Time-Dependent Schrödinger Equation with Magnetic Field

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1 Introduction

1.1 Mathematic model

In this report we consider a spinless particle in $\mathbb{R}^d$ with mass $m \in \mathbb{R}_{\geq 0}$ and charge $e \in \mathbb{R}$ in a homogeneous magnetic field $B(t)$. We follow the notation introduced in [1] and quickly recapulate that derivation. In quantum mechanics, the time evolution of a particle subject to a magnetic field is governed by the Pauli equation

$$i\hbar\partial_t \Psi(x,t) = H_P(t)\Psi(x,t) \tag{1}$$

$$H_P(t) := \frac{1}{2m}\sum_{k=1}^{d}(p_k - eA_k(x,t))^2 + e\phi(x,t) + \tilde{V}(x,t) \tag{2}$$

where $\tilde{V}(x,t)$ is some external potential. The magnetic field 2-form dA associated with $B(t)$ is independent of x because of the homogeneity of $B(t)$ and we can thus rewrite the magnetic vector potential to

$$A(x,t) := \frac{1}{2}B_{jk}(t)x^j \mathrm{d}x^k, \tag{3}$$

where $B(t) = (B_{jk}(t))_{j,k=1}^d$ is a real, skew-symmetric matrix. Using the operators

$$L_{jk} := x_j p_k - x_k p_j \tag{4}$$

$$H_B(t) := -\sum_{j,k=1}^{d} B_{jk}(t)L_{jk} \tag{5}$$

the Pauli-Hamiltonian takes the form

$$H_P(t) = \frac{1}{2m}\left(\hbar^2(-\Delta) - e\sum_{1\leqslant j<k\leqslant d} B_{jk}(t)L_{jk} + \frac{e^2}{4}\|B(t)x\|^2_{\mathbb{R}^d}\right) + e\phi(x,t) + \tilde{V}(x,t). \tag{6}$$

1.2 Numerical model

We introduce $\epsilon^2 := \hbar$ and redefine t, x and B to find the simplified form

$$H_P(t) = -\Delta + H_B(t) + V(x,t) \tag{7}$$

where $V(x,t) := \frac{1}{2m}\frac{e^2}{4}\|B(t)x\|^2_{\mathbb{R}^d} + e\phi(x,t) + \tilde{V}(x,t)$ is the total potential. The Schrödinger equation is then split up into three separate parts that can be solved numerically.

$$i\epsilon^2\partial_t\Psi = -\Delta\Psi \tag{K}$$

$$i\epsilon^2\partial_t\Psi = H_B(t)\Psi \tag{M}$$

$$i\epsilon^2\partial_t\Psi = V(x,t)\Psi \tag{P}$$

(K) can be solved discretely in Fourier-space and (P) by pointwise multiplication with $e^{-i/\epsilon^2\int_{t_0}^t dtV(x,t)}$. (M) is reduced to the linear differential equation

$$\frac{d}{dt}y(t) = B(t)y(t) \tag{B}$$

[2] proves the existence of a solution $U(t,t_0)$ to (B). The unitary representation

$$\rho : SO(d) \longrightarrow U(L^2(\mathbb{R}^d)) \tag{8}$$

$$R \longmapsto (\rho(R)\Psi)(x) = \Psi(R^{-1}x) \tag{9}$$

maps the solution $U(t,t_0)$ of (B) to a solution of (M). The proof of this statement can be found in [1]. The exact flow map $U(t,t_0)$ is approximated through a Magnus expansion proposed by [3].

2 Setup and Method

3 Results

4 Summary and Conclusion

References

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