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SCHRÖDINGER BASE STATES IN STRONG PERIODIC MEDIA

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We separate the two-dimensional Schrödinger equation in a spatially sinusoidal potential and find a series of orthogonal base states, all of the same energy, consisting of a Mathieu function in one Cartesian axis and a characteristic exponential in the other. Superpositions of these base states can rigorously satisfy boundary conditions when the medium has a sharp edge illuminated by perfect-Bragg radiation. The new states hold even when the potential peaks are higher than the transverse energy of the particle and hence extend existing weak-potential solutions of dynamical diffraction theory. The new states are applicable to current experiments with atoms in standing light and they reduce to the dynamical diffraction states when the potential is weak..

1 Introduction

When an atom moves through a standing light wave, it experiences a spatially-sinusoidal and time-independent potential due to the interaction of the atom's electric dipole with the electric field of the light. If the direction of the atom's motion is appropriate, Bragg diffraction will occur.[1-3] The situation is similar to that of a neutron moving through a perfect crystal, where, at least to lowest orders in a Fourier expansion, the potential can also be described as a simple sinusoid. There already exist well-developed theoretical treatments of neutron diffraction in crystals (dynamical diffraction theory[4-5]) and the wavefunctions developed in these treatments can be used to describe some cases of atom diffraction in standing light. Some, but not all cases. As we shall see below, an important dimensionless parameter in the Schrödinger theory of Bragg diffraction is q - the ratio of the heights of the peaks of the sinusoidal potential to the transverse kinetic energy of the particle, i.e. the kinetic energy in the direction perpendicular to the periodic lattice. For neutrons Bragg diffracting in crystals, q is of the order of 10^{-5} and consequently the base states in dynamical diffraction theory are derived under the assumption that $q \ll 1$. However for an atom Bragg diffracting in standing light, q can easily exceed 1 or 10 or more with ordinary laboratory light intensities and hence the existing base states, valid only for $q \ll 1$, do not apply. The purpose of this paper is to derive Schrödinger base states applicable to q values order of 1, 10, or larger.

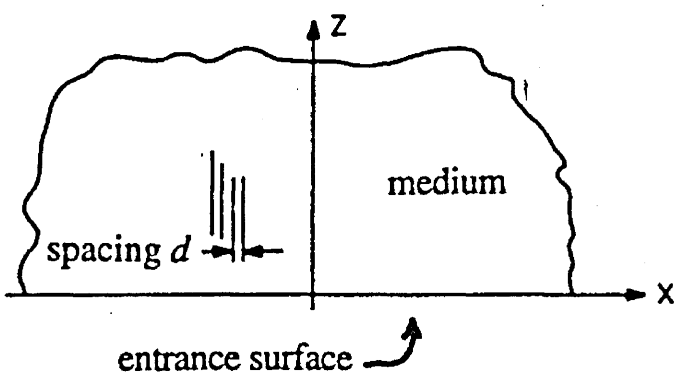

Figure 1 The coordinates, the position of the medium and its entrance surface $z = 0$, and the orientation and spacing d of the planes of the periodic potential.

Fig. 1 sets the stage for the discussion. The plane $z = 0$ is the entrance surface of the medium; the region $z < 0$ has zero potential, the region $z > 0$ is the periodic medium with a potential given by

$$V(x) = V_0 + 2V_1 \cos Gx \; . \tag{1}$$

Here the x-axis is along the entrance surface, $G \equiv 2\pi / d$ with d the spacing of the potential peaks and V_0 and V_1 are constants. Thus the surfaces of constant potential are planes perpendicular to both the plane of the figure and the entrance surface, i.e. a situation called Laue-case in crystal diffraction. In addition to satisfying Schrödinger's eq. within the potential of Eq. 1, the wavefunctions we seek must also satisfy boundary conditions at the entrance surface. We will assume that the incident particle has mass m and energy E, and that the incident wavefunction is simply a plane wave whose wavevector has magnitude k, lies on the x-z plane, and has a negative x-component $-G/2$. The z-component of the incident wavevector is then

$$k_z = \left[k^2 - \left(\frac{G}{2}\right)^2\right]^{\frac{1}{2}}. \tag{2}$$

In short, the plane-wave illumination in Fig. 1 is from the lower right at the Bragg angle.

Since V_0 and V_1 are zero for $z < 0$ and constants for $z > 0$, the medium has an abrupt or sharp edge. To describe a gentle or soft edged medium one would have to let V_0 and V_1 be functions of z. We will not consider soft edges here.

2 Background

As background for the large q wavefunctions, let us recall the two small q wavefunctions, Ψ^+ and Ψ^-, used as base states in dynamical diffraction.[4-5] These each have the factored form

$$\Psi^{\pm}(x,z,t) = \psi^{\pm}(x) e^{iK_z^{\pm} z} e^{-iEt/\hbar}, \tag{3}$$

but, as indicated, their x-axis wavefunctions, $\psi^+(x)$ and $\psi^-(x)$, and their z-axis wavenumbers, K_z^+ and K_z^-, are distinct. Specifically, the states, normalized over one potential period d, are

$$\psi^{\pm}(x) = \left(\frac{G}{4\pi}\right)^{\frac{1}{2}} \left(e^{iGx/2} \pm e^{-iGx/2}\right), \tag{4}$$

and their z-axis wavenumbers are

$$K_z^{\pm} \equiv \left[k^2 - \left(\frac{2m}{\hbar^2}\right)(V_0 \pm V_1) - \left(\frac{G}{2}\right)^2\right]^{\frac{1}{2}}. \tag{5}$$

