Hamiltonian Dynamics of Semiclassical Gaussian Wave Packets in Electromagnetic Potentials

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Abstract

We extend our previous work on symplectic semiclassical Gaussian wave packet dynamics to incorporate electromagnetic interactions by including a vector potential. The main advantage of our formulation is that the equations of motion derived are naturally Hamiltonian. We obtain an asymptotic expansion of our equations in terms of $\hbar$ and show that our equations have $\mathcal{O}(\hbar)$ corrections to those presented by Zhou, whereas ours also recover the equations of Zhou in the case of a linear vector potential and quadratic scalar potential. One and two dimensional examples of a particle in a magnetic field are given and numerical solutions are presented and compared with the classical solutions and the expectation values of the corresponding observables as calculated by the Egorov or Initial Value Representation (IVR) method. We numerically demonstrate that the $\mathcal{O}(\hbar)$ correction terms improve the accuracy of the classical or Zhou's equations for short times in the sense that our solutions converge to the expectation values calculated using the Egorov/IVR method faster than the classical solutions or those of Zhou as $\hbar \to 0$.

1 Introduction

1.1 Motivation

Gaussian wave packets have historically been used to solve the time-dependent semiclassical Schrödinger equation [3, 6–9, 15]. While the Schrödinger equation is computationally non-trivial to solve in the semiclassical regime, those methods using the Gaussian wave packets provide an alternative set of differential equations that may be solved for the time-dependent parameters of the Gaussian wave packet. The Gaussian wave packet is an ansatz for an exact solution in the case of linear vector potentials with quadratic scalar potentials (see Hagedorn [6]), and gives a good short time approximation of the solution for other potentials in the semiclassical regime as shown by Zhou [30].

However, the set of differential equations of Zhou for the parameters is not a Hamiltonian system in general. Given that the equations of motion for a classical particle is a Hamiltonian system and also that the Schrödinger equation is a (infinite-dimensional) Hamiltonian system as we will explain in a moment, it is rather natural to seek a Hamiltonian formulation of the dynamics of the Gaussian wave packet. This was the main motivation of our previous work [26] on the symplectic/Hamiltonian formulation of the Gaussian wave packet dynamics.

In this paper, we utilize the same symplectic-geometric framework to derive a Hamiltonian system of equations governing the evolution the wave packet parameters under the influence of electromagnetic fields by taking into account a vector potential. Semiclassical dynamics under the influence of electromagnetic fields has been of great interest recently because of its significance in quantum control and solid state physics.

1.2 Hamiltonian Formulation of Classical Dynamics

It is well known that the equations of motion of a classical particle in $\mathbb{R}^d$ is a Hamiltonian system. From the symplectic-geometric point of view, one takes the cotangent bundle $T^*\mathbb{R}^d \cong \mathbb{R}^{2d} = \{(q,p) \,|\, q,p \in \mathbb{R}^d\}$ as the phase space and define the classical symplectic form $\Omega_0 := \mathbf{d}q_i \wedge \mathbf{d}p_i$ (the Einstein summation convention is assumed). This renders $T^*\mathbb{R}^d$ a symplectic manifold. We also define a Hamiltonian function $H_0\colon T^*\mathbb{R}^d \to \mathbb{R}$ as

$$H_0(q,p) := \frac{1}{2m}(p - \boldsymbol{A}(q))^2 + V(q), \tag{1}$$

where $V\colon \mathbb{R}^d \to \mathbb{R}$ and $\boldsymbol{A}\colon \mathbb{R}^d \to \mathbb{R}^d$ are scalar and vector potentials respectively, and we set the charge to be 1 for simplicity.

Now let $X_{H_0} = \dot{q}_i \frac{\partial}{\partial q_i} + \dot{p}_i \frac{\partial}{\partial p_i}$ be the vector field on $T^*\mathbb{R}^d$ defined by $\mathbf{i}_{X_{H_0}}\Omega_0 = \mathbf{d}H_0$ where $\mathbf{i}$ stands for the contraction. Then the equation yields the equations of motion of the classical particle in the electromagnetic field:

$$\dot{q} = \frac{1}{m}(p - \boldsymbol{A}(q)), \qquad \dot{p} = -\frac{1}{2m}\boldsymbol{\nabla}_q \left(|\boldsymbol{A}(q)|^2 - 2\boldsymbol{A}(q)\cdot p\right) - \boldsymbol{\nabla}V(q), \tag{2}$$

where $\boldsymbol{\nabla}_q$ stands for the gradient with respect to the variable q, and $|\cdot|$ stands for the Euclidean distance in $\mathbb{R}^d$.

1.3 Hamiltonian Formulation of the Schrödinger Equation

We may generalize the notion of Hamiltonian system as follows: Let P be a symplectic manifold, i.e., a manifold equipped with a closed non-degenerate 2-form Ω, and let $H\colon P \to \mathbb{R}$ be a smooth function. Then we define the *Hamiltonian vector field* X_H on P corresponding to the Hamiltonian function H by setting $\mathbf{i}_{X_H}\Omega = \mathbf{d}H$. The vector field X_H then defines the evolution equation on P. We may take it as the definition of a generalized Hamiltonian system; see, e.g., Marsden and Ratiu [17] for more details.

We may now formulate the time-dependent Schrödinger equation as a Hamiltonian system as follows: Let $\mathcal{H} := L^2(\mathbb{R}^d)$ with the standard (right-linear) inner product $\langle\cdot,\cdot\rangle$, and equip it with the symplectic form $\Omega_{\mathcal{H}}(\psi_1,\psi_2) := 2\hbar\,\mathrm{Im}\langle\psi_1,\psi_2\rangle$, and take the expectation value $\langle H\rangle\colon \mathcal{H} \to \mathbb{R}$ of the Hamiltonian operator as the Hamiltonian function. Then the Hamiltonian vector field $X_{\langle H\rangle}$ on $\mathcal{H}$ defined by $\mathbf{i}_{X_{\langle H\rangle}}\Omega_{\mathcal{H}} = \mathbf{d}\langle H\rangle$ yields the usual time-dependent Schrödinger equation

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\psi = \hat{H}\psi, \tag{3}$$

where $\hat{H}$ is the Hamiltonian operator defined below.

1.4 Geometry of Reduced Models

Given that the basic equations of classical and quantum dynamics are both Hamiltonian systems, it is natural to expect that the basic equations of semiclassical dynamics—or more generally approximation/reduced models of quantum dynamics—are Hamiltonian as well. Is there a way to exploit the above symplectic structure $\Omega_{\mathcal{H}}$ on $\mathcal{H} = L^2(\mathbb{R}^d)$ to find a Hamiltonian formulation of reduced models?

Lubich [16] (see also Kramer and Saraceno [13]) came up with a general prescription to achieve this by geometrically interpreting approximation models of quantum dynamics. Suppose that we have an ansatz $\varphi\colon M \to \mathcal{H} := L^2(\mathbb{R}^d); y \mapsto \varphi(y;\cdot)$ for the solution of the Schrödinger equation, where M is a finite-dimensional manifold (where the parameters for the ansatz live). The parameters y evolve in time according to the dynamics in M to be determined, and the time evolution $t \mapsto \varphi(y(t);\cdot)$ gives an approximation to the solution of the Schrödinger equation (3). Lubich [16] (see also Ohsawa and Leok [26]) showed that one can achieve the best approximation in M as follows: Consider the embedding $\iota\colon M \to \mathcal{H}$ defined by the ansatz φ as $\iota(y) := \varphi(y;\cdot)$. Then we can pull back the symplectic form $\Omega_{\mathcal{H}}$ to M to obtain a 2-form $\Omega := \iota^*\Omega_{\mathcal{H}}$ on M. Under a certain technical condition (see [16] and [26, Proposition 2.1] for details), Ω

defines a symplectic form on M. One may also define the pull-back $H := \langle H \rangle \circ \iota$ of the Hamiltonian function, i.e., $H(y) := \left\langle \varphi(y;\,\cdot\,), \hat{H}\varphi(y;\,\cdot\,) \right\rangle$. Then we may define the Hamiltonian vector field X_H on M by setting $\mathbf{i}_{X_H}\Omega = \mathbf{d}H$. Lubich [16] showed that this gives the least squares approximation of the vector field $X_{\langle H \rangle}$ in the following sense: For any $y \in M$ and any $V_y \in T_yM$,

$$\|X_{\langle H \rangle}(\iota(y)) - T_y\iota(X_H(y))\| \leq \|X_{\langle H \rangle}(\iota(y)) - T_y\iota(V_y)\|$$

in terms of the L^2 norm in $\mathcal{H} = L^2(\mathbb{R}^d)$; see Fig. 1.

