EUROPHYSICS LETTERS

OFFPRINT

Vol. 68 • Number 5 • pp. 632–638

Quantum chaos in the Bose-Hubbard model

* * *

A. R. Kolovsky and A. Buchleitner

Published under the scientific responsibility of the

EUROPEAN PHYSICAL SOCIETY

Incorporating

JOURNAL DE PHYSIQUE LETTRES • LETTERE AL NUOVO CIMENTO

Europhys. Lett., **68** (5), pp. 632–638 (2004)
DOI: 10.1209/epl/i2004-10265-7

Quantum chaos in the Bose-Hubbard model

A. R. Kolovsky[1,2] and A. Buchleitner[1]

[1] *Max-Planck-Institut für Physik Komplexer Systeme - D-01187 Dresden, Germany*
[2] *Kirensky Institute of Physics - 660036 Krasnoyarsk, Russia*

received 15 June 2004; accepted in final form 13 October 2004
published online 5 November 2004

PACS. 05.45.Mt – Quantum chaos; semiclassical methods.
PACS. 05.30.Jp – Boson systems.
PACS. 03.75.Kk – Dynamic properties of condensates; collective and hydrodynamic excitations, superfluid flow.

Abstract. – We present a numerical study of the spectral properties of the 1D Bose-Hubbard model. Unlike the 1D Hubbard model for fermions, this system is found to be non-integrable, and exhibits Wigner-Dyson spectral statistics under suitable conditions.

During the last two decades much attention has been paid to the spectral properties of quantum systems which exhibit chaotic dynamics in the classical limit. The intrinsic complexity of these systems (due to underlying chaos) leads to an irregular energy spectrum with universal statistical properties —a phenomenon often referred to as "quantum chaos" [1]. One of the recent developments in the field is related to "many-body quantum chaos" [2]. Here the systems of interest consist of many interacting (identical) particles and may have no classical counterpart. Notwithstanding this, numerical studies of some simple models (like, for example, a 1D chain of interacting spins [3,4]) have shown that also the spectrum of a deterministic many-body system(1) can exhibit universal statistics. In the present paper we numerically study the spectrum of the 1D Bose-Hubbard model [5,6]. Our particular interest in this system stems from its possible laboratory realization with cold atoms loaded into optical lattices [7]. We will show that, unlike the 1D Hubbard model for fermions, the 1D Bose-Hubbard model is generally non-integrable. Moreover, in a certain parameter regime, its spectrum obeys the Wigner-Dyson statistics for Gaussian Orthogonal Ensembles characteristic of quantum chaotic systems. Let us also stress that here we focus on the limit of an infinite lattice with filling factor (this is the average number of atoms per lattice site) $\bar{n} \simeq 1$. This condition allows for direct comparison of the Hubbard model for bosons with that for fermions and distinguishes the present contribution from refs. [8–12], devoted to the properties of the two- and three-site Bose-Hubbard model in the limit $\bar{n} \to \infty$.

The Hamiltonian of the 1D Bose-Hubbard (BH) model reads

$$\widehat{H} = -\frac{J}{2}\left(\sum_l \hat{a}^\dagger_{l+1}\hat{a}_l + \text{H.c.}\right) + \frac{W}{2}\sum_l \hat{n}_l(\hat{n}_l - 1). \tag{1}$$

(1)By "deterministic system" we understand that, on the level of the Hamiltonian, the system does not exhibit any randomness.

Having in mind spinless atoms in a quasi-1D optical lattice, the creation, $\hat{a}_l^\dagger$, or annihilation, $\hat{a}_l$, operator in (1) "creates" or "annihilates" an atom in the l-th well of the optical potential, in a Wannier state $\psi_l(x)$. The parameter J is the hopping matrix element, the parameter W the on-site interaction energy for atoms sharing one and the same well. The Hilbert space of the system (1) is spanned by Fock states given by symmetrised products of single-particle Wannier states in the coordinate representation. Assuming a finite size of the lattice, $l = 1, \ldots, L$, and a finite (conserved) number N of the atoms, the dimension of the Hilbert space is $\mathcal{N} = (N + L - 1)!/N!(L - 1)!$.

