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LETTER TO THE EDITOR

Zero-eigenenergy state of the Aubry model

K A Chao

Department of Physics and Measurement Technology, University of Linköping, S-58183 Linköping, Sweden

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Abstract. The Aubry model with site energy $V\cos(Qn+\varphi)$ is analysed. We have proved that the zero-eigenenergy state (ZES) exists only if the system contains an odd number of sites and if $\varphi = \pm\frac{1}{2}\pi$. The eigenfunction of the ZES has a definite symmetry. In the vicinity of the critical value $V=2$, the characteristic features of this wavefunction have been demonstrated.

The one-dimensional Aubry Hamiltonian (Aubry 1978)

$$H(Q,\varphi)=\sum_{n=-\infty}^{\infty}[V\cos(Qn+\varphi)a_n^\dagger a_n+t(a_{n+1}^\dagger a_n+a_{n-1}^\dagger a_n)] \tag{1}$$

contains two incommensurate periods when Q is incommensurate to π. Though some important aspects of the model are well understood, this is not so for the zero-eigenenergy state (ZES) of $H(Q,\varphi)$. Recently the ZES has been investigated by several authors (Bulka 1981, Avron and Simon 1982, Sokoloff 1984, Ostlund and Pandit 1984, Zdetsis *et al* 1986, Liu 1987) with various approaches. However, the characteristic features of the ZES still remain unclear. Since it is difficult to derive the eigenfunction of the ZES analytically, one must turn to a numerical solution. However, boundary conditions cannot be imposed on a system with incommensurate periods. Therefore, in principle one must consider an infinite system, which is of course an impossible task. Almost every author believes that his numerical study on the ZES is reliable if the system he considers is sufficiently long. In this letter we will first show that the ZES exists only if the phase φ is properly chosen so that the Hamiltonian $H(Q,\varphi)$ has the required symmetry. Otherwise the ZES does not exist at all, regardless of the size of the system. With the correct choice of the phase φ, the eigenfunction of the ZES will then be derived.

Let us first study the role of the phase φ. The eigenenergy $E(Q,\varphi)$ of the Hamiltonian $H(Q,\varphi)$ is obtained by solving the determinantal equation

$$\begin{vmatrix} \ddots & & & & \\ t & V\cos(-Q+\varphi)-E(Q,\varphi) & t & & \\ & t & V\cos(\varphi)-E(Q,\varphi) & t & \\ & & t & V\cos(Q+\varphi)-E(Q,\varphi) & t \\ & & & & \ddots \end{vmatrix}=0. \tag{2}$$

Here the rows and columns are labelled from $-\infty$ to $+\infty$ according to the value of n. First we multiply the 2μth row and the $(2\mu+1)$th column by -1, where $\mu = -\infty, \ldots, -1, 0, 1, \ldots, \infty$. Next we exchange the νth row with the $-\nu$th row, as well as the νth column with the $-\nu$th column, where $\nu = 1, 2, \ldots, \infty$. Then (2) becomes

$$\begin{vmatrix} \ddots & & & & \\ & t-V\cos(Q+\varphi)+E(Q,\varphi) & t & & \\ & t & -V\cos(\varphi)+E(Q,\varphi) & t & \\ & & t & -V\cos(-Q+\varphi)+E(Q,\varphi) & t \\ & & & & \ddots \end{vmatrix} = 0. \qquad (3)$$

Equations (2) and (3) have the same set of eigenenergies. If the ZES exists, then (2) and (3) can be expanded in powers of t/V as $\Sigma_{\mu=0}^{\infty} X_\mu(Q,\varphi)(t/V)^\mu = 0$ and $\Sigma_{\mu=0}^{\infty} X_\mu(-Q,\varphi)(-t/V)^\mu = 0$, respectively. Since the value of t/V is arbitrary, we have the condition $X_\mu(Q,\varphi) \equiv (-1)^\mu X_\mu(-Q,\varphi)$. The explicit form of $X_\mu(Q,\varphi)$ is very tedious. However, it can be shown that the above condition implies that, for $E(Q,\varphi)=0$ and t/V arbitrary, the two determinants in (2) and (3) are identical. Since the dimensions of both determinants are infinite, we can set $n=0$ at any diagonal element in (2) and set $n=0$ at any other diagonal element in (3). Consequently, if the ZES exists, the necessary condition is