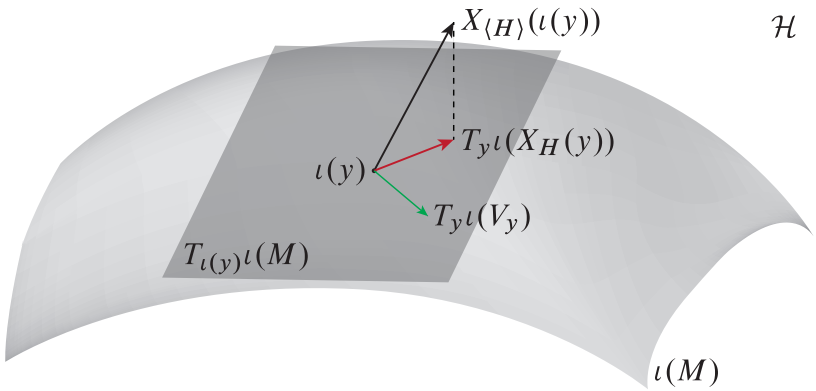


Figure 1: The Hamiltonian Vector Field X_H gives the best approximation on M of the vector field $X_{\langle H \rangle}$.

2 Hamiltonian Dynamics of Gaussian Wave Packets in Electromagnetic Potentials

2.1 Gaussian Wave Packet in Electromagnetic Potentials

Our ansatz or approximation/reduced model is the Gaussian wave packet of Heller [7, 8, 9] and Hagedorn [3, 6] (see also Littlejohn [15]):

$$\chi_M(q, p, \mathcal{A}, \mathcal{B}, \phi, \delta; x) := \exp\left\{ \frac{\mathrm{i}}{\hbar} \left(\frac{1}{2}(x - q)^T (\mathcal{A} + \mathrm{i}\mathcal{B})(x - q) + p \cdot (x - q) + \phi + \mathrm{i}\delta \right) \right\}, \tag{4}$$

where $(q, p) \in T^*\mathbb{R}^d \cong \mathbb{R}^{2d}$ is the phase space center, $\phi \in \mathbb{S}^1$ is the phase factor, $\delta \in \mathbb{R}$ controls the norm, and $\mathcal{A} + \mathrm{i}\mathcal{B} \in \Sigma_d := \{\mathcal{A} + \mathrm{i}\mathcal{B} \in \mathbb{C}^{d\times d} \mid \mathcal{A}, \mathcal{B} \in \mathrm{Sym}_d(\mathbb{R}), \mathcal{B} - \text{positive definite}\}$. Note that the above Gaussian is not normalized:

$$\mathcal{N}(\mathcal{B}, \delta) := \|\chi(y;\,\cdot\,)\|^2 = \sqrt{\frac{(\pi\hbar)^d}{\det \mathcal{B}}} \exp\left(-\frac{2\delta}{\hbar} \right), \tag{5}$$

where we set $y = (q, p, \mathcal{A}, \mathcal{B}, \phi, \delta)$. We will address this issue later.

Following the geometric picture of Lubich [16] described above, we define M to be the space of the above parameters:

$$M := T^*\mathbb{R}^d \times \Sigma_d \times \mathbb{S}^1 \times \mathbb{R},$$

and consider the embedding $\iota\colon M \to \mathcal{H}$ defined as $\iota(y) := \chi_M(y;\,\cdot\,)$. Then one can show that the pull-back $\Omega_M := \iota^*\Omega_{\mathcal{H}}$ is in fact a symplectic form on M; see Ohsawa and Leok [26, Section 3].

In this paper, we would like to incorporate the effect of electromagnetic fields to the dynamics of the Gaussian wave packet. So we take Hamiltonian operator $\hat{H}$ to be

$$\hat{H} := \frac{1}{2m}\Big(-\mathrm{i}\hbar\boldsymbol{\nabla} - \boldsymbol{A}(x) \Big)^2 + V(x),$$

where we assume that the scalar and vector potentials $V\colon \mathbb{R}^d \to \mathbb{R}$ and $\boldsymbol{A}\colon \mathbb{R}^d \to \mathbb{R}^d$ are smooth functions; we write the i-th component of $\boldsymbol{A}_i$ as opposed to the more conventional A_i in order to make it more conspicuous and to avoid possible confusions with the components of $\mathcal{A}$.

One may then evaluate the pull-back $H_M := \langle H \rangle \circ \iota\colon M \to \mathbb{R}$ of the Hamiltonian $\langle H \rangle$ by evaluating the expectation value of the Hamiltonian operator as follows:

$$\begin{aligned} H_M(y) := \langle H \rangle \circ \iota(y) &= \left\langle \chi_M(y;\,\cdot\,), \hat{H}\chi_M(y;\,\cdot\,) \right\rangle \\ &= \mathcal{N}(\mathcal{B},\delta)\biggl(\frac{p^2}{2m} + \frac{\hbar}{4m}\operatorname{Tr}\bigl(\mathcal{B}^{-1}(\mathcal{A}^2+\mathcal{B}^2)\bigr) - \frac{1}{m}\left\langle \boldsymbol{A}(x)\cdot p \right\rangle \\ &\quad + \frac{\hbar}{2m}\left\langle \operatorname{Tr}\Bigl(D\boldsymbol{A}^T(x)\mathcal{A}\mathcal{B}^{-1}\Bigr) \right\rangle + \frac{1}{2m}\left\langle |\boldsymbol{A}(x)|^2 \right\rangle + \left\langle V(x) \right\rangle \biggr), \end{aligned} \tag{6}$$

where $\boldsymbol{A}$ is regarded as a column vector, $D\boldsymbol{A}(x)$ is the $d \times d$ matrix whose (i,j)-component is $\frac{\partial \boldsymbol{A}_i}{\partial x_j}(x)$, and $\langle\,\cdot\,\rangle$ stands for the expectation value of an observable with respect to the *normalized* Gaussian $\chi_M/\|\chi_M\|$: For any smooth function $\mathcal{U}\colon \mathbb{R}^d \to \mathbb{R}$ satisfying a certain growth condition (see Section 3.1),

$$\begin{aligned} \langle \mathcal{U}(x) \rangle &:= \frac{1}{\mathcal{N}(\mathcal{B},\delta)} \left\langle \chi_M(y;\,\cdot\,), \mathcal{U}(\,\cdot\,)\chi_M(y;\,\cdot\,) \right\rangle \\ &= \frac{1}{\mathcal{N}(\mathcal{B},\delta)} \int_{\mathbb{R}^d} \mathcal{U}(x) \exp\left(-\frac{1}{\hbar}(x-q)^T \mathcal{B}(x-q) \right) \mathrm{d}x. \end{aligned} \tag{7}$$

2.2 Hamiltonian Formulation of Gaussian Wave Packet Dynamics

One may now certainly formulate a Hamiltonian system on M using the above pull-backs of the symplectic form and the Hamiltonian. However, the pull-back of the symplectic form turns out to be very cumbersome; neither does it provide much insight into its relationship with the symplectic form Ω_0 of classical dynamics; see Ohsawa and Leok [26, Eq. (10)].

Fortunately, there is a way around it to obtain a simpler and more appealing formulation by exploiting the inherent symmetry of the system [26, Section 4]. First observe that the Hamiltonian (6) does not depend on the phase factor variable ϕ; that is, the Hamiltonian is invariant under the following $\mathbb{S}^1$-action on the manifold M:

$$\mathbb{S}^1 \times M \to M; \quad (\theta, (q,p,\mathcal{A},\mathcal{B},\phi,\delta)) \mapsto (a,p,\mathcal{A},\mathcal{B},\phi+\hbar\,\theta,\delta).$$

This action turns out to be symplectic and the corresponding momentum map (Noether conserved quantity) is

$$\mathbf{N}\colon M \to \mathbb{R}; \qquad \mathbf{N}(y) := -\hbar\mathcal{N}(\mathcal{B},\delta).$$

It is natural to look at the level set $\mathbf{N}^{-1}(-\hbar)$ because, in view of the definition (5) of $\mathcal{N}$, this level set corresponds to the choice of the parameter δ so that the Gaussian χ_M is normalized, i.e., $\|\chi(y;\,\cdot\,)\| = 1$. Furthermore, one may eliminate the variables (ϕ,δ) from the formulation, because now we may apply the Marsden–Weinstein reduction [18] (see also Marsden et al. [19, Sections 1.1 and 1.2]) to obtain the reduced symplectic manifold

$$\overline{M} := \mathbf{N}^{-1}(-\hbar)/\mathbb{S}^1 = T^*\mathbb{R}^d \times \Sigma_d.$$

See [26, Section 4] for the details of this reduction.