Note that, instead of the Wannier basis, one can use a basis given by symmetrised products of Bloch waves $\phi_\kappa(x) = (1/\sqrt{L}) \sum_l \exp[i\kappa l]\psi_l(x)$, where $\kappa = 2\pi k/L$ is the single-particle quasimomentum ($\kappa = 2\pi$ corresponds to the centre of the Brillouin zone). In second quantisation, this change of the basis amounts to the substitution $\hat{b}_k = (1/\sqrt{L}) \sum_l \exp[i2\pi kl/L]\hat{a}_l$. Then the Hamiltonian (1) takes the form (up to an additive term $WN/2$)

$$\widehat{H} = -J\sum_k \cos\left(\frac{2\pi k}{L}\right)\hat{b}_k^\dagger \hat{b}_k + \frac{W}{2L}\sum_{k_1,k_2,k_3,k_4} \hat{b}_{k_1}^\dagger \hat{b}_{k_2} \hat{b}_{k_3}^\dagger \hat{b}_{k_4} \tilde{\delta}(k_1 - k_2 + k_3 - k_4), \tag{2}$$

where $\tilde{\delta}(k) = 1$ if k is a multiple of L, and $\tilde{\delta}(k) = 0$ otherwise (conservation of total quasimomentum).

Let us proceed with our analysis of the spectrum of the BH model. In the limiting cases $J = 0$ (no hopping) and $W = 0$ (non-interacting bosons), the BH model is completely integrable, with eigenstates given by symmetrised products of single-particle Wannier states, $|n_1, \ldots, n_l, \ldots, n_L\rangle$, or Bloch states, $|n_1, \ldots, n_k, \ldots, n_L\rangle$, respectively. The corresponding eigenvalues are

$$E_\mu = W\mu, \quad \mu = \frac{1}{2}\sum_{l=1}^{L} n_l(n_l - 1), \sum_{l=1}^{L} n_l = N, \tag{3}$$

for $J = 0$, and

$$E_\nu = -J\nu, \quad \nu = \sum_{k=1}^{L} \cos\left(\frac{2\pi k}{L}\right) n_k\,, \sum_{k=1}^{L} n_k = N, \tag{4}$$

for $W = 0$. Note that in both cases the majority of the energy levels are multiply degenerate, *i.e.* different combinations of integers n_l (n_k) may result in the same values of μ (ν).

We now demonstrate the non-integrability of the BH model for J, $W \neq 0$. The left panel in fig. 1 shows the BH spectrum for finite size $L = N = 5$ as a function of the parameter $u = W$ with $J = 1 - u$. The first step of the analysis is to account for the trivial symmetry of the spectrum, due to the translational invariance of the Hamiltonian. This implies that the Hamiltonian (1), (2) factorises as

$$H = \bigoplus_{k=1}^{L} H^{(\kappa)}, \tag{5}$$

where $\kappa = 2\pi k/L$ is now the *total* quasimomentum. Thus, the spectrum in fig. 1(a) is a superposition of L independent spectra. Next we account for the "odd-even" symmetry of the $\kappa = \pi$ and $\kappa = 2\pi$ subspaces. The levels of the odd $\kappa = 2\pi$ symmetry are shown in the right panel of fig. 1. No crossings between levels are left (on the scale of the figure, some tiny avoided crossings are not resolved), and, thus, no further decomposition of the spectrum is possible. This proves the non-integrability of the system(2). Note that, in contrast, the 1D Hubbard

(2)For a brief discussion of the non-crossing scenario see, *e.g.*, ref. [13], which also contains an extended list of related references.

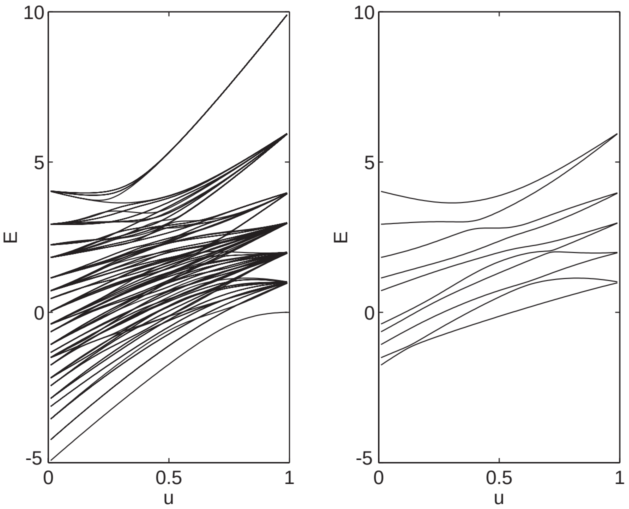

Fig. 1 – Energy level dynamics of the BH model as a function of the parameter $u \equiv W$, $J = 1 - u$, for $L = N = 5$ and periodic boundary conditions. The left panel shows the complete spectrum, the right panel singles out the "odd $\kappa = 2\pi$" symmetry component.

