Solutions – Sheet 4

1) With $S_j^x = \frac{1}{2}(\sigma_j^+ + \sigma_j^-)$ and $S_j^y = \frac{i}{2}(\sigma_j^- - \sigma_j^+)$

we have $$H = -\frac{J}{2}\sum_{j=1}^{L-1}\left(\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+\right) + \Delta\sum_{j=1}^{L-1} S_j^z S_{j+1}^z .$$

JW

$$\xrightarrow{\text{JW}} \tilde{H}_{JW} = -\frac{J}{2}\sum_{j=1}^{L-1}\left(c_j^\dagger c_{j+1} + h.c.\right) + \Delta\sum_{j=1}^{L-1}\left(c_j^\dagger c_j - \frac{1}{2}\right)\left(c_{j+1}^\dagger c_{j+1} - \frac{1}{2}\right)$$

$$\boxed{\begin{aligned} &F_j = e^{i\pi\sigma_j^+\sigma_j^-} = e^{i\pi c_j^\dagger c_j} = (-1)^{n_j},\quad F_j = F_j^\dagger = F_j^2 = 1,\quad [F_j, c_i] = 0,\ i\neq j \\ &c_j^\dagger F_j = -F_j c_j^\dagger = c_j^\dagger,\quad \sigma_j^+ = F_1\cdots F_{j-1}c_j^\dagger,\quad S_j^z = c_j^\dagger c_j - \frac{1}{2} \end{aligned}}$$

- PBC: $$H_{JW}^{PBC} = \frac{J}{2}(-1)^{\sum_j c_j^\dagger c_j}\left(c_L^\dagger c_1 + h.c.\right) + \Delta\left(c_L^\dagger c_L - \frac{1}{2}\right)\left(c_1^\dagger c_1 - \frac{1}{2}\right).$$

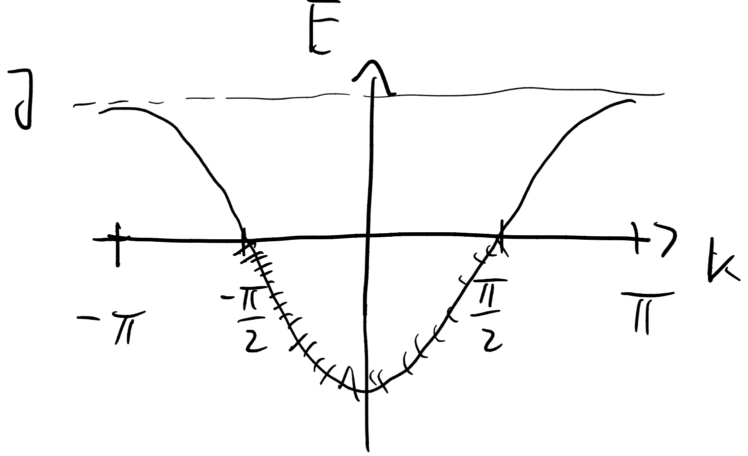
- Cleary $[H, S_z] = 0$ since H only contains products of S_j^z's and $\sigma_i^+ \sigma_j^-$, i.e. terms with the same number of increasing and lowering operators.

  Analogously $[H_{JW}, N] = 0$, since H_{JW} contains only terms with the same number of creation and annihilation operators.

- Limiting cases: (i) $\Delta \to -\infty$, then $H \approx -|\Delta| \sum_j S_j^z S_{j+1}^z$,
  (J finite) i.e. a classical Ising ferromagnet with degenerate ground states $|\uparrow, \dots, \uparrow\rangle$, $|\downarrow, \dots, \downarrow\rangle$ with $S_z = \pm \frac{L}{2}$.

  (ii) $\Delta \to +\infty$, then $H \approx |\Delta| \sum_j S_j^z S_{j+1}^z$, i.e. a classical anti-ferromagnet with degenerate ground states $|\uparrow\downarrow\uparrow\downarrow\ldots\rangle$, $|\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\ldots\rangle$ with $S_z = 0$ (even L).

