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Quantum mechanical bound rotator as a generalized harmonic oscillator

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Abstract. We report quantum mechanical studies of an entity of importance in the dynamics of the rotational polaron which arises in non-linear physics. The rotational polaron consists of a particle such as an electron or exciton in interaction with an oscillator subject to a sinusoidal potential which binds it to a ring. Our investigation focuses on the oscillator. Energy eigenvalues and eigenfunctions are computed and related to those for a harmonic oscillator. The time evolution under the action of a perturbing potential is also examined.

1. Introduction

In the study of non-linear excitations in condensed matter systems [1–6], an entity called the rotational polaron has been introduced recently [5, 6]. It is a rotational counterpart of the ordinary polaron and has been shown [5, 6] to exhibit curious features such as saturation of self-trapping with increasing non-linearity, multiple stationary states, and the counterintuitive disappearance of symmetry breaking on *increasing* non-linearity. A rotational polaron consists of a quantum mechanical particle interacting with a rotational oscillator. In the semiclassical approximation wherein the oscillator is treated classically, it obeys the following equations of motion:

$$i\hbar\dot{c}_m = \sum_n V_{mn}c_n + E(\theta_m)c_m \quad (1.1a)$$

$$\ddot{\theta}_m + \Omega^2 f(\theta_m) + RE'(\theta_m)|c_m|^2 = 0 \quad (1.1b)$$

where c_m and θ_m are the amplitude of the particle and the rotational coordinate of the oscillator at the m th site respectively, V_{mn} is the intersite matrix element describing transfer of the particle, and Ω and R are measures of the restoring force and the moment of inertia of the rotator, respectively. Equations (1.1) are generalizations of equations in which the functions f and E are assumed linear in θ_m . Among the several choices that have been studied [5, 6], the simplest non-trivial one is

$$f(\theta_m) = (1/\Lambda) \sin(\Lambda\theta_m) \quad (1.2a)$$

$$E(\theta_m) = (E_0/\Lambda) \sin(\Lambda\theta_m) \quad (1.2b)$$

with the limit of $\Lambda \rightarrow 0$ giving the standard non-linear Schrödinger equation [1, 3]

$$i\hbar\dot{c}_m = \sum_n V_{mn}c_n + E_0\theta_m c_m \quad (1.3a)$$

$$\ddot{\theta}_m + \Omega^2\theta_m + RE_0|c_m|^2 = 0. \quad (1.3b)$$

Existing results on the rotational polaron are based on a classical description of the oscillator part of the Hamiltonian describing the rotational polaron. It is obviously of interest to generalize the description of the oscillator to include quantum mechanics. As an initial attempt at this problem, we study in this paper the quantum mechanics of the oscillator part alone, without paying attention to the moving particle. Such systems are of interest also in the problem of liquid crystals [7]. We concentrate here on a single oscillator consisting of a quantum mechanical particle constrained to move in a ring bound by a sinusoidal potential. In section 2, we present the equation of motion, indicate its relation to that obeyed by a harmonic oscillator, and provide expressions which clarify the relation, both in the context of the energy spectrum and the eigenfunctions. In section 3, we investigate the time evolution of the system under the action of a perturbation and study transitions analogous to transitions between the number states of the harmonic oscillator when a linear displacement is added to it. In section 4, we present concluding remarks.

2. Energy eigenvalues and eigenfunctions

We consider a particle constrained to move on a ring of length L and bound to a point on the ring by a potential which is similar to a harmonic oscillator potential, and thus write the equation for the wavefunction ψ of the particle as

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + \frac{m\omega^2 L^2}{4\pi^2} \left(1 - \cos \frac{2\pi x}{L}\right) \psi = \mathcal{E}\psi. \quad (2.1)$$

Here the particle has mass m and energy \mathcal{E} . In the limit of large L , equation (2.1) reduces to the Schrödinger equation for a harmonic oscillator of frequency ω . Equation (2.1) can be written in the standard Mathieu form [8],

$$\frac{d^2\psi}{d\phi^2} + \left(b - \frac{s}{2}\right) \psi + \frac{s}{2} \cos(2\phi)\psi = 0 \quad (2.2)$$

where

$$\phi = \frac{\pi x}{L} \quad b = \frac{2m\mathcal{E}L^2}{\hbar^2\pi^2} \quad s = \frac{m^2\omega^2 L^4}{\hbar^2\pi^4}. \quad (2.3)$$

