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## LETTER TO THE EDITOR

## A variational sinc collocation method for strong-coupling problems

**Paolo Amore**

Facultad de Ciencias, Universidad de Colima, Bernal Díaz del Castillo 340, Colima, Mexico

E-mail: [paolo@ucol.mx](mailto:paolo@ucol.mx)

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### Abstract

We have devised a variational sinc collocation method (VSCM) which can be used to obtain accurate numerical solutions to many strong-coupling problems. Sinc functions with an optimal grid spacing are used to solve the linear and nonlinear Schrödinger equations and a lattice  $\phi^4$  model in  $(1 + 1)$ . Our results indicate that errors decrease exponentially with the number of grid points and that a limited numerical effort is needed to reach high precision.

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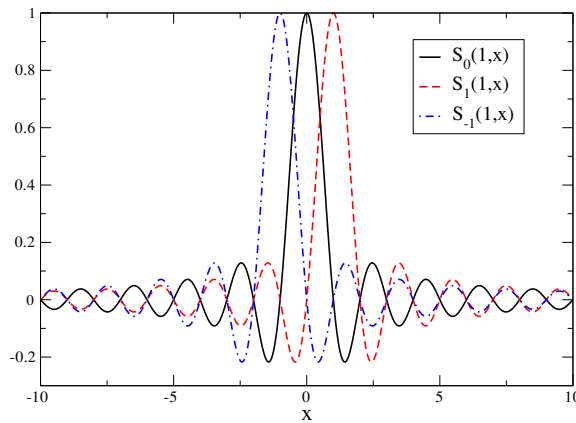
(Some figures in this article are in colour only in the electronic version)

Due to the inapplicability of perturbation theory in the strong-coupling regime, a number of different techniques have been devised in the past to deal with strong-coupling problems. Particular attention has gone into developing new methods, in which variational principles are used to improve perturbation theory, leading to results which are valid on a much larger domain. The linear delta expansion (LDE) [1] and the variational perturbation theory (VPT) [2] are probably the best-known examples of such efforts: in many cases these methods allow us to obtain series with finite (or even infinite) radius of convergence, in contrast with the divergent series which are usually obtained using perturbation theory [3].

In this letter we wish to show that the variational ideas which have inspired both the LDE and VPT methods can also be applied to improve the performance of numerical techniques. The numerical method that we are using is the sinc collocation (SCM) [4], which uses sinc functions to efficiently ‘discretize’ a problem in a given region. Sinc functions are used in different areas of physics and mathematics (see, for example [5] and references therein).

A sinc function is defined as

$$S_k(h, x) \equiv \frac{\sin(\pi(x - kh)/h)}{\pi(x - kh)/h}. \quad (1)$$



**Figure 1.** Sinc functions corresponding to different values.

and obeys the integral representation

$$S_k(h, x) = \frac{h}{2\pi} \int_{-\pi/h}^{+\pi/h} e^{\pm i(x-kh)t} dt. \quad (2)$$

Here  $h$  is the spacing between absolute maximas of neighbouring sinc functions, while the integer index  $k$  controls the location of such maximas.

The reader interested in a more detailed account of the properties of the sinc function should refer to [4]; here we only state the main properties which will be useful in the following.

Using equation (2) it is straightforward to evaluate the integrals

$$\mathcal{I}_1 \equiv \int_{-\infty}^{+\infty} S_k(h, x) dx = h \quad (3)$$

$$\mathcal{I}_2 \equiv \int_{-\infty}^{+\infty} S_k(h, x) S_l(h, x) dx = h \delta_{kl}. \quad (4)$$

A function  $f(x)$  analytic on a rectangular strip centred on the real axis can be approximated in terms of sinc functions as

$$f(x) \approx \sum_{k=-\infty}^{+\infty} f(kh) S_k(h, x). \quad (5)$$

Using equation (5) together with equation (3) one obtains

$$\int_{-\infty}^{+\infty} f(x) dx \approx h \sum_{k=-\infty}^{\infty} f(k, h). \quad (6)$$

An expression for the error in equation (5) has been obtained by Stenger [4], showing that it decays exponentially as the spacing  $h$  is reduced.