(iii): $\Delta \to 0$: $H_{JW} = -\frac{J}{2} \sum_j c_j^\dagger c_{j+1} + h.c.$



$$\underset{L\to\infty}{=} \int_{-\pi}^{+\pi} \frac{dk}{2\pi}\, c_k^\dagger (-J\cos k)\, c_k$$

$\rightsquigarrow$ Ground state is Slater determinant with states $|k| < k_F = \frac{\pi}{2}$ filled with free fermions.

In spin language, this state has magnetization $S_z = 0$ (half-filling).

2.) ED with total S_z conservation.

(i) List all states with fixed $N_\uparrow = L - N_\downarrow$ from smaller to larger integers to build the $I[J]$ lookup table.

↳ Example $L=4$, $N_\uparrow = 2$

				I	J
$\vert\downarrow\downarrow\uparrow\uparrow\rangle$ →	0011 →	$0\cdot 2^3 + 0\cdot 2^2 + 1\cdot 2^1 + 1\cdot 2^0$	$=$	3	0
$\vert\downarrow\uparrow\downarrow\uparrow\rangle$ →	0101 →	— — — — —	$=$	5	1
$\vert\downarrow\uparrow\uparrow\downarrow\rangle$ →	0110 →	— — — — —	$=$	6	2
$\vert\uparrow\downarrow\downarrow\uparrow\rangle$ →	1001 →	— — — —	$=$	9	3
$\vert\uparrow\downarrow\uparrow\downarrow\rangle$ →	1010 →	— — — — —	$=$	10	4
$\vert\uparrow\uparrow\downarrow\downarrow\rangle$ →	1100 →		$=$	12	5

↳ Generally, start from $\underbrace{00\ldots0}_{L-N_\uparrow}\underbrace{1\ldots1}_{N_\uparrow} \simeq \sum_{j=0}^{N_\uparrow - 1} 2^j$

and use the function next_permutation (in C++, similar routines exist in all languages) to generate all other permutations.

(ii) Use two-table method to build $\hat{J}[I] = \hat{J}_a[I_a] + \hat{J}_b[I_b]$ lookup tables. (See Lecture 10 for details and the example $L=4, N_\uparrow = 2$).

- Note that (i), (ii) are independent of the concrete model (assuming only S_z/N-conservation).
- Quick and dirty (slower) version (extra cost $\mathcal{O}(\log(\dim \mathcal{H}))$): Use map data structure (containers.Map in Matlab).
  C++, python
  No significant extra cost in memory.

(iii) Build sparse-matrix of Hamiltonian (or on the fly $H|\psi\rangle$-routine) following the scheme in Lecture 9 (see also sheet 3).

(iv) Implement Lanczos-routine (see Lecture 8) or use internal routine of your favorite language with the sparse matrix from (iii) as an input.

3. Detecting phase transitions in the XXZ-chain from energy levels in different symmetry sectors ($J = 1.0$)

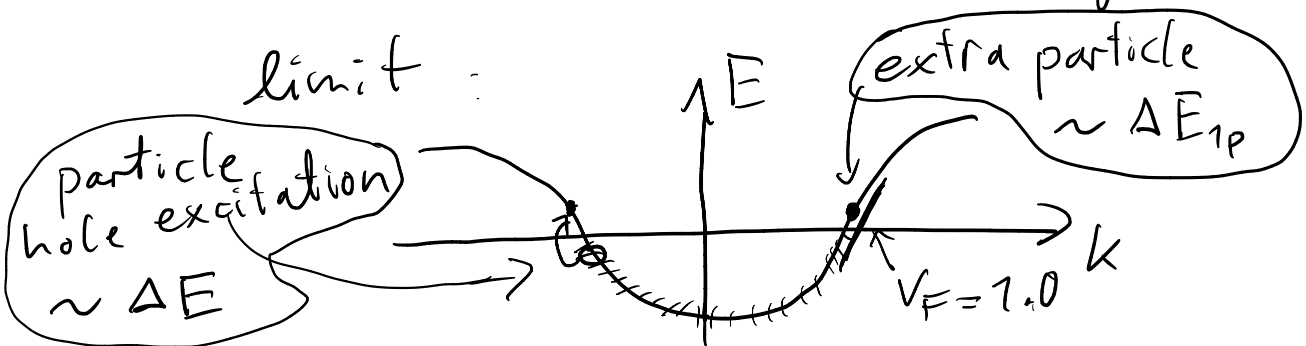
(i) Phase transition to Ising ferromagnet at $\Delta = -1$, detected by crossing of the lowest eigenvalue in the $S_z = \pm \frac{L}{2}$ and the $S_z = 0$ sector.