$$V\cos(-nQ+\varphi) = -V\cos[(n-p)Q+\varphi] \qquad (4)$$

where p is an arbitrary integer. Therefore φ can only take the values

$$\varphi_0 = \tfrac{1}{2}pQ \pm \tfrac{1}{2}\pi. \qquad (5)$$

By a shift of the origin $n=0$, it is easy to see that the Hamiltonian (1) associated with any even p is equivalent to the Hamiltonian with $\varphi_0 = -\frac{1}{2}\pi$, and the Hamiltonian associated with any odd p is equivalent to the Hamiltonian with $\varphi_0 = -\frac{1}{2}\pi - \frac{1}{2}Q$. For $\varphi_0 = -\frac{1}{2}\pi$, the Hamiltonian can be rewritten as

$$\begin{aligned} H(Q,-\tfrac{1}{2}\pi) = {} & E_0 a_0^\dagger a_0 + t(a_0^\dagger a_1 + a_1^\dagger a_0 + a_0^\dagger a_{-1} + a_{-1}^\dagger a_0) \\ & + \sum_{n=1}^{\infty} [V\sin(Qn)(a_n^\dagger a_n - a_{-n}^\dagger a_{-n}) \\ & + t(a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1} + a_{-n-1}^\dagger a_{-n} + a_{-n}^\dagger a_{-n-1})] \end{aligned} \qquad (6)$$

where $E_0 = 0$. On the other hand, for $\varphi_0 = -\frac{1}{2}\pi - \frac{1}{2}Q$ we have

$$\begin{aligned} H(Q,-\tfrac{1}{2}\pi-\tfrac{1}{2}Q) = {} & \sum_{n=1}^{\infty} \{V\sin[(n-\tfrac{1}{2})Q]a_n^\dagger a_n + t(a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n)\} \\ & + t(a_m^\dagger a_1 + a_1^\dagger a_m)|_{m=0} \\ & + \sum_{m=0}^{-\infty} \{V\sin[(m-\tfrac{1}{2})Q]a_m^\dagger a_m + t(a_m^\dagger a_{m-1} + a_{m-1}^\dagger a_m)\}. \end{aligned} \qquad (7)$$

For those sites with site indices $m \leqslant 0$, we redefine the old mth site as the new $(m-1)$th site. Hence, the sites are now labelled as $n = -\infty, \ldots, -2, -1, 1, 2, \ldots, \infty$. Equation (7) is then re-expressed as

$$\begin{aligned} H(Q,-\tfrac{1}{2}\pi-\tfrac{1}{2}Q) = {} & t(a_{-1}^\dagger a_1 + a_1^\dagger a_{-1}) + \sum_{n=1}^{\infty} \{V\sin[Q(n-\tfrac{1}{2})](a_n^\dagger a_n - a_{-n}^\dagger a_{-n}) \\ & + t(a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1} + a_{-n-1}^\dagger a_{-n} + a_{-n}^\dagger a_{-n-1})\}. \end{aligned} \qquad (8)$$

Under the condition (4), we see from (2) and (3) that if $E(Q, \varphi_0)$ is an eigenenergy of $H(Q, \varphi_0)$, then $-E(Q, \varphi_0)$ is also an eigenenergy of $H(Q, \varphi_0)$. If $\varphi_0 = -\frac{1}{2}\pi$, the corresponding Hamiltonian (6) has an odd number of sites. Therefore, the total number of eigenenergies is odd and the ZES must exist. On the other hand, if $\varphi_0 = -\frac{1}{2}\pi - \frac{1}{2}Q$, the corresponding Hamiltonian (8) has an even number of sites. In this case, if the energy spectrum contains the zero eigenenergy then the zero eigenenergy must be at least doubly degenerate. However, the Hamiltonian (8) does not have the symmetry to cause such degeneracy. Consequently, the Hamiltonian (8) does not have the ZES. We have also performed a detailed numerical calculation to confirm this conclusion.

To summarise the above analysis, the necessary and sufficient condition for the existence of the ZES is $\varphi_0 = -\frac{1}{2}\pi$ in a system with an odd number of sites. The requirement of an odd number of sites is a topological condition and cannot be removed even if the number of sites approaches infinity. It is important to point out that this condition applies to any value of the ratio V/t.

