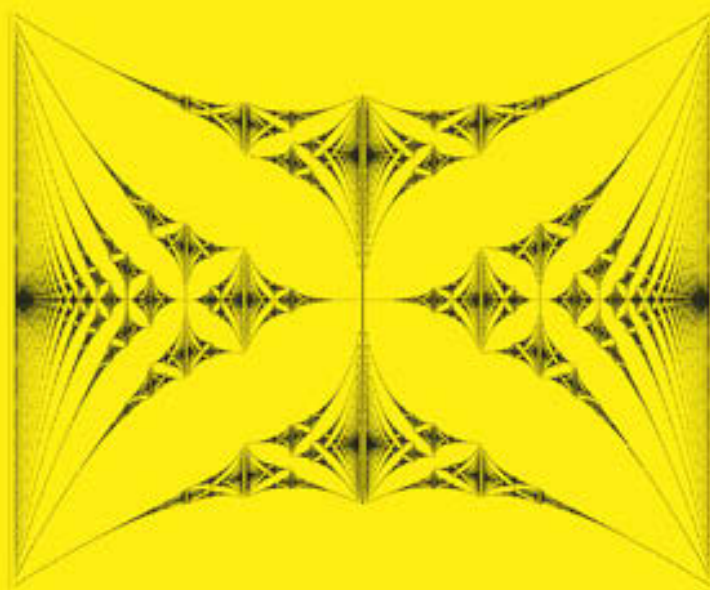


low-dimensional nanoscale systems on discrete spaces



erhardt papp · codrutza micu

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In the memory of
Siri and Eduard

... ..

Preface

Quantum systems on discrete spaces represent to date a rapidly growing research field lying at the interface between tight binding models in solid-state physics and theoretical developments like discrete and q -difference equations. The interplay between such directions provides a deeper understanding of nanoscaled structures which, since more than one decade look increasingly promising for technological applications in electronic devices. Such systems concern the two-dimensional (2D) electron gas under the influence of transversal magnetic fields, the conductor on the 1D lattice in the presence of electric fields, 1D rings in external fields and at last, but not at least, junctions between rings and leads, rings and quantum dots or dots and leads. Promising developments have also been done in the field of quantum LC-circuits. The space discretization has been successful in providing explanations needed for several phenomena like the dynamical localization on the 1D lattice under the influence of time dependent electric fields. It should be remarked, quite satisfactorily, that such phenomena have received evidence in high precision experiments with GaAl/GaAlAs, or other self assembled heterostructures. We also succeeded to establish period doubling in the flux dependent oscillations of total persistent currents in discretized Aharonov-Bohm rings, which deserve further attention.

From the theoretical point of view our main emphasis in this volume is on solvable quantum mechanical systems on the discrete space. Besides the discrete Schrödinger-equation, the most typical example is the second order discrete Harper-equation serving to the description of Bloch-electrons on 2D lattices threaded by a transversal and homogeneous magnetic field. Handling such systems is intimately connected with a lot of mathematical subtleties like orthogonal polynomials of a discrete variable, commensuration and incommensurability effects, periodic and quasiperiodic struc-

tures, q -deformed and discrete equations or relationships between localization effects and Lyapunov exponents. Such issues are able to be used for an updated study of thermodynamic and transport properties, but useful details concerning the quantum Hall effect are also included. We would like to emphasize that the presented matter reveals the increasing perspective concerning the role of space-discreteness for a deeper understanding of nanoscaled systems. To this aim mathematical details needed have been introduced in as transparent a manner as possible.

We found it reasonable to restrict ourselves to 11 chapters. In addition, there are more than 300 alphabetically ordered citations, titles of papers included. It is understood that other special matters, such as discrete Klein-Gordon and Dirac equations, or nonlinear lattices, go beyond the immediate scope of this volume. However, the main point remains, namely to solve discrete Schrödinger-equations and especially tight binding models under the influence of external fields. Accordingly, there are reasons to say that we succeeded in reviewing interesting developments within a reasonable amount of space. For the sake of complementary information in the field of semiconductor superlattices monographs by Bastard (1992), Datta (1995) and Akkermans and Montambaux (2004) are quite useful.

The present volume can be recommended first of all to graduate students and doctoral fellows dealing with Theoretical Physics and its applications. The presented matter is also profitable for advanced students in solid-state physics, applied mathematics and microelectronics. Moreover, useful information for researchers interested in the field is also provided. This volume originates from the updated and revised formulation of our previous lecture in the field (Papp and Micu (2005)).

Interesting discussions with I. Cotaescu, H. Scutaru, I. Bica, D. Grecu, M. Visinescu, E. Burzo, G. Adam, N. Avram, G. Zet, M. Coldea, I. Gottlieb, D. Vangheli, V. Viman and D. Vulcanov, are deeply acknowledged. The technical help by D. Racolta and L. Aur in processing the file is much appreciated. We are also indebted to W. Bestgen, H. D. Doebner, R. M. Weiner and F. Gebhardt for kind hospitality, as well as to CNCISIS/Bucharest for financial support.

Timisoara, Baia Mare
December 2006

E. Papp
C. Micu

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Chapter 1

Lattice Structures and Discretizations

Quantum systems on discrete spaces have received much interest in many areas like electrons on lattices under the influence of external fields, quantum optics, electronics, neuronal networks, signal processing, mesoscopic systems and superlattices. Starting with the discrete space or time one gets faced with the formulation of appropriate discretization schemes. For this purpose discrete variables $x \in \mathbf{Z}$ are almost useful. Other related equations, such as q -difference ones are able to be implied by modern mathematical developments such as quantum groups, the covariant calculus on noncommutative spaces, and R -matrix descriptions (see Chari and Pressley (1994), Faddeev et al (1990)). Here $0 < q < 1$, stands for the generic deformation parameter, but complex q -values and especially roots of unity can also be considered. In addition, there are q -difference equations which are incorporated naturally into the description of actual physical systems such as Bloch-electrons on two- or three-dimensional lattices threaded by a magnetic field, as already referred to above. Moreover, many systems are able to be characterized by inherent length scales which can be used, at least in principle, for subsequent discretizations, too.

1.1 Discrete derivatives

Assuming a function on a lattice with the spacing a , say $f(x)$, we may introduce left and right hand difference quotients as

$$\delta_- f(x) = \frac{f(x) - f(x-a)}{a} = \frac{1}{a} \left(1 - \exp \left(-a \frac{d}{dx} \right) \right) f(x) \quad (1.1)$$

and

$$\delta_+ f(x) = \frac{f(x+a) - f(x)}{a} = \frac{1}{a} \left(\exp \left(a \frac{d}{dx} \right) - 1 \right) f(x) \quad (1.2)$$

respectively. Such quotients, which can also be viewed as discrete derivatives, reproduce the usual one to $O(a^2)$ -order. The discretization proceeds in terms of the identification $x = n_i a$, where x_i is an integer, i.e. $n_{i+1} = n_i + 1$. Then the above quotients are replaced by the discrete derivatives

$$\nabla f(x) = f(x) - f(x-1) \quad (1.3)$$

and

$$\Delta f(x) = f(x+1) - f(x) \quad (1.4)$$

respectively, where x stands hereafter for n_i . Accordingly

$$\nabla \Delta f(x) = \Delta \nabla f(x) = f(x+1) - 2f(x) + f(x-1) \quad (1.5)$$

represents the discretized version of the second derivative. On the other hand one starts from the common assumption that the usual dimensionless momentum operator $i\partial/\partial x$ is Hermitian, so that the discrete derivative Δ behaves as $\Delta^+ = -\nabla$ under Hermitian conjugation. Accordingly, the second order discrete derivative operator $\nabla \Delta$ displayed above is itself Hermitian.

We have to remark that the Leibniz-rule for the differentiation of a product is modified as follows

$$\nabla (f(x)g(x)) = f(x)\nabla g(x) + g(x-1)\nabla f(x) \quad (1.6)$$

and

$$\Delta (f(x)g(x)) = f(x)\Delta g(x) + g(x+1)\Delta f(x) \quad (1.7)$$

respectively, whereas

$$\Delta^n f(x) = \sum_{k=0}^n \frac{n! (-1)^k}{(n-k)! k!} f(x+n-k) \quad (1.8)$$

and

$$\nabla^n f(x) = \sum_{k=0}^n \frac{n! (-1)^k}{k! (n-k)!} f(x-k) \quad . \quad (1.9)$$

Such formulae are quite useful for concrete computations. In this context hypergeometric type second-order difference equations like

$$\sigma(x) \nabla \Delta P_n(x) + \tau(x) \Delta P_n(x) + \lambda_n P_n(x) = 0 \quad (1.10)$$

where $\sigma(x)$ ($\tau(x)$) is an at most second-degree (first degree) polynomial, have been studied in some more detail by Nikiforov, Suslov and Uvarov (1991).