As the reader can appreciate in figure 1 for a fixed  $h$  a given sinc function selects a point on the real line, corresponding to its maximum value, where all the other sinc functions vanish. This property, which allows us to obtain a proper ‘discretization’ of a problem in the continuum, is at the basis of the SCM.

We now describe the SCM in detail by considering the stationary Schrödinger equation

$$-\frac{1}{2} \frac{d^2 \psi}{dx^2} + V(x) \psi(x) = E \psi(x). \quad (7)$$

The matrix elements  $H_{kl}$  of the Hamiltonian evaluated in the set of sinc functions are given by

$$H_{kl} \approx \left[ -\frac{1}{2}c_{kl}^{(2)} + \delta_{kl}V(kh) \right]. \quad (8)$$

Note that the kinetic term has been obtained by using the property

$$\frac{d^2}{dx^2}S_k(h, x) = 0 \sum_{l=-\infty}^{\infty} c_{lk}^{(2)}S_k(h, x), \quad (9)$$

where

$$c_{lk}^{(2)} = \begin{cases} -\frac{\pi^2}{3h^2} & \text{if } k = l \\ -\frac{2}{h^2} \frac{(-1)^{k-l}}{(k-l)^2} & \text{if } k \neq l \end{cases}, \quad (10)$$

while the potential matrix has been approximated by the diagonal matrix of the potential evaluated over the grid. To understand this approximation we must realize that a sinc function converts into a Dirac delta in the limit  $h \rightarrow 0$  and that the overlap between distinct sinc functions is minimal unless they coincide.

Once  $h$  is specified the diagonalization of  $H_{kl}$  allows us to obtain numerical approximations to the energies and wave functions of the problem: this strategy was used in [6] to solve the Schrödinger equation corresponding to different potentials. Although the choice of  $h$  strongly affects the precision of the numerical results, no procedure to determine  $h$  is discussed in [6]. Using a different method, the author and collaborators [7] have solved numerically the Schrödinger equation for the anharmonic oscillator using an arbitrary basis of Gauss–Hermite functions, depending upon a scale factor. In that paper it was proved that the arbitrary scale factor can be chosen optimally by applying the principle of minimal sensitivity (PMS) [8] to the sub-trace of the Hamiltonian matrix.

Using the same procedure we regard  $h$  as a variational parameter and consider the trace

$$\text{Tr}[H] = \frac{\pi^2}{6h^2}(2k_{\max} + 1) + \sum_{k=-k_{\max}}^{k_{\max}} V(kh), \quad (11)$$

where  $2k_{\max} + 1$  is the number of sinc functions (grid points) used in the evaluation.

The solution to the PMS equation

$$\frac{d}{dh} \text{Tr}[H] = 0 \quad (12)$$

provides the optimal spacing<sup>1</sup>. Once that  $h$  has been determined using the PMS our method allows us to obtain quite rapidly the numerical approximations<sup>2</sup>.

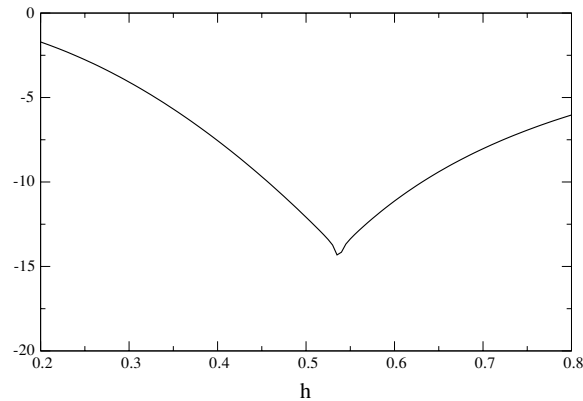
In figure 2 we display the  $\log_{10}|E_0 - E_0^{\text{exact}}|$  as a function of the spacing  $h$  using 21 grid points ( $k_{\max} = 10$ ) for the harmonic oscillator  $V(x) = x^2/2$ . The PMS condition, equation (12), yields  $h_{PMS} = 0.547$ , which is remarkably close to the minimum of the curve.

