# Comments about energies of parameter-dependent systems

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It is shown that the proper dependence of eigenvalues with respect to the parameters and quantum numbers can be found by calculating the extremum of the energy functional.

Recently, Rosen[1] has shown that the quantity $E$ defined by

$$E = \min_{\vec{q}} \epsilon(\vec{q}), \quad \vec{q} = (q_1, q_2, \ldots, q_N) \ , \tag{1}$$

$$\epsilon(\vec{q}) = 2A\left(\sum_{i=1}^{N} q_i^2\right)^{-1} + \sum_{i=1}^{N} \xi_i q_i^2 + \sum_{i=1}^{N}\sum_{j=1}^{N} \gamma_{ij} q_i^2 q_j^2 \ , \tag{2}$$

satisfies the following equations:

$$E = 2\sum_{i=1}^{N} \xi_i \frac{\partial E}{\partial \xi_i} + 3\sum_{i=1}^{N}\sum_{j=1}^{N} \gamma_{ij} \frac{\partial E}{\partial \gamma_{ij}} \ , \tag{3}$$

$$\frac{\partial E}{\partial \xi_i}\frac{\partial E}{\partial \xi_j} = \frac{\partial E}{\partial \gamma_{ij}} \ . \tag{4}$$

The real constants $\xi_i$ are positive or negative and $\gamma_{ij} = \gamma_{ji}$ constitute a positive-definite array.

Using the Hellmann-Feynman theorem (HFT) and the quantum-mechanical virial theorem (VT), it is easy to show that the eigenvalues of the Hamiltonian operator

$$H = \sum_{i=1}^{N}\left(\frac{-\partial^2}{\partial q_i^2} + \xi_i q_i^2\right) + \sum_{i=1}^{N}\sum_{j=1}^{N} \gamma_{ij} q_i^2 q_j^2 \tag{5}$$

fulfill (3), while Eq. (4) follows from the semiclassical relation $\langle q_i^2 q_j^2\rangle = \langle q_i^2\rangle \langle q_j^2\rangle$.

This result is very interesting and it should be able to find important applications for determining the dependence of eigenvalues with respect to the parameters included in the Hamiltonian. However, we consider that the demonstration presented by Rosen for Eq. (3) seems to be too cumbersome in order to perform its extension without additional difficulties for more complex problems.

In this paper we will show that Eq. (3) can be demonstrated in a very simple way, so that it offers an appropriate manner by means of which Rosen's conclusions may be applied to more complex problems.

Let us suppose that the energy functional $\epsilon(\vec{q})$ possesses the form

$$\epsilon(\vec{q}) = T(\vec{q}) + V(\alpha, \vec{q}) \ , \tag{6}$$

where $T(\vec{q})$ is a homogeneous function of degree $-2$, and $\alpha$ is an arbitrary parameter. Besides, we assume that the form of $V(\alpha, \vec{q})$ is such that it allows the existence of an extremum value for $\epsilon(\vec{q})$, i.e.,

$$\frac{\partial \epsilon}{\partial q_i}(\vec{q} = \vec{q}_0) = 0; \quad i = 1, 2, \ldots, N \ . \tag{7}$$

From a physical point of view it is necessary that $\epsilon(\vec{q})$ has only one extremum value, a minimum, but our mathematical result is independent of this assumption. Equation (7) leads us at once to the VT:

$$2T(\vec{q}_0) = \vec{q}_0 \cdot \vec{\nabla} V(\alpha, \vec{q}_0) ; \quad \vec{\nabla} = \left(\frac{\partial}{\partial q_1}, \frac{\partial}{\partial q_2}, \ldots, \frac{\partial}{\partial q_N}\right) \ . \tag{8}$$

Furthermore, the condition of variational extremum (7) assures us the fulfillment of the HFT:

$$\frac{\partial E}{\partial \alpha} = \sum_{i=1}^{N}\left(\frac{\partial \epsilon}{\partial q_i}\right)_{\alpha}(\vec{q} = \vec{q}_0)\frac{\partial q_{i0}}{\partial \alpha} + \left(\frac{\partial \epsilon}{\partial \alpha}\right)_{\vec{q}}(\vec{q} = \vec{q}_0)$$

$$= \frac{\partial V}{\partial \alpha}(\alpha, \vec{q} = \vec{q}_0) \ , \tag{9}$$

where $E = \epsilon(\vec{q}_0)$. Equations (8) and (9) enable us to generalize at once Rosen's results.