As a result, the symplectic form Ω_M on M gives rise to the following symplectic form $\Omega_\hbar$ on $\overline{M}$:

$$\begin{aligned} \Omega_\hbar &= \mathbf{d}q_i \wedge \mathbf{d}p_i + \frac{\hbar}{4}\mathcal{B}_{ik}^{-1}\mathcal{B}_{lj}^{-1}\mathbf{d}\mathcal{A}_{ij} \wedge \mathbf{d}\mathcal{B}_{kl} \\ &= \mathbf{d}q_i \wedge \mathbf{d}p_i + \frac{\hbar}{4}\mathbf{d}\mathcal{B}_{ij}^{-1} \wedge \mathbf{d}\mathcal{A}_{ij}. \end{aligned} \tag{8}$$

Notice that the symplectic form is very simple and also appealing because it has an additional $\mathcal{O}(\hbar)$ correction term compared to the classical symplectic form Ω_0. It is also clear from the above expressions that $\mathcal{B}^{-1}$ and $\mathcal{A}$ are conjugate variables. The corresponding Poisson Bracket is then

$$\{F,G\}_\hbar := \frac{\partial F}{\partial q_i}\frac{\partial G}{\partial p_i} - \frac{\partial G}{\partial q_i}\frac{\partial F}{\partial p_i} + \frac{4}{\hbar}\left(\frac{\partial F}{\partial \mathcal{B}^{-1}_{jk}}\frac{\partial G}{\partial \mathcal{A}_{jk}} - \frac{\partial G}{\partial \mathcal{B}^{-1}_{jk}}\frac{\partial F}{\partial \mathcal{A}_{jk}}\right).$$

Since we are now looking at the normalized Gaussian, we have $\mathcal{N}(\mathcal{B},\delta) = 1$, and thus the reduced Hamiltonian $H\colon \overline{M} \to \mathbb{R}$ becomes

$$\begin{aligned} H(q,p,\mathcal{A},\mathcal{B}) &= \frac{p^2}{2m} + \frac{\hbar}{4m}\operatorname{Tr}\big(\mathcal{B}^{-1}(\mathcal{A}^2+\mathcal{B}^2)\big) - \frac{1}{m}\left\langle \boldsymbol{A}(x)\cdot p\right\rangle \\ &\quad + \frac{\hbar}{2m}\left\langle \operatorname{Tr}\Big(D\boldsymbol{A}^T(x)\mathcal{A}\mathcal{B}^{-1}\Big)\right\rangle + \frac{1}{2m}\left\langle |\boldsymbol{A}(x)|^2\right\rangle + \left\langle V(x)\right\rangle. \end{aligned} \tag{9}$$

The Hamiltonian vector field X_H on $\overline{M}$ defined by the Hamiltonian system $\mathbf{i}_{X_H}\Omega_\hbar = \mathbf{d}H$ or equivalently $\dot{y} = \{\bar{y}, H\}_\hbar$ with $\bar{y} = (q,p,\mathcal{A},\mathcal{B})$ gives the following set of ordinary differential equations:

$$\begin{aligned} \dot{q}_i &= \frac{1}{m}\left(p_i - \left\langle \boldsymbol{A}_i(x)\right\rangle\right), \\ \dot{p}_i &= -\frac{1}{2m}\left(\left\langle D_i|\boldsymbol{A}(x)|^2\right\rangle - 2\left\langle D_i\boldsymbol{A}_j(x)p_j\right\rangle\right) - \frac{\hbar}{2m}\left\langle \boldsymbol{A}_k(x)\mathcal{A}_{kj}\mathcal{B}^{-1}_{ji}\right\rangle - \left\langle D_iV(x)\right\rangle, \\ \dot{\mathcal{A}}_{ij} &= -\frac{1}{m}(\mathcal{A}^2-\mathcal{B}^2)_{ij} + \frac{1}{m}\left\langle D^2_{ij}\boldsymbol{A}_k(x)p_k - D_k\boldsymbol{A}_i(x)\mathcal{A}_{kj} - \mathcal{A}_{ik}D_j\boldsymbol{A}_k(x) - \frac{1}{2}\left\langle D^2_{ij}|\boldsymbol{A}(x)|^2\right\rangle\right\rangle, \\ &\quad - \frac{\hbar}{2m}\left\langle D^2_{ij}(D_l\boldsymbol{A}_k(x)\mathcal{A}_{lm}\mathcal{B}^{-1}_{mk})\right\rangle - \left\langle D^2_{ij}V(x)\right\rangle, \\ \dot{\mathcal{B}}_{ij} &= -\frac{1}{m}(\mathcal{A}\mathcal{B}+\mathcal{B}\mathcal{A})_{ij} + \frac{1}{m}\left\langle \mathcal{B}_{ik}D_j\boldsymbol{A}_k(x) + D_k\boldsymbol{A}_i(x)\mathcal{B}_{kj}\right\rangle, \end{aligned} \tag{10}$$

where $(D\boldsymbol{A})_{ij} = D_j\boldsymbol{A}_i = \frac{\partial \boldsymbol{A}_i}{\partial x_j}$, and $D^2_{ij}\boldsymbol{A}_k = \frac{\partial \boldsymbol{A}_k}{\partial x_i \partial x_j}$.

3 Asymptotic Expansion

3.1 Asymptotic Expansion of Hamiltonian

While the above set (10) of equations is Hamiltonian by construction, it has the drawback that it is not in a closed form: The potential terms—involving either the scalar potential V or the vector potential $\boldsymbol{A}$—appear as expectation values (with respect to the normalized Gaussian). Unfortunately, it is impossible to explicitly evaluate these expectation values unless V and $\boldsymbol{A}$ are polynomials.

So we apply Laplace's method to obtain an asymptotic expansions of the integrals as $\hbar \to 0$ (see, e.g., Miller [20, Chapter 3]). Assuming that the Gaussian is normalized, i.e., $\mathcal{N}(\mathcal{B},\delta) = 1$, each potential term is of the form (see (7)):

$$\left\langle \mathcal{U}\right\rangle(q,\mathcal{B}) = \int_{\mathbb{R}^d} \mathcal{U}(x)\exp\left(-\frac{1}{\hbar}(x-q)^T\mathcal{B}(x-q)\right)\,\mathrm{d}x,$$

As is proved in Ohsawa and Leok [26, Proposition 7.1] (see also Miller [20, Section 3.7]), if $\mathcal{U}$ satisfies a certain growth condition as $|x| \to \infty$, then $\langle \mathcal{U}\rangle$ has the following asymptotic expansion:

$$\left\langle \mathcal{U}\right\rangle(q,\mathcal{B}) = \mathcal{U}(q) + \frac{\hbar}{4}\operatorname{Tr}\big(\mathcal{B}^{-1}D^2\mathcal{U}(q)\big) + \mathcal{O}(\hbar^2) \quad \text{as} \quad \hbar \to 0, \tag{11}$$

where $D^2\mathcal{U}(q)$ is the Hessian matrix of $\mathcal{U}(x)$ evaluated at $x = q$. We note in passing that this asymptotic expansion is exact (i.e., the $O(\hbar^2)$ term vanishes) if $\mathcal{U}$ is quadratic.

As a result, we have the following asymptotic expansion for the Hamiltonian H from (6):

$$H = H_\hbar + \mathcal{O}(\hbar^2) \quad \text{as} \quad \hbar \to 0$$

with

$$\begin{aligned} H_\hbar(q, p, \mathcal{A}, \mathcal{B}) := {}& \frac{1}{2m}(p - \boldsymbol{A}(q))^2 \\ & + \frac{\hbar}{4m} \operatorname{Tr}\left(\mathcal{B}^{-1}\left(\mathcal{A}^2 + \mathcal{B}^2 - D\boldsymbol{A}^T(q)\mathcal{A} - \mathcal{A}D\boldsymbol{A}(q) - D^2(\boldsymbol{A}(q)\cdot p) + \frac{1}{2}D^2|\boldsymbol{A}(q)|^2\right)\right) \\ & + V(q) + \frac{\hbar}{4}\operatorname{Tr}\bigl(\mathcal{B}^{-1}D^2V(q)\bigr). \end{aligned} \tag{12}$$

Notice that, just as for the symplectic form Ω in (8), this semiclassical Hamiltonian H has an additional $\mathcal{O}(\hbar)$ correction term compared to the classical Hamiltonian H_0 from (1).

