

# 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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a specific problem where a blend of spectral techniques and Lanczos' method allows to relate the splitting of the first Landau level to the geometrical invariants of the Riemannian manifold where the quantum particle is confined.

## 2. Feynman path integral, Trotter formula and the FFT

The dynamics of any (bosonic) quantum system relies on Feynman's path integral formula for the propagator, which in the phase space formulation reads

$$\langle \mathbf{q}'t' | \mathbf{q}''t'' \rangle = \int_{\substack{q(t')=q' \\ q(t'')=q''}} \mathcal{D}q \mathcal{D}p \exp \left\{ \frac{i}{\hbar} \int_{t'}^{t''} [\mathbf{p}(t) \cdot d\mathbf{q}(t) - H(\mathbf{p}(t), \mathbf{q}(t), t) dt] \right\}. \quad (2.1)$$

The integral here is meant as a shorthand for the following limit:

$$\lim_{T \rightarrow \infty} \prod_{l=1}^T \int d\mathbf{q}_l \prod_{l=0}^T \int d\mathbf{p}_l \exp \left\{ \frac{i}{\hbar} \sum_{l=0}^T [\mathbf{p}_l \cdot (\mathbf{q}_{l+1} - \mathbf{q}_l) - \tau H(\mathbf{p}_l, \mathbf{q}_l, t_l)] \right\}, \quad (2.2)$$

where the variables with subscript  $l$  are evaluated at time  $t_l = t' + l\tau$ ,  $\tau = (t'' - t')/(T + 1)$ . Multiplying by  $f(\mathbf{q}')$  and integrating over  $\mathbf{q}'$ , the formula gives an algorithm to compute the solution  $\psi(\mathbf{q}, t)$  of the Schroedinger equation  $i\hbar \partial \psi / \partial t = H(-i\hbar \nabla, \mathbf{q})\psi$  with initial condition  $\psi(\mathbf{q}, 0) = f(\mathbf{q})$ . The amount of computation required even for the simplest quantum system makes the algorithm impractical *in general*. (Actually each step  $\psi(t_l) \rightarrow \psi(t_{l+1})$  requires  $O(N^2)$  operations where  $N$  is the number of lattice points in the phase space  $(\mathbf{q}, \mathbf{p})$ .) Even if the Hamiltonian is quadratic in the momenta, in which case the momentum variables  $\mathbf{p}$  can be integrated out, we are left with a  $O(N^2)$  algorithm. The clue to speed up the computation lies in the fact that the integration over  $\mathbf{q}$  and  $\mathbf{p}$  with phase factors  $\exp(\pm i\mathbf{p} \cdot \mathbf{q})$  can be performed in  $O(N \log N)$  operations by a Fast Fourier Transform (FFT) [11] provided that the Hamiltonian  $H(\mathbf{q}, \mathbf{p}, t)$  has a special form, to be discussed below. Another starting point to derive the algorithm, which proves to be more general, is the one provided by Trotter's formula, also called *the splitting method* in numerical analysis. Let us assume that the (quantum) Hamiltonian be of the form

$$H(\mathbf{q}, \mathbf{p}, t) = \sum_{\alpha=1}^r h_{\alpha}(\mathcal{L}_{\alpha}(\mathbf{q}, \mathbf{p}), t), \quad (2.3)$$

where  $\mathcal{L}_{\alpha}$  is a Lagrangian subset of  $\{q_1, \dots, q_n, p_1, \dots, p_n\}$ , i.e., a set of  $n$  variables in involution under the quantum commutator ( $[q_i, p_j] = i\hbar \delta_{ij}$ ,  $[q_i, q_j] = [p_i, p_j] = 0$ ). Trotter's formula gives (hereafter we adopt units such that  $\hbar = 1$ )

$$T \left( \exp \left\{ -i \int_{t'}^{t'+\tau} H(\mathbf{q}, \mathbf{p}, t) dt \right\} \right) \sim \exp \{ -i\tau h_1 \} \cdots \exp \{ -i\tau h_r \}. \quad (2.4)$$

Since  $p_j = -i\partial/\partial q_j$ , each exponential involving the momenta  $\mathbf{p}$  can be evaluated to machine precision by diagonalizing  $h_i$  through a Fourier transform.

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<sup>1</sup> 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  $H = h_1(\mathbf{p}) + h_2(\mathbf{q})$  the algorithm<sup>2</sup> is just given as follows.