It is understood that (1.10) can be rewritten equivalently as a second-order discrete equation:

$$(\sigma(x) + \tau(x)) P_n(x+1) + \sigma(x) P_n(x-1) + (\lambda - \tau(x) - 2\sigma(x)) P_n(x) = 0 \quad (1.11)$$

which produces hypergeometric type solutions like Hahn, Chebyshev, Meixner, Krawtchouk or Charlier polynomials for selected forms of $\sigma(x)$ - and $\tau(x)$ -functions (Nikiforov, Suslov and Uvarov (1991)). Main formulae concerning such polynomials are presented in section 1.7 as well as in Appendix A.

1.2 The Jackson derivative

Proceeding in a different manner, Jackson (1909) proposed long ago the generalized q -derivative

$$\partial_x^{(q)} f(x) \equiv \frac{d_q(x)}{d_q x} = \frac{f(qx) - f(x)}{x(q-1)} \quad (1.12)$$

working irrespective of x , which reproduces the usual one if $q \rightarrow 1$. Now the Leibniz-rule is modified as

$$\partial_x^{(q)} (f(x)g(x)) = f(x)\partial_x^{(q)} g(x) + g(qx)\partial_x^{(q)} f(x) \quad (1.13)$$

which looks like (1.6). In particular the q -derivative of a power-like function x^n is given by

$$\partial_x^{(q)} x^n = [[n]]_q x^{n-1} \quad (1.14)$$

where

$$[[n]]_q = \frac{q^n - 1}{q - 1} \quad (1.15)$$

denotes the related quantum number. It is clear that $[[n]]_q \rightarrow n$ as $q \rightarrow 1$. Relatedly, one says that under q -deformation the c -number n is replaced by the quantum-number $[[n]]_q$. We have to be aware that (1.12) opens the way to the formulation of q -analysis. Accordingly special functions are substituted by q ones, and the same concerns, of course the hypergeometric series (Gasper and Rahman (1990)). One realizes that the q -derivative written down above is not unique. Indeed, we can also introduce the symmetrized derivative (see e.g. Kulish and Damaskinsky (1990))

$$\mathcal{D}_x^{(q)} f(x) = \frac{f(qx) - f(q^{-1}x)}{x(q - q^{-1})} \quad (1.16)$$

which yields

$$\mathcal{D}_x^{(q)} x^n = [n]_q x^{n-1} \quad (1.17)$$

instead of (1.14), where now

$$[n]_q = \frac{q^n - q^{-n}}{q - q^{-1}}. \quad (1.18)$$

However, one has

$$[n]_q = q^{1-n} [[n]]_{q^2} \quad (1.19)$$

which shows that such quantum numbers are actually inter-related. Moreover, we have to remark that

$$\Delta f(x) = z(q - 1) \partial_z^{(q)} \varphi(z) \quad (1.20)$$

where $z = q^x$ and $f(x) = \varphi(z)$. This relationship is able to serve to the conversion of discrete equations into a q -difference ones and conversely.

Needless to say that q -analysis is far from being trivial. So, the q -binomial theorem reads (see Bailey (1935))

$$\sum_{n=0}^{\infty} \frac{(a; q)_n}{(q; q)_n} x^n = \frac{(ax; q)_{\infty}}{(x; q)_{\infty}} \quad (1.21)$$

in which “ a ” denotes a constant parameter. Accordingly, a q -analog of the gamma function is given by

$$\Gamma_q(x) = \frac{(q; q)_{\infty}}{(q^x; q)_{\infty}} (1 - q)^{1-x} \quad (1.22)$$

which has also been expressed before in terms of the q -integral proposed by Jackson (1910). For the convergence sake one should consider that $0 < q < 1$ both in (1.21) and (1.22). In the above formulae $(a; q)_n$ denotes the q -shifted factorial

$$(a; q)_n = (1 - a)(1 - aq) \cdots (1 - aq^{n-1}) \quad (1.23)$$

where $(a; q)_0 = 1$ so that

$$(a; q)_{\infty} = \prod_{n=0}^{\infty} (1 - aq^n) \quad . \quad (1.24)$$

We have to remark that the present q -Gamma function satisfies the typical functional equation

$$\Gamma_q(x + 1) = [[x]]_q \Gamma_q(x) \quad (1.25)$$

which confirms in turn the relevance of its definition via (1.22). The infinite products quoted above yield a shifted factorial as follows

$$(a; q)_n = \frac{(a; q)_{\infty}}{(aq^n; q)_{\infty}} \quad (1.26)$$

which is now valid for arbitrary complex n -values.

Before proceeding further we would like to say that the Jackson derivative has also been rediscovered recently in terms of the radial reduction of the covariant derivative characterizing the quantum-group $SO_q(N)$, as illustrated by q -deformed radial Schrödinger equations established before (Carow-Watamura and S. Watamura (1997), Papp (1997)).

1.3 The q -integral

In order to perform scalar products and suitable normalizations we have to apply the Jackson q -integral (Gasper and Rahman (1990), Jackson (1910)). So one has

$$\int_0^a f(x) d_q x = a(1-q) \sum_{k=0}^{\infty} f(aq^k) q^k \quad (1.27)$$

if $0 < q < 1$, but

$$\int_0^a f(x) d_q x = a(1-q) \sum_{k=0}^{\infty} \frac{1}{q^{k+1}} f\left(\frac{a}{q^{k+1}}\right) \quad (1.28)$$

if $q > 1$. Inserting e.g. $f(x) = x^n$ yields

$$\int_0^a x^n d_q x = \frac{a^{n+1}}{[[n+1]]_q} \quad (1.29)$$

in both cases. One sees that (1.14) and (1.29) express inverse operations, as one might expect. Furthermore, there is

$$\int_0^{\infty} f(x) d_q x = (1-q) \sum_{k=-\infty}^{+\infty} f(q^k) q^k \quad (1.30)$$

if $0 < q < 1$, which can be generalized on the whole real axis as

$$\int_{-\infty}^{+\infty} f(x) d_q x = (1-q) \sum_{k=-\infty}^{+\infty} [f(q^k) + f(-q^k)] q^k \quad (1.31)$$

Of course, one realizes that convergence conditions $0 < q < 1$ and $q > 1$ mentioned above can be generalized as $|q| < 1$ and $|q| > 1$, respectively.

The symmetrized versions of (1.27) and (1.28) are given by

$$\int_0^a f(z) D_q z = \left(\frac{1}{q} - q\right) \sum_{k=0}^{\infty} a q^{2k+1} f(a q^{2k+1}) \quad (1.32)$$

and

$$\int_0^a f(z) D_q z = \left(q - \frac{1}{q}\right) \sum_{k=0}^{\infty} \frac{a}{q^{2k+1}} f\left(\frac{a}{q^{2k+1}}\right) \quad (1.33)$$

if $|q| < 1$ and $|q| > 1$, respectively. So, one obtains

$$\int_0^a z^n D_q z = \frac{a^{n+1}}{[n+1]_q} \quad (1.34)$$

which is valid again in both cases. This reproduces, of course, (1.29) up to the selection of the appropriate quantum number. Integrations by parts can also be easily done. Using (1.13) one finds e.g.

$$\int_0^a f d_q g = f(x) g(x)|_0^a - \int_0^a g(qx) d_q f \quad (1.35)$$

which works both for $|q| < 1$ and $|q| > 1$. One remarks that the discrete counterpart of (1.35) reads

$$\sum_{x=a}^{b-1} f(x) \Delta g(x) = f(x) g(x)|_a^b - \sum_{x=a}^{b-1} g(x+1) \Delta f(x) \quad (1.36)$$

where x stands again for the discrete variable and which proceeds in accord with (1.7). A similar equation can be derived for the left difference operator ∇ .

1.4 Generalized q -hypergeometric functions

Many solutions of discrete equations are expressed in terms of the generalized hypergeometric function (Gasper and Rahman (1990), Gradshteyn and Ryzhik (1965))

$${}_{p_1}F_{p_2} \left(\begin{matrix} \alpha_1, \alpha_2, \dots, \alpha_{p_1} \\ \beta_1, \beta_2, \dots, \beta_{p_2} \end{matrix} \middle| z \right) = \quad (1.37)$$

$$= \sum_{k=0}^{\infty} \frac{(\alpha_1)_k \cdots (\alpha_{p_1})_k}{(\beta_1)_k \cdots (\beta_{p_2})_k} \frac{z^k}{k!}$$

where p_1 and p_2 are indices and where α_j and β_j are parameters. The classical shifted factorial is given by

$$(a)_k = \frac{\Gamma(a+k)}{\Gamma(a)} = a(a+1)\cdots(a+k-1) \quad (1.38)$$

as usual, where $(a)_0 = 1$. Recall that the usual Gaussian hypergeometric function is

$$F(\alpha, \beta, \gamma; z) = {}_2F_1\left(\begin{matrix} \alpha, \beta \\ \gamma \end{matrix} \middle| z\right) \quad (1.39)$$

whereas the confluent one is given by

$$F(\alpha, \gamma; z) = {}_1F_1\left(\begin{matrix} \alpha \\ \gamma \end{matrix} \middle| z\right) \quad (1.40)$$