One may now replace the Hamiltonian H by $H_\hbar$ to define the Hamiltonian vector field $X_{H_\hbar}$ as $\mathbf{i}_{X_{H_\hbar}}\Omega_\hbar = \mathbf{d}H_\hbar$. Then the vector field $X_{H_\hbar}$ yields

$$\begin{aligned} \dot{q}_i &= \frac{p_i}{m} - \frac{\boldsymbol{A}_i(q)}{m} - \frac{\hbar}{4m}\mathcal{B}^{-1}_{jk}D^2_{kj}\boldsymbol{A}_i(q), \\ \dot{p}_i &= -\frac{1}{2m}D_i\left(|\boldsymbol{A}(q)|^2 + \frac{\hbar}{4}(\mathcal{B}^{-1}_{jk}D^2_{kj}|\boldsymbol{A}(q)|^2) - 2\boldsymbol{A}_k(q)p_k - \frac{\hbar}{2}\mathcal{B}^{-1}_{jk}D^2_{kj}\boldsymbol{A}_l(q)p_l\right) \\ &\quad - D_i\left(V(q) + \frac{\hbar}{4}(\mathcal{B}^{-1}_{jk}D^2_{kj}V(q))\right), \\ \dot{\mathcal{A}}_{ij} &= -\frac{1}{m}(\mathcal{A}^2 - \mathcal{B}^2)_{ij} + \frac{1}{m}\left(D_i\boldsymbol{A}_k(q)\mathcal{A}_{kj} + \mathcal{A}_{ik}D_j\boldsymbol{A}_k(q) + D^2_{ij}\boldsymbol{A}_k(q)p_k - \frac{1}{2}D^2_{ij}|\boldsymbol{A}(q)|^2\right) - D^2_{ij}V(q), \\ \dot{\mathcal{B}}_{ij} &= -\frac{1}{m}(\mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A})_{ij} + \frac{1}{m}(D_i\boldsymbol{A}_k(q)\mathcal{B}_{kj} + \mathcal{B}_{ik}D_j\boldsymbol{A}_k(q)). \end{aligned} \tag{13}$$

If we define those terms involving scalar and vector potentials with $O(\hbar)$ corrections as

$$V_\hbar(q, \mathcal{B}) := V(q) + \frac{\hbar}{4}\operatorname{Tr}\bigl(\mathcal{B}^{-1}D^2V(q)\bigr),$$

$$\boldsymbol{A}_{\hbar,i}(q, \mathcal{B}) := \boldsymbol{A}_i(q) + \frac{\hbar}{4}\operatorname{Tr}\bigl(\mathcal{B}^{-1}D^2\boldsymbol{A}_i(q)\bigr), \qquad |\boldsymbol{A}|^2_\hbar(q, \mathcal{B}) := |\boldsymbol{A}(q)|^2 + \frac{\hbar}{4}\operatorname{Tr}\bigl(\mathcal{B}^{-1}D^2|\boldsymbol{A}(q)|^2\bigr),$$

we can rewrite the first two of the above set of equations in a slightly more succinct form:

$$\begin{aligned} \dot{q} &= \frac{1}{m}\left(p - \boldsymbol{A}_\hbar(q, \mathcal{B})\right), \\ \dot{p} &= -\frac{1}{2m}\boldsymbol{\nabla}_q\left(|\boldsymbol{A}|^2_\hbar(q, \mathcal{B}) - 2\boldsymbol{A}_\hbar(q, \mathcal{B})\cdot p\right) - \boldsymbol{\nabla}_q V_\hbar(q, \mathcal{B}). \end{aligned}$$

Notice also its similarity to the classical equations (2).

3.2 Linear Vector Potential with Quadratic Scalar Potential

As mentioned in the Introduction, when the vector potential $\boldsymbol{A}$ is linear ($\boldsymbol{A}(x) = Ax$, where A is a constant $d \times d$ matrix) and the scalar potential V is quadratic, the Gaussian wave packet (4) gives an exact solution to the Schrödinger equation if the parameters satisfy the following set of equations (along with additional equations for ϕ and δ):

$$\begin{aligned} \dot{q}_i &= \frac{1}{m}(p_i - \boldsymbol{A}_i(q)), \\ \dot{p}_i &= -\frac{1}{2m}D_i\left(|\boldsymbol{A}(q)|^2 - 2\boldsymbol{A}_j(q)p_j\right) - D_iV(q), \\ \dot{\mathcal{A}}_{ij} &= \frac{1}{m}(D_i\boldsymbol{A}_k(q)\mathcal{A}_{kj} + \mathcal{A}_{ik}D_j\boldsymbol{A}_k(q)) - \frac{1}{2m}D^2_{ij}|\boldsymbol{A}(q)|^2 - \frac{1}{m}(\mathcal{A}^2 - \mathcal{B}^2)_{ij} - D^2_{ij}V(q), \\ \dot{\mathcal{B}}_{ij} &= \frac{1}{m}(\mathcal{B}_{ik}D_j\boldsymbol{A}_k(q) + D_i\boldsymbol{A}_k(q)\mathcal{B}_{kj}) - \frac{1}{m}(\mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A})_{ij}. \end{aligned} \tag{14}$$

This result is a special case of the more general result of Hagedorn [6] on quadratic Hamiltonians, and also is equivalent to the set of equations given by Zhou [30]; see also the earlier work by Kim and Weiner [12] in which the authors obtained a similar set of equations for the expectation values of the tensor products of $\hat{x}$ and $\hat{p} - \boldsymbol{A}(q)$ in this particular special case where $\boldsymbol{A}$ is linear and V is quadratic.

We note that both Hagedorn and Zhou use, instead of $(\mathcal{A}, \mathcal{B})$, parameters (Q, P) that are $d \times d$ complex matrices satisfying $Q^T P - P^T Q = 0$ and $Q^* P - P^* Q = 2\mathrm{i} I_d$; more precisely, Hagedorn uses parameters $A, B \in \mathbb{C}^{d \times d}$, which are related to Q and P as $A = Q$ and $B = -\mathrm{i}P$. In fact, these two sets of parameters are related by $\mathcal{A} + \mathrm{i}\mathcal{B} = PQ^{-1}$; see Ohsawa [25] for the geometric interpretation of these two different parametrizations. It is straightforward calculations using this relation to check that Zhou's equations imply the above set of equations.

Our set of equations, either (10) or (13), recovers the above set of equations under the above assumptions on the potentials. In fact, as mentioned above, the asymptotic expansion (11) is exact if $\mathcal{U}$ is quadratic. This implies that the Hamiltonian (9) and its $\mathcal{O}(\hbar^2)$ approximation (12) coincide, and thus so do the equations (10) and (13). Now, if the vector potential $\boldsymbol{A}$ is linear and the scalar potential V is quadratic, many of the terms in (13) involving the Hessians of the potentials vanish, hence recovering (14).

4 Semiclassical Angular Momentum in Electromagnetic Potentials

One advantage of the Hamiltonian formulation using the language of symplectic geometry is that it is amenable to the geometric treatment of symmetry. Specifically, if the Hamiltonian function of the system is invariant under some Lie group action, it is desirable to investigate any conserved quantities in the system via Noether's Theorem. Particularly, in this section, we show that the semiclassical angular momentum found in our previous work [24] is conserved if the electromagnetic potentials possess a rotational symmetry.

4.1 Symmetry in Electromagnetic Potentials

Suppose that the scalar and vector potentials V and $\boldsymbol{A}$ possess the rotational symmetry in the following sense: For any $R \in \mathsf{SO}(d)$ and any $x \in \mathbb{R}^d$,

$$V(Rx) = V(x) \quad \text{and} \quad \boldsymbol{A}(Rx) = R\boldsymbol{A}(x); \tag{15}$$

that is, V is $\mathsf{SO}(d)$-invariant whereas $\boldsymbol{A}$ is $\mathsf{SO}(d)$-equivariant. We note that the latter condition implies $D\boldsymbol{A}(Rx) = R\boldsymbol{A}(x)R^T$ for any $R \in \mathsf{SO}(d)$ and any $x \in \mathbb{R}^d$.