**Algorithm 1.** Iterate  $N$  times:

**begin**

$$\psi \leftarrow \psi \times \exp\{-i\tau h_2(\mathbf{q})\}$$

$$\text{FFT}(\psi)$$

$$\psi \leftarrow \psi \times \exp\{-i\tau h_1(\mathbf{p})\}$$

$$\text{FFT}^{-1}(\psi)$$

**end**

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

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

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**

$$\psi \leftarrow \psi \times \exp\{-i\tau h_2(\mathbf{q})\}$$

$$\text{FFT}_{q_1}(\psi)$$

$$\psi \leftarrow \psi \times \exp\{-i\tau p_1 A^1(q_2)\}$$

$$\text{FFT}_{q_2}(\psi)$$

$$\psi \leftarrow \psi \times \exp\{-i\tau h_1(\mathbf{p})\}$$

$$\text{FFT}_{q_1}^{-1}(\psi)$$

$$\psi \leftarrow \psi \times \exp\{-i\tau p_2 A^2(q_1)\}$$

$$\text{FFT}_{q_2}^{-1}(\psi)$$

**end**

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

<sup>1</sup> See [12] for the one-dimensional case; the code to deal with the three-dimensional Dirac equation has been produced in the meanwhile.

<sup>2</sup> We assume that FFT overwrites  $\psi$  with its Fourier transform.

In three degrees of freedom *if* we can get rid of one component of the potential, say  $A^1$ , by a gauge transformation, then we can cycle around the path  $(q_1 q_2 q_3) \rightarrow (q_1 p_2 q_3) \rightarrow (p_1 p_2 p_3) \rightarrow (q_1 q_2 p_3) \rightarrow (q_1 q_2 q_3)$ . Otherwise we have to double the number of FFTs per step. A simpler, actually entirely general, strategy is the following.

Let us find potentials  $\chi_\mu$  such that  $A_\mu = \partial \chi_\mu / \partial q_\mu$  (not summed). We then write

$$p_\mu - A_\mu = \exp\{i\chi_\mu\} p_\mu \exp\{-i\chi_\mu\}, \quad (2.6)$$

and the single Trotter step can be written as

$$\prod_\mu \left( \exp\{i\chi_\mu\} \exp\left\{-\frac{1}{2}i\tau p_\mu^2\right\} \exp\{-i\chi_\mu\} \right) \exp\{-i\tau V(\mathbf{q})\}, \quad (2.7)$$

$H = \sum_\mu (p_\mu - A_\mu)^2 + V(\mathbf{q})$  being the quantum Hamiltonian. This is actually the simplest way to define the Hamiltonian with Dirichlet boundary condition, since in this case  $p_\mu$  is *not* diagonalizable via a Fourier sine transform, while its square does. We can thus apply the splitting method to *any* magnetic field as follows.

**Algorithm 3.** *Iterate  $N$  times:*

**begin**

$\psi \leftarrow \psi \times \exp\{-i\tau V(\mathbf{q}) - i\chi_1(\mathbf{q})\}$

$\text{FFT}_{q_1}(\psi)$

$\psi \leftarrow \psi \times \exp\{-i\tau p_1^2\}$

$\text{FFT}_{q_1}^{-1}(\psi)$

$\psi \leftarrow \psi \times \exp\{i\chi_1(\mathbf{q}) - i\chi_2(\mathbf{q})\}$

$\text{FFT}_{q_2}(\psi)$

$\psi \leftarrow \psi \times \exp\{-i\tau p_2^2\}$

$\text{FFT}_{q_2}^{-1}(\psi)$

$\psi \leftarrow \psi \times \exp\{i\chi_2(\mathbf{q})\}$

**end**

Practical implementations of these algorithms must face the problem of optimizing various cutoffs: the system is put into a cubic box of size  $S$ , partitioned into  $N$  slices in each degree of freedom and the total evolution time is subdivided into  $T$  steps. The parameters  $S$ ,  $N$  and  $T$  should be chosen in order to minimize the errors of the algorithm. The rule of the thumb is the following. *Assume that we want to represent correctly the eigenmodes of the problem up to some energy  $E$ , then*

(i)  $\tau \leq \frac{1}{2}\pi E^{-1}$ ;

(ii) *the typical length scale of the eigenfunctions of energy  $\sim E$  should be smaller than  $S$ ; and*

(iii) *its Fourier transform should be essentially contained in a region  $\pm \frac{1}{2}\pi NS^{-1}$ .*

It was shown in [4] how to extract the spectrum and the eigenstates of a time-independent Hamiltonian by analyzing the signal

$$F(t) = \int dq \psi(q, 0)^* \psi(q, t), \quad (2.8)$$

paying due attention to the alias problem. In this context the spectral method should be compared with other methods (like finite element, conjugate gradient and Lanczos' methods) and

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<sup>3</sup>. 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<sup>4</sup> 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.