Note that for positive V_0 and V_1 and for $V_1 < V_0$, both K_z^+ and K_z^- are less than the incident k_z given by Eq. 2, i.e. the particle must loose z-momentum climbing into the positive potential medium. Note also that while the $\psi^{\pm}(x)$ wavefunctions are each an equal-weight superposition of left and right running Bragg waves, $\psi^+(x)$ is a cosine with maximum probability for the particle to be at the peaks of the potential of Eq. 1. and $\psi^-(x)$ is a sine with maximum probability at the valleys of the potential. Consequently, $\psi^+(x)$ experiences more potential than $\psi^-(x)$, which explains why $\psi^+(x)$ is associated with a smaller value of K_z than is $\psi^-(x)$. In fact, it has been noted[5] that the values K_z^+ and K_z^- given in Eq. 5 can be derived from the general energy constraint

$$K_z^{\pm} = \left[k^2 - \left(\frac{2m}{\hbar^2}\right)\langle V\rangle^{\pm} - \left(\frac{G}{2}\right)^2\right]^{\frac{1}{2}}, \tag{6}$$

where $\langle V\rangle^{\pm}$ is the expectation value of the potential of Eq. 1 for the state $\psi^{\pm}(x)$.

The two complete base states $\Psi^{\pm}(x,z,t)$ of Eq. 3 are a sufficient basis to match at the boundary $z = 0$ any perfect Bragg illumination of the medium. By perfect Bragg illumination we mean a plane wave with k_x either $+G/2$ or $-G/2$ or an arbitrary superposition of both of these plane waves. For example, if the illumination is the single Bragg plane wave mentioned above which approaches the entrance surface from the lower right in Fig. 1 with x-momentum $-\hbar G/2$, then the resulting wavefunction in the medium is

$$\Psi_{total}(x,z,t) = \frac{1}{\sqrt{2}}\left[\Psi^+(x,z,t) - \Psi^-(x,z,t)\right], \tag{7}$$

the minus sign removing the unwanted right-going waves at $z = 0$ and thereby matching the incident left going wave. Because of the different values of K_z^+ and K_z^-, a beating effect occurs with increasing depth z in the medium so that, even though the particle definitely had negative x-momentum at $z = 0$, it will definitely have positive x-momentum at a depth Δ given by

$$\Delta = 2\pi\left(K_z^- - K_z^+\right)^{-1}, \tag{8}$$

will return to negative x-motion at twice Δ, etc. The depth Δ is known as the pendelösung length and the oscillations of the direction of propogation are known as pendelösung oscillations. Fig. 2 shows the probability distribution of the total state over two potential periods in the x-direction, i.e. there is a potential peak at the center of the horizontal axis and one at each edge of the Fig., and over three pendelösung depths Δ in the z-direction ($\Delta = 625$ of the arbitrary vertical units). Note that as the particle enters at $z = 0$ going left, the intensity is uniform across the entrance surface, then it piles up on the left side of each channel at $z = \Delta/2$, and then it is uniform again at depth Δ. But now the the particle is propogating to the upper right, i.e. it has been turned by Bragg diffraction.

The base states $\Psi^{\pm}$ out of which the total state of Eq. 7 is constructed are clearly not exact solutions of Schrödinger's eq. in the potential of Eq. 1, but, as we shall see, they are approximate solutions when the potential V_1 is small compared to the x-axis kinetic energy $\hbar^2 (G/2)^2/(2m)$. For use below let us introduce the dimensionless ratio of these energies as the parameter q,

$$q \equiv \frac{8mV_1}{\hbar^2 G^2}. \tag{9}$$

3 From Schrödinger To Mathieu

To find base wavefunctions for large q, consider the two-dimensional Schrödinger equation in the potential of Eq 1,

$$i\hbar \frac{\partial \Psi}{\partial t} + \frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial z^2}\right)\Psi - V_0 \Psi - 2V_1 \cos(Gx)\Psi = 0. \tag{10}$$

We seek factored base states just as in Eq. 3, i.e.

$$\Psi(x,z,t) = \psi(x)\, e^{iK_z z} e^{-iEt/\hbar}, \tag{11}$$

except that for large q, $\psi(x)$ and K_z are no longer given by Eqs. 4 and 5 and, as we shall see, more than two base states will be needed at large q. Insertion of Eq. 11 into Eq. 10 and introduction of a dimensionless coordinate, $Gx/2 \rightarrow x$, leads to the equation