model for fermions is integrable for arbitrary u. In the latter case, in addition to the trivial (u-independent) symmetries (like quasimomentum and odd-even symmetry), the system has a number of non-trivial (u-dependent) integrals [13, 14]. Therefore, the spectrum of the 1D (Fermi) Hubbard model can be decomposed further until only one (possibly degenerate) level is left.

The non-integrability of our present system (manifest in the avoided crossings in the right panel of fig. 1) does not yet guarantee that the spectrum of the BH model has the universal statistical properties associated with quantum chaos. Loosely speaking, the latter requires a delocalisation of the eigenfunctions of the system in any generic basis. To quantify such delocalisation, we consider the Shannon entropy

$$S(u) = \left\langle -\frac{1}{\log \mathcal{N}} \sum_{j=1}^{\mathcal{N}} \left|c_j\right|^2 \log\left(|c_j|^2\right) \right\rangle, \tag{6}$$

where the c_j are the expansion coefficients of an arbitrary eigenstate of the system in a given basis, and the angular brackets denote an average over all eigenstates. It is reasonable to choose as a basis the "ν-basis", when our starting point is $u = 0$ (no interaction), or the "μ-basis", when starting at $u = 1$ (no hopping). First, let us clarify the notion of ν- and μ-basis. As mentioned above, and as apparent from fig. 1, the spectrum of the system at $u = 1$ ($J = 0$) consists of a number of degenerate levels with energies given in eq. (3). An arbitrarily small J removes this degeneracy, and the levels split into a μ-band with a width proportional to J. Moreover, there is a vicinity of $J = 0$ where the widths of the μ-bands are much smaller than the distance between them and, hence, the eigenfunctions of the system do not depend on J. These states form the μ-basis. More formally, the μ-basis is given by the eigenstates of the Hamiltonian (1), where the matrix elements between Fock states with different μ are set to zero (by hand). Analogously, the ν-basis is given by the eigenstates of the Hamiltonian (2) where the matrix elements between states with different ν are set to zero.

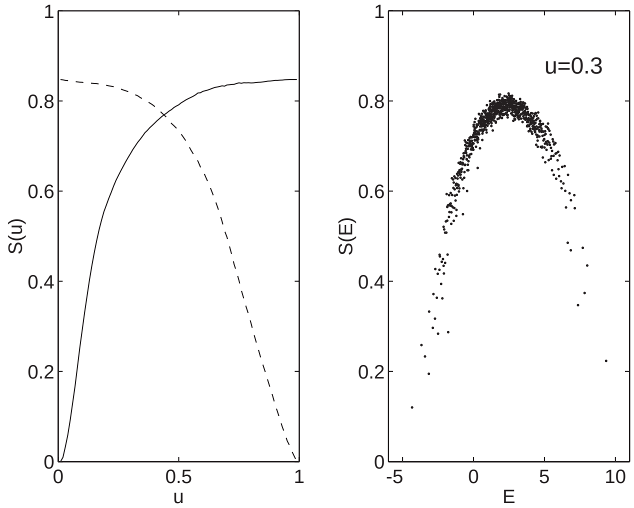

Fig. 2 – Left panel: mean entropy (6) in the ν-basis (solid line) and in the μ-basis (dashed line) as a function of the interaction parameter u ($N = L = 8$). Right panel: entropy (10) of the individual eigenstates (dots), for $u = 0.3$.

