. However, we need to carefully treat the absolute values of the Gaussian wave packet, since they contain ε in the denominator. By the chain rule, it is sufficient to first calculate the derivatives of averages of some arbitrary potential $\widehat{U}$, which is independent of the parameters. Then, the average has the form

$$\begin{aligned} \langle \widehat{U} \rangle_u &= \int \widehat{U}(x) |u(x)|^2 \,\mathrm{d}x \\ &= \frac{\sqrt{\det(\mathcal{C}_\mathrm{I})}}{(\pi\varepsilon)^{\frac{d}{2}}} \int \widehat{U}(x) \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I} (x-q)\right) \,\mathrm{d}x, \end{aligned}$$

from which we see that, in this case, the average only depends on q and $\mathcal{C}_\mathrm{I}$. Let u be a Gaussian wave packet with $\|u\|_{L^2} = 1$. By (4.1) we obtain

$$\begin{aligned} \partial_q \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I} (x-q)\right) &= \frac{2}{\varepsilon} \mathcal{C}_\mathrm{I}(x-q) \exp\left(-\frac{1}{\varepsilon}(x-q)^T \mathcal{C}_\mathrm{I} (x-q)\right) \\ &= -\nabla |u(x)|^2, \end{aligned}$$

thus, using integration by parts, the derivative of the average with respect to to q is given by

$$\partial_q \langle \widehat{U}(x) \rangle_u = \langle \nabla \widehat{U}(x) \rangle_u.$$

We continue with derivatives with respect to $\mathcal{C}_\mathrm{I}$. For a differentiable matrix function $F : \mathbb{R}^{d\times d} \to \mathbb{R}$ and a general invertible, symmetric matrix $M = (m_{ij})_{i,j=1,\dots,d}$ we define the componentwise derivation matrix

$$\partial_M F(M) \coloneqq (\partial_{m_{ij}} F(M))_{i,j=1,\dots,d} \in \mathbb{R}^{d\times d}.$$

By [23, Part 0.8.10] we have

$$\partial_M a^T M b = a b^T \quad \text{and} \quad \partial_M \det(M) = \det(M) M^{-1}$$

and consequently,

$$\partial_M \sqrt{\det(M)} = \frac{1}{2}\sqrt{\det(M)}M^{-1}.$$

Hence, it follows that

$$\partial_{\mathcal{C}_\mathrm{I}} \exp\left(-\frac{1}{\varepsilon}(x-q)^T\mathcal{C}_\mathrm{I}(x-q)\right) = -\frac{1}{\varepsilon}(x-q)(x-q)^T \exp\left(-\frac{1}{\varepsilon}(x-q)^T\mathcal{C}_\mathrm{I}(x-q)\right)$$

and

$$\partial_{\mathcal{C}_\mathrm{I}}\langle \widehat{U}(x)\rangle_u = -\frac{1}{\varepsilon}\big\langle (x-q)(x-q)^T\widehat{U}(x)\big\rangle_u + \frac{1}{2}I^{-1}\big\langle\widehat{U}(x)\big\rangle_u.$$

By Lemma 5.1 we have $\big|\big\langle (x-q)(x-q)^T\widehat{U}(x)\big\rangle_u\big| \le C\varepsilon$ for parameters on a bounded domain.

For potentials depending on the parameters, we use again that we are on a bounded domain and that the dependence on ε of the potentials in (3.2) is such that ε does not enter the denominator. □

We now turn to the L^2-error bound and adapt the proof of [25, Lemma 3.5] to the magnetic case and note that the multiplication potential $\widetilde{V}$ is already covered. In order to demonstrate the dependence of the constant in the error bound, we carry out the proof for the advection term.

Proof of Theorem 3.8. From the proof of [25, Lemma 3.5] with the potentials $\widetilde{V}$ and

$$Y \coloneqq A \cdot (\mathcal{C}(x-q) + p) \tag{5.1}$$

we know that

$$\big\|\psi(t) - u(t)\big\|_{L^2} \le \int_0^t \frac{1}{\varepsilon}\,\big\|\widetilde{W}_q u + W_q u\big\|_{L^2}\,\mathrm{d}s,$$

where

$$W_q = \frac{1}{2}\sum_{|\alpha|=3}(x-q)^\alpha \int_0^1 (1-\theta)^2\partial^\alpha Y\big(q+\theta(x-q)\big)\mathrm{d}\theta$$

denotes the remainder of the second order Taylor polynomial of Y around the q and $\widetilde{W}_q$ is the remainder for $\widetilde{V}$. Following the proof of [25], we bound $\big\|W_q u\big\|_{L^2}$ by finding a bound on $\partial^\alpha Y\big(q+\theta(x-q)\big)$, which then leads us to

$$|W_q(\cdot,x)|^2 \le C|x-q|^6.$$

By norm conservation and Lemma 5.1 the claim then follows. For the third derivative of $\partial_{lmn}Y$ where $l,m,n = 1,\dots,d$, we have

$$\begin{aligned}\partial_{lmn}Y = &\sum_{j,k=1}^d \partial_{lmn}A_j\big(\mathcal{C}_{jk}(x_k-q_k)+p_j\big)\\ &+\sum_{j=1}^d \partial_{lm}A_j\mathcal{C}_{jn} + \sum_{j=1}^d \partial_{ln}A_j\mathcal{C}_{jm} + \sum_{j=1}^d \partial_{mn}A_j\mathcal{C}_{jl}.\end{aligned} \tag{5.2}$$

The term $x-q$ in (5.2) evaluated at $q+\theta(x-q)$ has the form

$$\sum_{j,k=1}^d \partial_{lmn}A_j\mathcal{C}_{jk}\theta(x_k-q_k).$$

By Lemma 5.1 we gain additional orders of ε, and we thus neglect the first summand in (5.2). The remaining terms are bounded again using Lemma 5.1. ☐

6. Expectation values: proof of Lemma 3.6

In this section we adapt the proofs of [25, Section 3.2] on conservation properties to the time-dependent, magnetic case. Due to time-dependence, the energy will not be a conserved quantity.