### 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

<sup>3</sup> The program is available for MSDOS systems with VGA or EGA.

<sup>4</sup> Tecchiolli has developed a version of fast Sine transform based on Rader-Brenner's algorithm which is as efficient as the corresponding FFT.

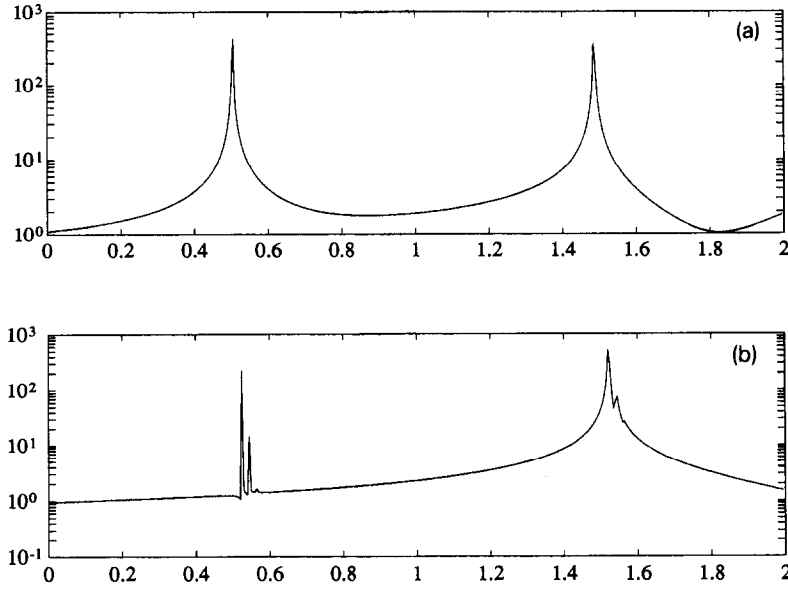


Fig. 1. The spectrum extracted from the signal  $\langle \psi(0) | \psi(t) \rangle$  in the case of a particle in a uniform magnetic field (a); with a small perturbation the degeneracy is removed (b).

checked that the degeneracy can be lifted by adding a small quadratic perturbation. Applying Algorithm 3 with a fast sine transform gives essentially identical results, owing to the fact that the box size  $S$  was chosen much larger than the typical length scale  $((\hbar c)/(eB))^{1/2}$ .

More complex situations arise if the magnetic field is *not* uniform and/or the surface is *not* flat. A problem originating in [8] is the following: given a  $(2n)$ -dimensional Riemannian manifold  $\mathcal{M}$  and a nondegenerate (symplectic) two-form  $\mathbf{B}$  on it, representing a magnetic field, under which circumstances does the Landau phenomenon take place at least for the ground state? By “Landau phenomenon” we mean a degeneracy with a multiplicity proportional to the volume of the manifold (infinite degeneracy for the noncompact case). It is clear that if  $\mathbf{g}$  and  $\mathbf{B}$  define a Kaehler structure, the Hamiltonian reduces to  $\Sigma \nabla_j^\dagger \nabla_j$ ; hence its ground state is locally represented by holomorphic functions and the problem is solved by the Riemann–Roch–Hirzebruch theorem, at least in the compact case [7,9]. Outside the class of Kaehler manifolds very little is known. Some general results on the spectrum in the flat case, two dimensions, nonuniform  $\mathbf{B}$  can be found in [2]. We have considered [10] the problem under the assumption that the metric  $g$  and the two-form  $\mathbf{B}$  define an *almost Kaehler manifold* [13] and we have shown how the infinite degeneracy of the ground state is broken in perturbation theory: a state  $|\psi_0\rangle$  belonging to the first Landau level gets an energy shift  $E_0$  given by

$$E_0 \sim \frac{1}{24} \langle \psi_0 | \nabla_\mu \mathbf{B}_{\rho\sigma} \nabla^\mu \mathbf{B}^{\rho\sigma} | \psi_0 \rangle. \quad (3.1)$$

The correction vanishes in the Kaehler case and it is proportional to the average scalar curvature<sup>5</sup>  $\langle R \rangle$  for a diagonal metric of the special form we will consider below. Higher-order

<sup>5</sup> In the sequel  $R_{\mu\nu\rho\sigma}$  denotes Riemann’s tensor,  $R_{\mu\nu}$  is Ricci’s tensor,  $R = g^{\mu\nu} R_{\mu\nu}$  is the scalar curvature and  $\nabla_\mu$  denotes covariant differentiation.

