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Hyperviral theorems applied to the linear oscillator with velocity-dependent anharmonicity

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Abstract. An alternative derivation is given of a perturbation theoretic scheme for the anharmonic oscillator recently proposed by Swenson and Danforth. The scheme uses the hypervirial and Hellmann–Feynman theorems. The calculation is extended to velocity-dependent perturbations. As a special case, the linear relativistic quantum oscillator is studied to second order, and the corresponding energies worked out. Various powers-of-momentum expectation values are also worked out in this order.

1. Introduction

The use of hypervirial and Hellmann–Feynman theorems in perturbation theory is well known (see eg Epstein and Hirschfelder 1961). Recently, Swenson and Danforth (1972) applied these theorems to the anharmonic oscillator with a perturbation of the form kq^m, where k is an infinitesimal parameter, and q is the position coordinate variable. They developed a specific procedure by means of which the eigenvalue problem may be solved in principle to any order of perturbation theory.

In this paper, we examine the extension of these authors' results to the case where the perturbation is of the velocity-dependent form kp^m, where p is the momentum variable. In so doing, we also present an alternative derivation of the result that the perturbations in energy and in the expectation values of the momentum and position coordinates, and of their powers, are expressible solely in terms of the unperturbed energy, E_0. For the linear oscillator which we are treating, this means of course that the inclusion of perturbations of the form kq^m or kp^m would not lift any degeneracy that might exist at the zeroth order.

As a special example, we investigate the linear relativistic harmonic oscillator defined by the hamiltonian

$$H = (p^2c^2+m^2c^4)^{1/2}-mc^2+\tfrac{1}{2}m\omega^2q^2 \simeq \frac{p^2}{2m}+\tfrac{1}{2}m\omega^2q^2-\frac{p^4}{8m^3c^2}.$$

2. General anharmonic oscillator

Let ω denote the characteristic angular frequency of a harmonic oscillator. We measure energy in units of $\frac{1}{2}\hbar\omega$, momentum in units of $(\hbar m\omega)^{1/2}$, and position coordinates in units of $(\hbar/m\omega)^{1/2}$. Let the added perturbation be $-kp^n$, where $n \geqslant 0$, and k is an infinitesimal parameter. Then the general anharmonic oscillator we investigate has hamiltonian

$$H = p^2+q^2-kp^n.$$

The eigenvalue equation is written

$$H|n(k)\rangle = E|n(k)\rangle;$$

$$\langle n(k)|n(k)\rangle = 1.$$

For any operator A, we denote $\langle n(k)|A|n(k)\rangle$ simply by $\langle A\rangle$. Let W be a time-independent operator-valued function of the dynamical variables p, q. Then from the Hellmann–Feynman theorem we have

$$\frac{\partial E}{\partial k} = -\langle p^n\rangle; \tag{1}$$

and from the hypervirial theorem we have

$$\langle [p^2+q^2-kp^n, W]\rangle = 0. \tag{2}$$

Following Swenson and Danforth (1972) we choose

$$W = q^b p^a, \qquad a, b \geqslant 0.$$

Now from the Weyl algebra

$$[q, p] = \mathrm{i}$$

we deduce

$$[q^m, p^n] = \mathrm{i}n \sum_{r=1}^{m} q^{m-r}p^{n-1}q^{r-1} \tag{3}$$

$$[p^n, q^m] = -\mathrm{i}m \sum_{r=1}^{n} p^{n-r}q^{m-1}p^{r-1} \tag{4}$$

$$p^{a-1}q = qp^{a-1}-\mathrm{i}(a-1)p^{a-2}. \tag{5}$$

We assume that the quantities E, $\langle p^c\rangle$ for $c > 0$ are expressible as a convergent power series in k, and put

$$P^c \equiv \langle p^c\rangle = \sum_{n=0} k^n\langle p^c\rangle_n \equiv \sum_{n=0} k^n P^c_n \tag{6}$$

$$E = \sum_{n=0} k^n E_n. \tag{7}$$

Also let

$$P^0_n = \delta_{n0}, \tag{8}$$

so that (6) is also true for $c = 0$.

Combining (6) with (1) and (7), we obtain

$$E_r = -r^{-1}P^n_{r-1}, \qquad r \geqslant 1. \tag{9}$$

Now using (5) in (2), the hypervirial theorem becomes

$$\left\langle a\sum_{r=1}^{2} q^{2+b-r}p^{a-1}q^{r-1} - b\sum_{r=1}^{2} p^{2-r}q^{b-1}p^{r+a-1} + kb\sum_{r=1}^{n} p^{n-r}q^{b-1}p^{r-1+a}\right\rangle = 0. \tag{10}$$

We shall consider two special cases, namely $b = 0$ and $b = 1$.

(i) For $b = 0$ we have

$$\left\langle \sum_{r=1}^{2} q^{2-r} p^{a-1} q^{r-1} \right\rangle = 0,$$

that is,

$$\langle qp^{a-1} \rangle = -\langle p^{a-1} q \rangle. \tag{11}$$

Using (5) in (11), we have

$$2\langle qp^{a-1} \rangle = \langle \mathrm{i}(a-1)p^{a-2} \rangle = -2\langle p^{a-1} q \rangle. \tag{12}$$

Equation (12) is the analogue of equation (6) of Swenson and Danforth (1972).