Let ψ be the exact solution of (1.1a) and u the variational solution (2.5) such that (3.1) holds.

Proof of Lemma 3.6. The proof of norm conservation and the energy formula can be done in the same way as in [25]. We only show the conservation of total linear and angular momentum.

By [26, Theorem 1.3] or [10, Lemma 4.1] it is sufficient to show that $H(t)$ commutes with P and L, respectively, for each $t \in [0,T]$. By [25] it follows that $\mathcal{P}A_{k_j} = 0$ for all $k \in \{1,\dots,N\}$ and $j \in \{1,2,3\}$. We further calculate

$$\mathcal{P}(A\cdot\nabla)\psi = \sum_{k=1}^{N}\sum_{j=1}^{3}(\mathcal{P}A_{k_j})\partial_{k_j}\psi + A_{k_j}\mathcal{P}\partial_{k_j}\psi = (A\cdot\nabla)\mathcal{P}\psi.$$

Furthermore, a tedious calculation shows that $(A\cdot\nabla)\mathcal{L}\psi = \mathcal{L}(A\cdot\nabla)\psi$ if and only if

$$\sum_{l=1}^{N}\begin{pmatrix}A_{l_2}\partial_{l_3} - A_{l_3}\partial_{l_2}\\ A_{l_3}\partial_{l_1} - A_{l_1}\partial_{l_3}\\ A_{l_1}\partial_{l_2} - A_{l_2}\partial_{l_1}\end{pmatrix}\psi = \sum_{k=1}^{N}\sum_{j=1}^{3}\sum_{l=1}^{N}\begin{pmatrix}x_{l_2}(\partial_{l_3}A_{k_j})\partial_{k_j} - x_{l_3}(\partial_{l_2}A_{k_j})\partial_{k_j}\\ x_{l_3}(\partial_{l_1}A_{k_j})\partial_{k_j} - x_{l_1}(\partial_{l_3}A_{k_j})\partial_{k_j}\\ x_{l_1}(\partial_{l_2}A_{k_j})\partial_{k_j} - x_{l_2}(\partial_{l_1}A_{k_j})\partial_{k_j}\end{pmatrix}\psi$$

holds true. This condition is fulfilled if

$$\partial_{l_m}A_{k_j} = \alpha\delta_{l_m,k_j} \quad \text{und} \quad A_{l_n} = \alpha x_{l_n}$$

holds true for some $\alpha \in \mathbb{R}$, $j,n,m \in \{1,2,3\}$, and $k,l \in \{1,\dots,N\}$ and thus, if $A(\cdot,x) = \alpha(\cdot)x$ holds. ☐

7. Error bound for averages of observables: proof of Theorem 3.10

In this section we give the proof of Theorem 3.10, which generalizes [25, Thm. 3.5] for the magnetic case. We consider the Weyl quantization introduced in Section 3, which maps a classical observable to a quantum operator. For our analysis we allow the classical observable to depend on the variable x, i.e.

$$\widetilde{\boldsymbol{a}} : \mathbb{R}^{3d} \to \mathbb{R}, \ (x,q,p) \mapsto \widetilde{\boldsymbol{a}}(x,q,p). \tag{7.1}$$

For the symbol classes including classical observables depending on x we use the same notation as before

$$S(k,l,m) \coloneqq \left\{ \widetilde{\boldsymbol{a}} \in C^\infty(\mathbb{R}^{3d}) \;\middle|\; \begin{array}{l}\forall\alpha \in \mathbb{N}_0^{3d}\ \exists C_\alpha > 0 \text{ s.t. } \forall x,q,p \in \mathbb{R}^d:\\ |\partial^\alpha\widetilde{\boldsymbol{a}}(x,q,p)| \le C_\alpha\langle x\rangle^k\langle q\rangle^l\langle p\rangle^m\end{array} \right\} \tag{7.2}$$

and $S^0 \coloneqq S(0,0,0)$.

For a bounded classical observable with bounded derivatives its Weyl quantization defines a bounded operator on $L^2(\mathbb{R}^d)$, cf. [8,27].

