AN APPROXIMATE METHOD TO CALCULATE ENERGY LEVELS

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ABSTRACT — An approximate method, to calculate energy levels of quantum systems bound by a potential, is introduced which uses the virial theorem and an independent minimization procedure at each energy level. Results obtained are presented and discussed.

I – INTRODUCTION

Recently, an approximate method to calculate energy levels of quantum systems bound by a large class of potentials was introduced by Gersch and Braden [1]. One of its most appealing features is the use of the Heisenberg uncertainty principle, one of the basic principles expressing the physical content of quantum mechanics. The careful and criterious application of approximate methods to deal with the Schrödinger equation is always wellcome, as such methods may help to develop an intuitive understanding of the behaviour of microscopic systems and of how such behaviour is affected by changes in the parameters defining the system.

The variation method is amongst the most powerful approximate methods and highly sophisticated generalizations of Ritz technique have been devised to calculate energy levels beyond the ground-state E_0. These calculations may, for example, start with a linear combination of functions, $\psi_{\text{trial}} = \Sigma_k \, c_k \, \chi_k$, not necessarily orthogonal among them, and, by a convenient minimization procedure with respect to the c_k's, successive approximate eigenvalues are then found. The closer these functions are to exact wave-functions, the closer to the exact eigenvalues are the successive E_i's [2].

Our purpose with this note is mainly pedagogical. We shall be dealing with a simple, non-orthodox, application of the variation method which we believe has some connection with the work of ref. [1]. We will enforce the virial theorem (as well as the Hellmann-Feynman theorem), by performing, at each level separately, an independent minimization procedure with respect to a convenient trial wavefunction and a variation parameter β

$$\partial E/\partial \beta = 0\,, \tag{1}$$

dropping the constraint of orthogonality among the trial wavefunctions corresponding to different levels. We, nevertheless, find that the calculated levels are in very good agreement with the exact ones. An effort is made to understand why this happens.

The great advantage of the technique is to give simple analytical expressions for the energies, in terms of the parameters of the system under study. Even when more than one term is taken in the potential, a simple pocket calculator can easily handle such expressions. The method can thus hopefully play a useful role, both at the pedagogical level and at the level of research, in estimates of energy levels of models under investigation (for example, in elementary particle spectroscopy). We only use knowledge that a student, having followed a basic course in Quantum Mechanics, should have.

In section II we introduce the method and apply it to some important types of potentials. In section III we put together and complete our arguments and draw conclusions.

II – THE METHOD AND APPLICATIONS

With straightforward dimensional arguments one can easily show how condition (1) fulfills the virial theorem as well as the Hellman-Feynman theorem [3]. (See the Appendix for a more general proof).

Consider a potential

$$V(x) \sim x^{p} \tag{2}$$

and a trial wavefunction depending on the minimization parameter β, $\psi(x, \beta)$, such that

$$\psi(x, \beta) = \sqrt{\beta} \quad \phi(\xi) \text{ (*)} \tag{3a}$$

with

$$\xi \equiv \beta x \tag{3b}$$

and

$$\int \bar{\psi}(x) \psi(x) \, dx = \int \bar{\phi}(\xi) \phi(\xi) \, d\xi = 1 \tag{3c}$$

The variable ξ is here a convenient dimensionless quantity. The energy eigenvalue, for any level, can be written as

$$<E>_\nu = \frac{1}{\mu} < \frac{1}{2} \frac{d^2}{dx^2} >_\nu + <V>_\nu = <T>_\nu + <V>_\nu , \tag{4}$$

ν designating the order of the level and μ the reduced mass.

With (2) and (3) the energy $<E>_\nu$ is a function of μ and β, $E = E(\mu, \beta)$, β itself being, through the Schrödinger equation, a function of μ.

We have

$$<T>_\nu \sim \beta^2 / \mu \quad \text{and} \quad <V>_\nu \sim 1 / \beta^p , \tag{5}$$

the dimensionless numerical constants of proportionality in (5) being obtained from integrals over ξ.

The minimization condition (1), then becomes, with the help of expressions (5),

$$\partial <E>_\nu / \partial \beta = 2 <T>_\nu \beta^{-1} - p <V>_\nu \beta^{-1} = 0 , \tag{6}$$

giving

$$2 <T>_\nu = p <V>_\nu , \tag{7}$$

the form of the virial theorem for power behaved potentials.