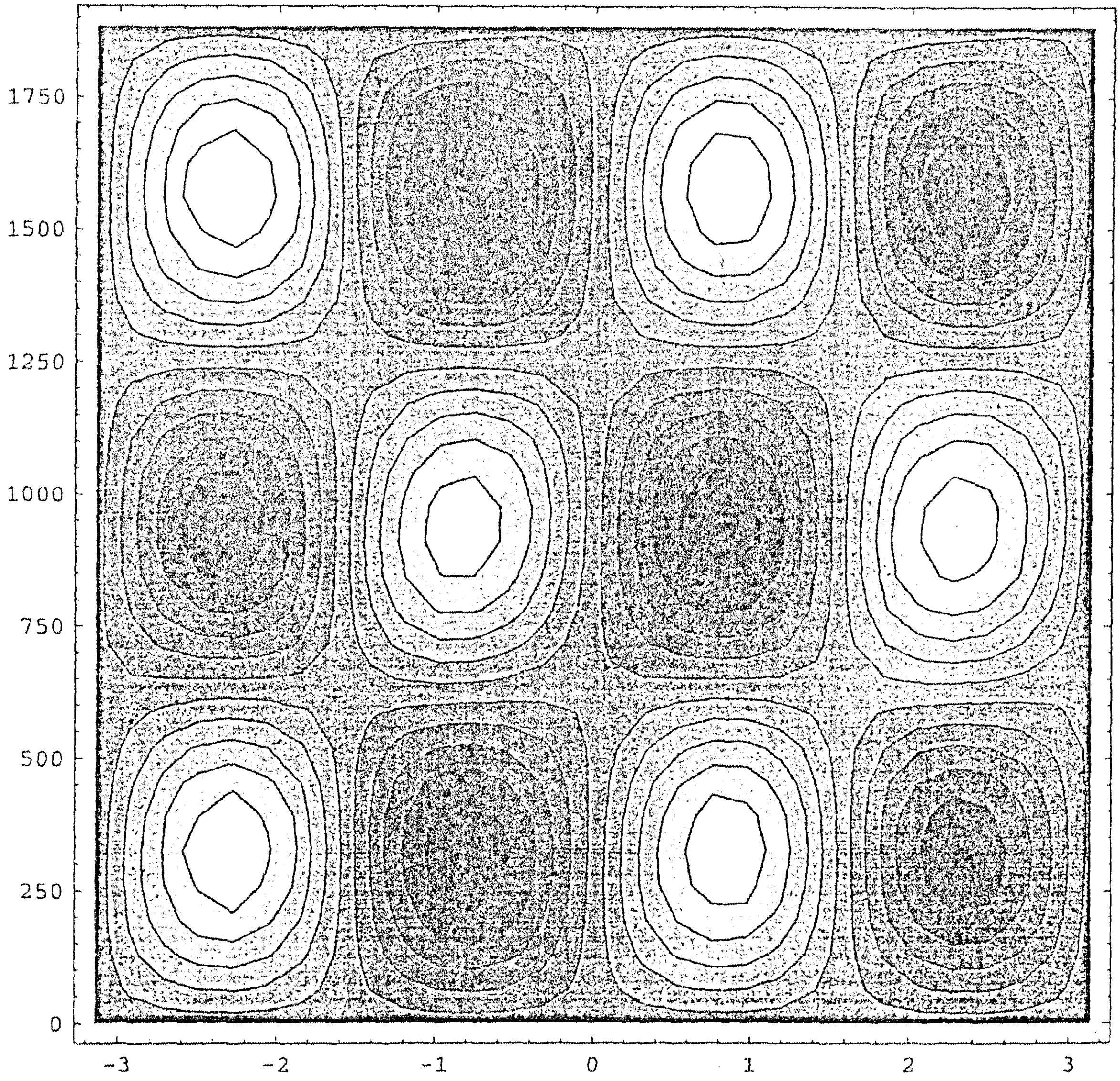

Figure 2 Probability density of the small q state of Eq. 7. The horizontal x-axis spans two lattice periods d, the vertical z-axis spans three pendelösung lengths Δ.

$$\frac{d^2\psi}{dx^2}+(a-2q\cos 2x)\psi=0 \tag{12}$$

for the x-axis wavefunction,where the new dimensionless parameter, a, is defined as

$$a=\frac{4}{G^2}\left[\left(\frac{2m}{\hbar^2}\right)(E-V_0)-K_z^2\right] \,. \tag{13}$$

Eq. 12 is the standard form of Mathieu's equation and its solutions are known as Mathieu functions.[6-7]

In the next section we consider integer order Mathieu functions since they are the states needed to develop wavefunctions generated by perfect-Bragg illumination. Before considering these functions let us first emphasize the wave-mechanical significance of the Mathieu parameter a. Consider a periodic Schrödinger probability amplitude ψ that obeys the Mathieu Equation. Multiply Eq. 12 by ψ^* and integrate over whatever period has been chosen for normalization, say π. (Note that in the dimensionless coordinate, the period of the potential is π ; the base state functions in the next section are all periodic over either π or 2π, but their squares are periodic over π , like the potential.) Use the normalization and solve for a to obtain

$$a=2q\int_0^\pi \psi^*(\cos 2x)\psi\,dx-\int_0^\pi \psi^*\frac{d^2\psi}{dx^2}dx \,. \tag{14}$$

The first term is the expectation value of the sinusoidal part of the potential and the second term (including the minus) is the expectation value of the kinetic energy in the x-direction, both terms in a dimensionless format. Eq. 14 implies that any specific periodic ψ that obeys Eq. 12 must be accompanied by a specific or characteristic value of the parameter a. And since K_z is the only free parameter in the Eq. 13 defining a, (G, E, and V_0 are assumed given and fixed), each specific solution will also be associated with a specific value of K_z. In short, the detail shape of an x-axis state will fix the the associated z-axis momentum, the same behavior seen earlier in Eq. 6 for the small q base states. Equating Eqs. 13 and 14 and solving for K_z, one obtains the generalization of Eq. 6 for base states of arbitrary q.

4 Mathieu Functions of Integer Order

For each positive integer, n, there exist two integer-order Mathieu functions[6-7] — the even one denoted $\mathrm{ce_n}(x,q)$ and the odd one denoted $\mathrm{se_n}(x,q)$. Each is real and has period either π or 2π. The even [odd] one $\mathrm{ce_n}(x,q)$ [$\mathrm{se_n}(x,q)$] can be expanded as a Fourier cosine [sine] expansion with real coefficients and with the lead term being $\cos nx$ [$\sin nx$]. There is also a single zeroth order function $\mathrm{ce_0}(x,q)$ that is even and periodic and has lead Fourier terms of a constant followed by $\cos 2x$. In all the Fourier expansions of integer Mathieu functions only alternate terms appear, e.g. $\cos x$, $\cos 3x$, $\cos 5x$, etc. in $\mathrm{ce_1}$. The shape of each function and hence its Fourier coefficients depend on the value of q.