Proposition 7.1 (Caldéron–Vaillancourt, [27, Thm. 2.8.1])**.** *Let $\widetilde{\boldsymbol{a}}$ be a classical observable as in (7.1) which is bounded with bounded derivatives. Then $\mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}})$ defines a bounded operator $\mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}}) : L^2(\mathbb{R}^d) \to L^2(\mathbb{R}^d)$,*

$$\left\|\mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}})\right\|_{L^2} \leq C_d \left(C_{\widetilde{\boldsymbol{a}}} + \widetilde{C}_{\widetilde{\boldsymbol{a}},d}\sqrt{\varepsilon}\right),$$

where

$$C_{\widetilde{\boldsymbol{a}}} = \max_{(x,q,p)\in\mathbb{R}^{3d}} |\widetilde{\boldsymbol{a}}(x,q,p)|,$$

the constant C_d depends on the dimension d, and $\widetilde{C}_{\widetilde{\boldsymbol{a}}}$ depends on higher order derivatives of $\widetilde{\boldsymbol{a}}$ and on d.

If we consider polynomially bounded symbols, Proposition 7.1 is not applicable. We will prove a variant, which is adapted to these kinds of symbols. A similar result without semiclassical scaling is shown in [30, Thm. 48].

Proposition 7.2. *Let $\boldsymbol{a} \in S(l,m)$ and $\varphi \in \Sigma^{\varepsilon}_{M(m,d),l}$ for $l,m \in \mathbb{N}_0$. Furthermore, for $\alpha \in \mathbb{N}_0^{2d}$ let C_α be the constants in (a) in Definition 2.2 and C_d the constant from Proposition 7.1. Then we have*

$$\left\|\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})\varphi\right\|_{L^2} \leq C_d C_0 C_{l,m} \|\varphi\|_{M(m,d),l;\varepsilon} + \mathcal{O}(\sqrt{\varepsilon}),$$

where C_α C_d and $\|\varphi\|_{k,l;\varepsilon}$ enter in $\mathcal{O}(\sqrt{\varepsilon})$, for $|\alpha| \geq 1$.

Before we give the proof, we need an auxiliary result. To this end we introduce the auxiliary differential operators, cf. [8, Thm. 4.14],

$$L_q \coloneqq \frac{1}{1+|p|^2}(1 + \mathrm{i}\varepsilon p \cdot \nabla_q) \quad \text{and} \quad L_p \coloneqq \frac{1}{1+|x-q|^2}(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p), \tag{7.3}$$

which satisfy

$$L_q \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} = \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} \quad \text{and} \quad L_p \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} = \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon}. \tag{7.4}$$

In the following lemma, we state how these operators map between the classes of classical symbols from Definition 2.2.

Lemma 7.3. *Consider a symbol $\boldsymbol{a} \in S(l,m)$, and the operators defined in (7.3). Then, there is a function $\boldsymbol{b}\colon \mathbb{R}^{3d} \to \mathbb{R}$ with*

$$\boldsymbol{b}\Big(x, \frac{x+q}{2}, p\Big) = L_q^k L_p^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big), \tag{7.5}$$

and the symbol

$$\widetilde{\boldsymbol{a}}(x,q,p) \coloneqq \langle 2q - x\rangle^{-l} \langle p\rangle^{k-m} \boldsymbol{b}(x,q,p) \tag{7.6}$$

satisfies $\widetilde{\boldsymbol{a}} \in S^0$, where the class of symbols was defined in (7.2).

For the sake of readability, we postpone the proof of Lemma 7.3 to Appendix A.

Proof of Proposition 7.2. First note that it suffices to consider Schwartz functions $\phi \in \mathcal{S}(\mathbb{R}^d)$. The idea is to reduce the problem such that we can make use of Proposition 7.1. Due to (7.4), we can rewrite the integral (3.11) for arbitrary $k, j \in \mathbb{N}_0$ as

$$\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})\varphi(x) = \frac{1}{(2\pi\varepsilon)^d} \int_{\mathbb{R}^{2d}} \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big) L_p^j L_q^k \left(\mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon}\right) \varphi(y)\, \mathrm{d}(q,p),$$

and apply the integration by parts formula to obtain

$$\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a})\varphi(x) = \frac{(-1)^{m+l}}{(2\pi\varepsilon)^d} \sum_{k=0}^{m} \int_{\mathbb{R}^{2d}} L_q^{m-k} L_p^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big) \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} L_q^k \varphi(q)\,\mathrm{d}(q,p).$$

We investigate the integrands

$$I_k(x,q,p) = L_q^{m-k} L_p^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big) \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} L_q^k \varphi(q)$$

separately in order to apply Proposition 7.1, and insert

$$\begin{aligned} I_k(x,q,p) &= \Big(\langle p\rangle^{-k}\langle q\rangle^{-l} L_q^{m-k} L_p^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big)\Big) \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} \langle q\rangle^l \langle p\rangle^k L_q^k \varphi(q) \\ &= \widetilde{\boldsymbol{a}}\Big(x, \frac{x+q}{2}, p\Big) \mathrm{e}^{\mathrm{i}p\cdot(x-q)/\varepsilon} \langle q\rangle^l \langle p\rangle^k L_q^k \varphi(q) \end{aligned}$$

where $\widetilde{\boldsymbol{a}}$ was defined in (7.6). Since it holds for $0 \le k \le m$

$$\big\|\langle q\rangle^l \langle p\rangle^k L_q^k \varphi\big\|_{L^2} \le C\|\varphi\|_{m,l;\varepsilon},$$

again Lemma 7.3 together with Proposition 7.1 yields the assertion. □

The following generalization of [25, Section 6.7] gives a useful representation for the observable error. To this end, let $U(t,s)$ be an evolution family and $\mathbf{A}$ a Weyl-quantized observable. We introduce the notation

$$\widetilde{\mathbf{A}}(t,s) \coloneqq U(s,t)\mathbf{A}U(t,s), \qquad t,s \in [0,T]. \tag{7.7}$$

