# Spectral methods in computational quantum mechanics

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*Abstract*

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We review some applications of spectral methods based on Fourier expansions to computational problems in quantum mechanics and we discuss a single topic in some detail, namely the case of a quantum (charged) spinless particle on a Riemannian manifold interacting with a magnetic field (the problem of Landau levels in a curved configuration space). We study the asymptotic expansion of the ground state around the flat metric and we give an estimate of the first few coefficients.

*Keywords:* Spectral methods, quantum mechanics, Landau levels.

## 1. Introduction

Spectral methods have gained a good reputation among numerical analysts as a robust numerical tool for a wide variety of problems in applied mathematics [1]. In this paper we discuss a certain class of applications initiated by Feit et al. [4] and later pursued by other authors [3,12]. The paper is divided into two parts. The first part introduces the general idea of spectral method as applied to quantum mechanics; it is meant to be a rather informal introduction to the subject, with a guide to the relevant references. In the second part we discuss

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While the first viewpoint (Feynman path integral) may be more appealing to physical intuition, this second one is more prosaic, but also more flexible — it can be applied for instance to the Dirac equation [1] where a classical description is, to say the least, problematic.

The algorithm which computes the quantum dynamics generated by the Hamiltonian $H$ is then constructed as a series of partial FFTs hopping from one $\mathcal{L}_\alpha$ to another, the wave function being multiplied by the phase factors $\exp\{-i\tau h_\alpha(\mathcal{L}_\alpha)\}$ appropriate to the current Lagrangian subspace. For the simplest case $H = h_1(p) + h_2(q)$ the algorithm [2] is just given as follows.

**Algorithm 1.** *Iterate $N$ times*:
**begin**
$\qquad \psi \leftarrow \psi \times \exp\{-i\tau h_2(q)\}$
$\qquad \text{FFT}(\psi)$
$\qquad \psi \leftarrow \psi \times \exp\{-i\tau h_1(p)\}$
$\qquad \text{FFT}^{-1}(\psi)$
**end**

A slightly more general Hamiltonian is given by the spinless particle in a magnetic field $B = \nabla \times A$ (in units such that $e/c \equiv 1$):

$$H = h_1(p) + h_2(q) + \sum_\mu p_\mu A^\mu(q), \quad \frac{\partial A^1}{\partial q_1} = \cdots = \frac{\partial A^n}{\partial q_n} = 0. \tag{2.5}$$

This is a rather special magnetic potential, the most general case can however be handled differently, as we show later. In two degrees of freedom the algorithm reads as follows.

**Algorithm 2.** *Iterate $N$ times*:
**begin**
$\qquad \psi \leftarrow \psi \times \exp\{-i\tau h_2(q)\}$
$\qquad \text{FFT}_{q_1}(\psi)$
$\qquad \psi \leftarrow \psi \times \exp\{-i\tau p_1 A^1(q_2)\}$
$\qquad \text{FFT}_{q_2}(\psi)$
$\qquad \psi \leftarrow \psi \times \exp\{-i\tau h_1(p)\}$
$\qquad \text{FFT}_{q_1}^{-1}(\psi)$
$\qquad \psi \leftarrow \psi \times \exp\{-i\tau p_2 A^2(q_1)\}$
$\qquad \text{FFT}_{q_2}^{-1}(\psi)$
**end**

In order of increasing complexity, we may consider the same problem of a splinless particle in a magnetic field moving on a manifold homeomorphic to $\mathbb{R}^n$ with a Riemannian metric $g$. The Hamiltonian is of the required form if $g$ is diagonal with $g_{jj}$ independent of $q_j$. Precisely this case will be considered in our application in Section 3.

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[1] See [12] for the one-dimensional case; the code to deal with the three-dimensional Dirac equation has been produced in the meanwhile.
[2] We assume that FFT overwrites $\psi$ with its Fourier transform.

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may turn out to be largely inferior. A simple variant of the algorithm, combined with Lanczos' method, can be dramatically faster, as we explain in the next section, at least in the case of spectra with well separated eigenvalues.

Where the method is really competitive is in the study of

(i) time dependent dynamics, i.e., $H = H(q, p, t)$; (in this case the system is interacting with its surroundings and we want to calculate transition rates far from the perturbative regime.)

(ii) barrier penetration (tunnel effect) in a time-dependent regime, which is generally hard to do outside the WKB approximation;

(iii) random perturbations: study of the quantum dynamics under an external random noise;

(iv) study of resonances (which are hard to detect otherwise).

