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LETTER TO THE EDITOR

The quantum harmonic oscillator on a lattice

E Chalbaud†, J-P Gallinar and G Mata

Departamento de Física, Universidad Simón Bolívar, Apartado 80659, Caracas 1080, Venezuela

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Abstract. We find the eigenvalue spectrum of a particle constrained to 'hop' between the sites of a simple cubic lattice in the presence of a spherically symmetric 'harmonic oscillator' potential. The eigenfunctions are found to be given in terms of the periodic Mathieu functions of period π. At low kinetic energies of hopping the solutions differ considerably from those of the continuum theory: the particle localises itself in a given shell around the origin and the virial theorem is thereby violated. At high kinetic energies we obtain the usual equidistant levels of the harmonic oscillator on the continuous manifold. We discuss in some detail the spectrum of the three-dimensional case and the associated degeneracies. It is seen that the well known accidental degeneracy of the harmonic oscillator wavefunctions is only partially lifted by the discretisation of space. Finally, mention is also made of the relevance of our solution to the physical problem of the inversion layer at the surface of a semiconductor when it is doped with a spatially constant electric charge density.

In a recent contribution to this journal, Gallinar and Mattis (1985) obtained an analytical solution, in terms of Bessel functions, for the eigenvalue spectrum of a particle constrained to 'hop' on a lattice (a 'Wannier' particle) when subjected to a constant force, i.e. subjected to a linear or piecewise linear potential (see the review by Mattis (1986)). Their solution is relevant to the problem of the inversion layer near the surface of a semiconductor in the presence of a constant electric field, or in the variously defined particles of lattice gauge theories (Kogut 1979). The following question then naturally arises. Are there any other privileged potentials on a 'lattice' for which an analytical solution in terms of known functions is also possible? Non-trivial analytical solutions in physics are so few in number, and are also so desirable, that a quest for them is clearly far from being an idle undertaking.

In this letter we point out another such special—and important—solution. This is the solution to what may be called a quantum harmonic oscillator defined on the points of a simple cubic lattice. Thus, we shall take as our Hamiltonian $\mathscr{H}$ the following:

$$\mathscr{H} = -A \sum_j [\exp(\mathrm{i}ap_j) + \exp(-\mathrm{i}ap_j)] + \tfrac{1}{2}k \sum_j x_j^2 \tag{1}$$

where $p_j = -\mathrm{i}\,\partial/\partial x_j$, j runs over the d dimensions of the simple cubic lattice, a is the lattice constant and x_j is the jth component of the position vector of the Wannier particle. The operators $\exp(\pm \mathrm{i}ap_j)$ in (1) generate finite lattice translations of the particle (the 'hops') with lattice constant a. In expression (1), $A \geqslant 0$ is the usual tight-binding matrix element for the 'hopping' of the Wannier particle and, finally, k measures the strength of the 'spring' of the oscillator.

† Presently on sabbatical leave at: Department of Physics, New York University, New York, NY 10003, USA.

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It might seem inappropriate to use a continuum Hamiltonian such as (1) for a particle in a lattice. However, for the present problem it is easier to solve the continuum form (1) and then project onto the discrete Hilbert subspace in which $(x_j/a) \equiv n_j$ takes on integer values n_j *only*. By so restricting the Hilbert space of (1) to wavefunctions localised at the lattice points, the appropriate spectrum is thereby obtained.