As an illustrative example, let us consider the functional

$$\epsilon(\vec{q}) = 2A\left(\sum_{i=1}^{N} |q_i|^{2\lambda}\right)^{-1/\lambda} + \sum_{i=1}^{N} q_i^2\left(\xi_i + \sum_{j=1}^{N} \gamma_{ij} q_j^2 + \sum_{j=1}^{N}\sum_{k=1}^{N} \gamma'_{ijk} q_j^2 q_k^2\right) \ , \tag{10a}$$

$$-1 < \lambda < 1 \ , \tag{10b}$$

where the real constants $\xi_i$, $\gamma_{ij} = \gamma_{ji}$ are positive or negative numbers, and $\gamma'_{ijk}$ is a positive-definite array, which

 

is symmetric with regard to the exchange of all the indices. Equations (8) and (9) make certain that

$$2A\left(\sum_{i=1}^{N}|q_{i0}|^{2\lambda}\right)^{-1/\lambda}=\sum_{i=1}^{N}q_{i0}^{2}\left(\xi_i+2\sum_{j=1}^{N}\gamma_{ij}q_{j0}^{2}+3\sum_{j=1}^{N}\sum_{k=1}^{N}\gamma'_{ijk}q_{j0}^{2}q_{k0}^{2}\right)\ , \tag{11}$$

$$\frac{\partial E}{\partial\xi_i}=q_{i0}^{2}\ ;\ \frac{\partial E}{\partial\gamma_{ij}}=q_{i0}^{2}q_{j0}^{2}\ ;\ \frac{\partial E}{\partial\gamma'_{ijk}}=q_{i0}^{2}q_{j0}^{2}q_{k0}^{2}\ . \tag{12}$$

Substituting (11) and (12) in (10) (with $\vec{q}=\vec{q}_0$), we obtain

$$E=\sum_{i=1}^{N}\left(2\xi_i\frac{\partial E}{\partial\xi_i}+3\sum_{j=1}^{N}\gamma_{ij}\frac{\partial E}{\partial\gamma_{ij}}+4\sum_{j=1}^{N}\sum_{k=1}^{N}\gamma'_{ikj}\frac{\partial E}{\partial\gamma'_{ijk}}\right)\ . \tag{13}$$

This last equation is satisfied too by the eigenvalues of the Hamiltonian

$$H=\sum_{i=1}^{N}\left(\frac{-\partial^2}{\partial q_i^{2}}+\xi_i q_i^{2}+\sum_{j=1}^{N}\gamma_{ij}q_i^{2}q_j^{2}+\sum_{j=1}^{N}\sum_{k=1}^{N}\gamma'_{ijk}q_i^{2}q_j^{2}q_k^{2}\right)\ . \tag{14}$$

Our demonstration makes self-evident the reason from which the extremum $E$ corresponding to the functional $\epsilon(\vec{q})$ fulfills the same differential Eq. (13) as do the eigenvalues associated to the operator (14): both satisfy the VT and HFT. Besides, Eqs. (8) and (9) are of a general nature and may be applied without further difficulites to a large class of physical problems.

Orland[2] showed that the HFT, the VT, and the semiclassical approximation fix the $\lambda$ dependence for the eigenvalues of the operator

$$H(\lambda)=p^2+V(x)+\lambda W(x)\ . \tag{15}$$

We shall show here that those theorems determine, too, in an approximate fashion, the dependence of the eigenvalues on the quantum number $n$.

As an illustrative example, we choose the $2k$ oscillators $[V(x)=0,\ W(x)=x^{2k}]$ and the $2k$-anharmonic oscillators $[V(x)=x^2,\ W(x)=x^{2k}]$. In the first case we have

$$\epsilon_n(q)=A(k,n)/q^2+\lambda q^{2k}\ , \tag{16}$$

where the constant $A(k,n)$ only depends on $k$ and on the quantum number $n$. The extremum condition (7) yields

$$E_n=\epsilon_n(q_0)=(k+1)[A(k,n)/k]^{k/(k+1)}\lambda^{1/(k+1)}\ . \tag{17}$$

When $k=1$, the exact result is $A(1,n)=(n+\frac{1}{2})^2$. This result suggests to us that, as a first approximation, we may choose

$$A(k,n)=C_k(n+\tfrac{1}{2})^2,\quad n=0,1,2,\ldots\ . \tag{18}$$

The substitution of (18) in (17) allows us to obtain the correct dependence for the eigenvalues in the large $n$ regime:

$$E_n=(k+1)(C_k/k)^{k/(k+1)}(n+\tfrac{1}{2})^{2k/(k+1)}\lambda^{1/(k+1)}\ . \tag{19}$$

Choosing $C_k$ in a convenient way, Eq. (19) and the WKB method yield identical results. This equation holds also for the Coulombic potential ($\lambda<0$, $2k=-1$).