It is generally known that there exist sets of values of b for which the solutions of (2.2) are periodic with period $n\pi$ where n is an integer [8–11]. Since the physics of our problem demands solutions of (2.1) which are periodic in x -space with period L , we restrict ourselves to those Mathieu function solutions of (2.2) which are periodic in ϕ -space with period π . It is clear that, as the length L of the ring approaches infinity, the sinusoidal potential tends to the harmonic oscillator potential, and (2.1) reduces to the familiar Schrödinger equation for the harmonic oscillator. The spectrum of the latter is of course equidistant:

$$\mathcal{E}_n^{\text{ho}} = \left(n + \frac{1}{2}\right)\hbar\omega \quad n = 0, 1, \dots \quad (2.4)$$

It is of interest to obtain the general spectrum represented by (2.1) in the limit of large L . As a meaningful dimensionless parameter to be used in the required expansions, we select

$$\xi \equiv s^{-1/2} = (\hbar/m\omega)(\pi/L)^2 \equiv \pi^2(\lambda/L)^2. \quad (2.5)$$

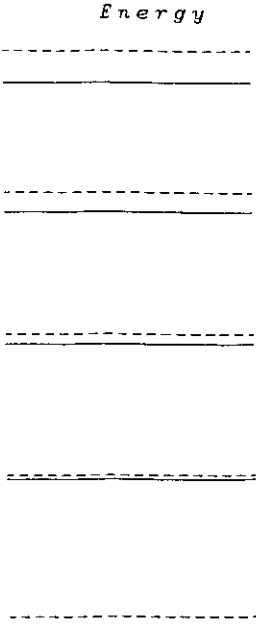


Figure 1. Comparison between the asymptotic spectrum (2.6, 2.7) and the harmonic oscillator spectrum (2.4). The energies are in units of $\hbar\omega$. The Mathieu spectrum is marked by the solid line and the dashed line denotes the harmonic oscillator spectrum. Note that the ground state energies for the asymptotic Mathieu Hamiltonian and the harmonic oscillator are practically the same and therefore a single dashed line has been used to show the coincidence of the two lines.

Except for the multiplying factor π^2 the parameter ξ is the square of the ratio of two characteristic lengths of the system. The first is $\lambda = \sqrt{\hbar/m\omega}$ which is the amplitude of the corresponding classical harmonic oscillator with a single quantum of the quantum mechanical oscillator. The second is the periodic length L of the ring. Following the method of [8], we can now write from (2.1) the energy eigenvalues as represented by

$$\mathcal{E}_n = \mathcal{E}_n^{\text{ho}} - \hbar\omega \sum_{k=1}^{\infty} G_k^m \xi^k. \tag{2.6}$$

We find the first few terms G in the expansion (2.6) to be

$$\begin{aligned} G_1^n &= \frac{(n + \frac{1}{2})^2}{4} \\ G_2^n &= \frac{(n + \frac{1}{2})[(n + \frac{1}{2})^2 + \frac{3}{4}]}{16} \\ G_3^n &= \frac{80(n + \frac{1}{2})^4 + 136(n + \frac{1}{2})^2 + 9}{2^{10}}. \end{aligned} \tag{2.7}$$

Figure 1 shows the harmonic oscillator limit of the spectrum along with the corrections we have obtained. One notices that the Mathieu spectrum starts out approximately equidistant like the harmonic oscillator spectrum but the higher energy levels become more closely spaced. It appears that the dominant correction to the oscillator potential coming from the Mathieu cosine potential is proportional to $-x^4$, and tends to flatten the harmonic oscillator potential and thus make the energy levels more closely spaced.