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

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

$$\mathbf{g} = \text{diag}[\lambda_1(\mathbf{q}), \dots, \lambda_n(\mathbf{q}), \lambda_1(\mathbf{q})^{-1}, \dots, \lambda_n(\mathbf{q})^{-1}], \quad (3.2)$$

with  $\partial\lambda_1/\partial q_1 = \dots = \partial\lambda_n/\partial q_n = 0$  in which case the Hamiltonian is of the general form<sup>6</sup> of (2.3). We also set  $\mathbf{B} = \sum \mathrm{d}p_j \wedge \mathrm{d}q_j = -\mathrm{d}(\sum q_j \mathrm{d}p_j)$  which is the *canonical two-form*. The Hamiltonian is then given (in suitable units) by

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

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

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

whose eigenvalues  $E_i(\mathbf{k})$  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  $E_0(\mathbf{k})$  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  $[\text{length}]^{-4}$  we restrict ourselves to the list

$$\begin{aligned} \mathcal{I}_0 &= R, & \mathcal{I}_1 &= R^2, & \mathcal{I}_2 &= R_{\mu\nu} R^{\mu\nu}, & \mathcal{I}_3 &= R_{\mu\nu\rho\sigma} R^{\mu\nu\rho\sigma}, \\ \mathcal{I}_4 &= \nabla^2 R, & \mathcal{I}_5 &= \nabla_\mu \nabla_\nu B_{\lambda\rho} \nabla^\mu \nabla^\nu B^{\lambda\rho}, \end{aligned} \quad (3.5)$$

and we try to fit the ground state  $E_0(\mathbf{k})$  with a linear combination<sup>7</sup>

$$E_0 \sim \sum_{i=0}^5 c_i \mathcal{I}_i. \quad (3.6)$$

To determine the six coefficients  $c_i$  through a best fit we need a rather large array  $\{E_0(\mathbf{k}^{(j)}) \mid j = 1, \dots, M\}$ . In practice we did the fit for  $M = 100$  with several choices of the functional form of  $\lambda_j(\mathbf{q})$ . 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  $t \rightarrow \infty$  the excited states are filtered out at a rate  $O(\exp\{-\delta E t\})$ , 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

<sup>6</sup> 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.

<sup>7</sup> Notice that we set the energy scale in such a way that the ground state energy is zero for the flat metric.

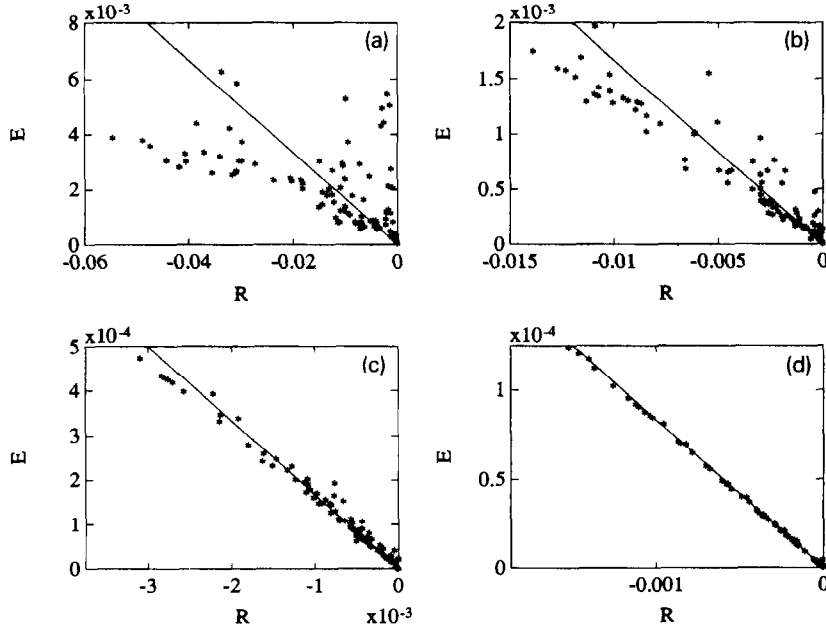


Fig. 2. A scatter plot  $E_0-R$  done for various choices of the parameter  $\rho$  which controls the average radius of curvature: (a)  $\rho = 1$ ; (b)  $\rho = 2$ ; (c)  $\rho = 4$ ; (d)  $\rho = 8$ . The continuous line represents  $E_0 = -\frac{1}{6}R$ .

