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LETTER TO THE EDITOR

Some comments on: The Kim–Sukhatme alternative approach to non-relativistic perturbation theory

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Abstract. The new perturbation theory expressions obtained by Kim and Sukhatme are commented on, and some new results are obtained starting from their expressions.

Recently Kim and Sukhatme [1] obtained some new expressions for ground- and excited-state wavefunctions and energies in perturbation theory, which do not involve infinite sums, and can be thought of as a generalization of LPT [2–5].

Consider a Hamiltonian

$$H = T + V + \lambda h = H_0 + \lambda h$$

where

$$H\Psi_n(x) = E_n\Psi_n(x) = \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \lambda^3 E_n^{(3)} + \cdots\right)\Psi_n(x).$$

Kim and Sukhatme define $f_n(x)$ according to the equation $\Psi_n(x) \equiv f_n(x)\phi_n(x)$, where the $\phi_n(x)$'s are eigenfunctions of the unperturbed Hamiltonian H_0. Expanding $f_n(x)$ in powers of λ

$$f_n(x) = 1 + \lambda f_n^{(1)}(x) + \lambda^2 f_n^{(2)}(x) + \lambda^3 f_n^{(3)}(x) + \cdots \tag{1}$$

and substituting in the Schrödinger equation, these authors obtain

$$f_n^{(1)}(x) = \int^x \frac{\mathrm{d}x'}{\phi_n^2(x')} \int_{-\infty}^{x'} \hat{h}(x'')\phi_n^2(x'')\,\mathrm{d}x'' \tag{2}$$

$$E_n^{(2)} = \int_{-\infty}^{\infty} \hat{h}(x) f_n^{(1)}(x)\phi_n^2(x)\,\mathrm{d}x = \langle n|\hat{h} f_n^{(1)}|n\rangle \tag{3}$$

$$f_n^{(2)}(x) = \int^x \frac{\mathrm{d}x'}{\phi_n^2(x')} \int_{-\infty}^{x'} \left[\hat{h}(x'') f_n^{(1)}(x'') - E_n^{(2)}\right]\phi_n^2(x'')\,\mathrm{d}x'' \tag{4}$$

$$E_n^{(k)} = \int_{-\infty}^{\infty} \left\{ \hat{h}(x) f_n^{(k-1)}(x) - \sum_{i=2}^{k-1} E_n^{(i)} f_n^{(k-i)}(x) \right\} \phi_n^2(x)\, \mathrm{d}x$$

$$= \langle n | \hat{h} f_n^{(k-1)} | n \rangle - \sum_{i=2}^{k-1} E_n^{(i)} \langle n | f_n^{(k-i)} | n \rangle \tag{5}$$

$$f_n^{(k)}(x) = \int^x \frac{\mathrm{d}x'}{\phi_n^2(x')} \int_{-\infty}^{x'} \left\{ \hat{h}(x'') f_n^{(k-1)}(x'') - \sum_{i=2}^{k} E_n^{(i)} f_n^{(k-i)}(x'') \right\} \phi_n^2(x'')\, \mathrm{d}x'' \tag{6}$$

where $\phi_n(x) = \langle x|n\rangle$, $\hat{h}(x) \equiv h(x) - E_n^{(1)}$ and $E_n^{(1)} = \int_{-\infty}^{\infty} h(x)\phi_n^2(x)\,\mathrm{d}x = \langle n|h|n\rangle$.

In the series expansion (1), $f_n^{(1)}(x)$ is *identical* to the Dalgarno–Lewis F_n function [6–9] (see for example [9, equation (21)]). Thus the approach of Kim and Sukhatme is very close to the Dalgarno–Lewis formalism.

Considering equations (3) and (5) (with $k = 3, 4, \ldots$) and summing these equations, one obtains

$$E_n - E_n^{(0)} - \lambda E_n^{(1)} = \langle n | \lambda \hat{h} (f_n - 1) | n \rangle - \langle n | f_n - 1 | n \rangle \{ E_n - E_n^{(0)} - \lambda E_n^{(1)} \}$$

i.e.