We now address the *eigenfunctions* through our comparative analysis. The eigenfunctions fall into two categories: even and odd. In terms of an expansion in powers of ξ (2.5) these eigenfunctions are

$$\begin{aligned}
 C e_{2n}(\phi, \xi) &= C \left[y_0^{(2n)} + \xi \frac{y_1^{(2n)}}{2} + \xi^2 \frac{y_2^{(2n)}}{4} + \dots \right] \\
 S e_{2n+2}(\phi, \xi) &= C \left[y_0^{(2n+1)} + \xi \frac{y_1^{(2n+1)}}{2} + \xi^2 \frac{y_2^{(2n+1)}}{4} + \dots \right]
 \end{aligned}
 \tag{2.8}$$

where

$$\begin{aligned}
 y_0^{(n)} &= H_n \\
 y_1^{(n)} &= -\frac{H_{n+4}}{16} - \frac{H_{n+2}}{4} - \frac{n(n-1)H_{n-2}}{4} - \frac{n(n-1)(n-2)(n-3)H_{n-4}}{16} \\
 y_2^{(n)} &= \frac{H_{n+8}}{512} + \frac{H_{n+6}}{64} - \frac{(n+2)H_{n+4}}{16} + \frac{(n^2-25n+16)H_{n+2}}{64} \\
 &\quad + \frac{n(n-1)(-n^2-27n+10)H_{n-2}}{64} + \frac{n(n-1)^2(n-2)(n-3)H_{n-4}}{16} \\
 &\quad - \frac{n(n-1)(n-2)(n-3)(n-4)(n-5)H_{n-6}}{64} \\
 &\quad + \frac{n(n-1)(n-2)(n-3)(n-4)(n-5)(n-6)(n-7)H_{n-8}}{512}
 \end{aligned}
 \tag{2.9}$$

where the H_n , having the dimensionless length $\eta = \sqrt{2}x/\lambda$ as their argument are the Hermite functions, which are the eigenfunctions for the harmonic oscillator, and C in the RHS of (2.8) is a normalization constant. The above expansion can be shown [8] to be good only for the first excited states, i.e. those whose spatial extent compared to λ is much smaller than the ratio of the characteristic lengths L/λ . In the limit of large L/λ we thus see that we obtain the harmonic oscillator wavefunctions as the first term in the asymptotic expansion (2.8, 2.9). The ground state and first excited wavefunctions are given by

$$\begin{aligned}
 C e_0(x) &= C e^{-x^2/2\lambda^2} \\
 S e_2(x) &= C(2)^{1/2}(x/\lambda)e^{-x^2/2\lambda^2}.
 \end{aligned}
 \tag{2.10}$$

Figure 2(a) shows the actual harmonic oscillator wavefunctions for the ground and first excited states as well as the first-order corrections due to finite L/λ . Specifically, L/λ has been taken to be equal to 15. For comparison, we show in figure 2(b) the actual oscillator wavefunctions alongside the Mathieu wavefunctions when $L/\lambda \ll 10$ so that one is far away from the harmonic oscillator limit. In particular s has been taken to be equal to 5 i.e. $L/\lambda = 4.698$. One thus finds that in the harmonic oscillator limit, the close similarity between the first few eigenfunctions of the Mathieu Hamiltonian and the harmonic oscillator wavefunctions parallels the similar nature of the first few energy lines displayed in figure 1. However from figure 2(b) one notices that especially for the first excited states, the departure of the Mathieu eigenfunctions from the exact harmonic oscillator wavefunctions is quite enormous.