Lemma 7.4. *Let ψ be the solution of (1.1a) and u the solution of (2.5). If the initial value $\psi_0 = u_0 \in \mathcal{M}$ is a Gaussian wave packet with $\|u_0\|_{L^2} = 1$, then the error of the observables takes the form*

$$\big\langle \psi(t)|\mathbf{A}\psi(t)\big\rangle - \big\langle u(t)|\mathbf{A}u(t)\big\rangle = \int_0^t \frac{1}{\mathrm{i}\varepsilon} \big\langle u(s)\big|\big[W_{u(s)}, \widetilde{\mathbf{A}}(t,s)\big] u(s)\big\rangle\,\mathrm{d}s. \tag{7.8}$$

The remainder potential W_u is given by

$$\begin{aligned} W_u &= (X(q) - \langle X\rangle_u - \varepsilon\widetilde{\alpha}) + (\nabla X(q) - \langle \nabla X\rangle_u)^T (x-q) \\ &\quad + \frac{1}{2}(x-q)^T \big(\nabla^2 X(q) - \langle \nabla^2 X\rangle_u\big)(x-q) + W_q + \widetilde{W}_q, \end{aligned} \tag{7.9}$$

with $X = Y + \widetilde{V}$ defined in (5.1) and (2.1), respectively, and W_q, $\widetilde{W}_q$ being the remainder potential of the Taylor expansion of Y and $\widetilde{V}$ around q, respectively.

Proof. Let $U(t,s)$ be the evolution family, such that the exact solution of (1.1a) is given by (2.3). Using $\psi_0 = u_0$ and $U(t,t) = \mathrm{Id}$ we calculate

$$\begin{aligned} &\langle u(t)|\mathbf{A}u(t)\rangle - \langle \psi(t)|\mathbf{A}\psi(t)\rangle \\ &\qquad = \langle u(t)|U(t,t)\mathbf{A}U(t,t)u(t)\rangle - \langle U(t,0)u(0)|\mathbf{A}U(t,0)u(0)\rangle \\ &\qquad = \langle u(t)|U(t,t)\mathbf{A}U(t,t)u(t)\rangle - \langle u(0)|U(0,t)\mathbf{A}U(t,0)u(0)\rangle \\ &\qquad = \int_0^t \frac{\partial}{\partial s}\langle u(s)|U(s,t)\mathbf{A}U(t,s)u(s)\rangle\,\mathrm{d}s. \end{aligned}$$

Employing the differential properties of the evolution family, we obtain

$$\begin{aligned} \frac{\partial}{\partial s}\widetilde{\mathbf{A}}(t,s)u(r) &= \frac{1}{\mathrm{i}\varepsilon}\big(H(s)U(s,t)\mathbf{A}U(t,s) - U(s,t)\mathbf{A}U(t,s)H(s)\big)u(r) \\ &= \frac{1}{\mathrm{i}\varepsilon}\big(H(s)\widetilde{\mathbf{A}}(t,s) - \widetilde{\mathbf{A}}(t,s)H(s)\big)u(r), \end{aligned} \tag{7.10}$$

for $r, s, t \in [0, T]$. From this, we can proceed in the same way as in [25] and arrive at (7.8). □

The key task in the proof of Theorem 3.10, is an estimate on the commutator in (7.8). The bound in Proposition 7.2 allows us to state the following extension of [25, Remark 6.2] to polynomially bounded symbols which is an intermediate step towards the desired result.

Lemma 7.5. *Let $W(\cdot, t)$ be an auxiliary smooth potential in y and $\boldsymbol{a}$ be a polynomially bounded classical observable, s.t. $\boldsymbol{a}W \in S(l, m)$. Then, there exists $C_{\boldsymbol{a},W} > 0$, such that for all $\varphi \in \Sigma^{\varepsilon}_{M(m,d),l}$ it holds that*

$$\Big\| \Big(\frac{1}{\mathrm{i}\varepsilon} \big[\mathrm{op}_{\mathrm{Weyl}}(\boldsymbol{a}), W \big] - \mathrm{op}_{\mathrm{Weyl}}(-\nabla_p \boldsymbol{a}) \nabla W \Big) \varphi \Big\|_{L^2} \leq \varepsilon C_{\boldsymbol{a},W} \|\varphi\|_{M(m,d),l;\varepsilon}.$$

The constant $C_{\boldsymbol{a},W}$ depends on second order derivatives of W and $\boldsymbol{a}$, but is independent of ε and t.

Further, to prove Theorem 3.10 we have to establish a variant of Egorov's theorem, which compares the Weyl quantization of a classical observable $\boldsymbol{a}$ along some flow to the evolution of the time-evolved quantum observable (7.7). The main difficulties are the time-dependence of the Hamiltonian operator $H(t)$, which prevents energy conservation, and the polynomial growth of the observables To the best of our knowledge, in the literature such a proof of such a variant is not available, and the results presented for example in [3] and [30, Thm. 12] do not cover our more general case.