The problem posed by (1) has been briefly outlined by Mattis (1986) in his recent review on 'The Few-Body Problem on a Lattice'. As pointed out by him, in one dimension (i.e. for $d = 1$) the spectrum of $\mathcal{H}$ is related to the eigenvalue spectrum of the inversion layer at the surface of a semiconductor, when the electrons or holes there 'hop' in a region of constant electric charge density. This constant charge density gives rise to a potential V that varies as $V \propto x^2$, where $x = na \geq 0$ is the perpendicular distance from the surface of the semiconductor, with n an integer that labels the plane indices and with a being the lattice constant or distance between the planes that are parallel to the surface. The presence of this last one at $x = 0$ forces the wavefunction to vanish for $x \leq 0$, and makes it natural to choose the odd-parity eigenfunctions of (1) as the appropriate physical solutions to the problem of the inversion layer. Aside from this relevant physical application to semiconductor physics, what makes (1) uniquely interesting from a mathematical viewpoint is its exact analytical solvability by separation of variables, for any d. For it must be stressed that the linear potential ($V \propto r$), or the Coulomb potential ($V \propto r^{-1}$), for example, *cannot* be so separated on the lattice if $d > 1$. This is, of course, in sharp contrast with the separability of the same potentials on the continuous manifold. For these non-separable potentials one may wish to resort to Bethe lattice constructs to obtain analytical results when $d > 1$ (Gallinar 1984).

Let us turn now to the solution of (1) by separation of variables. We first set $d = 1$ and find that the eigenvalue equation $\mathcal{H}|\Psi\rangle = E|\Psi\rangle$ may be readily solved by writing it in the momentum or p representation, with $x = i\partial/\partial p$, as

$$-2A\cos(p)\Psi(p) - \frac{k}{2}\frac{d^2\Psi}{dp^2} = E\Psi(p) \tag{2}$$

or

$$\frac{d^2\Psi(v)}{dv^2} + (\alpha - 2q\cos 2v)\Psi(v) = 0 \tag{3}$$

where

$$v \equiv \tfrac{1}{2}ap \qquad q \equiv -\frac{8A}{ka^2} \qquad \alpha \equiv \frac{8E}{ka^2}.$$

Equation (3) is the canonical form of Mathieu's differential equation (Abramowitz and Stegun 1965). Since x/a has to be an integer number because the particle 'exists' only on the lattice points, the basis wavefunctions in the momentum representation will be plane waves with the periodicity $p = (2\pi/a)$ of the reciprocal lattice. Hence, of all solutions of Mathieu's equation in (3), only those periodic with period $v = ap/2 = \pi$ will be acceptable. In particular, according to well known properties, the so-called characteristic exponent of Floquet will then be zero (or an integer) to ensure the periodicity of $\Psi(v)$. The eigenfunctions $\Psi_r(v)$ of (3) shall be given, accordingly, in terms of the *Mathieu functions* $\mathrm{ce}_{2r}(v; q)$ and $\mathrm{se}_{2r}(v; q)$ (Abramowitz and Stegun 1965) as

$$\Psi_r^e(v) = N_r^e\,\mathrm{ce}_{2r}(v; q) \qquad (r = 0, 1, 2, \ldots) \tag{4}$$

for the even periodic functions of period π, and

$$\Psi_r^0(v) = N_r^0 \, \mathrm{se}_{2r}(v; q) \qquad (r = 1, 2, \ldots) \tag{5}$$

for the odd periodic functions of period π, N_r^e and N_r^0 being appropriate normalisation constants. The corresponding energy eigenvalues will be

$$E_r^e = \tfrac{1}{8}ka^2 a_{2r}(q) \qquad (r = 0, 1, 2, \ldots) \text{ (even)} \tag{6}$$

and

$$E_r^0 = \tfrac{1}{8}ka^2 b_{2r}(q) \qquad (r = 1, 2, \ldots) \text{ (odd)} \tag{7}$$

with $a_{2r}(q)$ and $b_{2r}(q)$ being the *characteristic values* of α in equation (3) for the even and odd periodic Mathieu functions of period π, respectively. The first five levels that arise from (6) and (7) are shown in figure 1 as a function of the dimensionless 'kinetic energy' parameter $2A/ka^2$. From the property $a_{2r}(0) = b_{2r}(0) = (2r)^2$ (Abramowitz and Stegun 1965), we find that for zero kinetic energy one has $E_r^e = E_r^0 = \frac{1}{2}ka^2r^2$, and the particle then 'sits' on the two rth nearest neighbours of the origin (or on the origin itself for $r = 0$), its total energy being entirely potential energy. We emphasise here

