Gaussian wave packets for the magnetic Schrödinger equation

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Abstract

In this talk, we consider the semiclassical magnetic Schrödinger equation, which describes the dynamics of particles under the influence of a magnetic field. Following [1], 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 will derive ODEs for the parameters of the variational solution. Moreover, we obtain L^2-error bounds and observable error bounds for the approximating Gaussian wave packet.

Keywords: magnetic Schrödinger equation, semiclassical analysis, variational approximation, observables

1 Introduction

We consider the semiclassical magnetic Schrödinger equation

$$i\varepsilon\partial_t\psi(t) = H(t)\psi(t), \quad \psi(0) = \psi_0, \qquad (1)$$

with Hamiltonian

$$H(t) = \big(i\varepsilon\nabla + A(t)\big)^2 + V(t),$$

for $t \in [0,T]$ on $\mathbb{R}^d$ and the semiclassical parameter $0 < \varepsilon \ll 1$. The scalar, subquadratic potential V and the vector valued, sublinear, magnetic potential A are assumed to be smooth and might be time-dependent. We approximate the solution of (1) on the manifold $\mathcal{M}$ of Gaussian wave packets of the form

$$u(x,\cdot) = \exp\left(\frac{i}{\varepsilon}\left(\frac{1}{2}{x_q}^T C x_q + x_q^T p + \zeta\right)\right) \qquad (2)$$

where $x_q = x - q$ with time-dependent parameters $q(t), p(t) \in \mathbb{R}^d$, $C(t) \in \mathbb{C}^{d\times d}$ symmetric with positive definite imaginary part, and phase $\zeta(t) \in \mathbb{C}$. To approximate in time we derive equations of motion (ODEs) for the parameters of the wave packet. Following the approach in [1], we derive L^2-error bounds and error bounds for observables.

Employing a perturbation result for relatively bounded operators, well-posedness of (1) is obtained via evolution families in the hyperbolic case, cf. [3–5].

2 Variational approximation

We consider the Dirac-Frenkel variational approximation introduced in [1, 2]: Seek $u \in \mathcal{M}$ such that $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$ and

$$\big\langle i\varepsilon\partial_t u(t) - H(t)u(t) | v\big\rangle = 0,\ v \in \mathcal{T}_{u(t)}\mathcal{M}, \qquad (3)$$

where we denote by $\mathcal{T}_u\mathcal{M}$ the tangent space of the manifold $\mathcal{M}$ at u. Using the orthogonal projection $P_u : L^2(\mathbb{R}^d) \to \mathcal{T}_u\mathcal{M}$ onto the tangent space, the variational approximation (3) can be reformulated as

$$i\varepsilon\partial_t u(t) = P_{u(t)}\big(H(t)u(t)\big), \qquad (4)$$

with initial value $u(0) = u_0 \in \mathcal{M}$.

The approximation by Gaussian wave packets seems appropriate due to the following exactness result shown in [1].

Proposition 1 ([1, Prop. 3.2]). *Let $V(\cdot,t)$ be quadratic and $A(\cdot,t)$ be linear in space, $t \in [0,T]$. If the initial value ψ_0 is a Gaussian wave packet, then the solution of (1) is given by the variational approximation satisfying (4).*

3 Equations of motion

The variational formulation (4) leads to ordinary differential equations for the parameters of the Gaussian wave packet. To see this we use the following projection formula from [1].

Proposition 2 ([1, Prop. 3.14]). *For a Gaussian wave packet u with $\|u\|_{L^2} = 1$ and a scalar smooth potential W we have*

$$P_u(Wu) = \big(\alpha + v^T x_q + \tfrac{1}{2}x_q^T B x_q\big)u,$$

where α, v, B are given by

$$\alpha = \langle W\rangle_u - \frac{\varepsilon}{4}\mathrm{tr}\left(\mathrm{Im}\, C^{-1}\left\langle\nabla^2 W\right\rangle_u\right),$$
$$v = \langle\nabla W\rangle_u, \quad B = \langle\nabla^2 W\rangle_u.$$

Here we used the notation $\langle W\rangle_u = \langle u|Wu\rangle$.