error and at the same time gives information on the excited states can be devised borrowing from spectral methods and from Lanczos' methods.

- (i) Apply Algorithm 1 modified to *imaginary*  $\tau$  ( $T$  steps);
- (ii) apply Lanczos' algorithm [6] starting with the vector  $\psi$  which has been prepared in step (i) ( $L$  iterations).

The spectral method is used here to filter out the higher states and subsequently to build the subroutine which generates  $H\psi$  from  $\psi$ . The iteration parameters  $T$  and  $L$  must be chosen empirically to get the desired accuracy in acceptable time. The leading correction to the flat case is given by

$$E_0 \sim c_0 R, \quad (3.7)$$

and  $c_0$  is known [10] to be  $-\frac{1}{6}$  by perturbation theory in any number of dimensions; numerically we obtain the value  $c_0 = -0.166668$ , which means that the first correction coefficient is reproduced with a relative error of  $10^{-5}$  with respect to the analytical result. We introduced a scale parameter  $\rho$  in the metric such that the flat metric is reached in the limit  $\rho \rightarrow \infty$ ; the data very clearly exhibit the simple correlation between  $E_0$  and  $R$  as the metric is deformed to the flat limit (see Fig. 2). The deviations from (3.7) are used to fit the other coefficients. These are of course affected by a larger error than  $c_0$ . The fits are based on samples of 100 values of the wave number  $k$  for several values of the control parameter  $\rho$  which allows us to extrapolate to the zero-curvature limit and to extract the expansion coefficients, e.g., by Romberg extrapolation (see Fig. 3). We have also tried a fit of a ground state in terms of  $\langle \psi_0(\mathbf{k}) | R | \psi_0(\mathbf{k}) \rangle$ ; the only modification should be found on the coefficient  $c_4$ , because to this order  $\langle \psi_0(\mathbf{k}) | R | \psi_0(\mathbf{k}) \rangle \sim R(\mathbf{k}) + \frac{1}{4}(\nabla^2 R)(\mathbf{k})$ . In this latter fit we find that the new coefficient