The entropy (6) calculated in the ν-basis (solid line) and in the μ-basis (dashed line), respectively, is depicted in the left panel of fig. 2, for a filling factor $\bar{n} = N/L = 1$. There is a relatively wide interval of u where the functions $S^{(\nu)}(u)$ and $S^{(\mu)}(u)$ *simultaneously* take large values(3). Thus, the eigenfunctions of the system are essentially delocalised in either of the two basis sets, and one may expect universal spectral statistics. Indeed, a statistical analysis of the spectrum confirms this expectation. The histogram in the upper panel of fig. 3 shows the distribution of eigenenergies E for $L = N = 8$ and $u = 0.3$. The numerically obtained density of states is well approximated by a Gaussian distribution, $\rho(E) \sim \exp[-(E-\bar{E})^2/\sigma^2]$, where $\bar{E}$ and σ are fitting parameters(4). Using $\bar{E}$ and σ from the best fit we unfold the spectrum and extract the nearest-neighbour level statistics for $\kappa = 2\pi$ and $\kappa = 2\pi/L$. The result is presented in the lower panel of fig. 3, by the integrated level spacing distribution $I(s)$, $s = \Delta E \rho(E)$ (solid line), and compared to the Random Matrix Theory predictions for the Poissonian (dash-dotted line),

$$I(s) = 1 - \exp[-s], \tag{7}$$

and the Gaussian orthogonal (dashed line) ensemble,

$$I(s) = 1 - \exp\left[-\frac{\pi s^2}{4}\right], \tag{8}$$

as well as for the case resulting from a superposition of two independent GOE spectra (dotted line),

$$I(s) = 1 + \exp\left[-\frac{\pi s^2}{16}\right]\left[-1 + \mathrm{erf}\left(\frac{\sqrt{\pi}s}{4}\right)\right]. \tag{9}$$

(3)Notice an analogy with the results of ref. [15] for the 1D chain of randomly interacting fermions.

(4)In the present case of moderate interaction strength, the parameters σ and $\bar{E}$ scale with the number of atoms N as $\sigma \sim J\sqrt{N}$ and $\bar{E} \sim W\bar{n}^2 N$. Let us also note that for strong interaction we observe an asymmetric density of states, and the approximation of $\rho(E)$ by a Gaussian is no longer valid.

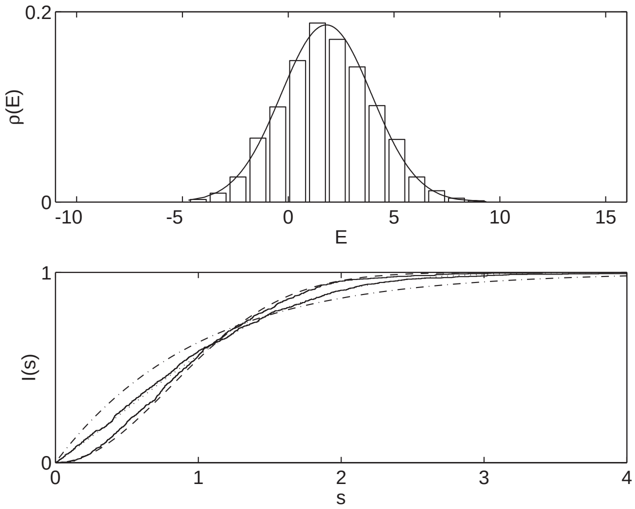

Fig. 3 – Density of states (upper panel) and integrated level spacing distributions (lower panel) for $L = N = 8$ and $u = 0.3$. The solid line in the upper panel is the best Gaussian fit to the numerically obtained density of states. The dash-dotted, dashed and dotted lines in the lower panel represent the random matrix predictions (7)-(9) for Poissonian, Gaussian orthogonal (GOE), and two superimposed, independent GOE ensembles, respectively. The solid lines are obtained from the numerical data for $\kappa = 2\pi$ (which reproduce the expectation for superimposed GOE spectra), and for $\kappa = 2\pi/8$ (which faithfully obey the GOE prediction).

The numerical data faithfully follow the distributions (8), (9) for quasimomentum $\kappa = 2\pi/L$ and $\kappa = 2\pi$, respectively, where the odd and the even part of the spectrum are superimposed in the latter case. Note that, since the present analysis involves the unfolding of the spectrum, the above results hold for arbitrary L.