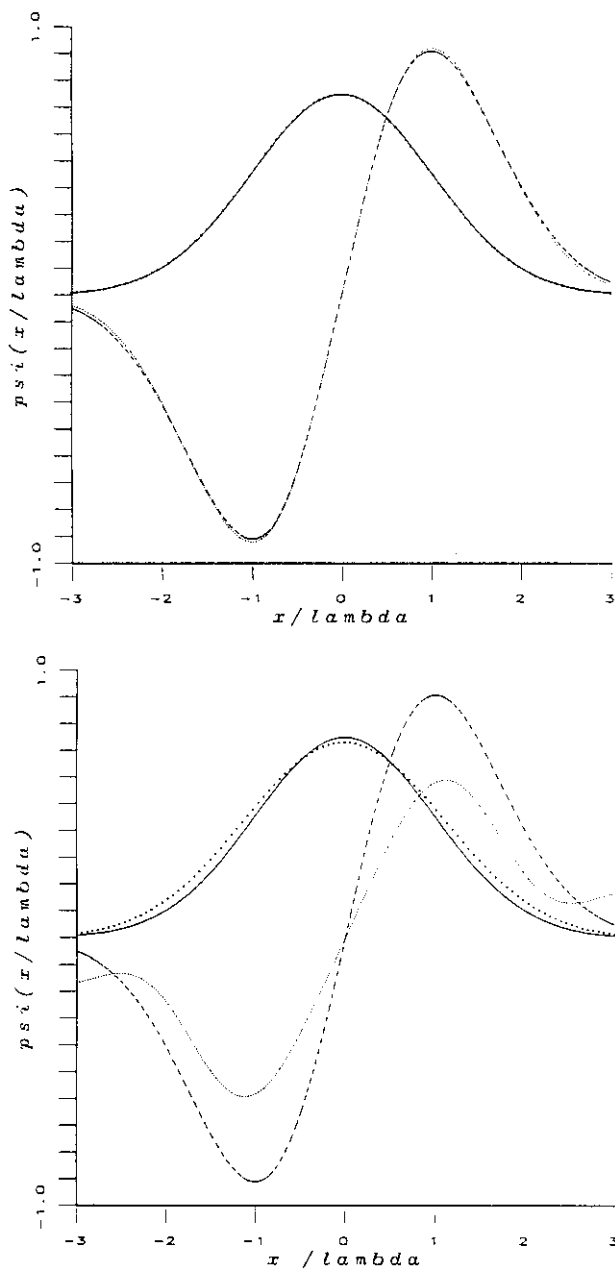


Figure 2. (a) Comparison between the asymptotic Mathieu wavefunctions and the harmonic oscillator wavefunctions for the ground and first excited states. L/λ has been taken to be equal to 15. The solid line shows the ground state Mathieu wavefunction and the line marked by bold dots gives the corresponding harmonic oscillator wavefunction, whereas the line with fine dots and the line with dashes mark the first excited state wavefunctions of the asymptotic Mathieu and the harmonic oscillator Hamiltonians respectively. (b) Comparison between the Mathieu wavefunctions and the harmonic oscillator wavefunctions for the ground and first excited states. s has been taken to be equal to five, i.e. $L/\lambda = 4.698$. The solid line shows the ground state Mathieu wavefunction, the line marked by bold dots gives the corresponding harmonic oscillator wavefunction, and the line marked by fine dots and the dashed line denote the first excited states of the Mathieu and harmonic oscillator Hamiltonians respectively.

3. Perturbations

We now present some calculations relevant to the situation in which a perturbation is added to the sinusoidal potential. This is analogous to applying a Hamiltonian perturbation linear in the displacement to the harmonic oscillator potential. Using a generalization of such an addition given earlier [12] in anharmonic contexts, the equation of motion can be obtained as

$$-\frac{\hbar^2}{2m} \frac{d^2 \tilde{\psi}}{dx^2} + \frac{m\omega^2 L^2}{4\pi^2} \left(1 - \cos \frac{2\pi x}{L}\right) \tilde{\psi} - \frac{V_1 L}{2\pi} \sin \frac{2\pi x}{L} \tilde{\psi} + (V_1 - m\omega^2) \frac{L^2}{4\pi^2} \tilde{\psi} = E \tilde{\psi} \quad (3.1)$$

which can be written as

$$-\frac{\hbar^2}{2m} \frac{d^2 \tilde{\psi}}{dx^2} + \frac{m\tilde{\omega}^2 L^2}{4\pi^2} \left(1 - \cos \frac{2\pi(x - \Delta)}{L}\right) \tilde{\psi} = \tilde{E} \tilde{\psi} \quad (3.2)$$

where the shift along the ring is Δ and the magnitude of the potential shift is such that in the harmonic oscillator limit, the strength of the shift is V_1 , and

$$\tilde{\omega} = \omega \left[1 + \frac{4V_1^2 \pi^2}{m^2 L^2 \omega^4}\right]^{1/4} \quad \tan\left(\frac{2\pi \Delta}{L}\right) = \frac{2\pi V_1}{m\omega^2 L}. \quad (3.3)$$

The Mathieu equation for the shifted potential then is of the form

$$\frac{d^2 \tilde{\psi}}{d\phi^2} + \left(\tilde{b} - \frac{\tilde{s}}{2}\right) \tilde{\psi} + \frac{\tilde{s}}{2} \cos 2(\phi - \phi_0) \tilde{\psi} = 0 \quad (3.4)$$

where

$$\tilde{b} = \frac{2m\tilde{E}L^2}{\hbar^2 \pi^2} \quad \tilde{s} = \frac{m^2 \tilde{\omega}^2 L^4}{\hbar^2 \pi^4} \quad \phi_0 = \frac{\pi \Delta}{L} \quad (3.5)$$

and can be solved immediately by comparison to (2.2)–(2.4).