Proposition 7.6 (time-dependent Egorov–theorem)**.** *Let $\mathbf{A}$ be a quantum observable stemming from a polynomially bounded classical observable $\boldsymbol{a}$ such that $\boldsymbol{a} \circ (\Phi^{t,s})^{-1} \in S(l, m)$. For $\varphi \in \Sigma^{\varepsilon}_{M(m,d),l}$ we have*

$$\Big\| \big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}} \left(\boldsymbol{a} \circ (\Phi^{t,s})^{-1} \right) \big) \varphi \Big\|_{L^2} \leq C\varepsilon^2 \|\varphi\|_{M(m,d),l;\varepsilon} (t-s)$$

for all $0 \leq s \leq t \leq T$. The constant C depends on derivatives of A, V and $\boldsymbol{a} \circ (\Phi^{t,s})^{-1}$, but not on ε.

Proof. (a) Let $\widetilde{\boldsymbol{a}} : \mathbb{R} \times \mathbb{R} \times \mathbb{R}^{2d} \to \mathbb{R}$, $(t, s, z) \mapsto \widetilde{\boldsymbol{a}}(t, s, z)$ be defined by

$$\widetilde{\boldsymbol{a}}(\tau, s, z) = \boldsymbol{a} \circ (\Phi^{\tau,s})^{-1}(z). \tag{7.11}$$

Since $\widetilde{\boldsymbol{a}}(t, t, \cdot) = \boldsymbol{a}$ and $U(t, t) = \mathrm{Id}$, we obtain similarly as for (7.10)

$$\begin{aligned}
&\mathrm{op}_{\mathrm{Weyl}} \left(\widetilde{\boldsymbol{a}}(t, s) \right) - \widetilde{\mathbf{A}}(t, s) \\
&= \int_s^t \partial_\tau \Big(U(\tau, t) \mathrm{op}_{\mathrm{Weyl}} \left(\widetilde{\boldsymbol{a}}(\tau, s) \right) U(t, \tau) \Big) \,\mathrm{d}\tau \\
&= \int_s^t U(\tau, t) \Big(-\frac{\mathrm{i}}{\varepsilon} \big[H(\tau), \mathrm{op}_{\mathrm{Weyl}} \left(\widetilde{\boldsymbol{a}}(\tau, s) \right) \big] + \mathrm{op}_{\mathrm{Weyl}} \left(\partial_\tau \widetilde{\boldsymbol{a}}(\tau, s) \right) \Big) U(t, \tau) \,\mathrm{d}\tau \\
&= \int_s^t U(\tau, t) \Big(-\mathrm{op}_{\mathrm{Weyl}}(\{ h(\tau), \widetilde{\boldsymbol{a}}(\tau, s) \}) + \mathrm{op}_{\mathrm{Weyl}} \left(\partial_\tau \widetilde{\boldsymbol{a}}(\tau, s) \right) \Big) U(t, \tau) \,\mathrm{d}\tau + \rho(t, s).
\end{aligned}$$

We first show that the remainder ρ is of order ε^2. To this end, we use an extension of [25, Prop. 6.2] to polynomially bounded observables in the spirit of Lemma 7.5. Together with Theorem 2.3, this bounds the remainder by the right-hand side of the estimate in the proposition. Thus, it remains to show that the integral vanishes.

In the following step we show that $\widetilde{\boldsymbol{a}}$ satisfies the transport equation

$$\partial_\tau \widetilde{\boldsymbol{a}}(\tau, s) = \{h(\tau), \widetilde{\boldsymbol{a}}(\tau, s)\}, \tag{7.12a}$$

$$\widetilde{\boldsymbol{a}}(s, s) = \boldsymbol{a} \tag{7.12b}$$

for $\tau \geq s$. Then the integrand vanishes, and we obtain

$$\widetilde{\mathbf{A}}(t, s) = \mathrm{op}_{\mathrm{Weyl}}(\widetilde{\boldsymbol{a}}(t, s)) + O(\varepsilon^2),$$

as claimed.

(b) We rewrite the transport equation (7.12) as

$$\begin{aligned} \partial_\tau \widetilde{\boldsymbol{a}}(\tau, s) &= J\nabla_z h(\tau) \cdot \nabla_z \widetilde{\boldsymbol{a}}(\tau, s), \\ \widetilde{\boldsymbol{a}}(s, s) &= \boldsymbol{a}. \end{aligned}$$

For $\tau \geq s$, $z \in \mathbb{R}^{2d}$ and $\widetilde{\boldsymbol{a}}$ defined in (7.11) we calculate

$$\begin{aligned} 0 &= \partial_\tau \boldsymbol{a}(z) \\ &= \partial_\tau \widetilde{\boldsymbol{a}}(\tau, s, \Phi^{\tau,s}(z)) \\ &= \partial_\tau \widetilde{\boldsymbol{a}}(\tau, s, \Phi^{\tau,s}(z)) + \partial_\tau \Phi^{\tau,s}(z) \cdot \nabla_z \widetilde{\boldsymbol{a}}(\tau, s, \Phi^{\tau,s}(z)) \\ &= \partial_\tau \widetilde{\boldsymbol{a}}(\tau, s, \Phi^{\tau,s}(z)) - J\nabla_z h(\tau, \Phi^{\tau,s}(z)) \cdot \nabla_z \widetilde{\boldsymbol{a}}(\tau, s, \Phi^{\tau,s}(z)), \end{aligned}$$

where we used in the last step that $\Phi^{\tau,s}$ solves (3.12). Since $\Phi^{\tau,s}$ is a diffeomorphism, this proves that $\widetilde{\boldsymbol{a}}$ indeed solves the transport equation (7.12). □

For polynomially bounded symbols scaled weighted Sobolev norms of a the variational solution, cf. [4,5] and [30, Prop. 123], will enter the error bounds. As we will see in the proof of Theorem 3.10, Egorov's estimate will be used on a scalar function of x times a Gaussian wave packet, which has been propagated in time by the evolution family. We therefore consider scaled weighted Sobolev norm of propagated initial data, see Theorem 2.3. For our error estimate the following observation will be useful.