Now we assume that the above-mentioned condition is satisfied and study the wavefunction of the ZES of (6). The eigenstate of $H(Q, -\frac{1}{2}\pi)$ can be created by the operator

$$A(E)^\dagger = \sum_{n=-\infty}^{\infty} f(E)_n a_n^\dagger \tag{9}$$

where the set of coefficients $\{f(E)_n\}$ satisfies the recursion relation

$$f(E)_{n+1} = [(V/t)\sin(Qn) - E]f(E)_n - f(E)_{n-1}. \tag{10}$$

For $E=0$, we have $f(0)_1 = -f(0)_{-1}$ and $f(0)_2 = f(0)_{-2} = [(V/t)\sin Q]f(0)_1 - f(0)_0$. It can be easily proved by mathematical induction that

$$f(0)_{2n} = f(0)_{-2n} = \{(V/t)\sin[(2n-1)Q]\}f(0)_{2n-1} - f(0)_{2n-2} \tag{11}$$

$$f(0)_{2n+1} = -f(0)_{-2n-1} = [(V/t)\sin(2nQ)]f(0)_{2n} - f(0)_{2n-1}. \tag{12}$$

These symmetry properties of the ZES wavefunction have been used to check the accuracy of the following numerical results.

To demonstrate the ZES wavefunction numerically, we set $t=1$ as our unit of energy. Because of the symmetry relations (11) and (12), we only need to show half of the wavefunction in the region $n \leq 0$. Since the interesting region is around the critical value $V/t = 2$, we will study three cases with $V = 1.99$, 2.0 and 2.01. For each value of V, we consider three values of $Q = 0.8$, 2.0 and 2.9.

Figure 1 shows the wavefunctions for $Q = 0.8$ in a finite system of 3001 sites. If we increase the size of the system, all wavefunctions retain their qualitative features. The insert for the case $V = 2.01$ illustrates the wavefunction around $n = 0$ in a large system of 100 001 sites.

Similar results for $Q = 2.0$, obtained with a system of 3001 sites, are plotted in figure 2. When we increase the size of the system, the characteristic features of the wavefunctions for $V = 1.99$ and $V = 2.0$ remain the same. However, there is a drastic change of the wavefunction for $V = 2.01$. The insert shows the wavefunction in the region $-5000 < n < 0$ in a system of 100 001 sites. Further increase of the size of the system does not alter the wavefunction qualitatively.

The most interesting case is shown in figure 3 for $Q = 2.9$. The plotted wavefunctions for $V = 1.99$ and $V = 2.0$ are derived with a system of 1001 sites. These two wavefunctions are similar and do not change their forms when the size of the system is increased.

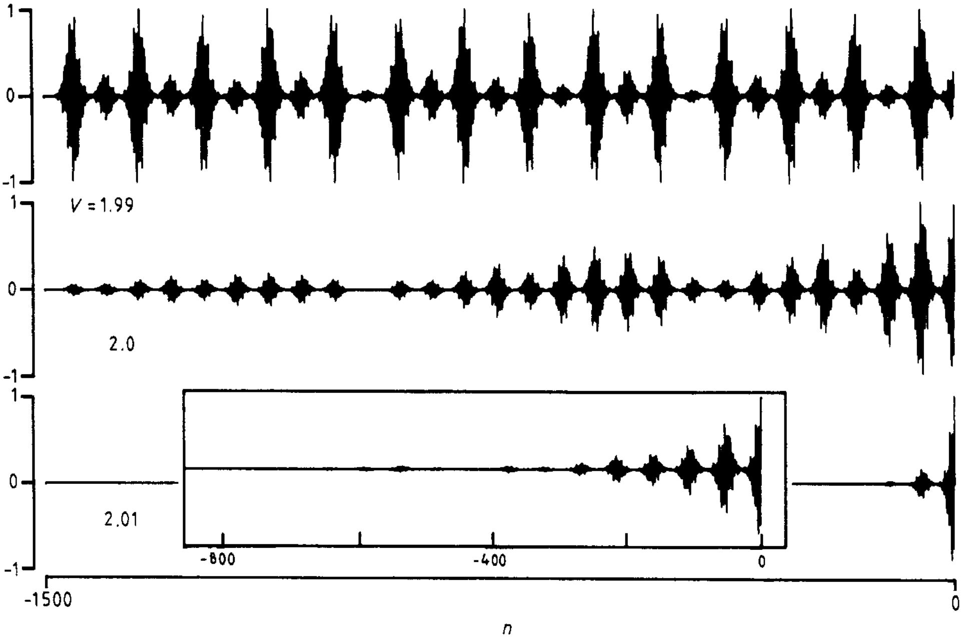

Figure 1. Wavefunctions for $Q = 0.8$ in a system of 3001 sites. The insert shows part of a wavefunction in a system of 100 001 sites.