Resorting for convenience, to the quantum number (1.15), we shall perform the q -generalization of (1.37) in terms of the substitutions

$$(a)_k \rightarrow \frac{(q^a, q)_k}{(1-q)^k} = \prod_{l=0}^{k-1} [[a+l]]_q \quad (1.41)$$

and

$$k! \rightarrow [[k]]_q! = \frac{(q, q)_k}{(1-q)^k} = \prod_{l=1}^k [[l]]_q \quad (1.42)$$

This leads to the q -generalization

$$\begin{aligned} & {}_{p_1}F_{p_2}^{(q)}\left(\begin{matrix} \alpha_1, \alpha_2, \dots, \alpha_{p_1} \\ \beta_1, \beta_2, \dots, \beta_{p_2} \end{matrix} \middle| \tilde{z}\right) = \\ & = \sum_{k=0}^{\infty} \frac{(q^{\alpha_1}, q)_k \cdots (q^{\alpha_{p_1}}, q)_k}{(q^{\beta_1}, q)_k \cdots (q^{\beta_{p_2}}, q)_k} \frac{\tilde{z}^k}{(q, q)_k} \end{aligned} \quad (1.43)$$

which reproduces (1.37) as $q \rightarrow 1$, where

$$\tilde{z} = (1-q)^{p_2-p_1+1} z \quad (1.44)$$

In order to identify the generalized q -hypergeometric function it is convenient to rewrite (1.43) as follows

$$\begin{aligned}
 {}_{p_1}F_{p_2}^{(q)} \left(\begin{matrix} \alpha_1, \alpha_2, \dots, \alpha_{p_1} \\ \beta_1, \beta_2, \dots, \beta_{p_2} \end{matrix} \middle| \gamma \tilde{z} \right) &= \\
 &= \sum_{k=0}^{\infty} C_k \tilde{z}^k
 \end{aligned} \tag{1.45}$$

where γ is an additional factor. One would then obtain the recurrence relation

$$C_{k+1} = \gamma \frac{(1-q)^{p_2-p_1+1} (1-q^{\alpha_1+k}) \dots (1-q^{\alpha_{p_1}+k})}{(1-q^{k+1}) (1-q^{\beta_1+k}) \dots (1-q^{\beta_{p_2}+k})} C_k \tag{1.46}$$

which can also be used in order to check the appearance of polynomial solutions for which $C_{n+1} = 0$. The q -exponential function is also of a special interest, but it will be discussed in section 3.6 in a close connection with the q -deformation of the time evolution.

1.5 The discrete space-time: a short retrospect

The basic idea about a discrete space and/or time is as old as the very beginning of the scientific thinking. The old Greeks speculated about the generalization of the atomistic structure of matter to space-time, as illustrated in an excellent volume by Vialtzew (1965). Such steps deserve an actual appreciation even from the perspective of contemporary physics. With the advent of quantum mechanics, the question of whether subdivisions of space and time intervals can be indefinitely performed or not, has focussed increasing interest. The latter alternative, which leads to the introduction of space-time quanta proceeding in a close connection with ultimate accuracies of space-time measurements, is looks almost promising. Pioneering work along this direction has been done by many authors, but here we would like just to remember specifically contributions done by Poincaré (1913), Planck (1913), Ambarzumian and Iwanenko (1930), March (1937), Heisenberg (1938a,1938b), Wheeler (1957), Brill and Gowdy (1970) and Finkelstein (1997). In “Physics and Reality” Einstein said:

“To be sure, it has been pointed out that the introduction of a spacetime continuum may be considered as contrary to nature in view of the molecular

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structure of everything which happens on a small scale. It is maintained that perhaps the success of the Heisenberg method points to a purely algebraical method of description of nature, that is to the elimination of continuum functions from physics. Then, however, we must also give up, by principle, the spacetime continuum" (see also Atakishiyev and Suslov (1990)).

Further developments rely on a celebrated paper by Snyder (1947) dealing with the introduction of a Lorentz invariant space-time. We then have to consider a discrete space-time in which there exists a smallest unit of length, say $a \neq 0$. The basic expectation is that accounting for a such length leads to the elimination of divergence difficulties plaguing quantum field theory. Introducing a such length in space-time yields, however, non-commutative relationships between x, y, z and t , so that space-time coordinates have to be considered by now as observables. More exactly, they are identified with the generators of the group of transformations leaving invariant the five-dimensional de Sitter quadratic form (see also Yang (1947))

$$R_5^2 = -\eta_0^2 + \eta_1^2 + \eta_2^2 + \eta_3^2 + \eta_4^2 \quad (1.47)$$

in which the η 's are assumed to be real variables. One would then obtain Hermitian space-time generators as follows

$$X_1 = ia \left(\eta_4 \frac{\partial}{\partial \eta_1} - \eta_1 \frac{\partial}{\partial \eta_4} \right) \quad (1.48)$$

$$X_2 = ia \left(\eta_4 \frac{\partial}{\partial \eta_2} - \eta_2 \frac{\partial}{\partial \eta_4} \right) \quad (1.49)$$

$$X_3 = ia \left(\eta_4 \frac{\partial}{\partial \eta_3} - \eta_3 \frac{\partial}{\partial \eta_4} \right) \quad (1.50)$$

and

$$\tilde{T}_0 = \frac{ia}{c} \left(\eta_4 \frac{\partial}{\partial \eta_0} - \eta_0 \frac{\partial}{\partial \eta_4} \right) \quad (1.51)$$

In addition, there are three operators like

$$L_k = -i\hbar \varepsilon_{kls} \eta_l \frac{\partial}{\partial \eta_s} \quad (1.52)$$

where $k, l, s = 1, 2, 3$ and where the usual summation convention is assumed. These latter operators correspond to the . Further three operators like

$$M_1 = i\hbar \left(\eta_0 \frac{\partial}{\partial \eta_1} + \eta_1 \frac{\partial}{\partial \eta_0} \right) \quad (1.53)$$

$$M_2 = i\hbar \left(\eta_0 \frac{\partial}{\partial \eta_2} + \eta_2 \frac{\partial}{\partial \eta_0} \right) \quad (1.54)$$

and

$$M_3 = i\hbar \left(\eta_0 \frac{\partial}{\partial \eta_3} + \eta_3 \frac{\partial}{\partial \eta_0} \right) \quad (1.55)$$

bearing on the Lorentz-boosts, have also to be considered. Accordingly, one finds the commutation relations

$$[X_k, X_l] = i \frac{a^2}{\hbar} \varepsilon_{kls} L_s \quad (1.56)$$

and

$$[\tilde{T}_0, X_k] = i \frac{a^2}{\hbar c} M_k \quad (1.57)$$

which are responsible for the discrete space-time and which reproduce the space-time continuum as soon as $a \rightarrow 0$. It is understood that L_k and M_k commutes with the Minkowski quadratic form

$$S_4^2 = c^2 \tilde{T}_0^2 - X_1^2 - X_2^2 - X_3^2 \quad (1.58)$$

provided (1.48)-(1.51) are valid. This means that the discrete space-time defined in this manner is itself Lorentz-invariant.

The eigenvalues, say x'_k , characterizing the discrete space are given by

$$x'_k = n_k a \quad (1.59)$$

where $n_k \in \mathbb{Z}$, which reveals the space discreteness in an explicit manner. The $\tilde{T}_0$ operator has, however, a continuous spectrum, which shows, so far, that the discreteness of space does not imply necessarily a discrete time. In this context a continuous time can be preserved, however, for reasons of mathematical simplicity. Either case, (1.59) shows that there are actual interplays between relativity and space-discreteness. Several ideas and approaches to the discrete space have also been sketched in an unpublished paper by Heisenberg in 1930 (see also Carazza and Kragh (1995)). In this

context the fundamental length has also been conceived as the absolute minimum of the position uncertainty of a particle.

Other manifestations of the fundamental length have been done by defining covariant space-time and four-momentum operators as (Hellund and Tanaka (1954))

$$X_\mu = \tilde{x}_\mu - a^2 \frac{\partial}{\partial \tilde{x}_\mu} \tilde{x}_\nu \frac{\partial}{\partial \tilde{x}_\nu} \quad (1.60)$$

and

$$P_\mu = \tilde{p}_\mu - i\hbar \frac{\partial}{\partial \tilde{x}_\mu} \quad (1.61)$$

respectively, where $\tilde{x}_\mu$ and $\tilde{p}_\mu$ are c -numbers like $\tilde{x}_\mu = (x, y, z, ict)$ and $\tilde{p}_\mu = (p_x, p_y, p_z, iE/c)$. For convenience, the same quotations for space-time operators have been preserved. This yields the commutation relations

$$[X_\mu, P_\nu] = i\hbar \left(\delta_{\mu\nu} + \frac{a^2}{\hbar^2} P_\mu P_\nu \right) \quad (1.62)$$

in which case Heisenberg's uncertainty principle is generalized as follows

$$\Delta X_\mu \Delta P_\nu \geq \hbar \left(1 + \frac{a^2}{\hbar^2} P_\mu^2 \right) \quad (1.63)$$

for $\mu = \nu$ (no summation). Moreover, there is

$$\Delta X_1 \Delta \tilde{T}_0 \geq \frac{a^2}{c} \quad (1.64)$$

which shows that elementary space-time volumes have also to be considered.