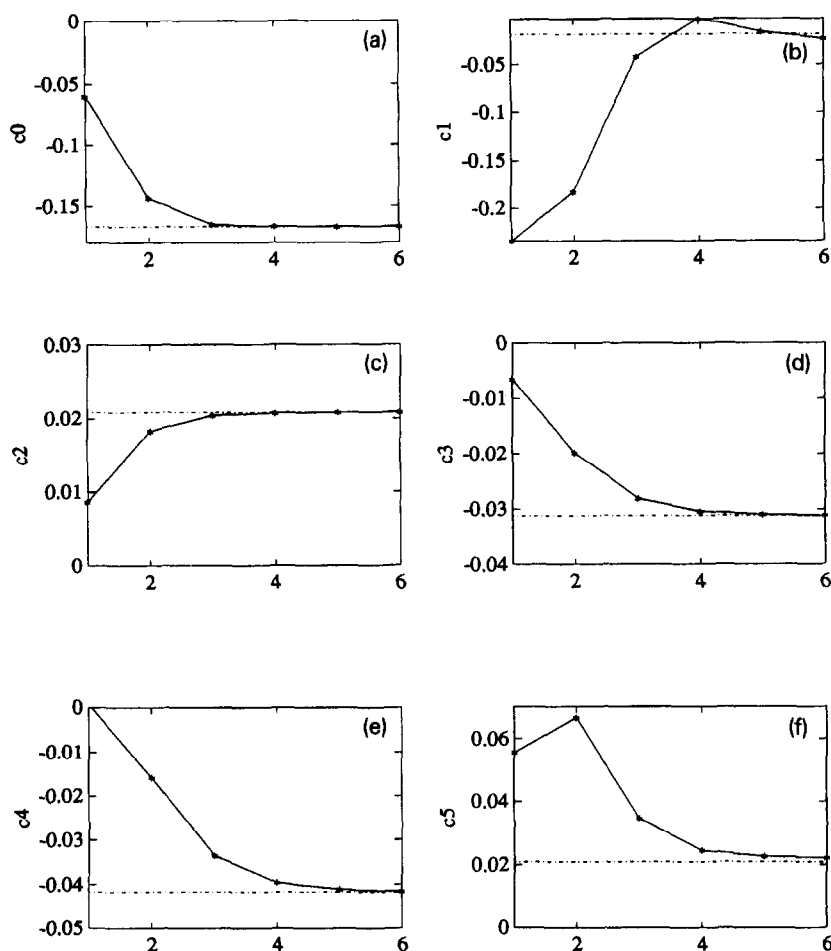


Fig. 3. Expansion coefficients of the ground state (3.6). The parameter  $\log_2(2\rho)$  is in abscissa, the last point being obtained by Romberg extrapolation. Dotted lines give the exact results from Table 1.

for  $\mathcal{J}_4$  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  $\mathcal{J}_2 - \frac{1}{4}\mathcal{J}_5$  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

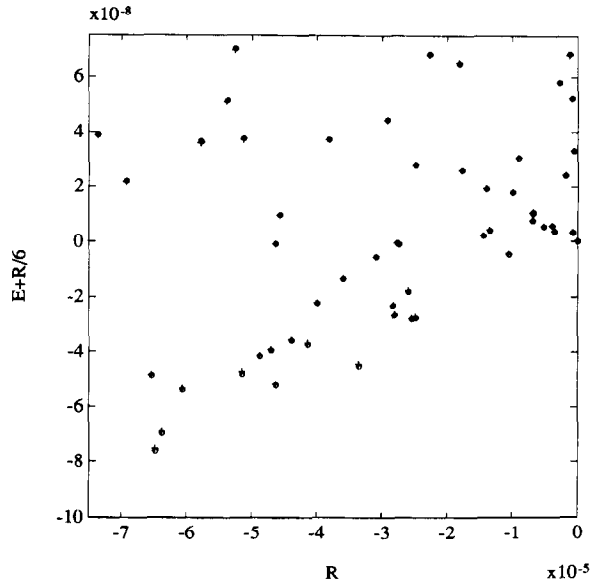


Fig. 4. Sample values of  $E_0(\mathbf{k})$ ; crosses denote the values of  $E_0 + \frac{1}{6}R$  while circles report the values of  $\sum c_i \mathcal{J}_i$  with the choice of coefficients given in the text.

$\mathcal{J}_5 = 4\mathcal{J}_2 + \delta$  but of course the coefficient of  $\delta$  is affected by a large error; likewise the average values of  $\mathcal{J}_1$  vary in the range  $10^{-9}$ – $10^{-10}$  in the sample with  $\rho = 16$ , hence *any* fitted value for  $c_1$  is hardly significant.

At this level of numerical accuracy there is no evidence for other invariants entering into the game (See Fig. 4 where we plot  $E_0 + \frac{1}{6}R$  in order to reveal the fine structure of the data), and indeed the five invariants can be shown to give a complete set *for this particular class of metrics*. An open problem is to determine the expansion to the same order of approximation for an arbitrary  $g_{\mu\nu}$  and for any number of dimensions.

#### 4. Conclusions

We have applied spectral methods to problems in elementary quantum mechanics concentrating to magnetic interaction of spinless particles. The case of a Dirac particle in 2 or 3 dimensions can also be studied with minor complications. Spectral methods proved to be very reliable, accurate and fast<sup>8</sup>. In particular the fact that momentum operators are represented exactly instead of in terms of finite differences allows to obtain high accuracy even with a small number of nodes (we did not find any differences between a  $64 \times 64$  and a  $128 \times 128$  grid to 12 digit precision).

The remarkable agreement of the numerical fit with the analytical calculation lets us hope that the methods presented here will prove to be useful also in other problems in “spectral geometry”.

<sup>8</sup> The CPU-time for a typical run (100 values of  $\mathbf{k}$ ) is just above one hour on a DEC  $\mu$ VAX 3900, which corresponds to roughly 40 seconds for each spectrum calculation. This means two orders of magnitudes faster than the method based on the Fourier analysis of the signal (2.8), which moreover needs lineshape fitting to attain our accuracy.

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