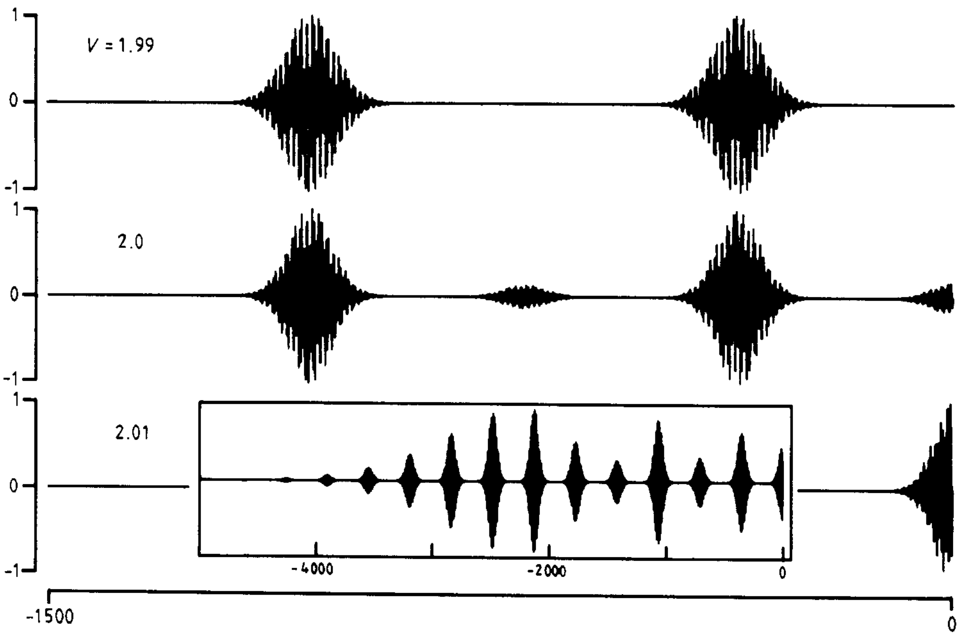

Figure 2. Wavefunctions for $Q = 2.0$ in a system of 3001 sites. The insert shows part of a wavefunction in a system of 100 001 sites.

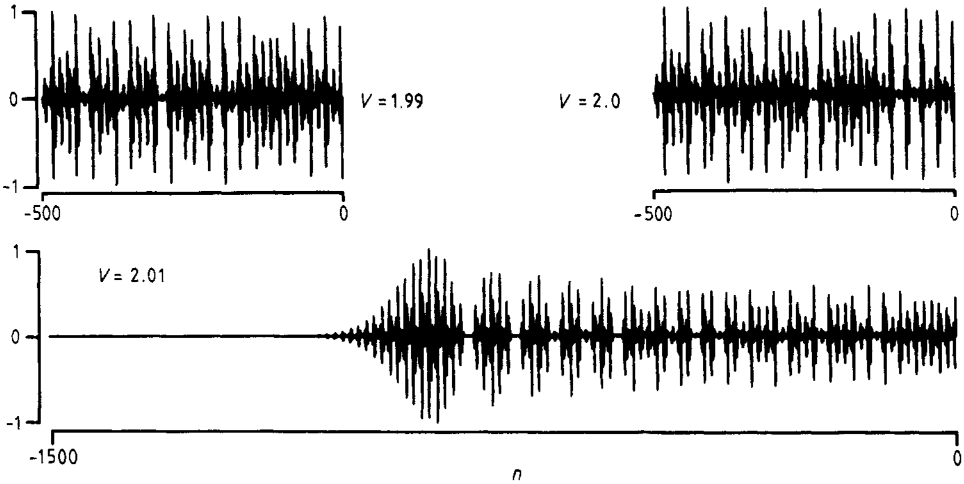

Figure 3. Wavefunctions for $Q = 2.9$ in a system of 1001 sites (for $V = 1.99$ and $V = 2.0$) and in a system of 3001 sites (for $V = 2.01$).

In a system of 1001 sites, the wavefunction for $V = 2.01$ is also similar to those plotted for $V = 1.99$ and $V = 2.0$. But with increasing size of the system, the wavefunction for $V = 2.01$ begins to localise around the middle of the system. For a system of 3001 sites, the localised wavefunction is shown in figure 3.

Before closing this letter, we would like to make two remarks. First, Sokoloff (1984) has argued that the ZES must exist even for the phase $\varphi = 0$, because the energy band is symmetric about $E = 0$. We have shown here that such an argument is incorrect. To study the ZES, one must consider a system with an odd number of sites and set $\varphi = -\frac{1}{2}\pi$. Second, Ostlund and Pandit (1984) detected the strange influence of the phase φ on the divergence of the transfer matrix elements which they could not explain. The present work suggests that the phase φ plays a role in the symmetry property of the whole system.

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