All these points were explored in [12]. In the case of one degree of freedom, the method is simple enough to allow for an efficient implementation on low-cost systems and can be used to explore the basic properties of quantum mechanics in an interactive way [3]. The strength of the algorithm lies in the fact that *unitarity* of time evolution is preserved to machine accuracy, while other numerical errors can be reduced as desired, at the price of speed. Also, the momentum-dependent parts of the Hamiltonian are treated much better than in any discretization scheme (finite differences); as a result one usually discovers that it is irrelevant to go below a certain lattice spacing ($a = S/N$). Another fine point is the treatment of boundary conditions. By adopting a complex fast sine (cosine) transform [4] one can simulate Dirichlet (Neumann) boundary conditions instead of periodic; this can be useful in order to estimate the finite-size effects on the results.

A last comment about *improving* Trotter's formula. In principle one could reduce the intrinsic error in Trotter's formula by several tricks, the simplest one [4] being to symmetrize the formula ($\exp A \exp B \sim \exp \frac{1}{2}A \exp B \exp \frac{1}{2}A$). Other methods are given in [3]. Whether it is convenient to *improve* the formula or rather cut down $\tau$ depends on how much overhead the improvement imposes on the algorithm. In our application in the next section it has been possible to completely symmetrize the formula without adding a single Fourier transform, but this is to be examined case by case.

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## 3. Landau levels on the computer

Landau levels are the discrete energy levels of a quantum particle of charge $e$ moving on a plane under the influence of a transversal uniform magnetic field $B$. The spectrum, identical to that of a harmonic oscillator with infinite degeneracy, was determined by Landau in 1930. The degeneracy of the Landau levels is forced by the peculiar realization of Euclidean invariance, namely a *projective* representation (the generators of the translation subgroup realize a Heisenberg algebra). We show in Fig. 1 the result of the standard spectral method (Algorithm 2); the accuracy of the method is such that even on a $64 \times 64$ grid the degeneracy is not broken; we

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[3] The program is available for MSDOS systems with VGA or EGA.

[4] Tecchiolli has developed a version of fast Sine transform based on Rader–Brenner's algorithm which is as efficient as the corresponding FFT.

corrections are given by a linear combination of invariants with physical dimension [length]$^{-4}$ or higher, built with the Riemann tensor, with $B$ and with their covariant derivatives.

A numerical study of the spectrum via spectral methods is particularly simple if the metric is diagonal:

$$g = \text{diag}\left[\lambda_1(q),\ldots,\lambda_n(q),\ \lambda_1(q)^{-1},\ldots,\lambda_n(q)^{-1}\right], \tag{3.2}$$

with $\partial\lambda_1/\partial q_1 = \cdots = \partial\lambda_n/\partial q_n = 0$ in which case the Hamiltonian is of the general form [6] of (2.3). We also set $B = \sum dp_j \wedge dq_j = -d(\sum q_j\, dp_j)$ which is the *canonical two-form*. The Hamiltonian is then given (in suitable units) by

$$H = \sum_{j=1}^{n}\left(\lambda_j(q)^{-1}\left(-i\frac{\partial}{\partial q_j}\right)^2 + \lambda_j(q)\left(-i\frac{\partial}{\partial p_j} - q_j\right)^2\right). \tag{3.3}$$

In each invariant (generalized) subspace $\mathscr{H}_k = \{\psi = \exp\{i k \cdot p\}\phi(q)\}$ it reduces to

$$H_k = \sum_{j=1}^{n}\left(-\lambda_j(q)^{-1}\frac{\partial^2}{\partial q_j} + \lambda_j(q)(q_j - k_j)^2\right), \tag{3.4}$$

whose eigenvalues $E_i(k)$ can be computed either in perturbation theory around the flat metric or numerically. We shall now describe the results obtained by numerical analysis; we work in *four dimensions* ($n = 2$) which is the lowest nontrivial case. The goal is now to relate the ground state $E_0(k)$ to the geometrical invariants which can be constructed in terms of the metric and the symplectic two-form. Since we do not have a complete classification of the invariants of physical dimension [length]$^{-4}$ we restrict ourselves to the list

$$\mathscr{I}_0 = R, \qquad \mathscr{I}_1 = R^2, \qquad \mathscr{I}_2 = R_{\mu\nu}R^{\mu\nu}, \qquad \mathscr{I}_3 = R_{\mu\nu\rho\sigma}R^{\mu\nu\rho\sigma},$$

$$\mathscr{I}_4 = \nabla^2 R, \qquad \mathscr{I}_5 = \nabla_\mu\nabla_\nu B_{\lambda\rho}\nabla^\mu\nabla^\nu B^{\lambda\rho}, \tag{3.5}$$

and we try to fit the ground state $E_0(k)$ with a linear combination [7]