For sufficiently small q, the Fourier coefficients can be expressed as power series in q. For $\mathrm{ce_1}$ and $\mathrm{se_1}$ these are[6-7]

$$\mathrm{ce_1}(x,q) = \left(1 - \frac{q^2}{128} - \frac{q^3}{512} + \cdots\right)\cos x - \left(\frac{q}{8} + \frac{q^2}{64} - \frac{q^3}{3072}\right)\cos 3x + \cdots,$$

$$\mathrm{se_1}(x,q) = \left(1 - \frac{q^2}{128} + \frac{q^3}{512} + \cdots\right)\sin x - \left(\frac{q}{8} - \frac{q^2}{64} - \frac{q^3}{3072}\right)\sin 3x + \cdots \quad . \tag{15}$$

To zeroth order in q, $\mathrm{ce_1}$ is $\cos x$ and $\mathrm{se_1}$ is $\sin x$ and hence we recover the dynamical diffraction states $\psi^{\pm}(x)$ of Eq. 4, but here unnormalized.

As anticipated in the previous section, each integer-order Mathieu function is a solution of the Mathieu equation 12 only if the parameter a has the appropriate characteristic value. The characteristic value for each specific type of function is q dependent.

For sufficiently small q, the characteristic values can be expressed as a power series in q. For $\mathrm{ce_1}$ and $\mathrm{se_1}$ these are[6-7], respectively,

$$a = 1 + q - \frac{q^2}{8} - \frac{q^3}{64} + \cdots \quad , \tag{16}$$

and

$$a = 1 - q - \frac{q^2}{8} + \frac{q^3}{64} + \cdots \quad . \tag{17}$$

To first order in q, when Eq. 13 for a and Eq. 9 for q are inserted in Eq. 16, the expression of Eq. 6 for K_z^+ is recovered. Similarly, Eq. 17 to first order in q yields the value of K_z^- . Thus the complete theory of dynamical diffraction at perfect Bragg conditions is contained in two Mathieu functions to zeroth order in q and in their characteristic values to first order in q.

For large q values the Fourier coefficients and the characteristic values cannot be determined from power series in q, such as in Eqs. 15, 16, and 17, and hence other techniques must be used. Suitable techniques were described in detail by McLachlan[6] and are available on Mathematica. Fig. 3 shows the characteristic values as a function of q for the first few integer-order Mathieu functions. Figs. 4, 5, 6 and 7 show graphs of these functions for several values of q.

Several features may be noted. First, at zero q the characteristic value for both the even and the odd function of order n is n^2. This is because, with no potential, the characteristic value is just the x-axis kinetic energy and, since only the lead term in the functions, i.e. $\cos nx$ or $\sin nx$, is present at $q = 0$, the (dimensionless) kinetic energy is just n^2. Second, with increasing q, the characteristic value for the odd function stays below that for the even function of the same order. This is because the even function "sees" the potential more. Third, with q sufficiently in excess of 1 the characteristic values of ce_0 and se_1, (and of ce_1 and se_2, etc.) asymptotically converge, indicating that these two functions tend toward the same energy expectation value. Since at large q the potential energy dominates the kinetic, the convergence of these characteristic values actually indicates that the two functions have the same expectation value for the potential, i.e. the squares of the functions must have the same shape. The graphs of ce_0 and se_1 at $q = 24$ confirm this, and a similar convergence can be seen in the pairs of functions in Figs. 5, 6, and 7. For the higher order pairs, the convergence doesn't fully develop until larger q values because of their greater kinetic energies. Fourth, the functions of even order n $=0,2,4,\cdots$ have period π; those of odd order $n=1,3,5,\cdots$ have period 2π. Fifth, for all the functions there is a general tendency, with increasing q, for the probability density to be pushed off the potential peaks and into the valleys, i.e. quantum mechanical channeling. To see this in the graphs, it is important to remember that the period of the potential is π, in the dimensionless coordinate, and thus the domain of the graphs is two periods of the potential, i.e. there is a potential peak at the center and at each edge of the graph. Finally, as the probability density gets more localized in the valleys with increasing q, higher order components are required in the Fourier expansions of the functions.