(*) This condition is fulfilled for (trial) wavefunctions of a power behaved potential (h. o. potential, for example).

From the very same condition (1), we still have, using (5) and (6),

$$\frac{d<E>_\nu}{d\mu} = \frac{\partial <E>_\nu}{\partial \mu} + \frac{\partial <E>_\nu}{\partial \beta_\nu} \, \frac{d\beta_\nu}{d\mu} = - \frac{<T>_\nu}{\mu} \; , \tag{8}$$

a statement of the Hellman-Feynman theorem.

The argument is independent of p, although in practice the method is most suitable and easily applied to cases when $p = n$ (integer), i. e., to polynomial potentials of the type $V(x) = \sum_{n \geq 0} a_n x^n$ (n even) or $V(r) = \sum_{n \geq 0} a_n r^n$.

We are still left with a large variety of possible trial functions. The 1-dimensional harmonic oscillator (h. o.) has the peculiarity that in this system the uncertainty relation for $\Delta p_x . \Delta x$ is maximally realized; by this we mean that $\Delta p_x . \Delta x = \hbar/2$ [6] ($\Delta p_x . \Delta x = (n + 1/2)\, \hbar$ for $n > 0$). Thus, its wavefunctions should be a good choice for variation calculations, either in 1- or in 3-dimensional problems, in agreement with ideas of Gersch and Braden and the interpretation of $\int p dq = n h$ (see ref [10]).

a) We start with a 1-dimensional system. In the spirit of the previous statements, the trial wavefunctions will be the h. o. wavefunctions

$$U_\nu = N_\nu \, H_\nu (\sqrt{\mu\omega}\, x) \; e^{-1/2 \mu\omega x^2} \; , \; N_\nu = \left(\frac{\sqrt{\mu\omega}}{\sqrt{\pi}\; 2^\nu \, \nu !} \right)^{1/2} , \tag{9}$$

where the integer ν gives the order of the level and H_ν are the Hermite polynomials; $\alpha = \sqrt{\mu\omega}$ is a strength parameter, ω the frequency of the oscillator and μ the reduced mass. We calculate equation (4) for $<E>_\nu$ and minimize the resulting equation with respect to ω (ω has dimensions of mass, but this is of no consequence here, as can be seen):

$$\partial <E>_\nu / \partial \omega = 0 \, . \tag{10}$$

The key point is the application of (10) to each level separately.

As an exercise, we apply the procedure to the quartic oscilator: $V(x) = a\,x^4$, for which accurate approximate methods have been developed [1, 4]. Using $u_0(x) = (\alpha/\sqrt{\pi})^{1/2} \exp(-1/2\ \mu\omega x^2)$ we calculate $\langle ax^4\rangle_0$ and $\langle T\rangle_0 = \langle -1/2\ \mu\ .\ d^2/dx^2\rangle$, corresponding to the ground-state:

$$\langle ax^4\rangle_0 = 3/4\ a\,(\mu\omega)^{-2}\,,\quad \langle p^2/2\,\mu\rangle_0 = \omega/4$$

Minimizing $\langle E\rangle_0$, we find $\omega = (6a/\mu^2)^{1/3}$ and, as our best estimate for E_0:

$$\langle E\rangle_0\ (a/\mu^2)^{-1/3} = 3/8\ .\ 6^{1/3}\,. \tag{11}$$

Continuing for the excited states we construct Table I, where we compare our results with accurate numerical calculations [9]; we also quote Gersch and Braden [1] and the results of Hioie and Montroll [4] (taken from ref. [1]). Our results compare very

