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COMMENT

Simple variational approaches to eigenvalues in quantum theory

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Abstract. We develop a very simple variational procedure for obtaining quite accurate analytical expressions for the eigenvalues of quantum mechanical models. It consists of finding the minimum value of a properly built functional form for the energy in the phase space. The method enables one to make use of available information about the analytic structure of the eigenenergies. Results are shown for the linear confining potential model.

Much effort has been devoted during the past few years to finding the analytical dependence of energy levels on the quantum numbers and parameters in the Hamiltonian operator. The simplest approach appears to be the scaling variational method (SVM), consisting of calculating the smallest energy expectation value with a properly scaled trial function (Fock 1930, McWeeny and Coulson 1948, Chen 1963, Gromes and Stamatescu 1976, 1979, Dias de Deus *et al* 1981, Fernández and Castro 1983a, b, Gerry and Silverman 1983, 1984, Mitter and Yamazaki 1984). When applying this method, the virial and Hellmann-Feynman theorems are satisfied (Fernández and Castro 1983a, b, Mitter and Yamazaki 1984) and it has been argued that the approximate eigenvalues obtained this way behave as the semiclassical JWKB energy levels disregarding the basis set used (Fernández and Castro 1983a, b). Since the SVM energy levels obey only first-order Rayleigh-Schrödinger perturbation theory they closely approach the exact eigenvalues only for small enough values of the perturbation parameter. It is also known that for the physically more interesting three-dimensional central field problems, the SVM is most successful when $l > n - l$, where $n = 1, 2, \ldots$ and $l = 0, 1, \ldots, n-1$ are the principal and angular quantum numbers, respectively. When the coupling parameter in the Hamiltonian operator is large enough, poor SVM results are found for the s states ($l = 0$).

An alternative promising approach to the eigenvalues of parameter-dependent systems has recently been proposed that consists of finding the minimum value of a functional form for the energy in the phase space (Rosen 1979). The eigenvalues so obtained prove to obey relationships resembling a sort of virial and Hellmann-Feynman theorem (Fernández and Castro 1983c), a fact that has led to a more general technique called the variational functional method (VFM) (Fernández *et al* 1984a, Arteca *et al* 1984a, b). Under certain conditions this procedure reduces to the SVM and, through simple geometrical reasoning (Fernández *et al* 1984b), enables one to explain why the SVM and JWKB eigenvalues have approximately the same analytical structure.

A quite different approximation scheme has been proposed by Banerjee (1979, 1982) who suggested the use of the JWKB eigenvalues to improve results in the large quantum number regime. However, his eigenenergies do not have the proper parameter

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dependence because they do not obey the Hellmann-Feynman theorem. These difficulties could be removed if this method were combined with another which provides approximate eigenvalues obeying that theorem as in the case of the SVM and VFM.

The purpose of this comment is to show that the SVM results can be improved in the large quantum number and parameter regimes by means of the VFM. This seems to be necessary since a recent investigation of the SVM properties (Mitter and Yamazaki 1984) has taken into account neither previous results on the subject nor the VFM. The VFM is briefly discussed next. For the sake of concreteness, and comparison purposes, it is applied to an example treated previously by means of the SVM, namely the linear confining potential model (Fernández and Castro 1983b, Mitter and Yamazaki 1984). We conclude with our results and a discussion.

In order to facilitate the discussion of the method let us consider the following quantum mechanical model:

$$H(Z, g) = p^2/2 - Z/r + gr^k \qquad p = -i\nabla \tag{1}$$

that has been very useful in describing quark-antiquark bound states, especially for $k = 1$ (Eichten *et al* 1978). The level ordering of its eigenvalues $E(Z, g)$ has been widely studied (Quigg and Rosner 1977, 1979, Martin 1977, 1982, Grosse 1977, Felman *et al* 1979, Grosse *et al* 1984). Therefore it is a good test problem for approximation methods. We can consider only the case $Z = 1$ without loss of generality.

An appropriate functional form for the energy levels of such a model is (Fernández *et al* 1984a, Arteca *et al* 1984a, b)

$$F_{nl}(g, q) = A_n q^{-2} - q^{-1} + gB_{nl}(g)q^k \tag{2}$$

where q is chosen so that $\partial F_{nl}/\partial q = 0$ and therefore it depends on g.

It can be easily shown from the Hellmann-Feynman and virial theorems that

$$\langle r^{-1} \rangle = q^{-1} + (k+2)g^2 q^k (\partial B_{nl}/\partial g) \tag{3a}$$

$$\langle p^2 \rangle = 2A_n q^{-2} + 2(k+1)g^2 q^k (\partial B_{nl}/\partial g) \tag{3b}$$

since A_n does not depend on g. We thus conclude that q^{-1} and $A_n q^{-2}$ are related to the Coulomb interaction and kinetic energy, respectively.