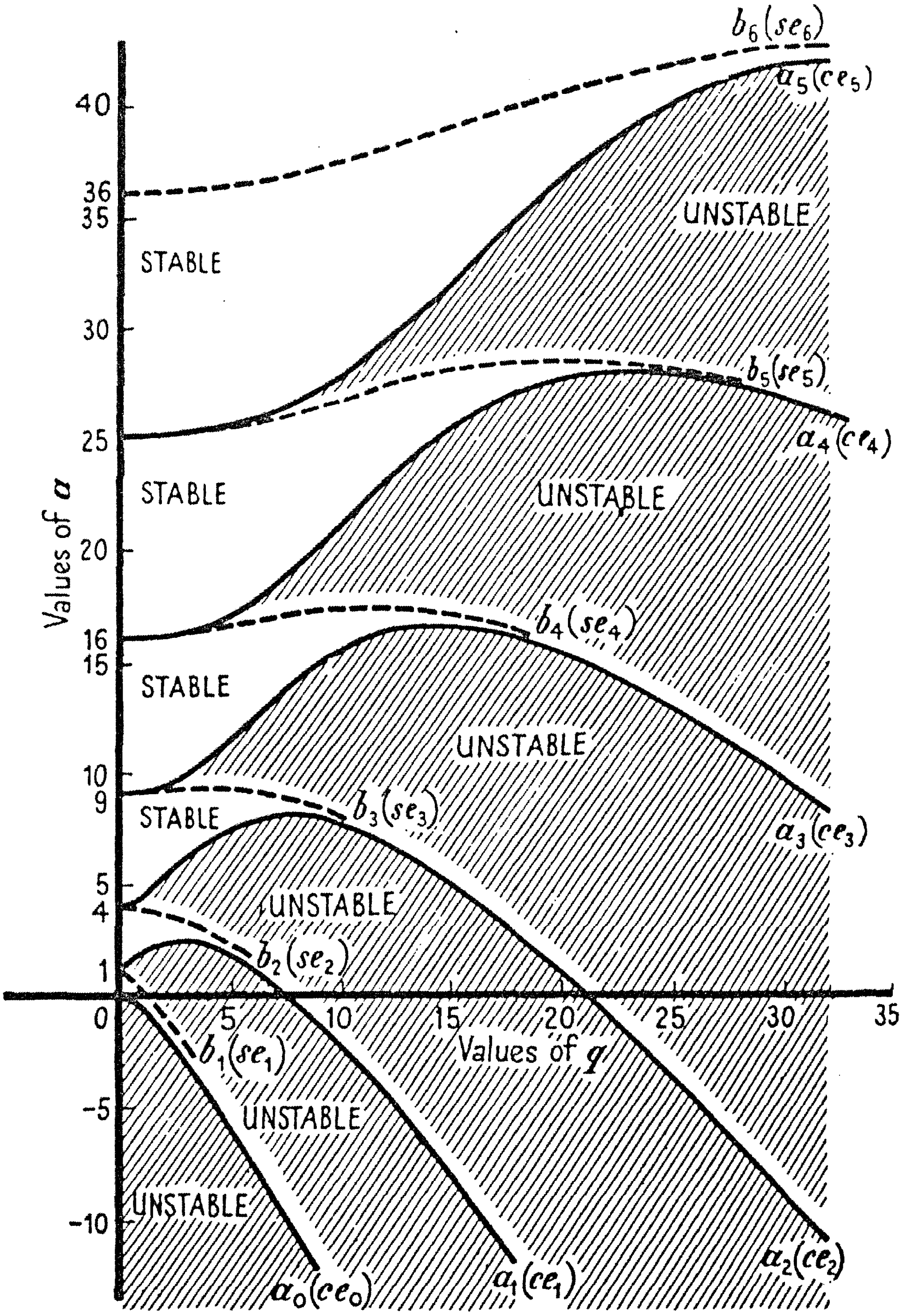

Figure 3 Characteristic values for integer order Mathieu functions. The values for the even and odd functions are labeled a_n and b_n, respectively, and are shown as solid and dotted curves, respectively.

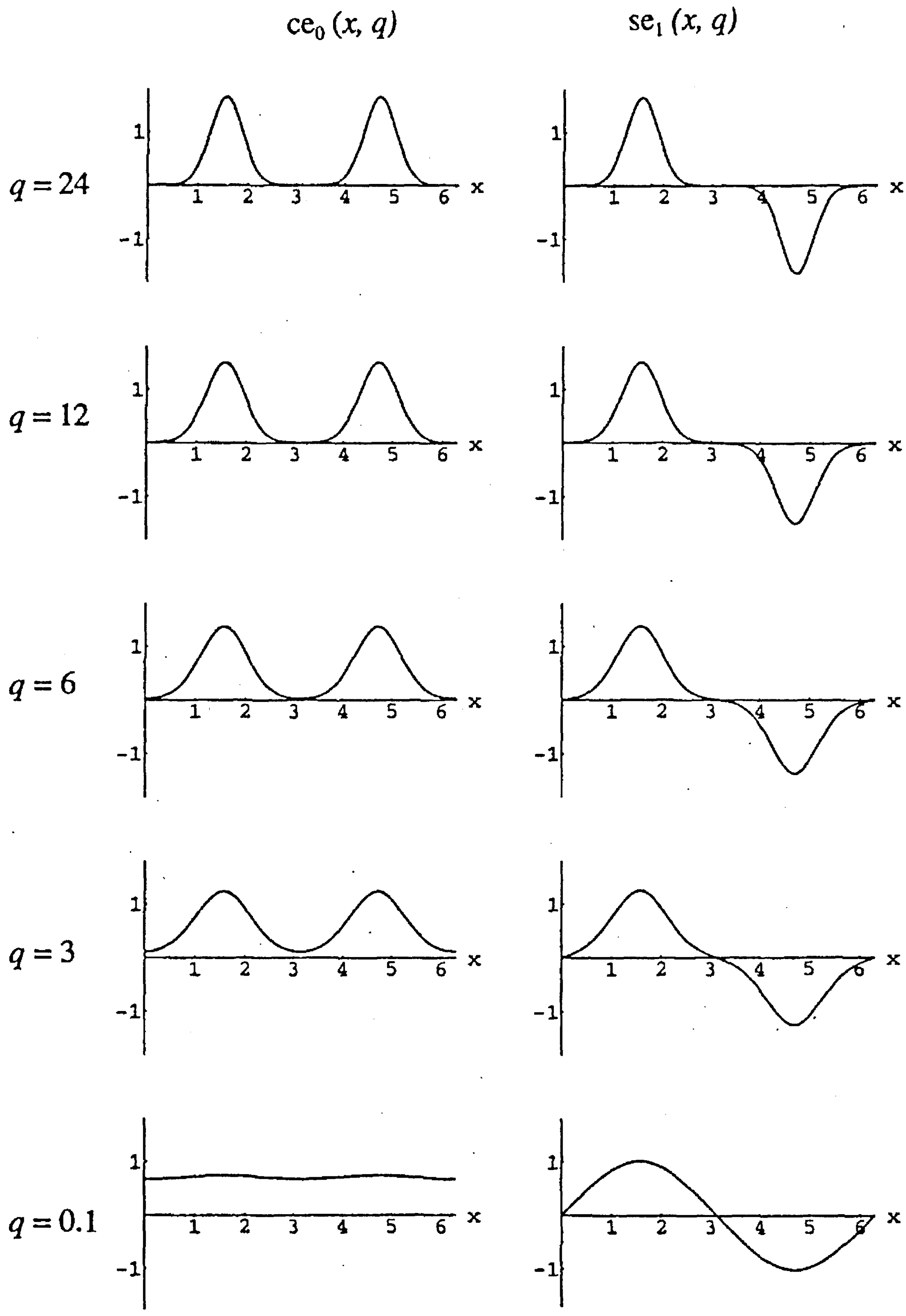

Figure 4 Mathieu functions ce_0 and se_1, over two periods of potential.