The anharmonic oscillator

$$H = -\frac{d^2}{dx^2} + x^2 + gx^4$$

<sup>1</sup> Usually this equation admits a unique real solution.

<sup>2</sup> All the examples considered in this letter have been obtained using a Mathematica code, running on a Linux desktop, with times of execution ranging from few seconds to few minutes.



**Figure 2.**  $\log_{10} |E_0 - E_0^{\text{exact}}|$  as a function of the spacing  $h$  using  $k_{\text{max}} = 10$  for the harmonic oscillator  $V(x) = x^2/2$ .

provides a more demanding test of our method. We have obtained the ground state energy corresponding to  $g = 2000$  using a grid of 101 points ( $k_{\text{max}} = 50$ ) and compared it with the precise results of [9], finding that the first 42 digits are correct (underlined):

$$E_0 = \underline{13.388\ 441\ 701\ 008\ 061\ 939\ 006\ 176\ 902\ 807\ 286\ 522\ 960\ 99}.$$

The result is also seen to converge exponentially to the exact answer as a function of the number of grid points.

We now consider the Gross–Pitaevskii (GP) equation

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + V_{\text{ext}}(x) + 4\pi a |\psi(x)|^2 \right] \psi(x) = E \psi(x),$$

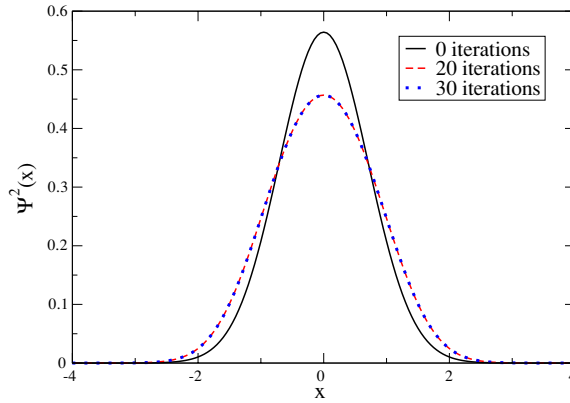
which is relevant in the study of Bose–Einstein condensation.  $V_{\text{ext}}(x)$  is the external confining potential and  $E$  is the energy of the condensate. The wave function  $\psi(x)$  is normalized to yield the number of particles in the condensate, i.e.  $\int dx |\psi(x)|^2 = N$ .

We have applied our method to the GP equation by first solving the corresponding linear equation,

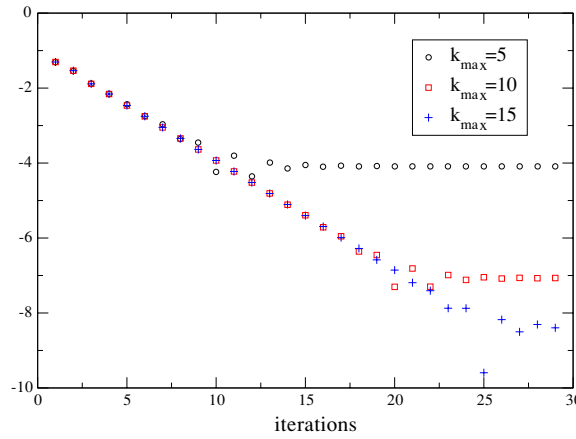
$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + V_{\text{ext}}(x) \right] \psi^{(0)}(x) = E^{(0)} \psi^{(0)}(x),$$

and by then implementing a self-consistent procedure in which the density term is evaluated taking the wave function calculated at the previous step and then it is used to build an effective potential  $V_{\text{eff}}^{(n)}(x) \equiv V_{\text{ext}}(x) + 4\pi a |\psi^{(n-1)}(x)|^2$  (here  $E^{(n)}$  and  $\psi^{(n)}(x)$  are the energy and wave function calculated after  $n$  iterations). In this potential the resulting Schrödinger equation is solved again and the procedure is iterated until self-consistency is reached.