(ii) For $b = 1$ we have

$$\left\langle a \sum_{r=1}^{2} q^{3-r} p^{a-1} q^{r-1} - \sum_{r=1}^{2} p^{a+1} + k \sum_{r=1}^{n} p^{n-1+a} \right\rangle = 0,$$

that is,

$$2a\langle q^2 p^{a-1} \rangle - 2\langle p^{a-1} \rangle + \tfrac{1}{2}a(a-1)(a-2)\langle p^{a-3} \rangle + nk\langle p^{n-1+a} \rangle = 0, \tag{13}$$

where we have used (5) and (12). We now use the (re-arranged) eigenvalue equation

$$q^2|n\rangle = (E - p^2 + kp^n)|n\rangle$$

to eliminate q^2 from (13). We obtain

$$2aEP^{a-1} - 2(a+1)P^{a+1} + \tfrac{1}{2}a(a-1)(a-2)P^{a-3} + k(2a+n)P^{n+a-1} = 0. \tag{14}$$

We now use (6) and (7) in (14). Then, by rewriting this as a power series in k, and equating the coefficients of k^n to zero, we obtain

$$\begin{aligned} P_i^{a+1} = \left(\frac{a}{4(a+1)}\right)\Bigg\{ & 4E_0 P_i^{a-1} - 4 \sum_{r=1} P_{i-r}^{a-1} P_{r-1}^{n} \theta(i-r^-) \\ & + \left(\frac{4a+2n}{a}\right) P_{i-1}^{n-1+a} \theta(i-1^-) + (a-1)(a-2) P_i^{a-3} \Bigg\} \end{aligned} \tag{15}$$

where

$$\theta(i-r^-) \begin{cases} = 0 & \text{if} \quad i < r \\ = +1 & \text{if} \quad i \geqslant r. \end{cases}$$

(It is to be noted that θ is defined at the origin $i = r$ as having the value $+1$.)

For any given value of n, equation (15) is the expression in terms of the unperturbed energy E_0 of the ith order perturbation theoretic correction to $\langle p^{a+1} \rangle$. The corresponding energy is given by (9).

3. Application to the linear relativistic quantal oscillator

The hamiltonian for this system is

$$\begin{aligned} H &= (p^2c^2 + m^2c^4)^{1/2} - mc^2 + \tfrac{1}{2}m\omega^2 q^2 \\ &= \frac{p^2}{2m} + \tfrac{1}{2}m\omega^2 q^2 - \frac{p^4}{8m^3c^2} + \frac{3p^6}{48m^5c^4} + \dots \end{aligned} \tag{16}$$

In the units of energy, momentum, and position coordinates which we are using, this becomes

$$H = p^2 + q^2 - kp^4 + O(p^6), \tag{17}$$

where

$$k = \frac{\hbar\omega}{4mc^2} \ll 1. \tag{18}$$

The condition $k \ll 1$ is always satisfied for vibrating physical systems, for if we take m to be of the order of the protonic mass, which is reasonable, then $k \ll 1$ implies $\omega \ll 4mc^2/\hbar$, that is, $\omega \ll 5{\cdot}7 \times 10^{24}$ Hz, which would be satisfied in practice.

Substituting $n = 4$ in equation (15) gives

$$P_i^{a+1} = \left(\frac{a}{4(a+1)}\right)\Bigg\{4E_0 P_i^{a-1} - 4\sum_{r=1} r^{-1} P_{i-r}^{a-1} P_{r-1}^4 \theta(i-r^-) + \left(\frac{4(a+2)}{a}\right) P_{i-1}^{a+3}\theta(i-1^-) + (a-1)(a-2)P_i^{a-3}\Bigg\} \tag{19}$$

(i) For $i = 0$ (ie first-order perturbation theory) direct substitution gives

$$P_0^2 = \tfrac{1}{2}E_0, \qquad E_0 = 2n+1, \qquad n = 0, 1, 2, \ldots$$

$$P_0^4 = \tfrac{3}{8}(E_0^2 + 1)$$

$$P_0^6 = \tfrac{5}{16}(E_0^3 + 5E_0)$$

$$P_0^8 = \tfrac{35}{128}(E_0^4 + 14E_0^2 + 9)$$

$$\ldots$$

and

$$P_0^{2r+1} = 0, \qquad r = 0, 1, 2, \ldots$$

$$E_1 = -\tfrac{3}{8}(E_0^2 + 1), \tag{20}$$

that is,

$$kE_1 = -\frac{3(\hbar\omega)^2}{16mc^2} n(n+1) - \frac{3(\hbar\omega)^2}{32mc^2} \qquad \text{(energy units).} \tag{21}$$

(ii) For $i = 1$ (ie second-order perturbation theory)

$$P_1^{2r+1} = 0, \qquad r = 0, 1, 2, \ldots$$

$$P_1^2 = \tfrac{3}{8}(E_0^2 + 1)$$

$$P_1^4 = \tfrac{1}{32}(17E_0^3 + 67E_0)$$

$$E_2 = -\tfrac{1}{64}(67E_0 + 17E_0^3)$$

$$\simeq -(E_0 + \tfrac{1}{4}E_0^3)$$

$$= -\tfrac{1}{4}(8n^3 + 12n^2 + 14n + 5). \tag{22}$$

4. Conclusion

We have extended Swenson and Danforth's scheme for using the hypervirial and

Hellmann–Feynman theorems in carrying out nth order perturbation theoretic calculations for an anharmonic oscillator to the case where the anharmonicity is velocity-dependent and of the form kp^n, where p is the momentum variable. In the process, we have rederived Swenson and Danforth's results in an alternative form. We apply the results to the linear relativistic quantal oscillator as an example, and solve the energy eigenvalue problem for this system up to second order. Expectation values of various powers of the momentum have also been derived up to this order.

As would be expected, expectation values of all odd powers of p vanish in all orders of perturbation theory if the perturbation is of the form kp^{2r}, $r = 0, 1, 2, \ldots$.

References

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