We can consider the Mathieu equations (2.2, 3.4) as eigenvalue problems with the solutions, $Ce(s, \phi)$, $Se(s, \phi)$ and $Ce(\tilde{s}, \phi - \phi_0)$, $Se(\tilde{s}, \phi - \phi_0)$ respectively, being looked upon as their eigenfunctions with respective eigenvalues $s/2 - be$, $s/2 - bo$ and $\tilde{s}/2 - \tilde{b}e$, $\tilde{s}/2 - \tilde{b}o$.

Let H_0 and $\psi_n(s, \phi)$ denote the Hamiltonian and the wavefunctions corresponding to equations (2.1) and (2.2) and let H and $\tilde{\psi}_n(\tilde{s}, \phi - \phi_0)$ label the Hamiltonian and wavefunctions corresponding to equations (3.1) and (3.2). Then if the system is placed initially in some eigenstate of the original Hamiltonian, ψ_n , the wavefunction will evolve under the action of the Hamiltonian H

$$\psi(\tilde{s}, \phi, t) = e^{-iHt/\hbar} \psi(s, \phi) \quad (3.6)$$

equivalently expressed as

$$\psi(\phi, t) = \sum_m f_{mn} e^{-i(\tilde{s}/2 - \tilde{b}_m)t/\hbar} \tilde{\psi}_m(\tilde{s}, \phi - \phi_0) \quad (3.7)$$

where the overlap integral is

$$f_{mn} = \int_0^{2\pi} d\phi \tilde{\psi}_m^*(\tilde{s}, \phi - \phi_0) \psi_n(s, \phi) \tag{3.8}$$

and the eigenstates have been normalized according to

$$\int_0^{2\pi} d\phi \tilde{\psi}_m^* \tilde{\psi}_n = 2\pi \delta_{mn} \quad \int_0^{2\pi} d\phi \psi_m^* \psi_n = 2\pi \delta_{mn}. \tag{3.9}$$

The probability that the system will be found at time t in an eigenstate ψ_p of the original Hamiltonian is given by

$$P_{pn}(t) = \left| \sum_m f_{mn} f_{pm}^* e^{-i(s/2 - \tilde{h}m)t/\hbar} \right|^2. \tag{3.10}$$

The eigenstate $\psi_n(\phi, s)$ can be written as an infinite sum of cosines or sines according to whether the eigenstate is even or odd. We can then write the following expressions for the overlap integral f_{mn} :

(i) m even, n even: $f_{mn} = \sum_k A_{2k}^{(n)}(s) \tilde{A}_{2k}^{(m)}(\tilde{s}) \cos 2k\phi_0$ (3.11)

(ii) m odd, n even: $f_{mn} = - \sum_k A_{2k}^{(n)}(s) \tilde{B}_{2k}^{(m)}(\tilde{s}) \sin 2k\phi_0$ (3.12)

(iii) m even, n odd: $f_{mn} = - \sum_k B_{2k}^{(n)}(s) \tilde{A}_{2k}^{(m)}(\tilde{s}) \sin 2k\phi_0$ (3.13)

(iv) m odd, n odd: $f_{mn} = \sum_k B_{2k}^{(n)}(s) \tilde{B}_{2k}^{(m)}(\tilde{s}) \cos 2k\phi_0.$ (3.14)

Figures 3(a) and (b) shows the self-propagators and transition probabilities for $s = 5$ and $\phi_0 = 0.3$. One sees that the ground state propagator exhibits ringing much like what one would see in a non-degenerate two-state system. The behaviour exhibited by the self-propagators for the first and second excited states has, on the other hand, far more structure. This suggests that these states are connected to the rest of the manifold in a more complicated way than the ground state. This may be for the following reason. In the case of the harmonic oscillator the behaviour of the ground state under the action of a linear perturbation is qualitatively different from the excited states because the ground state is a coherent state. In the present rotational case, a similar thing could be occurring. The ground state could be acting as a ‘coherent state’ for this problem, making its behaviour completely different from that of the other states both in the case of the propagators and the transition probabilities. The probability of transition from the ground to the first excited states is similar to the behaviour one could expect between the states of a non-degenerate two-state system, but the behaviour of the probability of transition from the first to second excited states is very different.