Lemma 7.7. *Let u be a Gaussian wave packet such that $\|u\|_{L^2} = 1$ and $\gamma \in \mathbb{N}_0^d$ be some multiindex. Then, it holds*

$$\left\| \varepsilon^{|\beta|} x^\alpha \partial^\beta \left((x-q)^\gamma u \right) \right\|_{L^2} \leq C \varepsilon^{|\gamma|} \|u\|_{|\alpha|,|\beta|;\varepsilon}, \tag{7.13}$$

where C depends on β and γ.

Proof. We calculate

$$\varepsilon^{|\beta|} \partial^\beta \left((x-q)^\gamma u(x) \right) = \sum_{\eta \leq \beta} \binom{\beta}{\eta} \varepsilon^{|\eta|} \partial^\eta (x-q)^\gamma \varepsilon^{|\beta-\eta|} \partial^{\beta-\eta} u(x).$$

and employ Lemma 5.1 to arrive at

$$\|\partial^\eta (x-q)^\gamma u\|_{L^2} \leq C(\gamma, \eta) \left\| |x-q|^{|\gamma-\eta|} u \right\|_{L^2} \leq C(\gamma, \eta) \varepsilon^{|\gamma-\eta|} c \, \|u\|_{L^2},$$

which proves (7.13). □

We now have everything at hand to estimate the error of observables and to conclude our final main result.

Proof of Theorem 3.10. By Lemma 7.4 we only have to bound the commutator in the representation formula (7.8).

(a) We apply Lemma 5.1 and [25, Lemma 3.15] to the remainder potential W_u in (7.9), which leads to

$$\|W_u u\|_{L^2} \le C\varepsilon \quad \text{and} \quad \|\nabla W_u u\|_{L^2} \le C\varepsilon, \tag{7.14}$$

where the constants depend on parameters and on potentials.

(b) We expand

$$\Big\langle \frac{1}{\mathrm{i}\varepsilon}\big[W_{u(s)}, \widetilde{\mathbf{A}}(t,s)\big]\Big\rangle_{u(s)} = \Big\langle \frac{1}{\mathrm{i}\varepsilon}\left[W_{u(s)}, \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\right]\Big\rangle_{u(s)} + r_1(s,t),$$

where the remainder is given by

$$r_1(s,t) = \Big\langle \frac{1}{\mathrm{i}\varepsilon}\big[W_{u(s)}, \widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\big]\Big\rangle_{u(s)}.$$

Using first Cauchy-Schwartz and then (7.14), we obtain

$$\begin{aligned}
|r_1(s,t)| &\le \frac{1}{\varepsilon}\left\|W_{u(s)}u(s)\right\|_{L^2}\left\|\big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\big)u(s)\right\|_{L^2} \\
&\qquad + \frac{1}{\varepsilon}\left\|\big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\big)W_{u(s)}u(s)\right\|_{L^2} \\
&\le c\left\|\big(\widetilde{\mathbf{A}}(t,s) - \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\big)u(s)\right\|_{L^2} \\
&\qquad + c\varepsilon\left\|W_{u(s)}u(s)\right\|_{M(m,d),j;\varepsilon} \\
&\le c\varepsilon^2,
\end{aligned}$$

where we used Proposition 7.6 and Lemma 7.7 for the last inequality.

(c) We write

$$\begin{aligned}
&\Big\langle \frac{1}{\mathrm{i}\varepsilon}\left[W_{u(s)}, \mathrm{op}_{\mathrm{Weyl}}\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\right]\Big\rangle_{u(s)} \\
&\qquad = \left\langle \mathrm{op}_{\mathrm{Weyl}}\left(-\partial_p\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\right)u(s) \,\middle|\, \nabla W_{u(s)}u(s)\right\rangle + \varepsilon r_2(s,t),
\end{aligned} \tag{7.15}$$

where by Lemma 7.5 the remainder term is bounded by

$$|r_2(s,t)| \le C_{q,\rho,X}\|u(s)\|_{M(n,d),j+l+3;\varepsilon}.$$

We can further bound the first term in (7.15) by employing Cauchy-Schwartz and estimate (7.14) to see

$$\begin{aligned}
&\left|\left\langle \mathrm{op}_{\mathrm{Weyl}}\left(-\partial_p\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\right)u(s) \,\middle|\, \nabla W_{u(s)}u(s)\right\rangle\right| \\
&\qquad\qquad \le C\varepsilon\left\|\mathrm{op}_{\mathrm{Weyl}}\left(-\partial_p\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\right)u(s)\right\|_{L^2}.
\end{aligned}$$

(d) Finally, we use Proposition 7.2 to estimate

$$\left\|\mathrm{op}_{\mathrm{Weyl}}\left(-\partial_p\left(\boldsymbol{a}\circ(\Phi^{t,s})^{-1}\right)\right)u(s)\right\|_{L^2} \le C\|u(s)\|_{M(m,d),j;\varepsilon},$$

which finishes the proof. □

Appendix A. Proof of Lemma 7.3

In this appendix, we show the bounds on the modified observables which are uniform in the spatial variable x.