TABLE I — Approximate energy levels of $V = a\,x^4$

State	Our results $\langle E\rangle_\nu / (a/\mu^2)^{1/3}$	Exact results (ref. 9)	Gersch, Braden (*) (ref. 1)	Hioie, Montroll (**) (ref. 4)
$\nu = 0$	$3/8.6^{1/3} \simeq 0.6814$	0.6680	1.1906	0.5461
1	$9/8.10^{1/3} \simeq 2.4237$	2.3936	3.0001	2.3627
2	$15/8.(78/5)^{1/3} \simeq 4.6850$	4.6968	5.1514	4.6688
3	$21/8.(150/7)^{1/3} \simeq 7.2911$	7.3367	7.5598	7.3121
4	$27/8.(83/3)^{1/3} \simeq 10.167$	10.244	10.179	10.222
5	$33/8.(366/11)^{1/3} \simeq 13.267$	13.379	12.980	13.358
6	16.565	16.712	15.943	16.692
7	20.037	20.221	19.050	20.201
8	23.668	23.890	22.289	23.869
9	27.446	27.706	25.651	27.685

(*) $\langle E\rangle_\nu / (a/\mu^2)^{1/3} \simeq 1.1906\ n^{4/3}\quad (n = 1, 2, \ldots\ ;\ n = \nu + 1)$

(**) $\langle E\rangle_\nu / (a/\mu^2)^{1/3} \simeq 1.376\ (\nu + 1/2)^{4/3}\quad (\nu = 0, 1, 2, \ldots)$

Our results can be put into a form $\sim (\nu + 1/2)^{4/3}$, except that the parameter in front of $(\nu + 1/2)^{4/3}$ slightly decreases with increasing ν.

well with the exact ones, the first level being much better than the values obtained in refs [1] and [4].

The case of several terms in $V(x)$ is handled in exactly the same way. When $V(x)$ has a part odd in x, an extension of the method is possible. In such cases the introduction of a second variation parameter is desirable in order to displace the origin of the variable $(x \rightarrow x - X_0)$. For a complete treatment of the double-well potential and the anharmonic potential using the present method, the reader is advised to consult ref [5].

b) For three-dimensional potentials the method is a straightforward generalization of the one-dimensional case. The wavefunctions of the three-dimensional h. o. are constructed from products of the one-dimensional wavefunctions

$$\psi_{\nu_1 \nu_2 \nu_3}(x, y, z) \propto e^{-1/2 \mu\omega r^2} H_{\nu_1}(\alpha x)\, H_{\nu_2}(\alpha y)\, H_{\nu_3}(\alpha z) \qquad (12)$$

with parity $(-1)^\nu$, $\nu = \nu_1 + \nu_2 + \nu_3$, and $r^2 = x^2 + y^2 + z^2$.

Taking linear combinations, we can form wavefunctions appropriate to levels with a given orbital angular momentum *l* and parity $(-1)^l$. As an example we quote for the first few levels:

State

(1S)	$\nu = 0$	$l = 0$	$(4(\mu\omega)^{3/2}/\sqrt{\pi})^{1/2}\ Y_{00}$
(1P)	1	1	$(8(\mu\omega)^{5/2}/3\sqrt{\pi})^{1/2}\ r\ Y_{1m}$
(2S)	2	0	$(2(\mu\omega)^{3/2}/3\sqrt{\pi})^{1/2}\ (2\ \mu\omega\ r^2 - 3)\ Y_{00}$
(2D)	2	2	$(4(\mu\omega)^{7/2}/15\sqrt{\pi})^{1/2}\ r^2\ Y_{2m}$
(3P)	3	1	$(20(\mu\omega)^{7/2}/75\sqrt{\pi})^{1/2}\ (2\ \mu\omega\ r^3 - 5r)\ Y_{1m}$
	l	l	$\sim\ r^l\ Y_{lm}$, etc;

all expressions are to be multiplied by $\exp(-1/2\ \mu\omega\ r^3)$ and the Y_{lm} refer to the spherical harmonics.

Let us calculate the energy levels of the linear potential $V(r) = ar$ which, as is well-known to particle physicists, has had a large application in quark models for mesons and baryons. To be definite, we assume two particles of mass m, bound by $V(r)$. Separating the centre-of-mass motion in the Schödinger equation, we are left with an equation in terms of the relative coordinates (r, θ, ϕ).