In figure 3 we have plotted the wave function in an harmonic trap, obtained after 0, 20 and 30 iterations of our method, assuming  $4\pi a = 1$  and  $\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 2$ . A grid of 21 points has been used. The 0 th order wave function corresponds to the usual harmonic oscillator wave function. In figure 4 we have plotted  $\log_{10} |E_0 - E_0^{\text{exact}}|$  as a function of the number of iterations for different grid sizes (11, 21 and 31, respectively): the data initially display an exponential decay— independent of the grid size—which is then followed by a plateau. The plateau signals that the maximal precision has been achieved for a given grid size.



**Figure 3.** Probability density for the ground state of the GP equation using  $V_{\text{ext}}(x) = x^2/2$ .



**Figure 4.**  $\log_{10} |E_0 - E_0^{\text{exact}}|$  as a function of the number of iterations for different grid sizes.

As a last example of application of our method we consider a lattice  $\phi^4$  in 1+1 dimensions. This model has been studied by Nishiyama in [10] and corresponds to the Hamiltonian

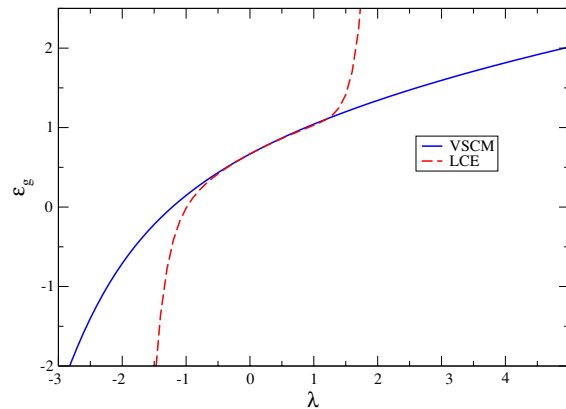
$$\mathcal{H} = \sum_i \left[ \frac{\pi_i^2}{2} + \frac{1}{2} (\phi_i - \phi_{i+1})^2 + \frac{1}{2} \phi_i^2 + g \phi_i^4 \right]. \tag{13}$$

The fields obey the canonical commutation relations  $[\phi_i, \pi_j] = i\delta_{ij}$  and  $[\phi_i, \phi_j] = [\pi_i, \pi_j] = 0$ . Following [10] we perform a rescaling of the fields  $\phi \rightarrow g^{-1/6}\phi$  and  $\pi \rightarrow g^{1/6}\pi$  and obtain

$$\mathcal{H} = g^{1/3} \sum_i \left[ \frac{\pi_i^2}{2} + \phi_i^4 + \lambda \left( \frac{1}{2} (\phi_i - \phi_{i+1})^2 + \frac{\phi_i^2}{2} \right) \right],$$

where  $\lambda \equiv g^{-2/3}$ . We express the ground state energy as  $E_g = g^{1/3}\epsilon_g$ .

Nishiyama has numerically solved this model using a linked cluster expansion (LCE) and the density matrix renormalization group (DMRG) [11]: using the LCE he has obtained a perturbation series in  $\lambda$ , up to order 11, whose convergence has then been improved using



**Figure 5.** Ground state energy for the lattice  $\phi^4$  model as a function of  $\lambda = g^{-2/3}$ .

Aitken's  $\delta^2$  process. The comparison with the DMRG results shows that LCE is valid up to  $\lambda \approx 2$ .