Comparing both sides of (4) and using Proposition 2 leads to ordinary differential equations for the parameters. The normalization is achieved by choosing an initial Gaussian wave packet of L^2-norm one and employing norm conservation. In order to apply Proposition 2 we make use of

$$\begin{aligned} i\varepsilon A \cdot \nabla u &= -A \cdot \big(Cx_q + p\big)u, \\ -\frac{\varepsilon^2}{2}\Delta u &= \left(\frac{1}{2}x_q^T C^2 x_q + p^T C x_q\right) u \\ &\quad + \left(\frac{1}{2}|p|^2 - \frac{i\varepsilon}{2}\mathrm{tr}(C)\right) u. \end{aligned}$$

For the equations of motion we use the notation

$$\begin{aligned} \widetilde{V} &= \frac{1}{2}|A|^2 + V, \\ J_A &= \big(\partial_j A_k\big)_{j,k=1}^d, \\ (D^2_{A,v})_{k,l} &= \textstyle\sum_{j=1}^d \partial_l \partial_k A_j v_j, \quad v \in \mathbb{C}^d. \end{aligned}$$

If the parameters of the Gaussian wave packet u defined in (2) satisfy

$$\begin{aligned} \dot{q} &= p - \langle A \rangle_u, \\ \dot{p} &= \big\langle J_A^T \mathrm{Re}\, C(x-q)\big\rangle_u + \langle J_A \rangle_u^T p - \langle \nabla \widetilde{V} \rangle_u, \\ \dot{C} &= -C^2 + \langle D^2_{A,\mathrm{Re}\, C(x-q)} \rangle_u + \langle D^2_{A,p} \rangle_u \\ &\quad + \langle J_A \rangle_u^T C + C \langle J_A \rangle_u - \langle \nabla^2 \widetilde{V} \rangle_u, \end{aligned}$$

then u is the variational solution (4). Moreover, ζ is defined by normalization of u.

4 L^2- and observable error bounds

If the potentials A and V can be approximated by linear or quadratic potentials, respectively, then by Proposition 1, the L^2-error is of order $\sqrt{\varepsilon}$, provided the following assumption holds.

Assumption *The parameters $q, p \in \mathbb{R}^d$, $C \in \mathbb{C}^{d\times d}$, and $\zeta \in \mathbb{C}$ of the Gaussian wave packet u satisfying* (2) *and* (4) *are bounded uniformly on* $[0, T]$.

For our analysis in [6], we assume that the equations of motion for the parameters are solved exactly and therefore use (4). With this, we can state the following bound.

Theorem 4. *Let ψ be the solution of* (1) *and u be the solution of* (4). *If the initial value ψ_0 is a Gaussian wave packet, then we have the error bound*

$$\|\psi(t) - u(t)\|_{L^2} \le tc\sqrt{\varepsilon},$$

where c depends on the parameters and on the potentials, but is independent of ε and t.

Next, we state the error of observables, i.e., selfadjoint operators on $L^2(\mathbb{R}^d)$, which are used to describe physical states. We consider operators $\mathbf{A} = \mathrm{op}_{\mathrm{Weyl}}(\mathfrak{a})$ corresponding to a classical observable $\mathfrak{a} = \mathfrak{a}(q,p) \in C^\infty(\mathbb{R}^{2d})$ via the Weyl-quantization satisfying

$$\mathrm{op}_{\mathrm{Weyl}}(p)\psi = i\varepsilon\nabla\psi, \quad \mathrm{op}_{\mathrm{Weyl}}(q)\psi = x\psi.$$

Theorem 5. *Let ψ be the solution of* (1) *and u be the solution of* (4). *If the initial value ψ_0 is a Gaussian wave packet, then we have the error bound*

$$\big|\big\langle \psi(t)|\mathbf{A}\psi(t)\big\rangle - \big\langle u(t)|\mathbf{A}u(t)\big\rangle\big| \le tc\varepsilon,$$

where c depends on the parameters, on the potentials, and on $\mathfrak{a}$, but is independent of ε and t.

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References

[1] Lasser, Caroline and Lubich, Christian, Computing quantum dynamics in the semiclassical regime, *Acta Numerica*, **29** (2020), pp. 229-401.

[2] Lubich, Christian, From quantum to classical molecular dynamics: reduced models and numerical analysis, *Zurich Lectures in Advanced Mathematics*, EMS, (2008), pp. x+144.

[3] Schmüdgen, Konrad, Unbounded self-adjoint operators on Hilbert space, *Graduate Texts in Mathematics*, **265**, Springer, Dordrecht, (2012), pp. xx+432.

[4] Engel, Klaus-Jochen and Nagel, Rainer, One-parameter semigroups for linear evolution equations, *Graduate Texts in Mathematics*, **194**, Springer-Verlag, (2000), pp. xxii+586.

[5] Pazy, A., Semigroups of linear operators and applications to partial differential equations, *Applied Mathematical Sciences*, **44**, Springer-Verlag, (1983), pp. viii+279.

[6] Burkhard, Selina, Gauß'sche Wellenpakete für die magnetische Schrödingergleichung, Master's Thesis, Karlsruhe Institue of Technology, (2021).