39. *Numerical Solution of an Unharmonic Oscillator Eigenvalue Problem by Milne's Method*

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1. In this note, we shall briefly report on our numerical solution of the quantum mechanical eigenvalue problem,

$$\mathcal{H}u_n(x)=\lambda_n u_n(x), \qquad (u_n \in L_2(-\infty, \infty), n=0, 1, 2, \cdots) \tag{1}$$

with the Hamiltonian,

$$\mathcal{H}=-\frac{d^2}{dx^2}+V(x), \qquad V(x)=-\nu x^2+x^4, \tag{2}$$

where ν is a parameter taking on either positive or negative values. One recognizes immediately that perturbation approach from the harmonic oscillator case cannot be useful even if there were a small parameter in front of the term x^4; when $\nu<0$ the perturbation series diverges! We have encountered the Hamiltonian (2) in our lattice space formulation of the $\lambda\phi^4$ field theory,[1] where the condition of mass-renormalization requires a large positive ν. The Hamiltonian of the same type has been studied by many authors in connection with the inversion vibration of NH_3 molecule[2] and the hydrogen-bonded solids; the 20-parameter variation calculation of Somorjai and Hornig[3] is perhaps the most elaborate, but on the one hand the precision they could obtain for eigenvalues was not high enough for our purpose (see Table below) and on the other they did not give the matrix elements due possibly to the limitation of the variation method.

2. In order to solve the eigenvalue problem (1), one normally attempts to connect smoothly the two solutions of the differential equation $(\mathcal{H}-\lambda)u(x)=0$, one started from $x=+\infty$ and the other from $x=-\infty$ (or from $x=0$ when the potential $V(x)$ is symmetric as ours is) by choosing appropriate value for λ on trial and error basis.

In our present problem, however, we have to determine the eigenvalues very accurately, in particular for the case of large $\nu>0$ because, due to the fact that the potential $V(x)$ is W-shaped having two deep valleys, the eigenvalue spectrum gets a doublet structure; the narrower the spacing becomes the larger the ν one takes.

We used the method proposed by W. E. Milne[4] in 1930; it is best

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