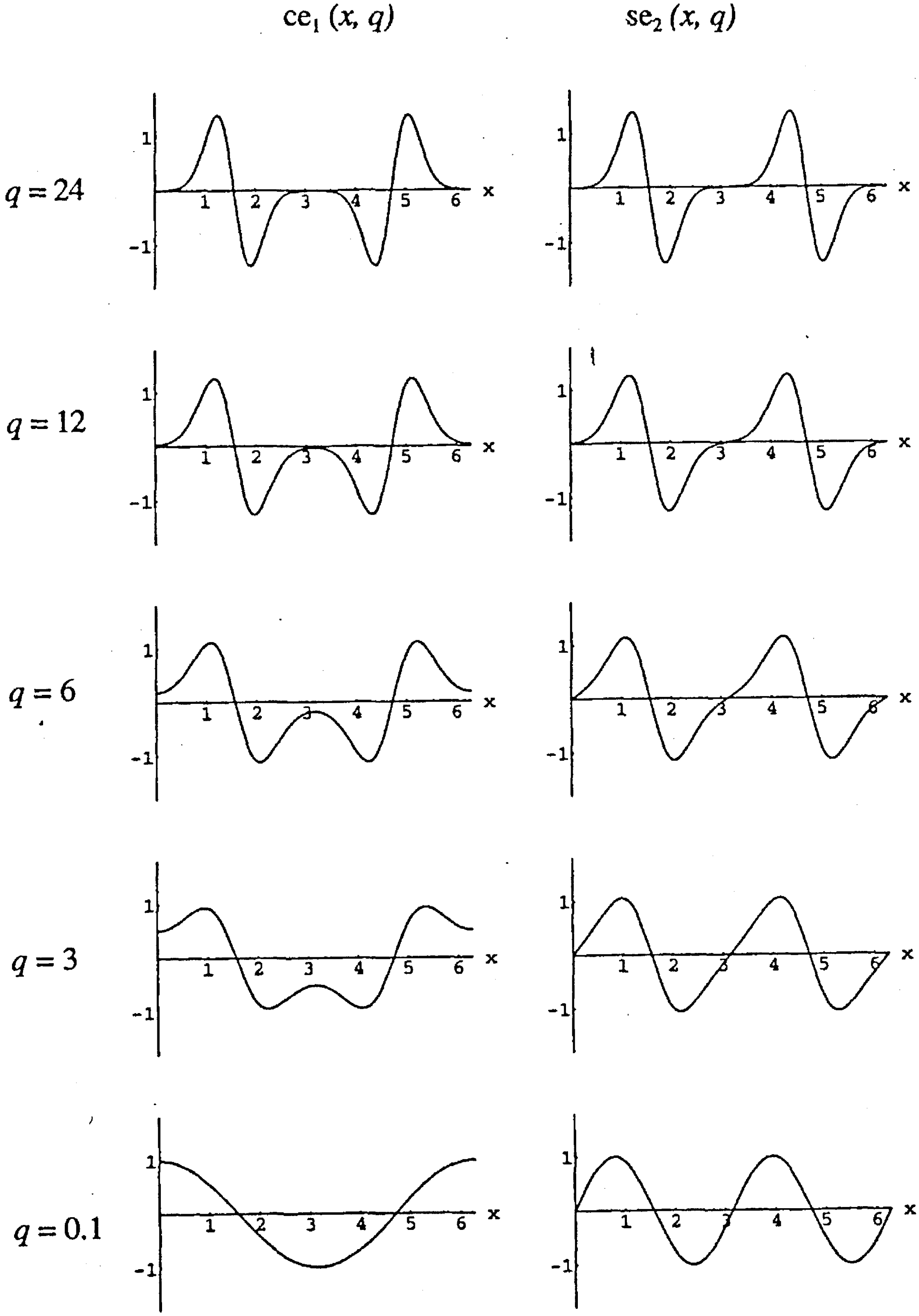

Figure 5 Mathieu functions ce_1 and se_2, over two periods of potential.