$$E_0 \sim \sum_{i=0}^{5} c_i\mathscr{I}_i. \tag{3.6}$$

To determine the six coefficients $c_i$ through a best fit we need a rather large array $\{ E_0(k^{(j)}) \mid j = 1,\ldots, M \}$. In practice we did the fit for $M = 100$ with several choices of the functional form of $\lambda_j(q)$. It is clear that the original spectral method based on the analysis of the signal (2.8) is too slow and inaccurate. Actually we are looking for small deviations from the standard Landau spectrum and we need a good accuracy (say 8-digit) to correlate the eigenvalues to the geometrical invariants. Since we are mainly interested in the ground state, we first of all convert the algorithm to *imaginary* time, in such a way to calculate $\exp\{-tH\}\psi$; in the limit $t \to \infty$ the excited states are filtered out at a rate $O(\exp\{-\delta Et\})$, where $\delta E = 2$ in the flat case. The systematic error in Trotter's formula, which is $O(\tau^2)$ for the symmetrized version, can be tamed by keeping $\tau$ small, at the expense of speed. Another strategy which avoids Trotter's intrinsic

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[6] Notice that this is the same class of metrics considered by Gilkey [5] in the study of the heat kernel expansion for a general second-order elliptic operator.

[7] Notice that we set the energy scale in such a way that the ground state energy is zero for the flat metric.

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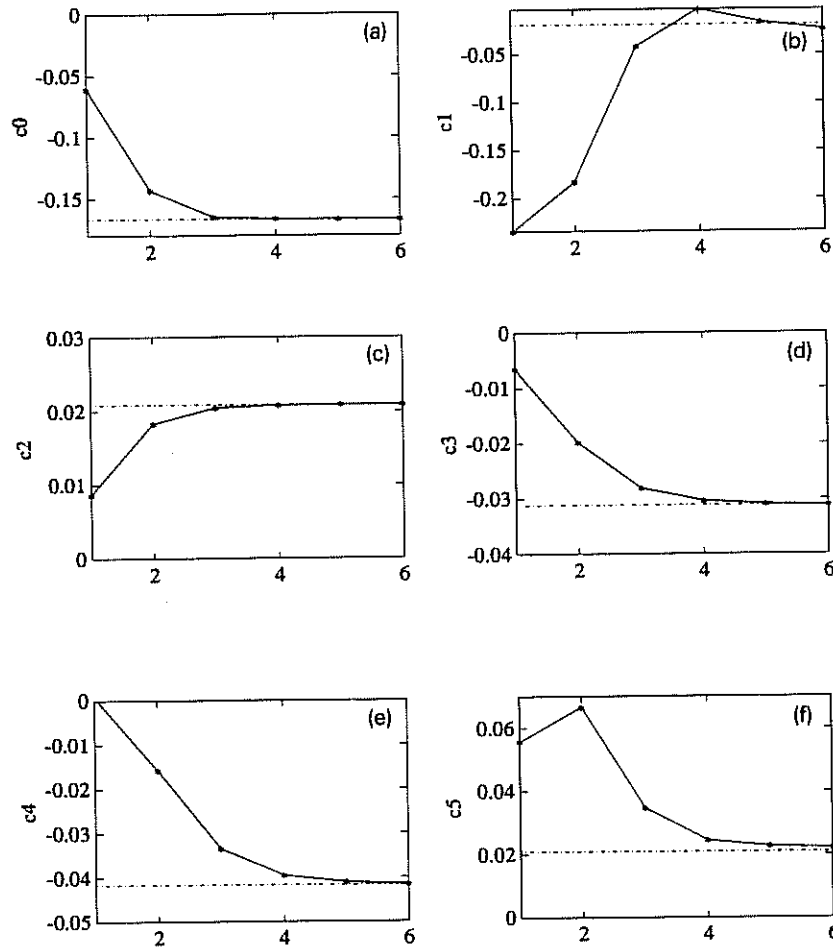ge scalar
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Fig. 3. Expansion coefficients of the ground state (3.6). The parameter $\log_2(2\rho)$ is in abscissa, the last point being obtained by Romberg extrapolation. Dotted lines give the exact results from Table 1.

for $\mathscr{I}_4$ is compatible with zero, a fact which already suggests the value $c_4 = -\frac{1}{24}$. The fitted coefficients are given in Table 1 together with the recently computed perturbative result [10]. Notice that numerically $\mathscr{I}_2 - \frac{1}{4}\mathscr{I}_5$ is very small but not negligible; in the fit we substitute

Table 1
Coefficients in (3.6) and their values obtained in perturbation theory

| $c_n$ | Fitted | Exact | Error (%) |
|---|---|---|---|
| 0 | $-0.166668$ | $-\frac{1}{6}$ | 0.001 |
| 1 | $-0.024305$ | $-\frac{17}{864}$ | 23.5 |
| 2 | $0.020853$ | $\frac{1}{48}$ | 0.1 |
| 3 | $-0.031221$ | $-\frac{1}{32}$ | 0.1 |
| 4 | $-0.041538$ | $-\frac{1}{24}$ | 0.3 |
| 5 | $0.022143$ | $\frac{1}{48}$ | 6.3 |

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