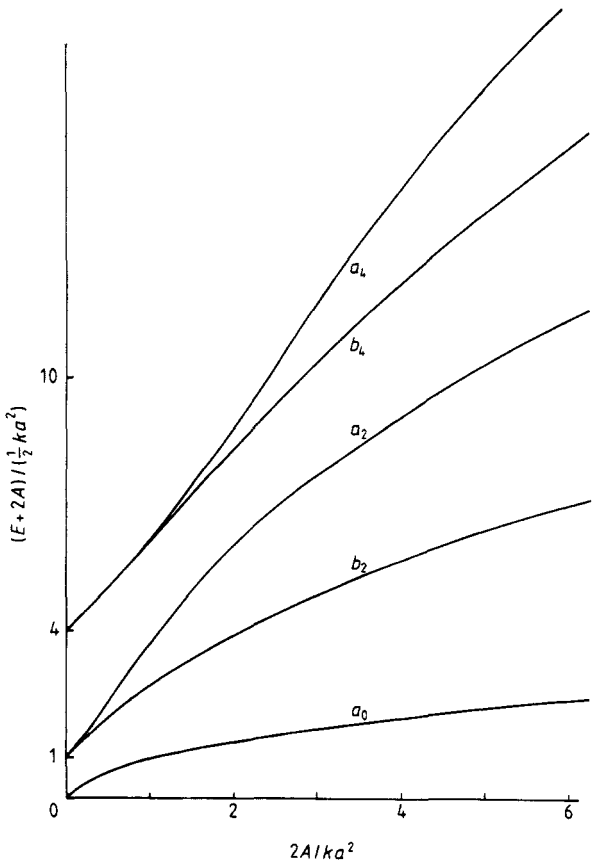

Figure 1. Plot of $(E+2A)/(\frac{1}{2}ka^2)$ against the 'kinetic energy' parameter $2A/ka^2$ for the first five levels of the one-dimensional discrete oscillator. The incipient equal spacing of the levels can already be discerned in this figure.

this result because it stands at odds (for $r \neq 0$) with what happens on the continuous manifold where, according to the virial theorem, the kinetic energy and the potential energy are equal and thus vanish simultaneously. In this same limit ($A = 0$), the wavefunctions $\mathrm{ce}_{2r}(v; 0)$ and $\mathrm{se}_{2r}(v; 0)$ in (4) and (5) behave respectively as $\cos(2rv)$ and $\sin(2rv)$, corresponding to complete delocalisation in momentum space. As A is then turned on, the double degeneracy present (for $r \neq 0$) opens up into even and odd levels, which interlace each other as shown in figure 1. In the continuum regime $|q| \to \infty$, and then we have that (Abramowitz and Stegun 1965), for either of the even or odd levels,

$$a_r \to -2|q| + 2(2r+1)(|q|)^{1/2}$$

which implies

$$E_r \to -2A + (r+\tfrac{1}{2})\left(\frac{k}{m}\right)^{1/2} \qquad (r = 0, 1, 2, \ldots). \tag{8}$$

To obtain (8) we have used the property $b_{2r}(q) \sim a_{2r-1}(q)$ for $|q| \to \infty$ and have made the natural identification $Aa^2 \equiv 1/2m$, with m being the usual mass of the particle on the continuous manifold. The continuum regime (8), characterised by equally spaced energy levels, can already be discerned in figure 1, although it is clear that for increasing quantum number r one has to go to ever higher values of the abscissa to bring this limit into evidence.

It is worthwhile remarking that, as previously argued, it is the odd eigenvalues given by (7) that yield the eigenvalues of the inversion layer problem with a constant charge density.

