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## A simple interpolation method for extracting quantal information from partially known potentials

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**Abstract.** From the sole knowledge of the numerical values of the potential  $V(x)$  at a finite number of points we are able to construct the potential as a function of the coordinate and infer approximate wavefunctions without in any way (numerically) dealing with Schrödinger's equation.

There are several interesting situations in which one knows the potential function, in the ordinary version of Schrödinger's equation, only in a finite set of points, say  $N$ . Examples include double quantum wells in relation to quantum Hall states [1, 2], layered multi-quantum-well structures which contain a number of identical, strictly two-dimensional electronic systems [3, 4], etc. From a different point of view, any self-consistent treatment of the quantum many-body problem will yield a numerical one-body potential that, as such, is given at a finite set of locations. For instance, this is the situation one encounters when solving the time-dependent Schrödinger equation by recourse to the cellular automata method [5].

We wish here to present an extremely simple algorithm that allows for a reasonable way of interpolating between the  $N$  points in which the potential is actually known, so as to construct a continuous potential function. We assume the potential to be a (piecewise) smooth and regular function and, consequently, the method cannot be applied to non-regular potentials (for instance, to the extreme case of a  $\delta$ -potential). Additionally, the mere knowledge of the potential at a finite set of locations allows one to construct a passable approximation to the wavefunction and yields, albeit in an approximate fashion, the energy spectrum, without having to (numerically) deal with Schrödinger's equation.

We start with the simple ansatz for an  $M$ -node excited state (we shall restrict ourselves, for the sake of simplicity, to the one-dimensional case)

$$\Phi_M(x) = P_M(x) \exp\left(-\frac{1}{2} \sum_{n=1}^{N-M-1} \lambda_n x^n\right) \quad (1)$$

where  $P_M$  is the general polynomial of the  $M$ th degree ( $x^M + c_M x^{M-1} + \dots + c_2 x + c_1$ ), whose coefficients are yet to be determined, and the  $\lambda$ s are parameters to be properly fixed according to the present algorithm. The form (1) can be justified on information-theoretic (IT) grounds [6, 7], as the one that maximizes the so-called relative entropy. However, we are not going to employ here IT techniques in order to determine the parameters  $\lambda_n$ .

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From Schrödinger's equation

$$\left[-\frac{1}{2} \frac{d^2}{dx^2} + V(x)\right] \Phi_M(x) = E_M \Phi_M(x) \quad (2)$$

we find, after setting  $\Phi_M(x)$  equal to our ansatz (1) and evaluating the quantity

$$\frac{1}{\Phi_M(x)} \frac{d^2 \Phi_M(x)}{dx^2} = 2 [V(x) - E_M] \quad (3)$$

the useful relationship

$$\begin{aligned} P_M(x) [V(x) - E_M] = & \frac{1}{4} \left( - \sum_{n=2}^{N-M-1} n(n-1) \lambda_n x^{n-2} + \frac{1}{2} \left[ \sum_{n=1}^{N-M-1} n \lambda_n x^{n-1} \right]^2 \right) P_M(x) \\ & + \frac{1}{2} \left( \frac{d^2 P_M(x)}{dx^2} - \frac{dP_M(x)}{dx} \sum_{n=1}^{N-M-1} n \lambda_n x^{n-1} \right). \end{aligned} \quad (4)$$

The idea is to write down (4) explicitly for the  $N$  points  $x_i$  where  $V(x)$  is known:

$$\begin{aligned} P_M(x_i) V(x_i) = E_M P_M(x_i) + & \frac{1}{4} \left( - \sum_{n=2}^{N-M-1} n(n-1) \lambda_n x_i^{n-2} + \frac{1}{2} \left[ \sum_{n=1}^{N-M-1} n \lambda_n x_i^{n-1} \right]^2 \right) P_M(x_i) \\ & + \frac{1}{2} \left( \left[ \frac{d^2 P_M(x)}{dx^2} \right]_{x=x_i} - \left[ \frac{dP_M(x)}{dx} \right]_{x=x_i} \sum_{n=1}^{N-M-1} n \lambda_n x_i^{n-1} \right) \quad i = 1, \dots, N \end{aligned} \quad (5)$$

