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A diatomic chain with a mass impurity

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It has a long history to study monatomic and diatomic chains with or without impurity as models for dynamics of lattices. By means of recurrence relations method, a diatomic chain with an impurity is studied. The Laplace transform of the momentum autocorrelation function of the impurity is derived. It has two pairs of resonant pole and three separated branch cuts. The poles lead to cosine function(s) and the cuts result in acoustic and optical branches. A frequency theorem is derived governing the upper and lower frequencies of the two branches; Criteria for resonant poles are established; general expres-sions for frequency and amplitude of cosine(s) are derived. The acoustic and optical branches can be expressed as inverse Laplace trans-forms which are not easy to be carried out in general. By means of convolu-tion theorem, *analytical expressions* for acoustic and optical branches are derived as expansions of even-order Bessel functions. The expansion coeffi-cients of the acoustic branch are integrals of real Jacobin elliptic functions. However, coefficients of the optical branch are integrals of *complex* elliptical functions. By addition theorem, the expansion coefficients for the optical branch are obtained as integrals of elliptic function along a contour parallel to the imaginary axis in a *complex* plane. A modulus theorem is derived relating the modulus of elliptic functions in the acoustic and optical branches.

Besides, a useful integral is obtained:

$$J=\int_0^{\phi}\frac{d\theta}{\sqrt{(1-r_1^2\sin^2\theta)(1-r_2^2\sin^2\theta)}} \qquad (r_2^2>r_1^2>1)$$

$$=tg\int_0^{\phi}\frac{d\varphi}{\sqrt{1-\kappa^2\sin^2\varphi}}=tg\int_0^{u_1}du=tgu_1, \qquad \sin\phi=snu_1,$$

with $g=1/\sqrt{r_2^2-1}$ and $\kappa^2=(r_2^2-r_1^2)/(r_2^2-1)<1$.

Biography

Ming B Yu has graduated from Jilin University, 1961. Before retiring, he worked as a Lecturer in Zhengzhou Coal Manage College, China, and a Visiting Adjunct Lecturer in University of Georgia, USA. Currently he is still active in studies in theoretical condensed matter physics and nonequilibrium statistical theory of closed and open systems.

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