As is done in [24], we define the action of the rotation group $\mathsf{SO}(d)$ on the symplectic manifold $\overline{M} = T^*\mathbb{R}^d \times \Sigma_d$ as follows:

$$\Gamma \colon \mathsf{SO}(d) \times \overline{M} \to \overline{M}; \qquad (q, p, \mathcal{A}, \mathcal{B}) \mapsto \Gamma_R(q, p, \mathcal{A}, \mathcal{B}) := \left(Rq, Rp, R\mathcal{A}R^T, R\mathcal{B}R^T\right).$$

It is easy to check that Γ is symplectic, i.e., $\Gamma_R^*\Omega = \Omega$ for any $R \in \mathsf{SO}(d)$. Then our Hamiltonian, either (9) or (12), is invariant under this action, i.e., for any $R \in \mathsf{SO}(d)$, $H \circ \Gamma_R = H$ and $H_\hbar \circ \Gamma_R = H_\hbar$. In fact, for the Hamiltonian (12), it follows from a straightforward calculation using the above symmetry assumptions on V and $\boldsymbol{A}$. For the Hamiltonian (9), note that the expectation values of the potentials maintain the same symmetry, i.e.,

$$\langle V \rangle (Rq, R\mathcal{B}R^T) = \langle V \rangle (q, \mathcal{B}), \quad \text{and} \quad \langle \boldsymbol{A} \rangle (Rq, R\mathcal{B}R^T) = R \langle \boldsymbol{A} \rangle (q, \mathcal{B}).$$

4.2 Semiclassical Angular Momentum

The momentum map $\mathbf{J}_\hbar \colon \overline{M} \to \mathfrak{so}(d)^*$ corresponding to the action Γ defined above is given by (see Ohsawa [24, Section 3] for the derivation)

$$\mathbf{J}_\hbar(q, p, \mathcal{A}, \mathcal{B}) = q \diamond p - \frac{\hbar}{2}[\mathcal{B}^{-1}, \mathcal{A}], \tag{16}$$

where $(q \diamond p)_{ij} = q_j p_i - q_i p_j$ (see Holm [11, Remark 6.3.3]), and we identified $\mathfrak{so}(d)^*$ with $\mathfrak{so}(d)$ via an inner product. Setting $\hbar = 0$ reduces the above to the classical angular momentum, hence we call the above the *semiclassical angular momentum*. Interestingly, this semiclassical angular momentum coincides with the expectation value of the angular momentum with respect to the normalized Gaussian, i.e., for $d = 3$,

$$\langle \hat{x} \times \hat{p} \rangle = \mathbf{J}_\hbar(q, p, \mathcal{A}, \mathcal{B}).$$

Now, assuming the symmetry (15) in the potentials, by Noether's Theorem (see, e.g., Marsden and Ratiu [17, Theorem 11.4.1]), we conclude that the semiclassical angular momentum (16) is a conserved quantity of our semiclassical equation (10) or (13).

5 Numerical Examples

Given that our set of equations (13) differs from that of Zhou by $\mathcal{O}(\hbar)$ correction terms, a natural question is whether these correction terms improve the accuracy of approximation. Specifically, we are interested in comparing the time evolution $t \mapsto z(t) = (q(t), p(t))$ of the phase space variables of our semiclassical equations with that of the expectation values $\langle \hat{z} \rangle$ of the position and momentum operators $\hat{z} = (\hat{x}, \hat{p})$, i.e., $t \mapsto \langle \hat{z} \rangle(t) = \langle \psi(t, \cdot\,), \hat{z}\psi(t, \cdot\,) \rangle$, where $t \mapsto \psi(t, \cdot\,)$ is a solution of the Schrödinger equation (3).

In the following, we compare numerical solutions of the classical equations (2), the semiclassical equations (13), as well as the time-dependent expectation values of observables as calculated by the Egorov [1, 2, 14] or Initial Value Representation [21–23, 28] (Egorov/IVR) method; see Section 5.1 below. Note that the time evolution of (q, p) of Zhou's equations (14) is identical to that of the classical equations (2). In all of the following, we solved our equations and the classical equations by the explicit Runge–Kutta method with a time step of 0.01. For the Egorov/IVR computations, we used 10^6 samples for each value of $\hbar$, with the exception of $\hbar = 0.01$ for which we used 10^7 samples.

5.1 The Egorov/IVR Method

It is computationally prohibitive to solve for the highly oscillatory wave functions numerically in the semiclassical regime $\hbar \ll 1$. Therefore, we employ the Egorov/IVR method instead of solving the Schrödinger equation (3) directly.

Let us first briefly describe Egorov's Theorem [2]. Given a wave function $\psi \in L^2(\mathbb{R}^d)$, define the corresponding *Wigner function* $\mathcal{W}_\psi \colon T^*\mathbb{R}^d \to \mathbb{R}$ on the phase space $T^*\mathbb{R}^d \cong \mathbb{R}^{2d}$ as follows:

$$\mathcal{W}_\psi(z) := \frac{1}{(2\pi\hbar)^d} \int_{\mathbb{R}^d} e^{-\frac{i}{\hbar} p \cdot x}\, \overline{\psi}(q - x/2)\, \psi(q + x/2)\, dx.$$

The Wigner function is used to define, for a given (classical) observable $a \colon T^*\mathbb{R}^d \to \mathbb{R}$ (such as the position, momentum, and energy in the classical sense), the corresponding operator $\hat{a}$ on the Hilbert space $L^2(\mathbb{R}^d)$ such that

$$\langle \psi, \hat{a}\psi \rangle = \int_{T^*\mathbb{R}^d} a(z)\, \mathcal{W}_\psi(z)\, dz.$$

Specifically, one obtains $\hat{a} = \hat{x}_i$ for $a = q_i$ for $\hat{a} = \hat{x}_i$, and $\hat{a} = \hat{p}_i$ for $a = p_i$. This procedure is called the *Weyl quantization* and is a standard quantization scheme on phase space $T^*\mathbb{R}^d$. Egorov's Theorem [2] states that, under some technical conditions on the Hamiltonian H and the observable a, the dynamics $t \mapsto \langle \psi(t), \hat{a}\psi(t) \rangle$ of the expectation value of $\hat{a}$ is approximated as follows: Given the initial wave function $\psi_0 \in L^2(\mathbb{R}^d)$,

$$\langle \psi(t), \hat{a}\psi(t) \rangle = \int_{T^*\mathbb{R}^d} (a \circ \Phi_t)(z)\, \mathcal{W}_{\psi_0}(z)\, dz + O(\hbar^2), \tag{17}$$

where $\Phi_{(\cdot)} \colon \mathbb{R} \times T^*\mathbb{R}^d \to T^*\mathbb{R}^d$ is the flow of the classical Hamiltonian system (2).

The Egorov/IVR method (see, e.g., [14]) numerically implements the above approximation by first sampling N initial conditions $\{z^{(k)}\}_{k=1}^N \subset T^*\mathbb{R}^d$ on the phase space, solve the classical Hamiltonian system (2) to obtain the solutions $\{\Phi_t(z^{(k)})\}_{k=1}^N$, and then take the average to approximate the above integral, i.e.,

$$\int_{T^*\mathbb{R}^d} (a \circ \Phi_t)(z)\, \mathcal{W}_{\psi_0}(z)\, dz \simeq \sum_{k=1}^N a \circ \Phi_t(z^{(k)}),$$

where the error of this Monte Carlo numerical integration is known to be proportional to $1/\sqrt{N}$.

The Egorov/IVR method is different from the well-known Herman–Kluk propagator [10] in the sense that it directly approximates the expectation values of observables without approximating the wave function or the propagator. We note that the Herman–Kluk propagator is known to have $O(\hbar)$ error—as opposed to $O(\hbar^2)$—in the propagator in terms of the operator norm in $L^2(\mathbb{R}^d)$ [27]; see also [29]. The Egorov/IVR method is also suited for our purposes because we are interested in the time evolution of expectation values.

5.2 1D Example

Here we let $d = 1$, $m = 1$, $V(x) = 1 - \frac{1}{2}\cos^2(x)$, $A(x) = \cos(x)$, subject to the initial conditions $q(0) = 0.5$, $p(0) = -1$, $\mathcal{A}(0) = 0$, $\mathcal{B}(0) = 1$; the scalar and vector potentials are taken from Zhou [30, Example 1]. In order to see how the error converges as $\hbar \to 0$, we ran the computations for $\hbar = 0.5, 0.3, 0.1, 0.05, 0.03, 0.01$.