and regard now the concomitant  $N$  relationships as posing a set of  $N$  coupled, *cubic* algebraic equations in the  $\lambda$ s,  $E_M$  and the  $M$  coefficients of  $P_M$ , which can be trivially solved by recourse to standard commercially available numerical algorithms (see, for instance, [8]). Actually, for the ground state one faces a merely *quadratic* system, since  $P_M$  equals unity and the second term in the first bracket on the RHS of (4), which gives the order of the system, acquires its simplest possible form.

In order to analyse the possibilities of the method proposed here, we have first investigated its validity for both the harmonic oscillator and the square-well potentials. In the case of the harmonic oscillator potential  $V(x) = x^2/2$  (we have taken  $\hbar = m = \omega = 1$ ), choosing  $P_0(x) = 1$  for the ground state,  $P_1(x) = x$  for the first excited state,  $P_2(x) = x^2 - c^2$  for the second excited state, etc, and  $N - M - 1 \geq 2$  for the number of  $\lambda$ s, it is easy to verify that from (4) one obtains  $\lambda_2^2 = 1$ ,  $\lambda_1 = \lambda_3 = \dots = \lambda_{N-M-1} = 0$ , and  $E_0 = \frac{1}{2}$ ,  $E_1 = \frac{3}{2}$ ,  $E_2 = \frac{5}{2}$ ,  $\dots$ . That is, we analytically recover the exact spectrum. Further, after selecting the positive root for  $\lambda_2$  (so as to guarantee the correct asymptotic behaviour) we obtain the exact wavefunctions. Of course, the same results can also be obtained in numerical fashion with the algorithm that we are here advancing.

In the case of the square-well potential

$$V(x) = \begin{cases} V_0 & \text{for } -a < x < a \\ \infty & \text{otherwise} \end{cases} \quad (6)$$

then choosing  $N = 3$  and  $P_0(x) = 1$  for the ground state ( $M = 0$ ), by substitution in (5) one obtains

$$V_0 = E_0 - \frac{1}{2}\lambda_2 + \frac{1}{8}\lambda_1^2 + \frac{1}{2}\lambda_1\lambda_2x_i + \frac{1}{2}\lambda_2^2x_i^2 \quad (7)$$

for any three points  $-a < x_i < a$ . The solution of this system of equations gives  $\lambda_2 = 0$  and  $\lambda_1^2 = 8(E_0 - V_0) < 0$ , so that we have obtained a plane wave as the solution for the wavefunction, of the form

$$\Phi_0(x) = \exp\left[-i\sqrt{2(E_0 - V_0)} x\right]. \quad (8)$$

If we now enforce the requirement that this wavefunction vanishes at  $x = \pm a$  we obtain the customary quantization prescriptions and, consequently, the exact results for both the spectrum and the wavefunctions.

That quite a considerable return is obtained for a very modest investment in information (the  $N$  values  $V(x_i)$ ) is illustrated with reference to the results displayed in figures 1–3. We have chosen two typical one-dimensional Hamiltonians, that is, those corresponding to the Morse and bistable potentials, respectively. The latter found many useful applications as, for instance, in connection with: (i) tunnel diodes and other switching devices [9]; (ii) lasers that above pumping threshold may operate in either one of two (or more) stable modes [10, 11]; (iii) chemical reactions in open systems that may have two stable stationary regimes separated by an unstable stationary solution [12]; (iv) the equilibrium position of the nitrogen atom in the ammonia molecule [13]; etc. The Morse potential is of some utility in modelling the interaction potential of diatomic molecules [14]. We have