In Table I we present the exact numerical eigenvalues for the quartic oscillator ($k=2$, $\lambda=1$) calculated by Banerjee *et al.*[3] ($E_n^a$) by means of a very accurate method (we only show their results up to the sixth decimal place), together with our approximate eigenvalues determined from Eq. (19). We have

TABLE I. Eigenvalues of the quartic oscillator ($H=p^2+x^4$).

| $n$ | $E_n$[a] | $E_n$[b] |
|---|---|---|
| 0 | 1.060 362 | 0.867 |
| 5 | 21.238 373 | 21.215 |
| 10 | 50.256 255 | 50.243 |
| 15 | 84.457 466 | 84.450 |
| 20 | 122.604 639 | 122.601 |
| 25 | 164.012 044 | 164.012 044 |
| 30 | 208.232 339 | 208.236 |
| 35 | 254.946 198 | 254.953 |
| 40 | 303.912 066 | 303.922 |
| 45 | 354.939 633 | 354.953 |
| 50 | 407.874 363 | 407.891 |
| 100 | 1 020.989 992 | 1 021. |
| 1 000 | 21 865.262 118 | 21 866. |
| 10 000 | 470 790.294 427 | 470 815. |

[a]Exact numerical (Ref. 3).
[b]Equation (18) with $C_2=1.243\,315\,5$.

chosen arbitrarily $C_2 = 1.243\,311\,55$ to perform the computations in order to obtain the exact result for $E_{25}$. Except for $E_0$, the exactness of our results is remarkable within the great range of values considered.

For the $2k$-anharmonic oscillators we have

$$\epsilon_n(q) = A(k,n)/q^2 + q^2 + \lambda q^{2k} , \tag{20}$$

and Eq. (7) leads to

$$\lambda k q_0^{2k+2} + q_0^4 - A(k,n) = 0 , \tag{21a}$$

$$E_n = \frac{k+1}{k} A(k,n) q_0^{-2} + \frac{k-1}{k} q_0^2 . \tag{21b}$$

In the large $n$ regime, Eqs. (21a) and (21b) give the following approximate result:

$$E_n \simeq (k+1)(C_k/k)^{k/(k+1)} \lambda^{1/(k+1)} (n+\tfrac{1}{2})^{2k/(k+1)} + (k-1)(C_k k^{1-k})^{1/(k+1)} \lambda^{-2/(k+1)} (n+\tfrac{1}{2})^{2/(k+1)} , \tag{22}$$

where we have used the approximation (18). The powers corresponding to $\lambda$ and $(n+\frac{1}{2})$ in the two right-hand side terms of Eq. (22) are identical to those provided by the WKB method.[4]

Our results deduced from Eqs. (18) and (21) for the anharmonic oscillator ($k=2$, $\lambda=1$) are compared in Table II with the exact numerical eigenvalues[3] for different $n$ values. In this case we have used $C_2 = 1.225$ with the purpose to obtain good results between $n=20$ and 25.

TABLE II. Eigenvalues of the anharmonic oscillator ($H = p^2 + x^2 + x^4$).

| $n$ | $E_n$[a] | $E_n$[b] |
|---|---|---|
| 0 | 1.392 351 | 1.325 |
| 5 | 23.297 441 | 23.572 |
| 10 | 53.449 102 | 53.739 |
| 15 | 88.610 349 | 88.816 |
| 20 | 127.617 778 | 127.673 |
| 25 | 169.817 528 | 169.673 |
| 30 | 214.779 684 | 214.394 |
| 35 | 262.195 757 | 261.534 |
| 40 | 311.831 518 | 310.863 |
| 45 | 363.501 895 | 362.200 |
| 50 | 417.056 263 | 415.396 |
| 100 | 1 035.544 183 | 1 029. |
| 1 000 | 21 932.783 711 | 21 736. |
| 10 000 | 471 103.777 791 | 466 575. |

[a]Exact numerical (Ref. 3). [b]Equation (21) with $C_2 = 1.225$.

In spite of the fact that we have employed a very simple model, the results possess in both cases an acceptable accuracy. Thus the present method could be very useful to estimate the eigenvalues in more complex problems, and to determine their functional dependence with the quantum numbers.

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