If we require $F_{nl}(g, q)(g \to 0) = E(1, 0)$, it follows that

$$A_n = n^2/2. \tag{4}$$

The function $B_{nl}(g)$ is useful in taking account of available information about the actual eigenvalues. Its form can be determined, for example, from perturbation theory (Arteca *et al* 1984a, b, Fernández *et al* 1983). As a first-order approximation it can be chosen to be independent of g which leads to the semiclassical relations (Orland 1979)

$$\langle p^2 \rangle = n^2 q^{-2} \qquad \langle r^{-1} \rangle = q^{-1} \qquad \langle r^k \rangle = B_{nl} q^k. \tag{5}$$

The requirement that

$$\lim_{g \to 0} [E_{nl}(1, g) - F_{nl}(g, q)] g^{-1} = 0 \tag{6}$$

leads to the SVM and first-order perturbation theory.

On the other hand, if B_{nl} is chosen so that

$$\lim_{g \to \infty} g^{-2/(k+2)} F_{nl}(g, q) = E_{nl}(0, 1)^{\text{JWKB}} \tag{7}$$

we obtain

$$B_{nl}=2^{k+1}k^{3k/2}(k+2)^{-(k+2)/2}\left[\pi^{1/2}\Gamma\left(\frac{3}{2}+\frac{1}{k}\right)\Gamma\left(\frac{1}{k}\right)^{-1}\left(n-\frac{l}{2}-\frac{1}{4}\right)n^{-1}\right]^{k} \tag{8}$$

and approximate eigenvalues that obey both the virial and Hellmann-Feynman theorems and approach the JWKB result (Quigg and Rosner 1977, 1979) as either g or the quantum numbers tend to infinity.

When $k=1$ (linear confining potential model) we have

$$F_{nl}=-\frac{1}{2q}+\tfrac{3}{2}B_{nl}gq \tag{9a}$$

where

$$gB_{nl}q^3+q=n^2 \tag{9b}$$

and

$$B_{nl}=3^{-1/2}(n-l/2-1/4)n^{-1}. \tag{9c}$$

The VFM results are much more accurate than Banerjee's (1979) ones because the former obey the Hellmann-Feynman theorem while the latter do not since his choice of scaling parameter does not fulfil the variational principle.

The VFM and SVM eigenvalues, together with those coming from numerical integration of the Schrödinger equation (Eichten *et al* 1978), are shown in table 1. It is worth noticing that both variational methods are complementary. In fact, the accuracy of the VFM increases as $n-l$ increases while the SVM behaves oppositely. For small

Table 1. Lowest eigenvalues of the linear confining potential model. (The three numbers for each g value are VFM, exact (Eichten *et al* 1978) and SVM results, respectively.

g	$E_{10}(1s)$	$E_{20}(2s)$	$E_{21}(1p)$	$E_{30}(3s)$	$E_{31}(2p)$	$E_{32}(1d)$	$E_{40}(4s)$	$E_{42}(2d)$
500	107.047	198.216	157.826	271.319	237.069	200.184	335.453	272.457
	108.366	198.509	162.909	271.268	240.094	208.517	335.237	278.168
	114.566	190.790	168.631	253.174	240.402	213.794	308.397	281.978
62.5	24.431	48.064	38.121	66.686	58.196	49.060	82.915	67.259
	24.856	48.125	39.413	66.612	58.979	51.146	82.776	68.706
	26.234	46.235	40.779	62.188	59.022	52.430	76.189	69.624
18.518 518 ...	9.778	20.690	16.339	29.125	25.385	21.362	36.428	29.510
	10.006	20.708	16.922	29.064	25.743	22.290	36.327	30.162
	10.550	19.889	17.502	27.143	25.749	22.845	33.456	30.555
7.8125	4.867	11.254	8.846	16.092	14.006	11.765	20.251	16.383
	5.014	11.258	9.177	16.040	14.214	12.267	20.171	16.754
	5.283	10.810	9.489	14.987	14.209	12.591	18.589	16.967
4.0	2.692	6.953	5.437	10.111	8.788	7.367	12.806	10.346
	2.796	6.950	5.651	10.066	8.924	7.701	12.740	10.586
	2.947	6.674	5.841	9.410	8.917	7.891	11.749	10.717
2.314 831 48 ...	1.562	4.653	3.617	6.890	5.979	5.002	8.786	7.087
	1.640	4.646	3.767	6.850	6.075	5.234	8.729	7.256
	1.732	4.462	3.893	6.407	6.068	5.362	8.055	7.343
1.457 725 948	0.911	3.287	2.539	4.965	4.302	3.590	6.375	5.135
	0.972	3.279	2.650	4.929	4.374	3.761	6.325	5.260
	1.030	3.149	2.738	4.613	4.366	3.852	5.842	5.322

enough g values the SVM is preferable as it satisfies first-order perturbation theory. Both procedures lead to the actual level ordering (Quigg and Rosner 1977, 1979, Martin 1977, 1982, Grosse 1977, Grosse and Martin 1980, Felman *et al* 1979, Grosse *et al* 1984) which is surprising in the case of the VFM since the JWKB eigenenergies with equal $n-l/2$ values are wrongly degenerate when $1/g=0$ (Quigg and Rosner 1977, 1979). It is then clear that the VFM removes such degeneracy correctly even for very large g values. In addition to this, it must be kept in mind that the SVM is merely a particular choice of B_{nl}.

Large-order scaling perturbation approximations are also possible even in the case of a continuous spectrum and more degrees of freedom as shown by Fernández *et al* 1984c, 1985). However, the first-order variational parameter does not prove to be the best choice and an appropriate convergence criterion has to be used.

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