$$V_{\text{Morse}}(x) = A [1 - \exp(-x)]^2 \quad (9)$$

where we adopt the value  $A = 10$ , and

$$V_{\text{bistable}}(x) = \frac{\alpha}{2}x^2 + \beta x^3 + \gamma x^4 \quad (10)$$

where we choose  $\gamma = 1$ ,  $\beta = -1$  and  $\alpha = -7.4293$ , as discussed in [15]. In figure 1 we display the inferred potential  $V(x)$  which is compared with the *exact* figures provided by (9) (full curve). The potential function inferred by taking  $M = 0$  (ground state) is represented by the broken curve, while the remaining curve (dotted) corresponds to results inferred by taking  $M = 2$  (second excited state). Notice that in this case we are able not only to interpolate, but also to *extrapolate* beyond the 'input-interval'  $[-3, 3]$ . Unfortunately, this is not always the case, as illustrated by the bistable potential case (figures 2(a) and 2(b)), where, however, the interpolation procedure works well enough. It is not surprising that the  $M = 2$  inference is better than the  $M = 0$  one, as it involves, in a way, more input information (the 'structure' of the ansatz wavefunction (1) is richer for  $M = 2$ ). To study the effect of different choices for the number and location of the points  $x_i$  of our sample, in the case of figure 2(a) we have used 10 non-equidistant points asymmetrically distributed in the interval  $[-3, 3]$ , while in figure 2(b) we have taken 18 equidistant points lying in the same interval. The quality of the results remains the same when changing the location of the points, but the inferred results approach better to the exact one when the number of sampling points increases. Figure 3 gives a typical example of the quality of our inferred wavefunctions (the ansatz provided by (1)). We depict there the second excited

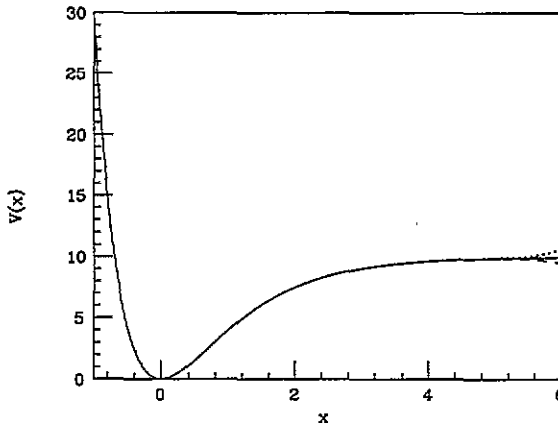


Figure 1. Inferred potential function  $V(x)$  is compared with the exact Morse potential (9) (full curve). Broken and dotted curves correspond to  $M = 0$  (ground state) and  $M = 2$  (second excited state), respectively. To solve (5), we have taken  $N = 18$ , the concomitant points symmetrically distributed around the origin in the interval  $[-3, 3]$ .

Table 1. Inferred energies are compared with exact results for several values of the parameter  $A$  of the Morse potential (9).  $E_0$  corresponds to the ground state and  $E_1$  and  $E_2$  to the first and second excited state, respectively. Technical details are as in figure 1.

	$A = 10$		$A = 20$	
	Exact	Inferred	Exact	Inferred
$E_0$	2.111 068	2.111 068	3.037 278	3.037 278
$E_1$	5.583 204	5.583 204	8.361 833	8.361 833
$E_2$	8.055 340	8.055 341	12.686 388	12.686 388

Table 2. Same as table 1 for several values of the parameter  $\beta$  of the bistable potential (10), using  $\alpha = -7.4293$  and  $\gamma = 1$ .

	$\beta = 0$		$\beta = -1$	
	Exact	Inferred	Exact	Inferred
$E_0$	-1.761 382	-1.761 320	-5.222 045	-5.222 259
$E_1$	-1.615 230	-1.615 205	-1.461 511	-1.462 125
$E_2$	0.660 254	0.660 235	-0.250 719	-0.250 930

state of the bistable potential. Within the interpolation interval, no differences with the exact wavefunction can be appreciated.