We now address the conditions for quantum chaos to prevail in the BH model. Obviously, the above criterion based on the mean entropy (6) provides only a rough estimate on the parameter region where one may expect an irregular spectrum. Moreover, besides the interaction parameter u and the filling factor $\bar{n}$, also the energy E should be considered as a relevant parameter. As an illustration of this statement, the right panel in fig. 2 shows the entropy of the individual eigenstates,

$$S(E) = \min\left[S^{(\nu)}(E), S^{(\mu)}(E)\right], \tag{10}$$

which are labeled here by the individual level's energy E. Obviously, there is a non-vanishing fraction of localised eigenstates associated with the lower and upper parts of the spectrum. Hence, one has to distinguish regular and chaotic spectral components [16]. In the presently considered case ($u = 0.3$, $\bar{n} = 1$), the regular component is negligible (less than 1/10 of the total number of levels) and, hence, the level spacing distribution follows the universal Wigner-Dyson law. However, when the ratio J/W approaches either one of the integrable limits, the regular component gradually increases at the expense of the irregular one, which causes a deviation from the universal distribution. The same holds true if we decrease the value of the filling factor. In this latter case, the chaotic component (typically located in the central part of the spectrum) is small even for $J/W \simeq 1$. Further studies are needed for a precise mapping of the chaotic region of the BH model in the parameter space spanned by u, $\bar{n}$, and E.

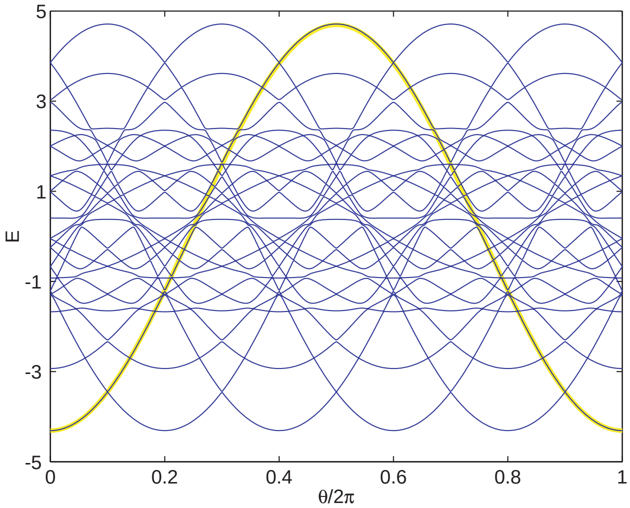

Fig. 4 – Level dynamics of the modified BH model (11) for $u = 0.1$, $\kappa = 2\pi$, and $L = N = 5$. The grey (yellow on-line) shaded energy level is the diabatic approximation for the ground-state evolution, which neglects the interaction-induced avoided crossings.

Let us finally discuss the physical manifestations of the irregular spectrum of the BH model, *i.e.* its relevance for ongoing experiments with cold atoms in optical lattices [7, 17–19]. Obviously, to probe the irregular part of the spectrum one has to excite the system. This can be done, for example, by applying a static force, *i.e.*, adding a term $F\sum_l l\hat{n}_l$ to the Hamiltonian (1). Note that the translational symmetry of the system, broken by this term, can be recovered by a suitable gauge transformation [20]. This leads to a time-dependent Hamiltonian of the form

$$\widehat{H}(t) = -\frac{J}{2}\left(e^{iFt}\sum_l \hat{a}^\dagger_{l+1}\hat{a}_l + \text{H.c.}\right) + \frac{W}{2}\sum_l \hat{n}_l(\hat{n}_l - 1), \tag{11}$$

and a parametric dependence of the eigenvalues of the Hamiltonian (11) on $\theta = Ft$, as illustrated in fig. 4 (for $L = N = 5$, $\kappa = 2\pi$, as in fig. 1, and $u = 0.1$). Let us assume for a moment that there are no atom-atom interactions and, thus, all avoided crossings in fig. 4 are true crossings. Then, in the course of time, the static force will drive the system along the continuation of the ground state (the grey shaded energy level in fig. 4), representing nothing else than *bona fide* Bloch oscillations, where the system comes back to its initial state after one Bloch period $T_\text{B} = 2\pi/F$. It is clear, however, that for $u \neq 0$ the system generally does not come back to the initial state, because of Landau-Zener transitions at the avoided crossings encountered during one Bloch cycle(5). In other words, after the Bloch cycle is completed, some excited states will be populated as a consequence of (a)diabatic transitions along the diabatic continuation of the ground state. (The branching ratio between diabatic and adiabatic transitions is obviously determined by the time derivative of θ, *i.e.*, by the field amplitude F.) In the case of strong static forcing, $F \gg J$, this excitation process is reversible, leading to *quasiperiodic* Bloch oscillations [21]. In contrast, for moderate forcing

(5)Note that all levels in fig. 3 anticross, at finite u, except for occasional exact crossings between even and odd symmetry states, at $\theta_j = (\pi/L)j$, $j = 0, \ldots, 2L-1$.

and chaotic instantaneous spectrum([6]) the excitation is irreversible, leading to decoherence of the one-particle density matrix and, as a consequence, to decay of the Bloch oscillations [22]. Since Bloch oscillations of the atoms are easily measured in laboratory experiments [17–19], their *irreversible decay* will provide a direct indication of chaos in the BH system.