We consider now the wavefunctions in real space. From the Fourier expansions of the Mathieu functions (Abramowitz and Stegun 1965)

$$\mathrm{ce}_{2r}(v; q) = \sum_{m=0}^{\infty} A_{2m}^{2r}(q) \cos(2mv) \tag{9}$$

and

$$\mathrm{se}_{2r}(v; q) = \sum_{m=0}^{\infty} B_{2m}^{2r}(q) \sin(2mv) \tag{10}$$

we obtain for the even wavefunctions $\Psi_r^e(x)$, in real space, that

$$\Psi_r^e(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}p \exp(\mathrm{i}px) \Psi_r^e(p) = \frac{N_r^e}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}p \exp(\mathrm{i}px)\, \mathrm{ce}_{2r}(\tfrac{1}{2}ap; q)$$

$$= \left(\frac{\pi}{2}\right)^{1/2} N_r^e \sum_{m=-\infty}^{+\infty} A_{2m}^{2r}(q) \delta(x + ma) \qquad (r = 0, 1, 2, \ldots) \tag{11}$$

where $A_{-2m}^{2r}(q) \equiv A_{2m}^{2r}(q)$ and for the odd wavefunctions we obtain

$$\Psi_r^0(x) = -\mathrm{i}\left(\frac{\pi}{2}\right)^{1/2} N_r^0 \sum_{m=-\infty}^{+\infty} B_{2m}^{2r}(q) \delta(x + ma) \qquad (r = 1, 2, \ldots) \tag{12}$$

with $B_{-2m}^{2r}(q) = -B_{2m}^{2r}(q)$.

From (11) and (12) we see that the probability of finding the particle in the rth eigenstate at a certain lattice site m is proportional to the coefficient $|A_{2m}^{2r}(q)|^2$ for the even states and to $|B_{2m}^{2r}(q)|^2$ for the odd ones. To lowest order in q, these coefficients

are given by (Abramowitz and Stegun 1965)

$$C^r_{r+2s} = \left(\frac{(-1)^s r!\, q^s}{4^s (r+s)!\, s!}\right) C^r_r + \ldots \tag{13}$$

with $C^r_m \equiv A^r_m$ or B^r_m, $rs > 0$, and by

$$C^r_{r-2s} = \left(\frac{(r-s-1)!\, q^s}{4^s s!\,(r-1)!}\right) C^r_r + \ldots . \tag{14}$$

Also, one has

$$A^r_r(0) = B^r_r(0) = 1 \qquad (r > 0). \tag{15}$$

Thus, to lowest order in $|q| = 8A/ka^2 \ll 1$, the probability of finding the particle (which is in the rth eigenstate) at a site that is s lattice constants away from the rth lattice site decays very rapidly (from nearly one) as s increases.

In figure 2 we show *part* of the eigenvalue spectrum for $d = 3$ obtained by separation of variables. The associated eigenstates, which are the product of the one-dimensional