Other evolutions could also be mentioned (see Kadyshevsky (1961)), but the main point is that accounting for (1.59) leads to the introduction of discrete-equations serving as starting points for an improved theoretical descriptions in several respects. Interestingly enough, similar results are provided by q -deformed oscillators for which q is a root of unity, as shown by Bonatsos et al (1994). Then position and momentum operators have discrete eigenvalues, which are the roots of certain q -deformed Hermite polynomials. This leads, in general, to a non-equidistant phase-space lattice. An exception is the parafermionic oscillator, for which an equidistant space-phase lattice can be readily derived.

In other words, there are theoretical supports to the existence of a discrete space in which the fundamental length plays a role which is similar, in a way or another, to the lattice spacing in solid state physics. Accordingly, discrete derivatives written down in section 1.1 are well motivated from a quantum mechanical point of view. From the mathematical perspective, similar developments can be traced back to the introduction of q -hypergeometric functions and Jackson-derivatives (see e.g. chapter 1 in Gasper and Rahman (1990)).

1.6 Quick inspection of q -deformed Schrödinger equations

The q -deformed Schrödinger-equation on the non-commutative quantum Euclidian space has been analyzed for the harmonic oscillator (see e.g. Carow-Watamura and Watamura (1994)), for the Coulomb potential (Song and Liao (1992)), Feigenbaum and Freund (1996), Micu (1999)), as well as for the free particle (Hebecker and Weich (1992), Ocampo (1996), Papp (1997)). For this purpose one resorts to the q -deformed Laplacian, which has been derived in terms of the $SO_q(N)$ -covariant calculus (Carow-Watamura and S. Watamura (1994)). Just mention that the non-commutative N -dimensional quantum Euclidian space is characterized by typical coordinate dependent realizations of $[x_j, x_k]$ commutators in terms of bilinear or quadratic monomials such as given e.g. by the $SO_q(3)$ relationships $[x_1, x_2] = (q - 1)x_2x_1$, $[x_2, x_3] = (q - 1)x_3x_2$ and $[x_1, x_3] = (1 - q)x_2^2/\sqrt{q}$. In addition, there are well defined q -difference realizations of annihilation and creation operators, such as done in the study of a different version of the q -deformed harmonic oscillator (Atakishiyev and Suslov (1990), Li and Sheng (1992)). An interesting q -deformation of the Schrödinger-equation has been established by resorting to a q -deformation of the Witt algebra (Twarock (1999)), in which case the non-linear Schrödinger-equation derived by Doebner and Goldin (1992) gets reproduced as $q \rightarrow 1$. Other issues, such as q -deformations of the phase-space (Zumino (1991), Ubriaco (1993), Kehagias and Zoupanos (1994), Celeghini et al (1995), Wess (1997)), can also be mentioned. We have to recognize, however, that a sound confirmation of the physical relevance of q -deformations referred to above is still lacking. Nevertheless, there are parameter dependent difference equations in which the q -parameter is implemented from the very beginning in terms of an appropriate physical description, such as the q -symmetrized Harper-equation (see chapter 9).

1.7 Orthogonal polynomials of hypergeometric type on the discrete space

Classical orthogonal polynomials of a discrete variable are of much interest for several applications. A systematic study of such polynomials has already been done by Nikiforov, Suslov and Uvarov (1991). These polynomials are specified by the $\sigma(x)$ - and $\tau(x)$ -functions in (1.10). In the case of hypergeometric type polynomials we have to choose $\sigma(x)$ and $\tau(x)$ as polynomials of at most second and of first degrees in x , respectively. So one has e.g.

$$\sigma(x) = x, \quad \tau(x) = \mu(\gamma - x) - x, \quad x \in [0, b] \quad (1.65)$$

for Krawtchouk polynomials, whereas

$$\sigma(x) = x, \quad \tau(x) = \mu(\gamma + x) - x, \quad x \in [0, \infty) \quad (1.66)$$

for Meixner-ones. In the first (second) case one has $\gamma = N_0 = b - 1$, $\mu = p/q$ with $p + q = 1$ ($0 < \mu < 1$ and $\gamma > 0$). Equation (1.10) can also be converted into the self-adjoint form

$$\Delta(\sigma(x)\rho(x)\nabla y(x)) + \lambda\rho(x)y(x) = 0 \quad (1.67)$$

where λ denotes the eigenvalue and where the weight function $\rho(x)$ is implemented via

$$\Delta(\sigma(x)\rho(x)) = \tau(x)\rho(x) \quad (1.68)$$

In addition, (1.67) can be generalized as

$$\Delta(\sigma(x)\rho_m(x)\nabla v_m(x)) + \mu_m\rho_m(x)v_m(x) = 0 \quad (1.69)$$

where

$$v_m(x) = \Delta^m y(x) \quad (1.70)$$

and where m is a positive integer. Accordingly, (1.68) becomes

$$\Delta(\sigma(x)\rho_m(x)) = \tau_m(x)\rho_m(x) \quad (1.71)$$

where

$$\tau_m(x) = \tau(x+m) + \sigma(x+m) - \sigma(x) \quad . \quad (1.72)$$

The generalized weight function reads

$$\rho_m(x) = \sigma(x+1)\rho_{m-1}(x) = \rho(x+m) \prod_{l=1}^m \sigma(x+l) \quad (1.73)$$

for which the eigenvalue becomes

$$\mu_m = \mu_{m-1} + \Delta\tau_{m-1}(x) \quad . \quad (1.74)$$

Furthermore, one finds the concrete realizations

$$\tau_m(x) = \tau(x) + m(\sigma'(x) + \tau'(x)) + \frac{m^2}{2}\sigma''(x) \quad (1.75)$$

and

$$\mu_m = \lambda + m\tau'(x) + \frac{m}{2}(m-1)\sigma''(x) \quad . \quad (1.76)$$

Other details are presented for interested readers in Appendix A.

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Chapter 2

Periodic Quasiperiodic and Confinement Potentials

Schrödinger equations with periodic potentials concern both continuous and discrete spaces, but the latter choice seems to be almost suitable from a general theoretical point of view. Indeed periodic lattice structures, such as the ones from solid state physics, give rise to actual periodic potentials, which produce in turn typical manifestations, such as the appearance of energy bands. The main ingredient is the Bloch-theorem (see also Ashcroft and Mermin (1976)) working in conjunction with the selection of the first Brillouin zone. Even if they are not an absolute novelty, such issues are well suited for a safe explanation of energy-bands, of persistent currents or of dynamic localization effects concerning low dimensional systems on discrete spaces. Preliminaries referring to confinement potentials for quantum dots and rings, as well as to persistent currents, are also addressed.

2.1 Short derivation of the Bloch-theorem

Let us consider the one-dimensional Schrödinger equation

$$\mathcal{H}\psi(x) = -\frac{\hbar^2}{2m_0} \frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x) \quad (2.1)$$

in which there is

$$V(x+a) = V(x) \quad (2.2)$$

irrespective of x . One then says that the potential is periodic, the period being denoted by a . The crystalline structure can be accounted for by inserting the effective mass m^* instead of m_0 . Here the coordinate is continuous, but dealing with the discrete space one inserts $x = na$, where n

is an integer while a stands for the lattice spacing. Looking for a square integrable wavefunction for which

$$\psi(x) \in \{L_2(-\infty, +\infty), dx\} \quad (2.3)$$

one sees immediately that the same holds for $\psi(x+a)$. Accordingly the translated wavefunction

$$\psi(x+a) \equiv T_0(a)\psi(x) = \exp(if(a))\psi(x) \quad (2.4)$$

is the by-product of an unitary transformation, in which case $f(a)$ is a pure phase. For definiteness, this phase may be located on the unit circle such that $f(a) \in [-\pi, \pi]$. The translation operator is given by

$$T_o(a) = \exp(a\partial/\partial x) = \exp(iap_{op}) \quad (2.5)$$

where $p_{op} = -i\partial/\partial x$ ($\hbar = 1$). Of course, one has the commutation relation

$$[H, T_0(a)] = 0 \quad (2.6)$$

which proceeds in accord with (2.2).