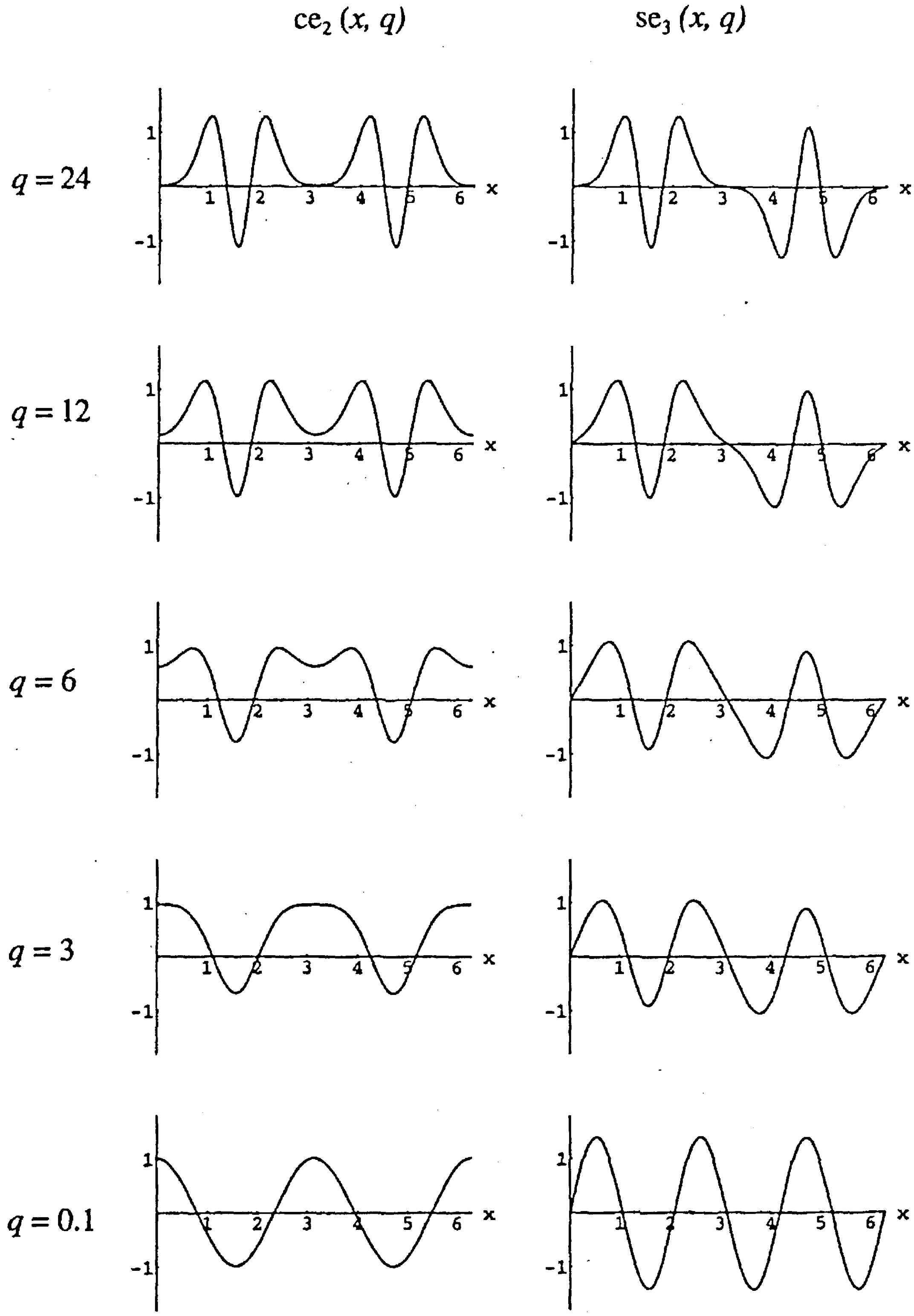

Figure 6 Mathieu functions ce_2 and se_3, over two periods of potential.