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \frac{\langle n | \lambda \hat{h} f_n | n \rangle}{\langle n | f_n | n \rangle}$$

$$= E_n^{(0)} + \lambda E_n^{(1)} + \frac{\langle n | \lambda \hat{h} (\lambda f_n^{(1)}(x) + \lambda^2 f_n^{(2)}(x) + \lambda^3 f_n^{(3)}(x) + \cdots) | n \rangle}{1 + \langle n | \lambda f_n^{(1)}(x) + \lambda^2 f_n^{(2)}(x) + \lambda^3 f_n^{(3)}(x) + \cdots | n \rangle} \tag{7}$$

which is as expected since, assuming $\langle n|f_n|n\rangle = \langle n|\Psi_n\rangle = 1$, i.e. cross normalization, equation (7) reduces to

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \langle En | \lambda \hat{h} | \Psi_n \rangle = \langle n | H | \Psi_n \rangle.$$

Integrating by parts, one can show that

$$\langle n | \hat{h} f_n^{(2)} | n \rangle = \langle n | f_n^{(1)} (\hat{h} f_n^{(1)} - E_n^{(2)}) | n \rangle \tag{8}$$

$$\langle n | \hat{h} f_n^{(3)} | n \rangle = \langle n | f_n^{(1)} (\hat{h} f_n^{(2)} - E_n^{(2)} f_n^{(1)} - E_n^{(3)}) | n \rangle \tag{9}$$

$$\langle n | \hat{h} f_n^{(k)} | n \rangle = \left\langle n \left| f_n^{(1)} \left(\hat{h} f_n^{(k-1)} - \sum_{i=2}^{k} E_n^{(i)} f_n^{(k-i)} \right) \right| n \right\rangle \tag{10}$$

etc. Thus the matrix elements of $f_n^{(k)}$ which arise in the numerator of (7) can be expressed in terms of matrix elements of $f_n^{(k-1)}$.

For instance

$$E_n^{(3)} = \langle n | \hat{h} f_n^{(2)} | n \rangle - E_n^{(2)} \langle n | f_n^{(1)} | n \rangle$$

$$= \langle n | f_n^{(1)} \hat{h} f_n^{(1)} | n \rangle - 2 E_n^{(2)} \langle n | f_n^{(1)} | n \rangle$$

$$E_n^{(4)} = \langle n | \hat{h} f_n^{(3)} | n \rangle - E_n^{(2)} \langle n | f_n^{(2)} | n \rangle - E_n^{(3)} \langle n | f_n^{(1)} | n \rangle$$

$$= \langle n | f_n^{(1)} \hat{h} f_n^{(2)} | n \rangle - E_n^{(2)} \{ \langle n | f_n^{(2)} | n \rangle + \langle n | f_n^{(1)2} | n \rangle \} - 2 E_n^{(3)} \langle n | f_n^{(1)} | n \rangle$$

etc.

Adding equations (8)–(10) (with $k = 4, 5, \ldots$) and using (7) one obtains

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \frac{\langle n|\lambda f_n^{(1)} \lambda \hat{h} f_n|n\rangle}{\langle n|f_n(1+\lambda f_n^{(1)})|n\rangle} \tag{11}$$

which suggests various approximations depending on how far one wishes to go in the f_n expansion (equation (1)).

The results, equations (7)–(11), may be looked upon as new results which supplement the derivations of Kim and Sukhatme.

Finally, Kim and Sukhatme use their techniques to investigate the $n = 2$ state of an infinite square well potential

$$V(x) = \begin{cases} 0 & |x| \leqslant \frac{1}{2}\pi \\ \infty & |x| > \frac{1}{2}\pi \end{cases} \tag{12}$$

subject to a perturbation $h(x) = Ax + B$, and using equation (3) obtain

$$E_2^{(2)} = \frac{A^2}{36}\left(\frac{\pi^2}{12} - \frac{5}{36}\right). \tag{13}$$

Equating this result to the standard term by term second-order energy expansion for this state

$$E_2^{(2)} = \frac{\langle 2|h|1\rangle^2}{3^2 - 2^2} + \frac{\langle 2|h|3\rangle^2}{3^2 - 4^2} + \frac{\langle 2|h|5\rangle^2}{3^2 - 5^2} + \cdots \tag{14}$$

one obtains

$$\pi^2\left(\frac{3\pi^2}{5} - 1\right) = \frac{2^{12}3^6}{5}\left\{\frac{1^2}{(1\times 5)^5} - \frac{2^2}{(1\times 7)^5} - \frac{3^2}{(3\times 9)^5} - \frac{4^2}{(5\times 11)^5} - \cdots\right\}$$

a quickly converging series relation (giving 5 digit agreement after five terms) which to the knowledge of the author is not quoted in the literature [10, 11].

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