In figure 4 we display the same quantities as in figure 3 but here we take the Mathieu Hamiltonian to be in the harmonic oscillator limit and compare it with the exact oscillator Hamiltonian. We find that the different probabilities approach the behaviour of the harmonic oscillator.

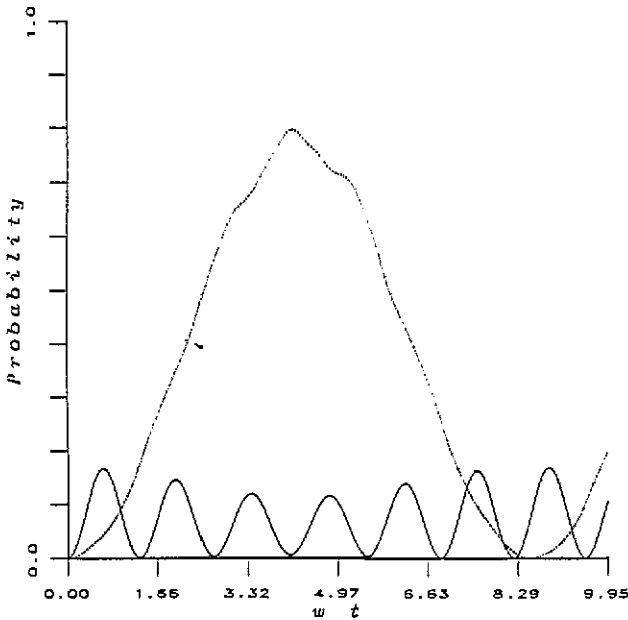
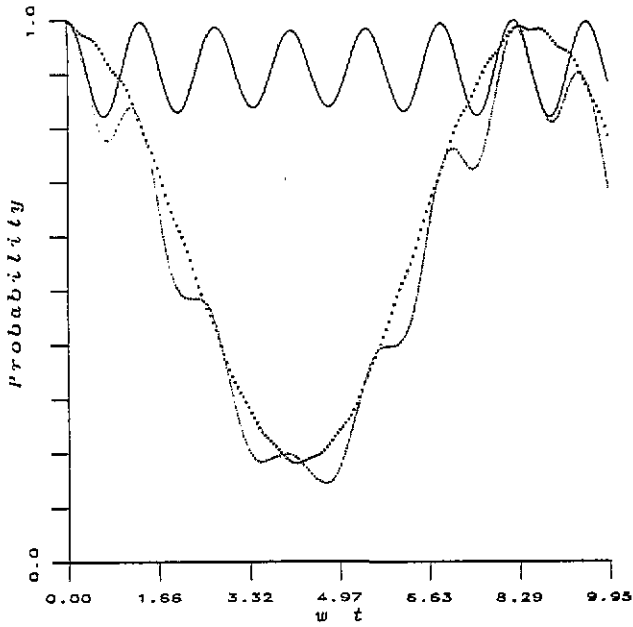


Figure 3. (a) Self propagators for the Mathieu Hamiltonian when $L/\lambda \ll 10$. In particular, s and ϕ_0 given in (3.5) are taken to be five and 0.3 respectively. The solid line gives the self-propagator for the ground state, whereas the dotted line and line marked with bold dots give the propagators for the first and second excited states respectively. (b) Transition probabilities for the same case. The solid line marks the transition probability between the ground and first excited states and the dotted line denotes the observable between the first and second excited states.