We wish to show that the same problem can be solved using our method. We have proceeded as follows: first we have solved the Schrödinger equation for the anharmonic oscillator, corresponding to setting  $\lambda = 0$ , and we have obtained the wave function  $\Psi(\phi) \approx \sum_{r=-k_{\max}}^{k_{\max}} \alpha_r S_r(h, \phi) / \sqrt{h}$ ; we have then used  $\Psi(\phi)$  to evaluate the matrix element  $\langle \Psi(\phi_{i+1}) | H | \Psi(\phi_{i+1}) \rangle$ , obtaining the effective potential felt by the  $i$ th site:

$$\tilde{V}(\phi) = \phi^4 + \lambda \left[ \frac{1}{2} \left( \phi^2 - 2\phi \sum_{r=-k_{\max}}^{k_{\max}} \alpha_r^2 r h + \sum_{r=-k_{\max}}^{k_{\max}} \alpha_r^2 (r h)^2 \right) + \frac{\phi^2}{2} \right]. \quad (14)$$

The Schrödinger equation is then solved again and the coefficients  $\alpha_r$  are recalculated. The procedure is repeated until self-consistency is reached.

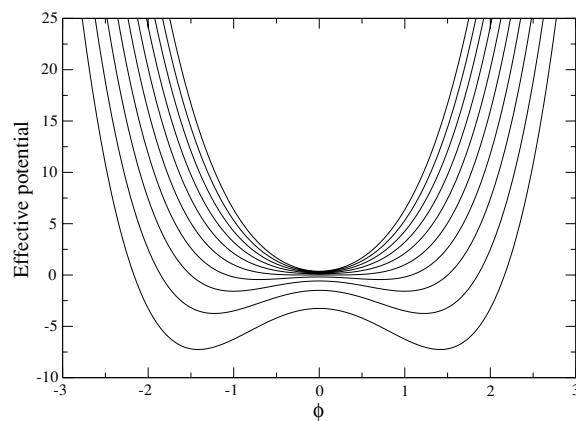
In figure 5 we have calculated the scaled ground state energy,  $\epsilon_g$ , as a function of  $\lambda$ , using a grid of 41 grid points ( $k_{\max} = 20$ ). The solid curve corresponds to the perturbative expansion of equation (6) of [10], to order  $\lambda^{11}$ , obtained with the LCE. Our result compares quite favourably also with the results obtained with the DMRG—see figure 2 of [10]—and have been obtained in few minutes of running time on a Linux desktop running Mathematica.

Note that in [10] it was speculated that there is a singularity around  $\lambda = -2$ , possibly related to the onset of a phase transition. Our numerical simulation *does not* show the presence of any discontinuity in  $\epsilon_g$ .

In figure 6 we show the effective potential for different values of  $\lambda$ , ranging from  $\lambda = -5$  to  $\lambda = 5$  (going from the lowest to the highest curves).

We wish to conclude this letter stressing few points, which we believe to be important: the VSCM provides errors which decrease exponentially with the number of grid elements; the grid spacings are obtained using the PMS and allow us to achieve optimal results with limited numerical effort; the diagonalization of the Hamiltonian matrix provides approximations for the energies and wave functions of part of the spectrum and can be used to study the time evolution of a wave packet (similarly to what done in [7]); finally, our method can also be applied *without modifications* to models with non-polynomial interactions.

The last example shows that VSCM can be a useful tool in the numerical solution of lattice quantum models and it could possibly provide an alternative to numerical methods already



**Figure 6.** Effective potential  $\tilde{V}(\phi)$  for values of  $\lambda$  going from  $-5$  to  $5$ . The curves differ by  $\Delta\lambda = 1$ .

present on the ‘market’. One interesting issue is the application of this method to problems in more than one dimension: in such cases, calling  $d$  the number of dimensions, we expect to deal with  $N^d \times N^d$  matrices (although the symmetries in the problem could help to reduce the number of elements of the Hamiltonian matrix, as in the case of spherical symmetry), while the procedure illustrated in this letter would essentially remain unchanged. In these cases our variational method could be essential to provide small errors with the least possible number of grid elements. Future work in this direction is expected.

### Acknowledgments

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