A similar agreement between inferred and exact figures can be found using other values of the potential parameters, and also looking at other quantal properties like energy spectra, expectation values  $\langle x^k \rangle$ , etc. As an illustration, we show in tables 1 and 2 the inferred and exact energy spectra up to the second excited state for the Morse potential (for different values of the parameter  $A$ ) and for the bistable potential (using different values of the parameter  $\beta$ ). A rapid glance to the pertinent figures confirms the quality of the results presented here. As one may expect the inferred results converge rapidly to the exact ones when an increasing number of points (in the same interval) are used, that is, when more input information on the discrete potential  $V(x_i)$  is assumed. Summing up, we have presented an extremely simple algorithm that, while avoiding any explicit numerical dealing with

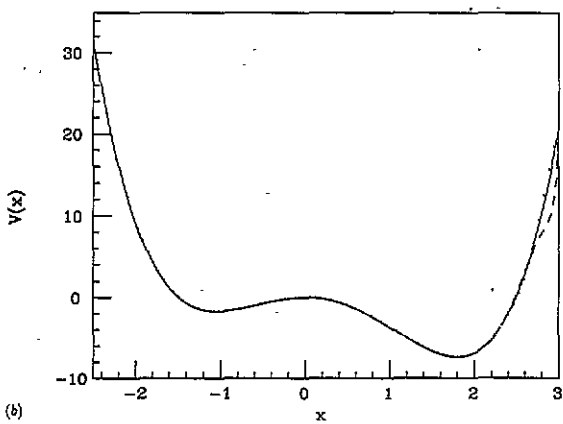
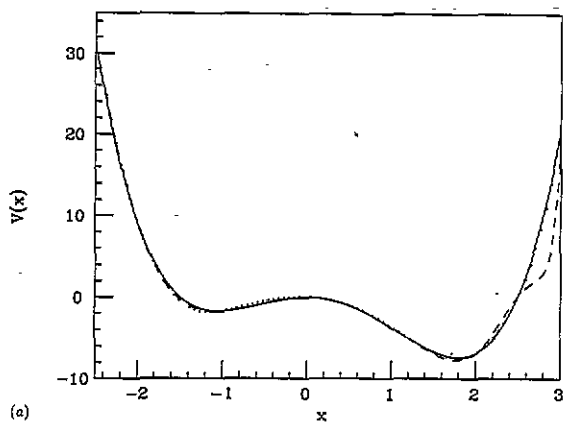


Figure 2. Same as figure 1 for the asymmetric bistable potential (10). To solve (5), we have taken: (a) 10 non-equidistant points asymmetrically distributed in the interval  $[-3, 3]$ ; (b) 18 equidistant points in the same interval.

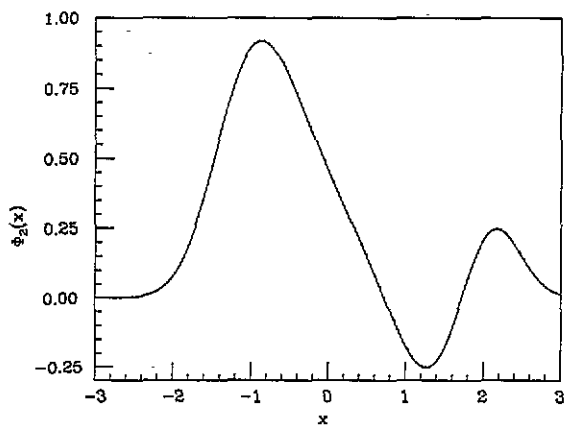


Figure 3. Inferred wavefunction (dotted curve) for the second excited state  $\Phi_2(x)$  of the bistable potential, (10), is compared with the exact result (full curve). Technical details are as in figure 1.

Schrödinger's equation, is able nonetheless to yield a wealth of new information, which is inferred from a very modest input information, without any undue effort.

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