Proof of Lemma 7.3. We first expand the expression as

$$L_q^k L_p^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big)$$
$$= \langle p\rangle^{-2k}\Big(1 + \mathrm{i}\varepsilon \sum_{j=1}^{d} p_j \partial_{q_j}\Big)^k \langle x-q\rangle^{-2l}\left(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p\right)^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big),$$

and consider the different orders of ∂_{q_j}. We obtain for $r \le k$

$$\partial_{q_j}^r \langle x-q\rangle^{-2l}\left(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p\right)^l \boldsymbol{a}\Big(\frac{x+q}{2}, p\Big)$$
$$= \sum_{n=0}^{r} \partial_{q_j}^n \Big(\langle x-q\rangle^{-2l}\left(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p\right)^l\Big)\partial_{q_j}^{r-n}\boldsymbol{a}\Big(\frac{x+q}{2}, p\Big).$$

Moreover, we can further expand the summands as

$$\partial_{q_j}^n \Big(\langle x-q\rangle^{-2l}\left(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p\right)^l\Big) = \sum_{i=0}^{n} \partial_{q_j}^i \langle x-q\rangle^{-2l} \partial_{q_j}^{n-i}\left(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p\right)^l.$$

Using the identity $x-q = 2\big(x - \frac{x+q}{2}\big)$, yields the representation in (7.5). Combining the following estimates for $k, \hat{k} \in \mathbb{N}$

$$\Big\langle \frac{x+q}{2} \Big\rangle \le \langle x-q\rangle\,\langle q\rangle, \qquad \Big|\partial_p^{\hat{k}}\langle p\rangle^{-k}\Big| \le C(k,\hat{k})\langle p\rangle^{-(k+\hat{k})},$$

and similarly for $\left|\partial_q \langle x-q\rangle^{-k}\right|$, with the fact that $\boldsymbol{a} \in S(l,m)$, we conclude

$$\Big|\partial_{q_j}^i \langle x-q\rangle^{-2l}\partial_{q_j}^{n-i}\left(1 - \mathrm{i}\varepsilon(x-q)\cdot\nabla_p\right)^l \partial_{q_j}^{r-n}\boldsymbol{a}\Big(\frac{x+q}{2}, p\Big)\Big| \le C\langle q\rangle^l \langle p\rangle^m,$$

which is equivalent to

$$\Big|\boldsymbol{b}\Big(x, \frac{x+q}{2}, p\Big)\Big| \le C\langle q\rangle^l\langle p\rangle^m = C\langle 2\frac{x+q}{2} - x\rangle^l \langle p\rangle^m.$$

Since the estimate holds for all $x, q, p \in \mathbb{R}^d$, we conclude

$$\big|\boldsymbol{b}(x,q,p)\big| \le C\langle 2q - x\rangle^l \langle p\rangle^m$$

Finally, with $|\langle p\rangle^{-2k} p^\alpha| \le \langle p\rangle^{-2k+|\alpha|}$, we obtain

$$\big|\widetilde{\boldsymbol{a}}(x,q,p)\big| \le C$$

for a constant $C > 0$ which is independent of x, q, p. By the very same arguments, one can deduce the bounds on the partial derivatives of $\widetilde{\boldsymbol{a}}$, which gives the claim. □

Acknowledgments

We thank Didier Robert for helpful discussions on the time-dependent Egorov theorem.

References

[1] S. Blanes and V. Gradinaru, *High order efficient splittings for the semiclassical time-dependent Schrödinger equation*, J. Comput. Phys. **405** (2020), 109157, 13. MR4045248

[2] J. P. Boris, *Relativistic plasma simulation-optimization of a hybrid code*, In: Proceeding of Fourth Conference on Numerical Simulations of Plasmas (1970), 3–67. https://apps.dtic.mil/sti/citations/ADA023511.

[3] A. Bouzouina and D. Robert, *Uniform semiclassical estimates for the propagation of quantum observables*, Duke Math. J. **111** (2002), no. 2, 223–252. MR1882134

[4] I. Burghardt, R. Carles, C. Fermanian Kammerer, B. Lasorne, and C. Lasser, *Separation of scales: dynamical approximations for composite quantum systems*, J. Phys. A **54** (2021), no. 41, Paper No. 414002, 36. MR4318625

[5] R. Carles, *On Fourier time-splitting methods for nonlinear Schrödinger equations in the semiclassical limit*, SIAM J. Numer. Anal. **51** (2013), no. 6, 3232–3258. MR3138106

[6] ______, *Semi-classical analysis for nonlinear Schrödinger equations—WKB analysis, focal points, coherent states* (2021), xiv+352. Second edition [of 2406566]. MR4274579

[7] R. D. Coalson and M. Karplus, *Multidimensional variational gaussian wave packet dynamics with application to photodissociation spectroscopy*, J. Chem. Phys. **93** (1990), no. 6, 3919–3930. https://doi.org/10.1063/1.458778.