Figure 2 shows the solutions on the classical phase space $T^*\mathbb{R} = \mathbb{R}^2$ from $t = 0$ to $t = 3$ as well as the error $|\langle \hat{z} \rangle(t) - z(t)|$ at $t = 1.6$ in terms of the Euclidean norm on the classical phase space. As can be seen, our solutions are closer to the Egorov/IVR than the classical solutions. Furthermore, as $\hbar \to 0$, our solutions converge to the Egorov/IVR solutions faster than the classical equations.

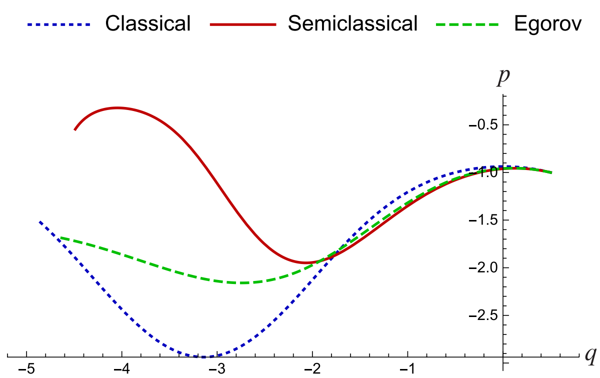
Figure 3 shows the time evolutions of the Hamiltonians for the classical, semiclassical, and Egorov/IVR solutions. Note that the Hamiltonians for all these three cases are different: It is H_0 in (1) for the classical case and $H_\hbar$ in (12) for the semiclassical case, whereas for the Egorov/IVR case, it is the expectation value $\langle \hat{H} \rangle$ of the Hamiltonian operator $\hat{H}$. In each of these cases, the corresponding Hamiltonian is a conserved quantity. Notice that the semiclassical Hamiltonian gives a better approximation to the expectation value of the Hamiltonian.

5.3 2D Example

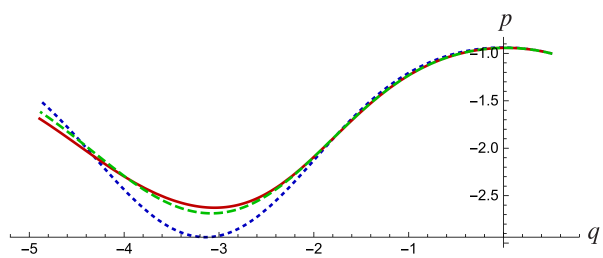
Here we let $d = 2$, $V(x) = \frac{1}{2}|x|^2 + \frac{1}{4}|x|^4$, $A(x) = (-x_2, x_1)$, subject to the initial conditions $q(0) = (1, 0)$, $p(0) = (0, 1)$, $\mathcal{A}(0) = \begin{pmatrix} -3 & -6 \\ -6 & -6 \end{pmatrix}$, $\mathcal{B}(0) = \begin{pmatrix} 1 & 1/2 \\ 1/2 & 1 \end{pmatrix}$.

Figure 4 shows the solutions on the classical configuration space $\mathbb{R}^2 = \{(q_1, q_2)\}$ from $t = 0$ to $t = 10$ as well as the error $|\langle \hat{z} \rangle(t) - z(t)|$ at $t = 2$ in terms of the Euclidean norm on the classical phase space $T^*\mathbb{R}^2 \cong \mathbb{R}^4$. Figure 5 shows the time evolutions of the Hamiltonians for the classical, semiclassical, and Egorov/IVR solutions just as in the 1D case. The same observations as above apply to these 2D results as well.

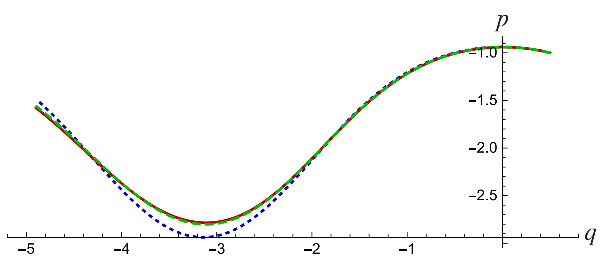
For this 2D example, the scalar and vector potentials chosen above satisfy the symmetry condition (15). Therefore, based on the result of Section 4, the semiclassical angular momentum (16) is also a conserved quantity of the semiclassical system (13) as well. Figure 6 shows the time evolutions of the classical angular momentum along the classical solutions, the semiclassical angular momentum (16) along the semiclassical