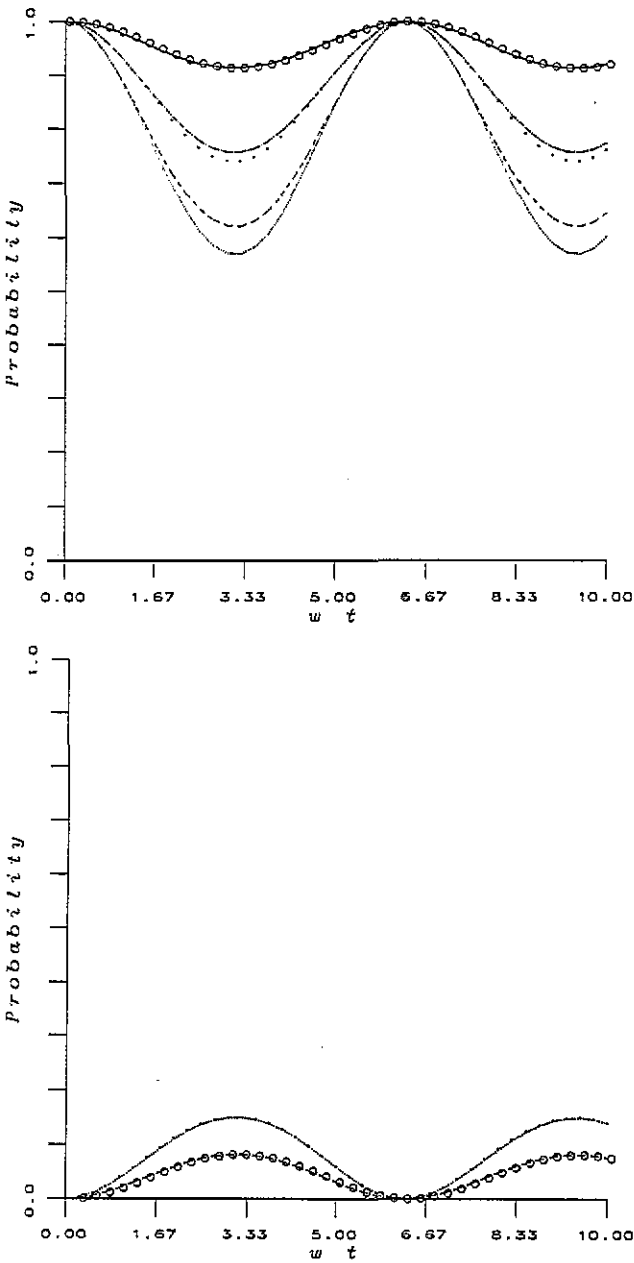


Figure 4. (a) Comparison of the self-propagators for the first three states between the Mathieu functions in the harmonic oscillator limit and the actual harmonic oscillator states. The solid line, the line marked by dots and dashes and the line with fine dots denote the propagators for the ground, first and excited states of the asymptotic Mathieu Hamiltonian respectively whereas the lines marked by circles, bold dots and light, fine dots denote the corresponding quantities for the harmonic oscillator. (b) Comparison of the transition probabilities between the states of the Mathieu problem in the harmonic oscillator limit and the exact harmonic oscillator problem. The bold dots and dotted line denote the transition probabilities between the ground and first excited states and between the first and second excited states of the asymptotic Mathieu Hamiltonian respectively whereas the line marked by circles and the dashed line denote the corresponding quantities for the harmonic oscillator Hamiltonian.

4. Concluding remarks

We have analysed the problem of a single oscillator bound by a sinusoidal potential on a ring and have explored its relation to the problem of a quantum mechanical harmonic oscillator. We have shown that the Mathieu Hamiltonian approaches its harmonic oscillator limit smoothly in the behaviour of the spectrum, the shape of the wavefunctions and the evolution of transitions between the states of the Hamiltonian on application of a perturbation. With this as a starting point, work on incorporating an interaction of a quantum mechanical excitation with the oscillator studied here is currently under way with applications to rotational polarons and liquid crystals. A few comments concerning the physical significance of the system might be relevant. Liquid crystals consist of partially ordered aggregates of molecules possessing directed shapes such as rods or discs [7]. A rod-like molecule can perform oscillations around its equilibrium direction. If an electronic excitation or an electron interacts strongly with this oscillation such that the presence of the excitation or charge affects the equilibrium direction of the molecule, the composite system is a rotational polaron.

The transport of the excitation or charge will be significantly affected [5] as a result of the strong attraction. Because the oscillation coordinate possesses a limited range (since it is an angle rather than a translational coordinate) novel physical effects such as saturation of non-linearity can occur. The present paper constitutes a beginning step in a fully quantum mechanical study of such phenomena.

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