[8] L. Evans and M. Zworski, *Lectures on semiclassical analysis*, 2007. https://math.berkeley.edu/~evans/semiclassical.pdf.

[9] E. Faou, V. Gradinaru, and C. Lubich, *Computing semiclassical quantum dynamics with Hagedorn wavepackets*, SIAM J. Sci. Comput. **31** (2009), no. 4, 3027–3041. MR2520310

[10] E. Faou and C. Lubich, *A Poisson integrator for Gaussian wavepacket dynamics*, Comput. Vis. Sci. **9** (2006), no. 2, 45–55. MR2247684

[11] V. Gradinaru and G. A. Hagedorn, *Convergence of a semiclassical wavepacket based time-splitting for the Schrödinger equation*, Numer. Math. **126** (2014), no. 1, 53–73. MR3149072

[12] V. Gradinaru and O. Rietmann, *Hagedorn wavepackets and Schrödinger equation with time-dependent, homogeneous magnetic field*, J. Comput. Phys. **445** (2021), Paper No. 110581, 18. MR4298183

[13] S. J. Gustafson and I. M. Sigal, *Mathematical concepts of quantum mechanics*, Third, Universitext, Springer, Cham, [2020] ©2020. MR4199124

[14] G. A. Hagedorn, *Semiclassical quantum mechanics. I. The $\hbar \to 0$ limit for coherent states*, Comm. Math. Phys. **71** (1980), no. 1, 77–93. MR556903

[15] ______, *Semiclassical quantum mechanics. III. The large order asymptotics and more general states*, Ann. Physics **135** (1981), no. 1, 58–70. MR630204

[16] ______, *Raising and lowering operators for semiclassical wave packets*, Ann. Physics **269** (1998), no. 1, 77–104. MR1650826

[17] E. Hairer and C. Lubich, *Long-term analysis of a variational integrator for charged-particle dynamics in a strong magnetic field*, Numer. Math. **144** (2020), no. 3, 699–728. MR4071828

[18] E. Hairer, C. Lubich, and B. Wang, *A filtered Boris algorithm for charged-particle dynamics in a strong magnetic field*, Numer. Math. **144** (2020), no. 4, 787–809. MR4081132

[19] B. C. Hall, *Quantum theory for mathematicians*, Graduate Texts in Mathematics, vol. 267, Springer, New York, 2013. MR3112817

[20] E. J. Heller, *Time dependent variational approach to semiclassical dynamics*, J. Chem. Phys. **64** (1976), no. 1, 63–73. MR446212

[21] ______, *Frozen Gaussians: a very simple semiclassical approximation*, J. Chem. Phys. **75** (1981), no. 6, 2923–2931. MR627226

[22] K. Hepp, *The classical limit for quantum mechanical correlation functions*, Comm. Math. Phys. **35** (1974), 265–277. MR332046

[23] R. A. Horn and C. R. Johnson, *Matrix analysis*, Second, Cambridge University Press, Cambridge, 2013. MR2978290

[24] N. King and T. Ohsawa, *Hamiltonian dynamics of semiclassical Gaussian wave packets in electromagnetic potentials*, J. Phys. A **53** (2020), no. 10, 105201, 17. MR4106520

[25] C. Lasser and C. Lubich, *Computing quantum dynamics in the semiclassical regime*, Acta Numer. **29** (2020), 229–401. MR4189293

[26] C. Lubich, *From quantum to classical molecular dynamics: reduced models and numerical analysis*, Zurich Lectures in Advanced Mathematics, European Mathematical Society (EMS), Zürich, 2008. MR2474331

[27] A. Martinez, *An introduction to semiclassical and microlocal analysis*, Universitext, Springer-Verlag, New York, 2002. MR1872698

[28] T. Ohsawa, *Approximation of semiclassical expectation values by symplectic Gaussian wave packet dynamics*, Lett. Math. Phys. **111** (2021), no. 5, Paper No. 121, 26. MR4318439

[29] O. Rietmann and V. Gradinaru, *Spawning semiclassical wavepackets*, Technical Report 2022-49, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2022. https://www.sam.math.ethz.ch/sam_reports/reports_final/reports2022/2022-49.pdf.

[30] D. Robert and M. Combescure, *Coherent states and applications in mathematical physics*, Theoretical and Mathematical Physics, Springer, Cham, 2021. Second edition [of 2952171]. MR4277789

[31] S. Waldmann, *Poisson-Geometrie und Deformationsquantisierung : Eine Einführung*, Springer Berlin Heidelberg, 2007. https://doi.org/10.1007/978-3-540-72518-3.

[32] Z. Zhou, *Numerical approximation of the Schrödinger equation with the electromagnetic field by the Hagedorn wave packets*, J. Comput. Phys. **272** (2014), 386–407. MR3212278

[33] Z. Zhou and G. Russo, *The Gaussian wave packet transform for the semi-classical Schrödinger equation with vector potentials*, Commun. Comput. Phys. **26** (2019), no. 2, 469–505. MR3939400

Institute for Applied and Numerical Mathematics, Karlsruhe Institute of Technology, 76149 Karlsruhe, Germany

Email address: {selina.burkhard, benjamin.doerich, marlis.hochbruck}@kit.edu

Department of Mathematics, Technical University of Munich, 85748 Garching bei München, Germany

Email address: classer@ma.tum.de