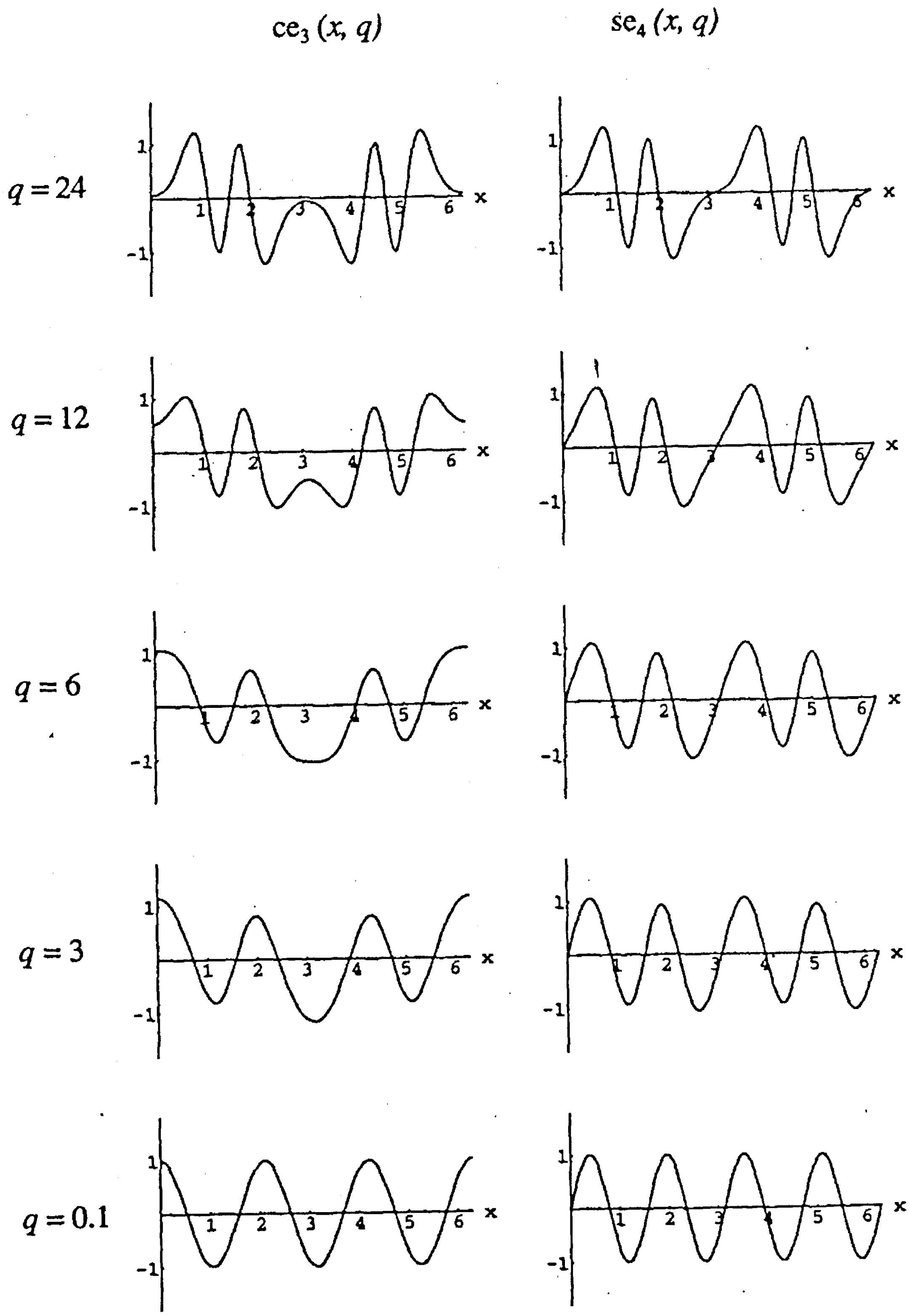

Figure 7 Mathieu functions ce_3 and se_4, over two periods of potential.

5 Total Wavefunctions

For a given q, the set of integer-order Mathieu functions are mutually orthogonal and form a complete set for expanding any function that shares the periodicity of the medium. The left-going and perfect-Bragg incident wave considered above in sections 1 and 2 presents just such a function at the entrance plane of the medium: its x-dependence in the dimensionless coordinate is simply

$$e^{-ix} = \cos x - i \sin x. \tag{18}$$

If the medium beyond the boundary has a Mathieu parameter of value q, expand Eq. 18 in integer-order Mathieu functions of that q value. Since Eq. 18 has period 2π,the cos x expands in odd order ce_n functions and the sin x in odd order se_n functions. Now each Mathieu function in the expansion is linked to a specific characteristic constant a and hence, via Eq. 13, to a specific z-axis wavenumber K_z. Therefore the complete in-medium wavefunction $\Psi(x,z,t)$ is obtained by multiplying each term by the appropriate z-dependent exponential, i.e. each term in the Mathieu expansion will have the form of Eq. 11 with a different K_z value for each term and, of course, the $\psi(x)$ in each term is an integer-order Mathieu function. Note that although each term factors into functions of x only, z only and t only, the complete wavefunction doesn't factor, just as in the small q state of Eq. 7. To prepare a factorable in-medium wavefunction, i.e. a single Mathieu function times a single z-axis exponential, one would need to illuminate the entrance surface with a coherent superposition of plane waves, $\exp(\pm ix), \exp(\pm 2ix), \exp(\pm 3ix), \cdots$, each with the proper amplitude and phase to build the specific Mathieu function.

The number of terms needed for an accurate Mathieu expansion of Eq. 18 increases with q and hence more coefficients must be calculated. Fortunately, because of the orthogonality of the Mathieu functions, a table of Fourier coefficients for various Mathieu functions (available on Mathematica) already contains the needed coefficients: if the table is arranged such that a row gives ascending Fourier coefficients for expanding a specific Mathieu function, then the columns give ascending Mathieu coefficients for expanding various sine and cosine functions.

Preliminary calculations of total wavefunctions generated by the incident state of Eq. 18 have been carried out up to $q = 24$. Even at q = 24 fewer than ten Fourier terms are required. Beyond $q = 1$, several new features emerge that are not present in the state of Eq.7 and the density of Fig. 2. In addition to a reduction of the principle pendelösung period, there are secondary pendelösung structures of even smaller z-periodicity and also an increasing localization of the density in the potential valleys.The reduction of the principle pendelösung period is because the difference in the characteristic constants for ce_1 and se_1 increases with q (see the a_1 and b_1 curves on Fig. 3). The finer pendelösung structures are due to beating of the various other K_z values that are now in the wavefunction and the x-localization is due to the higher x-momenta that are in the Mathieu functions with increasing q. These higher x-momenta imply additional outgoing beams at the exit surface of the medium and their relative brightness exhibits an interesting dependence on the thickness of the medium via the K_z beating. More details and density displays of these high-q total wavefunctions will be presented elsewhere.

6 Conclusions and Extensions

The base states presented in section 4 and the total wavefunctions outlined in section 5 solve the problem posed in the introduction: find the Schrödinger wavefunction generated in a medium with a strong sinusoidal potential when the medium has a sharp boundary and is illuminated by a perfect-Bragg plane wave of definite energy. The wavefunctions are built by superposition of products of integer-order Mathieu functions in x and complex exponentials in z with wavenumbers characteristic of each Mathieu function. Each term in the superposition is a rigorous solution of the Schrödinger equation in the periodic medium and the superposition rigorously matches the incident plane wave at the boundary. When the potential is weak the wavefunctions reduce to the familiar perfect-Bragg wavefunctions of dynamical diffraction theory

Several extensions are called for. First, in current experiments with atoms impinging on standing light, the incident radiation is not a single perfect-Bragg plane wave but typically is a mixture of many plane waves whose directions span a substantial fraction of the mean Bragg angle. Such off-Bragg waves can be handled via the same techniques as above but one must use fractional-order Mathieu functions.[6] These functions have characteristic-value curves that lie in the white regions of Fig. 3 marked "stable". Second, the sharp-edged boundary may not apply. In general, a soft-edged boundary calls for a z-dependent q. Third, if the detuning of the light is small [or zero], the potential is complex [or imaginary] and hence at least partially absorbing.[2] Mathieu functions do exist for complex q.[6] Fourth, the potential can be made time dependent.[8] Theoretical consideration of these situations will be presented elsewhere. But it seems clear that in all these extensions products of Mathieu functions and characterisitic exponentials in z will play a central role, since these are the base states in a sinusoidal medium.

Acknowledgments

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