We find

$$<E>_{1S} = 3\omega/4 + 2a/\sqrt{\pi\mu\omega} \tag{13}$$

After minimization $(\partial <E>_{1S} / \partial \omega = 0)$, we get the best estimate for the ground-state: $<E>_{1S} = 9/4\ (4a/3\sqrt{\pi\mu})^{2/3}$. In Table II we compare our estimates for S-wave states with the

TABLE II — Linear Potential

$(M = <T> + <V> + 2m)$

State	Our results	Exact results ref. 6
1S	3.111	3.105 (input)
2S	3.695	3.695
3S	4.175	4.182
4S	4.599	4.609
5S	4.987	5.000
1P	3.456	
2P	3.966	

$(a = 0.211\ \text{GeV}^2,\ \ m = 1.16\ \text{GeV})$

exact solutions of the Schrödinger equation, obtained from the poles of the Airy functions – ref [6]. This paper deals with a simple application of the linear potential to the charmonium system and the values quoted are very approximately the masses of the first few S-resonances: ψ, ψ', ψ'', etc. For completeness, we show our results for the 1P and 2P-wave states. The results have an error smaller than 0.4 %.

How well behaves the method, with h. o. wavefunctions in the case of the Coulomb potential? The results are not as good as the previous ones and we can hint at that from the following detail: in a Coulomb potential there is a degeneracy between, for instance, levels 1P and 2S, 2P and 3S, etc. If we calculate $<E>$ with h. o. functions this degeneracy is artificially lifted, although by a small amount; the best approximation will be to take average values. In Table III we present the results for the first levels.

TABLE III — Coulomb Potential

(We take $m = 1$, $\alpha = 1$)

State		Our results	average	Exact results ($E_n = -1/4n^2$; $n = 1, \ldots$)
$\nu = 1$,	$l = 0$	$-\frac{3}{4}\left(\frac{2\sqrt{2}}{3\sqrt{\pi}}\right)^2 \simeq -0.212$	-0.212	-0.250
2	0	$-\frac{7}{4}\left(\frac{5\sqrt{2}}{21\sqrt{\pi}}\right)^2 \simeq -0.06316$	-0.0599	-0.0625
1	1	$-\frac{5}{4}\left(\frac{4\sqrt{2}}{15\sqrt{\pi}}\right)^2 \simeq -0.05659$		
3	0	$-\frac{11}{4}\left(\frac{89\sqrt{2}}{660\sqrt{\pi}}\right)^2 \simeq -0.03184$	-0.0287	-0.0278
3	1	$-\frac{9}{4}\left(\frac{2\sqrt{2}}{15\sqrt{\pi}}\right)^2 \simeq -0.02547$		

One detail in the table is worth mentioning. We do not get upper bounds for the excited states when working with S-wave h. o. functions, but do get them using P-wave functions. This comes from the fact that the last functions are, due to their parity, orthogonal to the S-wave functions of the lower level.

The method should, nevertheless, still be reliable when the Coulomb interaction appears as a perturbation to the main potential: $V(r) = V_o + V_{coul}$.

In the phenomenological models of particle physics, V_o is often taken to be the linear potential. Such models do work very well, as far as mass spectroscopy is concerned, and work along these lines can be found in refs [3] and [8], which provide an intructive example of the influence, on the behaviour of the system, of the different terms of a potential.

III – CONCLUSIONS

We now put together those of the previous arguments which, in our view, justify the good results obtained with the method described.

In the first place, the application of the independent minimization procedure (1), with an appropriate choice of variation parameter, compels the expectation values of T and V to satisfy the virial theorem. There is an adaptation of the trial function to each state, in order to obtain the proper balance between the kinetic and potential energies of the state, as is required in spherically symmetric potentials. Certainly, both sides of the equality can still be wrong, differing from their exact values by the same amount, and we have to make sure that this difference is not large.

It is important, at this point, to understand the role of the uncertainty principle in reducing the possibility of a wrong estimate of the energy eigenvalues. Having used as trial wavefunctions solutions of the Schrödinger equation with harmonic oscilator potential, the constraint $<\Delta x>. <\Delta p> = (<\Delta x> \cdot <\Delta p>)_{h.o.} \geq \hbar/2$ is naturally enforced. Intead of introducing an ad hoc, although quite reasonable, rule to fix $<\Delta x> \cdot <\Delta p>$, as in ref [1], we have in our case $<\Delta x> \cdot <\Delta p>$ given by the wavefunctions of the h. o. potential. As these trial wavefunctions are solutions of the Schrödinger equation they have the correct limiting behaviour as $x \rightarrow 0$ and $x \rightarrow \infty$ ($r \rightarrow 0$ and $r \rightarrow \infty$ in three dimensions) and the correct nodal structure for the various eigenstates. They look like as wavefunctions should look: $<\Delta x> \cdot <\Delta p>$ cannot come very wrong. This provides an additional constraint that guarantees, with the viral theorem, that the energy levels are reasonably estimated.