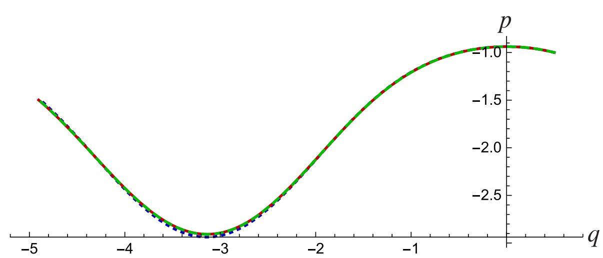
(a) $\hbar = 0.5$



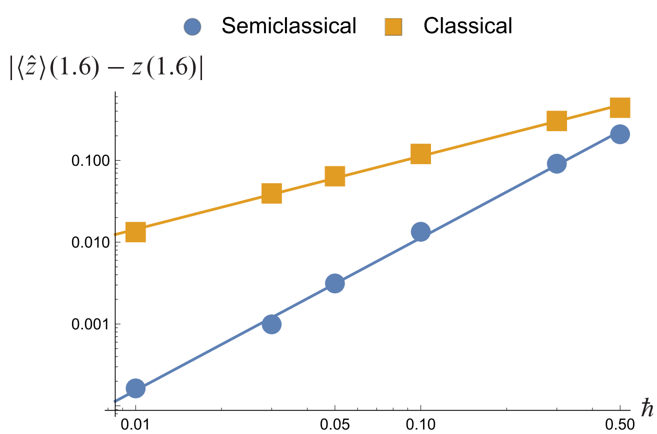
(b) $\hbar = 0.1$



(c) $\hbar = 0.05$

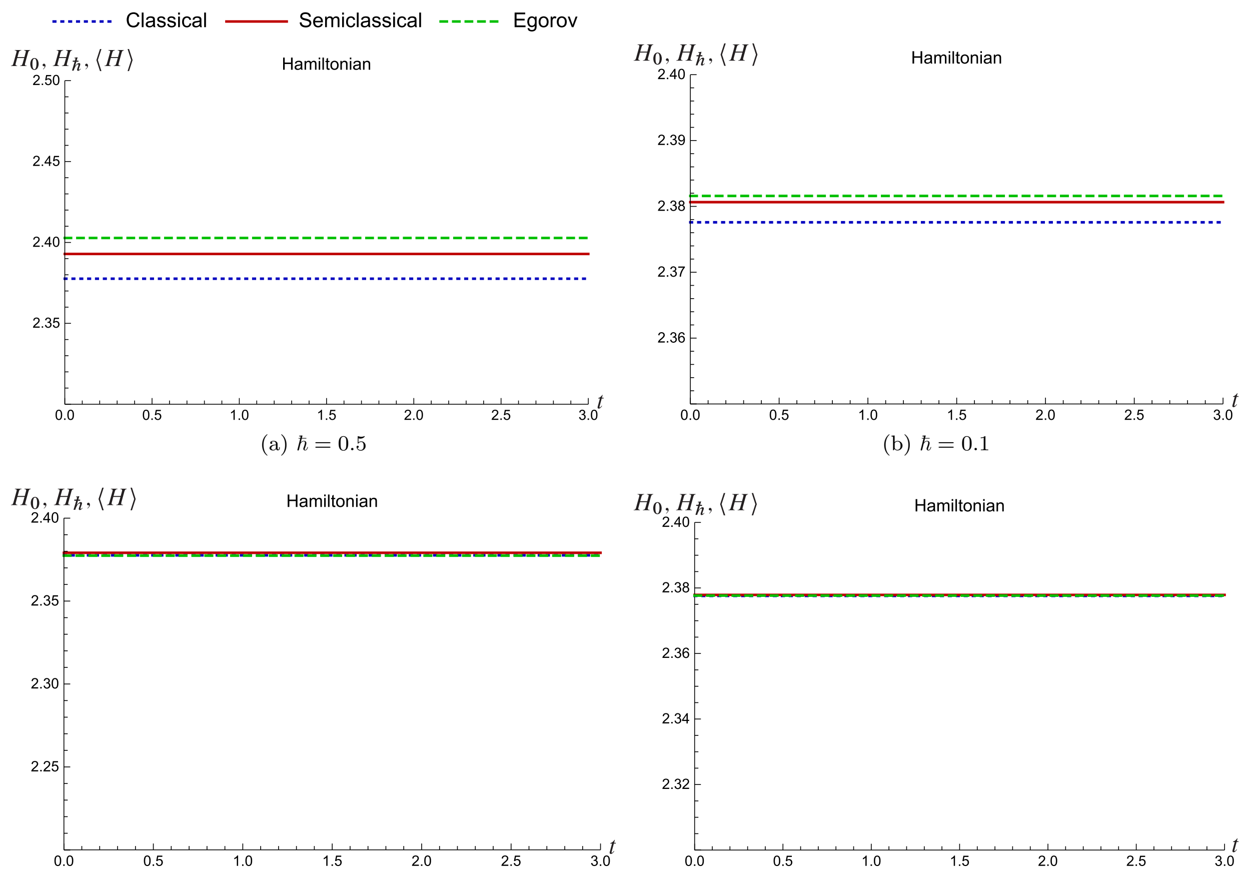


(d) $\hbar = 0.01$



(e) Convergence of errors as $\hbar \to 0$

Figure 2: Results of 1D computations with $m = 1$, $V(x) = 1 - \frac{1}{2}\cos^2(x)$, $A(x) = \cos(x)$. (a)–(d): Parametric plots of $t \mapsto q(t) = (q_1(t), q_2(t))$ in the classical phase space $T^*\mathbb{R} \cong \mathbb{R}^2$ for $\hbar = 0.5, 0.1, 0.05, 0.01$ from $t = 0$ to $t = 3$. Our solutions are closer to the Egorov/IVR than the classical solutions. (e): The error $|\langle \hat{z} \rangle(t) - z(t)|$ for several values of $\hbar$ at $t = 1.6$. As $\hbar \to 0$, our solutions converge to the Egorov/IVR solutions faster than the classical equations. The equation of the best fit line for the semiclassical error is $\exp(-0.190) * \hbar^{1.864}$, and $\exp(-0.125) * \hbar^{0.894}$ for the classical.



(a) $\hbar = 0.5$ (b) $\hbar = 0.1$ (c) $\hbar = 0.05$ (d) $\hbar = 0.01$

Figure 3: Time evolution of the Hamiltonian for the above 1D system solutions for $\hbar = 0.5, 0.1, 0.05, 0.01$. The semiclassical Hamiltonian (12) more closely approximates the Egorov/IVR expectation value $\langle \hat{H} \rangle$ of the Hamiltonian operator than the classical Hamiltonian (1).

solutions, and the expectation value of the angular momentum operator along the Egorov/IVR solutions. We see that the semiclassical angular momentum gives a better approximation to the expectation value of the angular momentum than the classical one does.

6 Conclusion and Future Work

We extended our earlier work on the Hamiltonian formulation of Gaussian wave packets to incorporate electromagnetic fields. Many of the results are extensions of our previous works to incorporate the electromagnetic effects. These results greatly expand the range of applications of semiclassical dynamics because of its importance in quantum control and solid state physics.

As seen in the above numerical results, our solutions converge to the the expectation value of the operator $z = (q, p)$ along the Egorov/IVR solution faster than the classical solution. Since the equations for q and p given by Zhou [30] are identical to the classical equations, our solutions also converge faster than those of Zhou. These results demonstrate that the $\mathcal{O}(\hbar)$ correction terms in our semiclassical equations (13) indeed improve the accuracy of the approximations of expectation values.

Our preliminary studies (under certain technical assumptions and without electromagnetic fields) indicate that the errors in the observables of the classical solution is $\mathcal{O}(\hbar)$ whereas $\mathcal{O}(\hbar^{3/2})$ for the semiclassical solution, despite the well-known fact that the Gaussian wave packet dynamics gives $\mathcal{O}(\hbar^{1/2})$ approximation *in terms of the wave functions* in L^2-norm established by Hagedorn [3, 4, 5, 6]. Our numerical results seem to support these claims. A proof of this error estimate remains for a future work.

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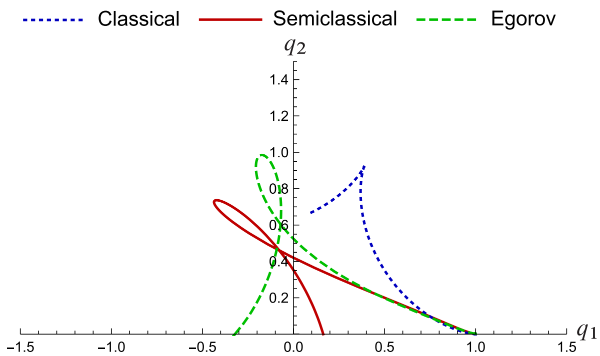
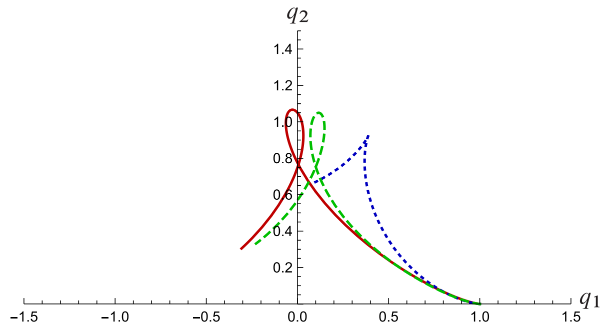
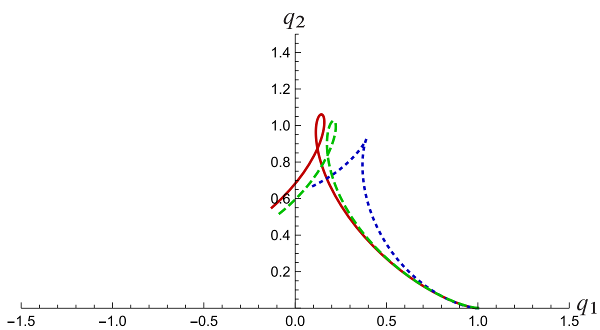


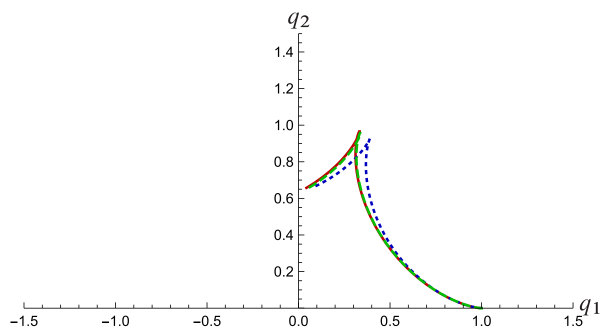
(a) $\hbar = 0.5$



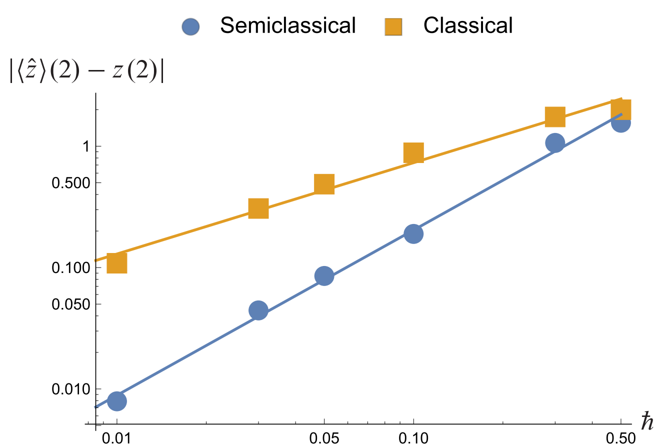
(b) $\hbar = 0.1$



(c) $\hbar = 0.05$



(d) $\hbar = 0.01$



(e) Convergence of errors as $\hbar \to 0$

Figure 4: Results of 2D computations with $d = 2$, $V(x) = \frac{1}{2}|x|^2 + \frac{1}{4}|x|^4$, $A(x) = (-x_2, x_1)$. (a)–(d): Parametric plots of $t \mapsto q(t) = (q_1(t), q_2(t))$ in the classical configuration space $\mathbb{R}^2$ for $\hbar = 0.5, 0.1, 0.05, 0.01$ from $t = 0$ to $t = 3$. (e): The error $|\langle \hat{z} \rangle(t) - z(t)|$ for several values of $\hbar$ at $t = 2$. Again, as $\hbar \to 0$, our solutions converge to the Egorov/IVR solutions faster than the classical equations. The equation of the best fit line for the semiclassical error is $\exp(1.544)\hbar^{1.3612}$, and $\exp(1.41845)\hbar^{0.752}$ for the classical.