Repeating the translation n -times one finds

$$\psi(x+na) = \exp(inf(a))\psi(x) \quad (2.7)$$

but one should also have

$$\psi(x+na) = \exp(if(na))\psi(x) \quad (2.8)$$

as the latter translation proceeds in terms of the rescaled period $a' = na$. Furthermore, there is $f(na) = nf(a)$, so that nothing prevents us from doing the identification

$$f(a) = ka \in [-\pi, \pi] \quad . \quad (2.9)$$

It is clear that the wavenumber k quoted above has been invoked on dimensionality grounds. So, the normalized eigenfunction of (2.1) exhibits itself a certain kind of twisted periodic behavior like

$$\psi(x+a) \equiv \psi_k(x+a) = \exp(ika)\psi_k(x) \quad . \quad (2.10)$$

This reproduces the 1D Bloch-theorem (see Ashcroft and Mermin (1976), Flügge (1971)) and corresponds, as it stands, to a forward translation. We have to remark that a modulated plane wave:

$$\psi_k(x) = \exp(ikx) u_k(x) \quad (2.11)$$

obeys (2.2) if

$$u_k(x+a) = u_k(x) \quad (2.12)$$

which shows that the modulation should be periodic, too. As a corollary, the energy becomes itself both k -dependent and periodic:

$$E = E(k) = E\left(k + \frac{2\pi}{a}\right) \quad (2.13)$$

where $2\pi/a$ has the meaning of a period characterizing the very existence of energy bands (see (2.24)).

2.2 The derivation of energy-band structures

In order to illustrate the appearance of energy bands, let us consider the periodic potential produced by an infinite sequence of identical barriers like (see also Davison and Steslicka (1992))

$$V(x) = \begin{cases} U_0, & x \in [na_1 + (n-1)b_1, n(a_1+b_1)] \\ 0, & x \notin [na_1 + (n-1)b_1, n(a_1+b_1)] \end{cases} \quad (2.14)$$

where $n = 0, \pm 1, \pm 2, \dots$. One sees that

$$V(x+a_1+b_1) = V(x) \quad (2.15)$$

so that now $a = a_1 + b_1$ plays the role of the lattice spacing. The depth of the potential barrier is b_1 , the length of the zero-potential cell is a_1 , whereas $U_0 > 0$ is a constant amplitude.

Next, let us choose three adjacent zones, say $\mathcal{D}_1$, $\mathcal{D}_2$, and $\mathcal{D}_3$, for which $x \in [-b_1, 0]$, $x \in [0, a_1]$ and $x \in [a_1, a_1 + b_1]$, respectively. Assuming at the beginning that $E > U_0$, one finds the solutions

$$\psi(x) = \psi_1(x) = A_1 \exp(ik_1x) + B_1 \exp(-ik_1x) \quad (2.16)$$

and

$$\psi(x) = \psi_2(x) = A_2 \exp(ik_2x) + B_2 \exp(-ik_2x) \quad (2.17)$$

in $\mathcal{D}_1$ and $\mathcal{D}_2$, where

$$k_1 = \sqrt{\frac{2m}{\hbar^2}(E - U_0)} \quad (2.18)$$

and

$$k_2 = \sqrt{\frac{2m}{\hbar^2}E} \quad (2.19)$$

respectively. On the other hand, one has

$$\psi(x) = \psi_3(x) = \exp(ikx) u_k(x) \quad (2.20)$$

for $x \in \mathcal{D}_3$, in which

$$u_k(x) = u_k(x - a) = \exp(-ik(x - a)) \psi_1(x - a) \quad (2.21)$$

Putting together (2.16) and (2.20), one finds immediately that

$$\psi_3(x) = \exp(ika) [A_1 \exp(ik_1(x - a)) + B_1 \exp(-ik_1(x - a))] \quad (2.22)$$

for $x \in \mathcal{D}_3$. Next, we have to apply continuity conditions concerning the wavefunction and its first derivative at $x = 0$ and $x = a_1$. This results in four homogeneous matching equations for the amplitudes A_1 , B_1 , A_2 and B_2 :

$$\begin{pmatrix} 1 & 1 & -1 & -1 \\ \exp(i(\theta - \theta_1)) & \exp(i(\theta + \theta_1)) & -\exp(i\theta_2) & -\exp(-i\theta_2) \\ k_1 & -k_1 & -k_2 & k_2 \\ k_1 \exp(i(\theta - \theta_1)) & -k_1 \exp(i(\theta + \theta_1)) & -k_2 \exp(i\theta_2) & k_2 \exp(-i\theta_2) \end{pmatrix} \cdot \quad (2.23)$$

$$\begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{pmatrix} = 0$$

where $\theta_1 = k_1 b_1$, $\theta_2 = k_2 a_1$ and $\theta = ka$. Denoting by $\mathcal{M}$ the matrix just displayed above, one finds the eigenvalue-condition

$$P(E; \theta_1, \theta_2) = \cos \theta \quad (2.24)$$

via $\det(\mathcal{M}) = 0$, where

$$P(E; \theta_1, \theta_2) = \cos \theta_1 \cos \theta_2 - \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin \theta_1 \sin \theta_2 \quad (2.25)$$

and where the r.h.s. of (2.24) agrees with (2.13). The interesting point concerning (2.24) is the remarkable separation of the θ -dependent term, i.e. of $\cos \theta$, on the r.h.s. of the equation. It is obvious that k_1 should be replaced by iK_1 , if $0 < E < U_0$, where

$$K_1 = \sqrt{\frac{2m}{\hbar^2} (U_0 - E)} \quad (2.26)$$

Then (2.25) becomes

$$P(E; i\tilde{\theta}_1, \theta_2) = \cosh \tilde{\theta}_1 \cos \theta_2 - \frac{k_2^2 - K_1^2}{2K_1 k_2} \sinh \tilde{\theta}_1 \sin \theta_2 \quad (2.27)$$

where $\tilde{\theta}_1 = K_1 b_1$. Invoking (2.8), one finds that unions over admissible energies are done by the inequalities

$$-1 \leq P(E; \theta_1, \theta_2) \leq 1 \quad (2.28)$$

and

$$-1 \leq P(E; i\tilde{\theta}_1, \theta_2) \leq 1 \quad (2.29)$$

respectively. In other words, we are ready to derive energy band structures for which the band edges are produced by the equality signs in (2.28) and (2.29). Conversely, one finds energy gaps in the complementary regions, i.e. at energies for which $|P(E; \theta_1, \theta_2)| > 1$ and $|P(E; i\tilde{\theta}_1, \theta_2)| > 1$, respectively.

Using for instance dimensionless variables like $\gamma_1 = \sqrt{2}b_1/l_c$, $\gamma_2 = \sqrt{2}a_1/l_c$, $W = E/mc^2$ and $u_0 = U_0/mc^2$ one sees that the energy-function exhibits the form

$$P(E; \theta_1, \theta_2) = \cos\left(\gamma_1 \sqrt{W - u_0}\right) \cos\left(\gamma_2 \sqrt{W}\right) - \frac{2W - u_0}{\sqrt{(W - u_0)W}} \sin\left(\gamma_1 \sqrt{W - u_0}\right) \sin\left(\gamma_2 \sqrt{W}\right) \quad (2.30)$$

where $l_c = \hbar/mc$ denotes the Compton wavelength. In particular, the W -dependence of $P(E; \theta_1, \theta_2)$ is displayed in figure 2.1, for $\gamma_1 = 2$, $\gamma_2 = 3$, $u_0 = 1$ and $0 < W < 10$. We have to remark that (2.28) and (2.29) yield four bands expressed approximately by the union

$$W \in [0.24, 0.57] \cup [1.08, 1.82] \cup [3.65, 4.86] \cup [7.23, 10] \quad (2.31)$$

in which the individual bandwidths increase with W .

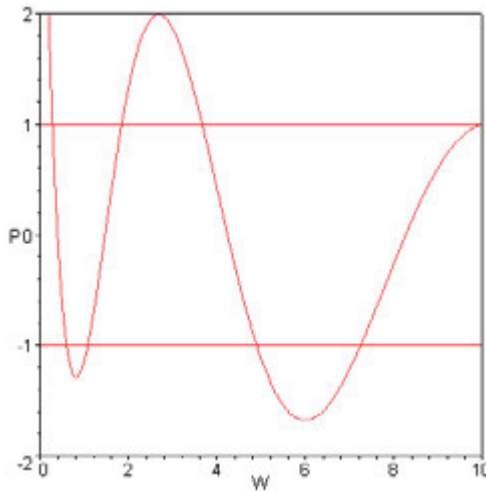


Fig. 2.1 The W -dependence of $P(E; \tilde{\theta}_1, \tilde{\theta}_2)$ for $\gamma_1 = 1$, $\gamma_2 = 3$ and $u_0 = 1$.