However, one should not trust in detail these trial functions. In the virial theorem and in the uncertainty relations one only makes use of some of the lowest moments of the distribution $|\psi(x)|^2$. Whenever the detailed structure of the wavefunctions is required, as it may happen in transition matrix elements, the optimized wavefunctions, in particular for the excited states, may give a poor approximation. It is clear that the closer the potential being studied is to the potential used to extract the trial wavefunctions, the higher are the chances of the optimized wavefunctions to simulate accurately the real ones.

Finally, we would like to finish by expressing the hope that our simple procedure will be useful for first estimates of energy levels for a large class of potentials.

APPENDIX

Let us write the trial wavefunction ψ_n showing explicitly the parameter dependence:

$$\psi_n = \psi_n\,(x\,;\,\alpha_n\,,\,\beta_n\,,\,\ldots).\,(^*) \tag{A.1}$$

Recalling that $|\psi|^2$ has the meaning of a probability distribution, it is wise to choose the parameters $\{\alpha_n\,,\,\beta_n\,,\ldots\}$ in connection with the moments of the distribution. For instances,

$$\alpha_n \sim \langle x \rangle_n \tag{A.2}$$

being related to the mean and

$$\beta_n^{-1} \sim (\langle x^2 \rangle_n - \langle x \rangle_n^2)^{1/2} \tag{A.3}$$

being related to the dispersion. We shall keep only these two parameters.

(*) True wavefunctions have no dependence of $\alpha, \beta, \cdots$ on *n*. Such no dependence on *n* is equivalent to the orthogonality condition.

If the trial wavefunctions are solutions of the Schrödinger equation with a power behaved potentital, $V_0 = a\,(x-b)^r$, with r even, it can be easily shown, from scaling and translation invariance properties of the Schrödinger equation, that

$$\psi_n\,(x\,;\,\alpha_n\,,\,\beta_n) \equiv \sqrt{\beta_n}\;\phi\,(\xi)\,, \tag{A.4}$$

with $\xi \equiv \beta_n\,(x - \alpha_n)$ and

$$\int_{-\infty}^{+\infty} |\,\psi_n(x)\,|^2\, dx = \int_{-\infty}^{+\infty} |\,\phi_n(\xi)\,|^2\, d\xi = 1\,. \tag{A.5}$$

The energy for the nth-level can be written

$$E_n = \frac{1}{2\,\mu}\beta_n^2 \int \bar{\phi}\,(\xi)\,\frac{d^2}{d\,\xi^2}\,\phi\,(\xi)\,d\,\xi + \int \bar{\phi}\,(\xi)\;V\,(\xi)\,\phi\,(\xi)\,d\,\xi \tag{A.6}$$

and the minimization conditions

$$\partial <\psi\,|\,H\,|\,\psi>_n /\, \partial\,\beta_n = 0 \quad \text{and} \quad \partial <\psi\,|\,H\,|\,\psi>_n /\, \partial\,\alpha_n = 0 \tag{A.7}$$

become

$$\frac{\partial <\psi\,|\,H\,|\,\psi>_n}{\partial\,\beta_n} = \frac{1}{\beta_n}\left[\,2 <T>_n - <x\,\frac{\partial\,V}{\partial\,x}>_n\right] + \frac{1}{\beta_n}\,\alpha_n\,\frac{\partial}{\partial\alpha_n}<V>_n = 0 \tag{A.8}$$

and

$$\frac{\partial <\psi\,|\,H\,|\,\psi>_n}{\partial\,\alpha_n} = \frac{\partial}{\partial\,\alpha_n}<V>_n = 0\,. \tag{A.9}$$

It is clear that (A.8), together with (A.9), implies the virial theorem.

An application of the two-parameter minimization procedure to the double-well problem is given in ref [5].

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