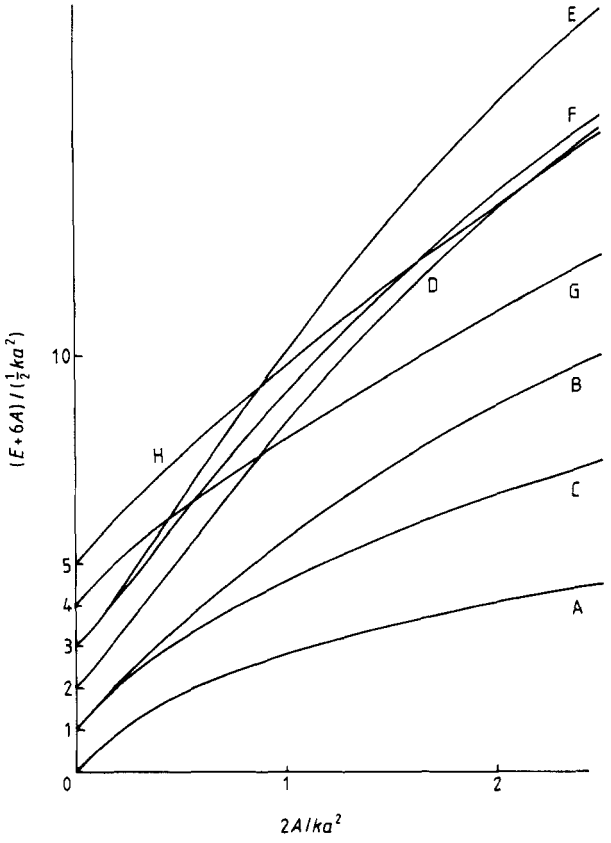

Figure 2. Plot of $(E+6A)/(\frac{1}{2}ka^2)$ against the 'kinetic energy' parameter $2A/ka^2$ for *some* of the levels of the three-dimensional discrete oscillator arising from the first six shells of the cubic lattice. The equal spacing of the continuum first six levels can also be discerned in the figure. As displayed, some of the levels of the discrete case have been omitted for visual convenience. Levels; A, $(a_0a_0a_0)$; B, $(a_0a_0a_2)$; C, $(a_0a_0b_2)$; D, $(a_0a_2a_2)$; E, $(a_2a_2b_2)$; F, $(a_2b_2b_2)$; G, $(a_0a_0b_4)$; H, $(a_0b_2b_4)$.

wavefunctions, are symbolically denoted by indicating on each curve the 1D levels from which they originate. These 3D wavefunctions are degenerate in general. As shown, the levels in figure 2 have been chosen so that all first six levels of the continuum can be seen to emerge on the right-hand side of the figure. For $q=0$, the degeneracy of the wavefunctions associated with the rth shell around the origin of the cubic lattice will be given by the number of rth nearest neighbours of the origin. This number is equal to the number of distinct integer solutions (n_x, n_y, n_z) of the Diophantine equation

$$N(r)=n_x^2+n_y^2+n_z^2=E/\tfrac{1}{2}ka^2 \tag{16}$$

where $N(r)\geqslant 0$ is an integer (function) that admits of the above decomposition. For instance, $N(r)=r$ if $0\leqslant r\leqslant 6$, $N(r)=r+1$ if $7\leqslant r\leqslant 11$, etc. The n_i $(i=x, y, z)$ can be associated with the wavefunctions ce_{2n} if n_i is positive and to the se_{2n} if n_i is negative, with $n=|n_i|$. The product wavefunction associated with (n_x, n_y, n_z) when $q=0$ will thus go over into an eigenstate of energy:

$$[2(|n_x|+|n_y|+|n_z|)+\tfrac{1}{2}(p_1+p_2+p_3)](k/m)^{1/2} \tag{17}$$

in the continuum harmonic oscillator, where p_i is the sign of n_i (zero being considered 'positive'). As can be seen from figure 2, there is considerable level crossing for $|q|\neq 0$ and different levels of the discrete case coalesce (for $|q|\to\infty$) onto a given level of the continuum oscillator, thus filling up the required degeneracy equal to $(n+1)(n+2)/2$ $(n=0, 1, 2, \ldots)$ for the nth energy level of the usual oscillator. For instance, we show in figure 2 the levels denoted by $(a_0a_2a_2)$, $(a_2b_2b_2)$ and $(a_0b_2b_4)$, which correspond to (n_x, n_y, n_z) equal to $(0, 1, 1)$, $(1, -1, -1)$ and $(0, -1, -2)$, respectively. All of these go to the level of energy $\frac{11}{2}(k/m)^{1/2}$ of the continuum oscillator. As A is turned on, a degenerate level of energy $(ka^2/2)N(r)$ in (16) splits into M levels, where M is the number of different associated triplets (n_x, n_y, n_z), disregarding internal permutations. The degeneracy of any of these resulting levels, apart from crossings, is 1, 3 or 6, depending upon whether the n_i in the triplet are all equal, two of them are equal, or all are different, respectively.

As is known, the point symmetry group of the cubic lattice is O_h. Since the irreducible representations of this group have a maximum dimension of three, whilst, on the other hand, here there are levels with sixfold degeneracy, it follows that the accidental degeneracies of the usual harmonic oscillator defined on the continuous manifold are not completely lifted in the discrete case studied here. The 'hidden symmetries' of (1) associated with this accidental degeneracy will be considered elsewhere.

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