2.3 Direct and reciprocal lattices

In solid state physics one gets faced with configuration space vectors like:

$$\vec{R}_n = n_1 \vec{a}_1 + n_2 \vec{a}_2 + n_3 \vec{a}_3 \quad (2.32)$$

referred to as Bravais-lattice vectors, where $n_j \in \mathbb{Z}$ ($j=1,2,3$) and where the $\vec{a}_j$'s are responsible for the primitive unit cell. Finite translations in the real space are then described by

$$\mathbf{T}_0(\vec{R}_n) = \exp\left(i \vec{p}_{op} \cdot \vec{R}_n\right) \quad (2.33)$$

where $\vec{p}_{op} = -i\nabla$. This yields

$$\mathbf{T}_0(\vec{R}_n) \psi_{\vec{k}}(\vec{x}) \equiv \psi_{\vec{k}}(\vec{x} + \vec{R}_n) = \exp\left(i \vec{k} \cdot \vec{R}_n\right) \psi_{\vec{k}}(\vec{x}) \quad (2.34)$$

where $\vec{k} \equiv \vec{k}_B$ is the Brillouin wavevector which incorporates the three-dimensional version of Bloch's theorem (see e.g. Ashcroft and Mermin (1976)).

The reciprocal lattice is characterized by the primitive vectors

$$\vec{g}_j = 2\pi \varepsilon_{jkl} \frac{\vec{a}_k \times \vec{a}_l}{V_1^{(3)}} \quad (2.35)$$

where $V_1^{(3)} = \vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)$ is the volume of the unit cell. A general reciprocal lattice vector is then given by

$$\vec{K}_m = m_1 \vec{g}_1 + m_2 \vec{g}_2 + m_3 \vec{g}_3 \quad (2.36)$$

where m_j 's are again integers. One sees that $\vec{a}_j \cdot \vec{g}_l = \delta_{jl}$, so that

$$\vec{R}_n \cdot \vec{K}_m = 2\pi n' \quad (2.37)$$

where

$$n' = n_1 m_1 + n_2 m_2 + n_3 m_3 \in \mathbb{Z} \quad . \quad (2.38)$$

Defining the wavefunction in the complementary wavevector representation by the discrete Fourier-transform

$$\tilde{\psi}_F(\vec{k}') = \sum_{\vec{R}_n} \psi(\vec{R}_n) \exp\left(-i \vec{k}' \cdot \vec{R}_n\right) \quad (2.39)$$

one has

$$\tilde{\psi}_F(\vec{k}' + \vec{k}_B) = \tilde{\psi}(\vec{k}') \quad (2.40)$$

where

$$\tilde{\psi}(\vec{k}') = \sum_{\vec{R}_n} \psi(\vec{R}_n) \exp\left(-i(\vec{k}' + \vec{k}_B) \cdot \vec{R}_n\right) \quad (2.41)$$

The sum in (2.39) and (2.41) is over all n_j 's. This shows the occurrence of a periodic behavior like

$$\tilde{\psi}(\vec{k}' + \vec{K}_m) = \tilde{\psi}(\vec{k}') \quad (2.42)$$

in which case

$$\tilde{\psi}_F(\vec{k}' + \vec{k}_B + \vec{K}_m) = \tilde{\psi}_F(\vec{k}' + \vec{k}_B) \quad (2.43)$$

On the other hand, (2.41) can be inverted as

$$\psi(\vec{x}) \exp\left(-i\vec{k}_B \cdot \vec{x}\right) = \sum_{\vec{K}_m} \tilde{\psi}(\vec{K}_m) \exp\left(i\vec{K}_m \cdot \vec{x}\right) \quad (2.44)$$

so that

$$\psi(\vec{x} + \vec{R}_n) = \exp\left(i\vec{k}_B \cdot \vec{R}_n\right) \psi(\vec{x}) \quad (2.45)$$

which concerns the three-dimensional form of Bloch's theorem (see Ashcroft and Mermin (1976)).

Inserting $\vec{k}_B = 0$, one sees that (2.43) exhibits the limiting form

$$\tilde{\psi}_F(\vec{k}') = \tilde{\psi}_F(\vec{k}' + \vec{K}_m) \quad (2.46)$$

which has been invoked in the study of the 1D harmonic oscillator on the lattice by Chabaud et al (1986) as

$$\tilde{\psi}_F(k') = \tilde{\psi}_F\left(k' + \frac{2\pi}{a}\right) \quad (2.47)$$

Related details are presented in section 4.1. The Bloch-theorem in N space dimensions is also expressed usually as

$$\psi_{\vec{k}}(\vec{x} + \vec{a}) = \exp\left(i \vec{k} \cdot \vec{a}\right) \psi_{\vec{k}}(\vec{x}) \quad (2.48)$$

in accord with (2.45), where

$$\vec{k} \cdot \vec{a} = \sum_{i=1}^N \theta_i \quad (2.49)$$

and where $\theta_i = k_i a_i \in [-\pi, \pi]$. Other details concerning the Bloch-theorem may be found in textbooks (Ashcroft and Mermin (1976), Flügge (1971)).

2.4 Quasiperiodic potentials

Let us now assume that the potential can be expanded in a multiple Fourier series as

$$V(x) = \sum_{\{m_k\}} a_{m_1, \dots, m_j} \exp\left(2\pi i \sum_{k=1}^j m_k \omega_k x\right) \quad (2.50)$$

where the m_k 's are integers. If the frequency ω_k can be expressed by a quotient of two prime integers P_k and Q_k :

$$\omega_k = \frac{P_k}{Q_k} \quad (2.51)$$

then $V(x)$ exhibits j periods for which

$$V(x + Q_k) = V(x) \quad (2.52)$$

where $k = 1, 2, \dots, j$. However, it may happen that the ω_k 's are incommensurate. This means that for any set of rational numbers $\{r_k\}$ the equation (Besicovitch (1932), Romerio (1971)) the equation

$$\sum_{k=1}^j r_k \omega_k = 0 \quad (2.53)$$

is able to be fulfilled for all k -values, if $r_k = 0$ only. This is e.g. the case if at least one of the frequencies is expressed by an irrational number. Then, one says that the potential is quasiperiodic, in which case the spectrum

becomes an infinite Cantor-set (Ostlund and Pandit (1984), Simon (1982)). However, there are certain circumstances under which generalized versions of the Bloch-theorem may be applied as shown by Ostlund et al (1983a). Moreover, the periodic behavior is restored as soon as one resorts to rational approximations of irrationals. So far irrationals have also been approached via $P_k \rightarrow \infty$, and $Q_k \rightarrow \infty$, but for this purpose continued fractions can also be considered (Azbel (1979), Aubry and Andre (1980), Sokoloff (1981), Thouless (1983a), Wilkinson and Austin (1994)). Nevertheless, a problem remains, namely the question of whether an irrational number can be discriminated in practice from a rational approximation, or not. Indeed, in order to reproduce in practice irrational frequencies an infinite experimental resolution would be necessary, but this latter point looks rather questionable. On the other hand there are fractal-like experimental realizations which can be viewed as competition effects between rational and irrational frequencies, in which case successive resolutions with increasing accuracy are in order.

It is also clear that potentials on a discrete space for which the period is incommensurate with the spacing of the underlying lattice are able to produce nontrivial manifestations. Choosing the dimensionless lattice spacing to be unity, we then have to consider potentials for which

$$V(x + Q_i) = V(x) \quad (2.54)$$

where now Q_i is irrational. In particular, we can then consider the cosine potential

$$V(x) = V_0 \cos\left(2\pi \frac{P_1}{Q_i} x + \delta\right) \quad (2.55)$$

or so called Maryland-model (see also section 4.5)

$$V(x) = V_0 \tan\left(\pi \frac{P_1}{Q_i} x + \delta\right) \quad (2.56)$$

Furthermore, let us assume that $V(x)$ provides the diagonal potential of an 1D tight binding model with nearest-neighbor (NN) hopping (see also chapters 6 and 7). Using (2.56) it has been found (interestingly enough), that the spectrum is discrete for irrational Q_i values, such that all the states are normalizable (see Grempel et al (1982)). Accordingly, one deals with localized states, which is reminiscent to the well-known influence of random

potentials (Anderson (1958)). This shows that quasiperiodic potentials are able to produce effects which are similar to the ones characterizing disordered systems, i.e. systems governed by diagonal random potentials specified above. In contradistinction, one obtains Q_1 bands as $Q_i \rightarrow Q_1$ approaches an integer, in which case the wavefunctions become increasingly extended. It is also been found that in the case of dissipative systems the transition from quasiperiodicity to chaos occurs both in a continuous and universal manner (Ostlund et al (1983b)).

In the sequel we shall confine, however, our attention on rational values of the commensurability parameter, with the understanding that irrationals are able to be handled as special limiting cases.