In conclusion, for small filling factors $\bar{n} \simeq 1$ and large lattices $L \gg 1$, the 1D Bose-Hubbard model reveals universal spectral statistics characteristic for quantum chaotic systems, provided tunnelling coupling and on-site interaction energy are of comparable magnitude. At these filling factors, the Bose-Hubbard model might appear rather reminiscent of the Hubbard model for fermions —which is known to be integrable— since the probability for more than two atoms to occupy the same site is strongly suppressed. Notwithstanding this, our results clearly illustrate the delicate role of the residual particle-particle interactions.

REFERENCES

[1] Giannoni M.-J., Voros A. and Zinn-Justin J. (Editors), *Chaos and Quantum Physics* (North-Holland, Amsterdam) 1991.
[2] Izrailev F. M., *New Directions in Quantum Chaos*, edited by Casati G., Guarneri I. and Smilansky U. (IOS Press, Amsterdam) 2000.
[3] Montambaux G., Poilblanc D., Bellissard J. and Sire C., *Phys. Rev. Lett.*, **70** (1993) 497.
[4] Berman G. P., Borgonovi F., Izrailev F. M. and Tsifrinovich V. I., *Phys. Rev. E*, **64** (2001) 056226.
[5] Fisher M. P. A., Weichman P. B., Grinstein G. and Fisher D. S., *Phys. Rev. B*, **40** (1989) 546.
[6] Sachdev S., *Quantum Phase Transitions* (Cambridge University Press, Cambridge) 2001.
[7] Greiner M., Mandel O., Esslinger T., Hänsch T. W. and Bloch I., *Nature*, **415** (2002) 39.
[8] Milburn G. J. *et al.*, *Phys. Rev. A*, **55** (1997) 4318.
[9] Anglin J. R. and Vardi A., *Phys. Rev. A*, **64** (2001) 013605.
[10] Polkovnikov A., Sachdev S. and Girvin S. M., *Phys. Rev. A*, **66** (2002) 053607.
[11] Mahmud K. W., Perry H. and Reinhardt W. P., *J. Phys. B*, **36** (2003) L265.
[12] Buonsante P., Franzosi R. and Penna V., *Phys. Rev. Lett.*, **90** (2003) 050404.
[13] Yuzbashyan E. A., Altshuler B. L. and Shastry B. S., *J. Phys. A*, **35** (2002) 7525.
[14] Shastry B. S., *Phys. Rev. Lett.*, **56** (1986) 1529.
[15] Jacquod Ph. and Varga I., *Phys. Rev. Lett.*, **89** (2002) 134101.
[16] Di Stasio M. and Zotos X., *Phys. Rev. Lett.*, **74** (1995) 2050.
[17] Ben Dahan M. *et al.*, *Phys. Rev. Lett.*, **76** (1996) 4508.
[18] Morsch O. *et al.*, *Phys. Rev. Lett.*, **87** (2001) 140402.
[19] Roati G. *et al.*, cond-mat/0402328 (2004).
[20] Kolovsky A. R. and Buchleitner A., *Phys. Rev. E*, **68** (2003) 056213.
[21] Kolovsky A. R., *Phys. Rev. Lett.*, **90** (2003) 213002.
[22] Buchleitner A. and Kolovsky A. R., *Phys. Rev. Lett.*, **91** (2003) 253002.

([6])A statistical analysis of the instantaneous spectrum (not presented here) suggests the following simple rule: If the spectrum at $\theta = 0$ exhibits universal random matrix statistics, it equally does so for $\theta \neq 0$. For the presently considered case, $\kappa = 2\pi$ and $L = N$, this means that the spectrum reproduces eq. (9) for $\theta = \theta_j$, interpolates between (9) and (8) in the vicinity of these symmetry points, and obeys eq. (8) for other values of θ.