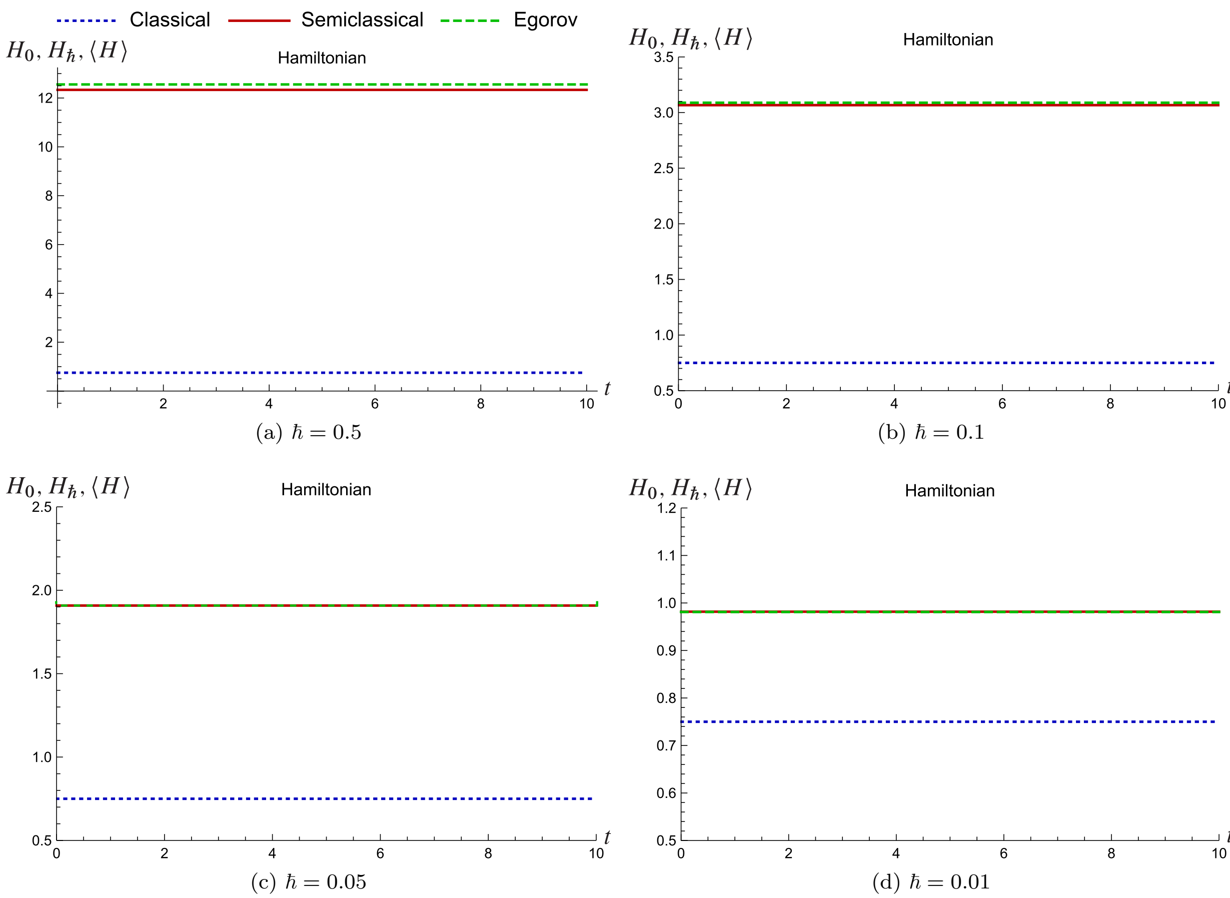


Figure 5: Time evolution of the Hamiltonian for the above 2D system solutions for $\hbar = 0.5, 0.1, 0.05, 0.01$. The semiclassical Hamiltonian (12) more closely approximates the Egorov/IVR expectation value $\langle \hat{H} \rangle$ of the Hamiltonian operator than the classical Hamiltonian (1).

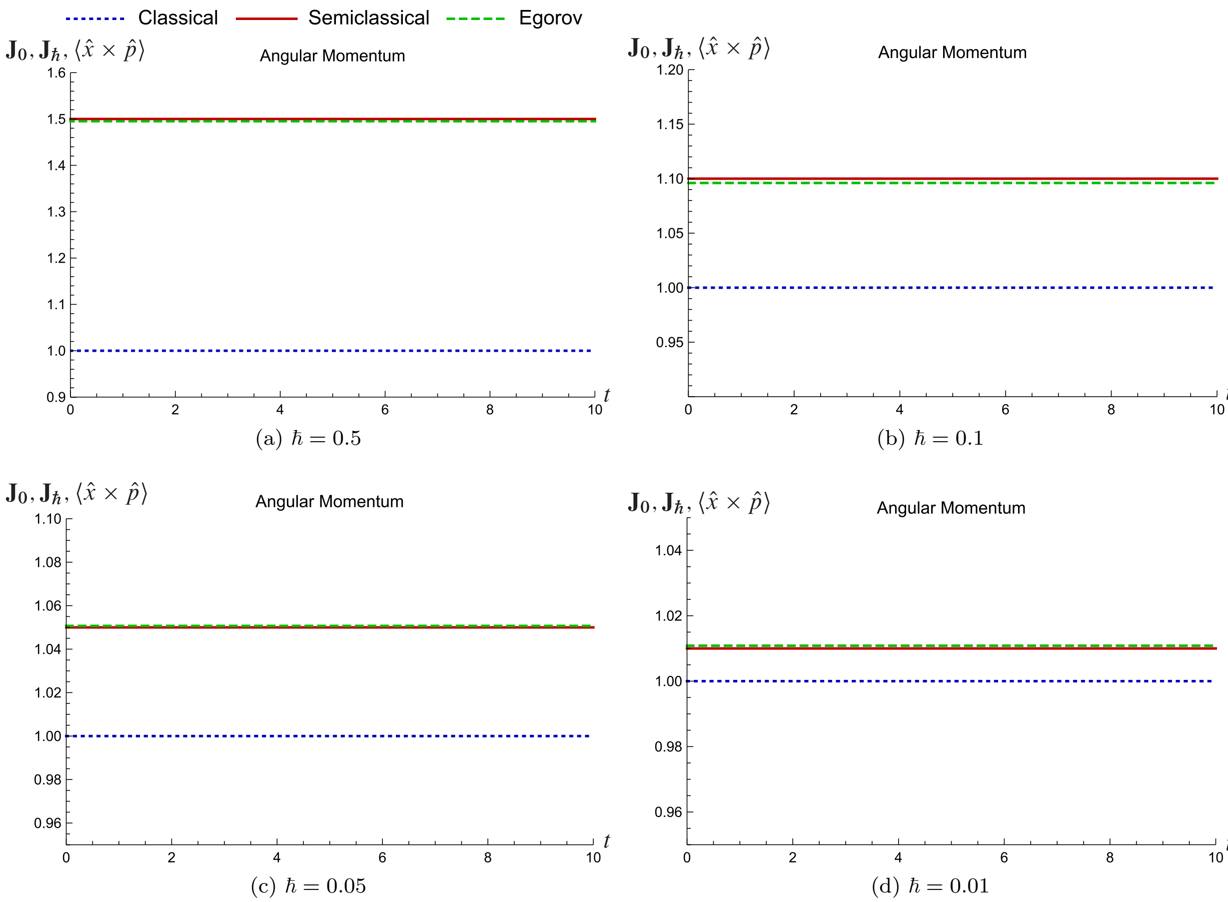


Figure 6: Time evolution of the classical angular momentum along the classical solution, the semiclassical angular momentum along the semiclassical solution, and the expectation value of the angular momentum operator for the 2D system. The semiclassical angular momentum is in far closer agreement than the angular momentum along the classical solutions.