2.5 A shorthand presentation of the elliptic Lamè-equation

Further mathematical details concerning periodic Schrödinger equations (Simon (1985), Dyakin and Petrukhovskii (1986)) are worthy of being mentioned. So there is an increasing interest in the application of non-unitary $SU(1, 1)$ - and $SU(2)$ -representations to the band-energy description of Scarf- and Lamè-Hamiltonians, respectively (Li and Kusnezov (2000a)). In this context, we would like to say that the usual elliptic Lamè-equation

$$\frac{d^2\psi}{dx^2} + \kappa^2 l(l+1) \operatorname{sn}^2 x \psi(x) = E \psi(x) \quad (2.57)$$

provides interesting applications in physics ranging from solitons to exactly solvable models (Li et al (2000b), Finkel et al (2000)). Here $\operatorname{sn} x = \operatorname{sn}(x|\kappa)$ is the Jacobi elliptic sine function with modulus $0 \leq \kappa \leq 1$, whereas l is a real parameter playing the role of the quantum number of the angular momentum. Along the real axis $\operatorname{sn}^2 x$ is periodic with period $2K$, where

$$K = \frac{\pi}{2} F\left(\frac{1}{2}, \frac{1}{2}, 1; \kappa^2\right) \quad (2.58)$$

denotes the complete elliptic integral. This equation can be converted into other systems, like Pöschl-Teller (Li and Kusnezov (2000a)) and Calogero-Moser (Enolskii and Eilbeck (1995)) systems, by resorting to suitable coordinate transformations and κ -selections. In this context, several classes of inter-related elliptic potentials and corresponding orthogonal polynomials have been discussed recently by Ganguly (2002). In addition, there are Scarf- and Mathieu-equation limits (Li et al (2000b)).

2.6 Quantum dot potentials

Nanoscaled systems such as quantum dots, nanorings, nanorings the 2D electron gas or the nanoconductors are multiparticle structures characterized by a reasonable small number of particles. Besides the single particle dynamics we then have to account for additional effects such as electron-electron interactions and the scattering of impurities. In addition, spin-orbit interactions can also be included. One recognizes that a complete description incorporating all these effects is computationally quite involved if not impossible. However, interactions referred to above may be less important in self assembled GaAs/GaAlAs-heterojunctions (Bastard (1992)), when the electrons occupy the lowest Landau-band only (Chakraborty et al (1994)). Under such conditions single particle electronic spectra are able to provide quite successfully useful information concerning thermodynamic and transport properties.

In this context there are reasons to say that the oscillator system is a useful tool to describe 2D- and 3D quantum dots (Simonin et al (2004)). The same concerns electrodynamic traps for the confinement of charged particles (Wuerker et al (1959), Wineland et al (1987)). The internal crystalline structure of quantum dots can be accounted for by resorting to the effective mass m^* , but descriptions on the discrete space remain desirable. To this aim discrete versions of the harmonic oscillator are presented in sections 4.1 and 5.6. A conceivable candidate for further developments, namely the q -deformed oscillator (Biedenharn (1989), Bonatsos et al (1994)), could also be proposed.

Of a special interest is the Fock-Darwin system, i.e. the single particle 2D parabolic quantum dot potential $kr_0^2/2$ supplemented by influence of a magnetic field $\vec{B}$ perpendicular to the plane of the dot. There is $r_0^2 = x^2 + y^2$, $k = m_0\omega_0^2/2$ and $q_e = -e < 0$, whereas the vector potential is selected in the symmetric gauge. This yields the Schrödinger-equation

$$\left[\frac{1}{2m_0} \left(-i\hbar \frac{\partial}{\partial x} - \frac{e}{2c} Bx \right)^2 + \frac{1}{2m_0} \left(-i\hbar \frac{\partial}{\partial y} + \frac{e}{2c} By \right)^2 + \right. \quad (2.59)$$

$$\left. + \frac{1}{2} kr_0^2 \right] \Psi(\vec{x}) = E \Psi(\vec{x}) \quad ,$$

which can be rewritten equivalently as

$$\mathcal{H}_{FD} \Psi(\vec{x}) = \left(-\frac{\hbar^2}{2m_0} \Delta_2 + \frac{m_0}{2} \omega^2 r_0^2 + \frac{1}{2} \omega_B L_z \right) \Psi(\vec{x}) = E \Psi(\vec{x}) \quad (2.60)$$

by resorting to the third component of the angular momentum operator. There is

$$\omega = \left(\omega_0^2 + \frac{1}{4} \omega_B^2 \right)^{1/2} = \omega_0 (1 + b^2)^{1/2} \quad (2.61)$$

where

$$\omega_B = \frac{eB}{m_0 c} = 2b\omega_0 \quad (2.62)$$

denotes the cyclotron frequency, while b is a transformation parameter. Using planar polar coordinates then gives the radial equation

$$\begin{aligned} & -\frac{\hbar^2}{2m_0} \left(\frac{d^2}{dr_0^2} + \frac{1}{r_0} \frac{d}{dr_0} \right) F(r_0) + \\ & + \left(\frac{m_\varphi^2}{2m_0 r_0^2} + \frac{m_0}{2} \omega^2 r_0^2 \right) F(r_0) = \left(E - \frac{\hbar}{2} m_\varphi \omega_B \right) F(r_0) \end{aligned} \quad (2.63)$$

where $m_\varphi = 0, \pm 1, \pm 2, \dots$ is the magnetic quantum number. So all that needs is the exact solution of the two dimensional isotropic oscillator (see e.g. Kostelevsky et al (1996)). Accordingly, the normalized wavefunction is given by

$$\Psi_n(r_0, \varphi; m_\varphi) = \left(\frac{2n_r!}{l_\omega (|m_\varphi| + n_r)!} \right)^{1/2} \frac{\exp(im_\varphi \varphi)}{\sqrt{2\pi}} F_n(r_0; |m_\varphi|) \quad (2.64)$$

where

$$F_n(r_0; |m_\varphi|) = \exp \left(-\frac{1}{2} \left(\frac{r_0}{l_\omega} \right)^2 \right) \left(\frac{r_0}{l_\omega} \right)^{|m_\varphi|} L_n^{(|m_\varphi|)} \left(\frac{r_0^2}{l_\omega^2} \right) \quad (2.65)$$

One has $n = n_r$ and

$$l_\omega = \left(\frac{\hbar}{m_0 \omega} \right)^{1/2} \quad (2.66)$$

where $n_r = 0, 1, 2, \dots$ denotes the radial quantum number, whereas $L_n^{(\alpha)}(x)$ stands for the Laguerre-polynomial. The corresponding energy reads

$$E = E_n(m_\varphi) = \hbar\omega_0 \left[\sqrt{1+b^2} (|m_\varphi| + 2n_r + 1) + bm_\varphi \right] \quad (2.67)$$

which proceeds in accord with (2.61) and (2.63). The dimensionless radial coordinate, say

$$r = \frac{r_0}{l_\omega} \quad (2.68)$$

can also be used, in which case (2.63) exhibits the typical form

$$\left[r^2 \frac{d^2}{dr^2} + r \frac{d}{dr} + 2(|m_\varphi| + 2n_r + 1)r^2 - r^4 \right] F(r) = m_\varphi^2 F(r) \quad . \quad (2.69)$$

So far, the wavefunction (2.64) obeys the periodic boundary condition

$$\Psi_n(r_0, \varphi; m_\varphi) = \Psi_n(r_0, \varphi + 2\pi; m_\varphi) \quad (2.70)$$

but an additional Aharonov-Bohm (AB) potential like (Aharonov and Bohm (1959))

$$A_\varphi = \frac{\Phi_A}{2\pi r_0}, \quad A_{r_0} = A_z = 0 \quad (2.71)$$

can also be inserted into (2.60). Here Φ_A stands for the thin magnetic flux confined along the Oz -axis. We can put, for convenience, $\Phi_A = \beta_A \Phi_0$, where $\Phi_0 = hc/e$ denotes the magnetic flux quantum, while β_A is a commensurability parameter. This amounts to replace m_φ by

$$m_\varphi \rightarrow m_\varphi + \beta_A \quad (2.72)$$

so that (2.70) becomes

$$\Psi_n(r_0, \varphi + 2\pi; m_A) = \exp(i2\pi\beta_A) \Psi_n(r_0, \varphi; m_A) \quad . \quad (2.73)$$

One remarks that (2.73) looks like the 1D Bloch-theorem (2.10), which opens the way to perform the identification

$$ka = 2\pi\beta_A \quad . \quad (2.74)$$

Now the lattice spacing a has to be viewed as a length scale which is proportional to a circumference.

On the other hand the velocity can be established as

$$v = \frac{1}{\hbar} \frac{dE}{dk} \quad (2.75)$$

where $E = E(k)$ is the related band energy, which is reminiscent to the parabolic energy dispersion law of the free particle. The corresponding current contribution is then given by (see also Chakraborty et al (1994))

$$I = -\frac{ev}{a} = -c \frac{dE}{d\Phi_A} \quad (2.76)$$

in accord with (2.74), which has the meaning of an equilibrium property at $T = 0$. This equation serves to the derivation of the persistent current by identifying E with the energies of quantum ring potentials, as we shall see later. The contribution of scattering states to the persistent current has also been established (Akkermans et al (1991)).

It should also be mentioned that inserting the cyclotron frequency (2.62) into (2.66) instead of ω yields the so called magnetic length

$$l_B = \sqrt{\frac{\hbar c}{eB}} \quad (2.77)$$

which serves as a typical length scale for systems threaded by a magnetic field. Competition effects between a and l_B would then be involved for systems on lattices pierced by a magnetic flux.

2.7 Quantum ring potentials

The displaced oscillator potential (Chakraborty et al (1994))

$$V_R(r_0) = \frac{1}{2}k(r_0 - R_0)^2 \quad (2.78)$$

is a useful candidate to the theoretical description of narrow nanoscopic semiconductor self-assembled rings for which the annular geometry effects are negligible. This potential exhibits a minimum at the ring radius $r_0 = R_0$. However, the quantum ring potential (2.78) is not exactly solvable, so that we have to resort to numerical or approximation methods. In contradistinction, the centrifugal “core” potential (Tan et al (1999))

$$V_R^{(c)}(r_0) = \frac{1}{2}k \left(r_0 - \frac{R_0^2}{r_0} \right)^2 \quad (2.79)$$

can be exactly solved. This proceeds by inserting

$$m_R = \left(m_\varphi^2 + \frac{m_0^2 \omega_0^2}{\hbar^2} R_0^4 \right)^{1/2} \quad (2.80)$$

instead of $|m_\varphi|$ in (2.64) and (2.65), with the understanding that $\exp(im_\varphi\varphi)$ in (2.64) is preserved as it stands. In order to reproduce data concerning actual GaAs-rings, selected numerical values like $m_0 = m^* = 0.067m_e$, $R_0 \cong 800nm$ and $k \cong 4.44 \times 10^{-5} meVnm^2$ have to be considered (Tan et al (1999)). The ring energy is then given by

$$E_R^{(\alpha)} = E_n(m_R) + kR_0^2 \quad (2.81)$$

which works in conjunction with (2.67) and (2.80), where α stands for the quantum numbers, i.e. $\alpha = \{m_\varphi, n_r\}$.

Moreover, the AB potential (2.71) piercing the ring can also be superimposed. The corresponding energy is then given by

$$\tilde{E}_R^{(\alpha)} = \hbar\omega_0 \left[\sqrt{1+b^2} (\tilde{m}_R + 2n_r + 1) + b(m_\varphi + \beta_A) \right] + kR_0^2 \quad (2.82)$$

where

$$\tilde{m}_R = \left((m_\varphi + \beta_A)^2 + \frac{m_0^2 \omega_0^2}{\hbar^2} R_0^4 \right)^{1/2} . \quad (2.83)$$

Azimuthal corrections to the ring potential like (Magnusdottir et al (1999))

$$V_R(r_0, \varphi) = \frac{1}{2} k_a \cos(2\varphi) r_0^2 \quad (2.84)$$

have also been considered.

2.8 Persistent currents and magnetizations

It can be readily verified that the derivative of the energy (2.82) with respect to the magnetic field is given by

$$\frac{\partial}{\partial B} \tilde{E}_R^{(\alpha)} = \frac{e\hbar}{2m_0c} \left[m_\varphi + \beta_A + \frac{\omega_B}{2\omega} (\tilde{m}_R + 2n_r + 1) \right] \quad (2.85)$$

whereas the one with respect to Φ_A reads

$$\frac{\partial}{\partial \Phi_A} \tilde{E}_R^{(\alpha)} = \frac{e\omega}{2\pi c \tilde{m}_R} \left[m_\varphi + \beta_A + \frac{\omega_B}{2\omega} \tilde{m}_R \right] \quad (2.86)$$

Fixing the number of electrons then gives the zero-temperature magnetization

$$M_\alpha = -\frac{\partial}{\partial B} \tilde{E}_R^{(\alpha)} \quad (2.87)$$

so that the total magnetization is given by the sum over states as (Tan et al (1999))

$$M = \sum_\alpha M_\alpha|_{T=0} = \sum_\alpha M_\alpha \theta(E_F - E_\alpha) \quad (2.88)$$

where now $E_\alpha = \tilde{E}_R^{(\alpha)}$ and where $\theta(x)$ denotes Heaviside's step function ($\theta(x) = 1$ for $x \geq 0$ and $\theta(x) = 0$ for $x < 0$). Furthermore, we can make the identification $E = \tilde{E}_R^{(\alpha)}$, in which case the persistent current such as specified by (2.76) is given by

$$I_\alpha = -\frac{e\omega}{2\pi \tilde{m}_R} \left[m_\varphi + \beta_A + \frac{\omega_B}{2\omega} \tilde{m}_R \right] \quad (2.89)$$

the total current being given again by the summation over states:

$$I = \sum_\alpha I_\alpha|_{T=0} = \sum_\alpha I_\alpha \theta(E_F - E_\alpha) \quad (2.90)$$

It is understood that the summations in (2.88) and (2.90) have to be performed by accounting for energies less than the Fermi-energy. Note that such currents have been observed in GaAs/GaAlAs self-assembled rings (Mailly et al (1993)). Next one sees that

$$cM_\alpha = \pi l_\omega^2 \tilde{m}_R I_\alpha - \frac{e\hbar\omega_B}{2m_0\omega} \left(n_r + \frac{1}{2} \right) \quad (2.91)$$

in which the first term from the r.h.s. is the magnetization produced by a current loop, whereas the second one represents a diamagnetic contribution. Applying the virial theorem, it can be easily verified that the expectation value of the squared radial coordinate with respect to the eigenfunction characterizing (2.82) is given by

$$\langle r_0^2 \rangle = l_\omega^2 (\tilde{m}_R + 2n_r + 1) \quad (2.92)$$

in accord with (2.66). So the magnetization produced by the current loop can be rewritten as

$$cM_\alpha^{(loop)} = \pi \langle r_0^2 \rangle \frac{\tilde{m}_R}{\tilde{m}_R + 2n_r + 1} \quad (2.93)$$

which approaches $\pi \langle r_0^2 \rangle$ as $\tilde{m}_R \rightarrow \infty$.

Choosing as an example free electrons on the 1D ring one obtains the number N_e of electrons as

$$N_e = \frac{2}{h} \int_0^L dx \int_0^{p_F} dp \quad (2.94)$$

where L denotes the ring circumference. The Fermi momentum $p_F = \hbar k_F$ is given by $E_F = p_F^2/2m_0$, as usual. Accordingly, there is

$$N_e = \frac{Lk_F}{\pi} \quad (2.95)$$

so that specifying the number of electrons amounts to consider a fixed value of the Fermi momentum.

Assuming that $T \neq 0$, we have to consider the canonical partition function

$$Z = \sum_\alpha \exp \left(-\frac{E_\alpha}{k_B T} \right) \quad (2.96)$$

for which the number of electrons is fixed. Inserting $E_\alpha = \tilde{E}_R^{(\alpha)}$ into (2.96), one realizes that Z is an even periodic function of the AB magnetic flux Φ_A (Byers et al (1961)). The underlying background is the summation over the magnetic quantum number from $-\infty$ to ∞ , which proceeds both for $T = 0$ and $T \neq 0$. This explains the appearance of AB-oscillations in the magnetic flux dependence of thermodynamic properties. So, the $T \neq 0$ counterpart of the $T = 0$ magnetization (2.88) is given by

$$M(\Phi, T) = -\frac{1}{Z} \sum_\alpha \frac{\partial}{\partial B} \exp \left(-\frac{E_\alpha}{k_B T} \right) \quad (2.97)$$

where Φ stands for the axial magnetic flux. Similarly, the temperature dependent persistent current reads

$$I(\Phi, T) = -\frac{1}{Z} \sum_{\alpha} \frac{\partial}{\partial \Phi} \exp\left(-\frac{E_{\alpha}}{k_B T}\right) \quad (2.98)$$

which is still a periodic, but an odd function of the magnetic flux Φ . We have to recognize that the derivation of temperature effects characterizing (2.95) and (2.96) is a lengthy job, but ingredients needed are presented in Appendix A in Cheung et al (1988). The influence of the electric field has also been considered (Barticevic et al (2002)). Thermodynamic properties relying on the grand canonical partition function are briefly discussed in section 8.6.

2.9 The derivation of the total persistent current for electrons on the 1D ring at $T = 0$

Let us consider as a next example free electrons on the planar 1D ring threaded by a magnetic flux Φ . The energies are given by Schrödinger equation

$$-\frac{\hbar^2}{2m_0 R_0^2} \frac{d^2}{d\varphi^2} \psi(\varphi) = E \psi(\varphi) \quad (2.99)$$

working in conjunction with the AB -type periodic boundary condition

$$\psi(\varphi + 2\pi) = \exp(i2\pi\beta) \psi(\varphi) \quad (2.100)$$

where $\beta = \Phi/\Phi_0$ and $\varphi \in [0, 2\pi]$. Proceeding in this manner gives the energy and the eigenfunction as

$$E = E_n = \frac{\hbar^2}{2m_0 R_0^2} (n + \beta)^2 \quad (2.101)$$

and

$$\psi = \psi_n(\varphi) = \frac{1}{\sqrt{2\pi}} \exp(i(\beta + n)\varphi) \quad (2.102)$$

respectively, where $n = 0, \pm 1, \pm 2, \dots$. The corresponding persistent current is then given by