(ii) $\Delta E(S_z=0) := E_1(S_z=0) - E_0(S_z=0)$ (excitation gap within the $S_z=0$ sector)

$$\Delta E_{1p} := E_0\left(S_z = \pm\tfrac{1}{2}\right) - E_0(S_z=0)$$ ("one-particle" gap)

At $\Delta = 1$, we see a crossing of $E_1(S_z=0)$ and $E_0(S_z=\pm\frac{1}{2})$, where for $\Delta >> 1$, $E_0(S_z=0)$ and $E_1(S_z=0)$ become degenerate (Ising AFM, $\Delta E(S_z=0)\to 0$).

For $\Delta < 1$, by contrast $\Delta E_{1p} < \Delta E(S_z=0)$. The latter can be understood from the $\Delta = 0$ (free fermion) limit :

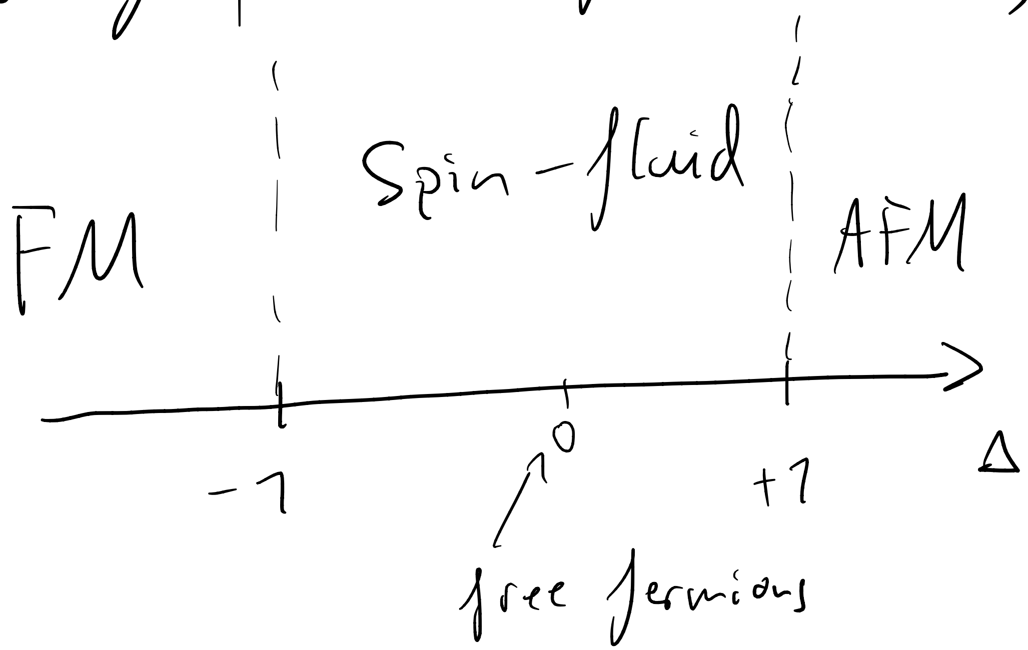


- Cost of putting extra particle $\geq \frac{2\pi}{L}\cdot v_F$
  $\leadsto \Delta E_{1p} \gtrsim \frac{2\pi}{L}$

- Cost of particle hole excitation $\geq 2 \cdot v_F \frac{2\pi}{L}$

$\rightsquigarrow \Delta E (S_z = 0) \gtrsim \frac{4\pi}{L}$.

- Resulting phase diagram $(J = 1)$



Benchmark Data: Lowest energy levels for L=16, J=1.0

Δ	PBC	OBC	S_z
-2	-8	-7.5	$\pm L/2$
-0.5	-4.413613	-4.190956	0
0.5	-6.042763	-5.835389	0
2	-9.906586	-9.510953	0

All following data for L=16, J=1.0

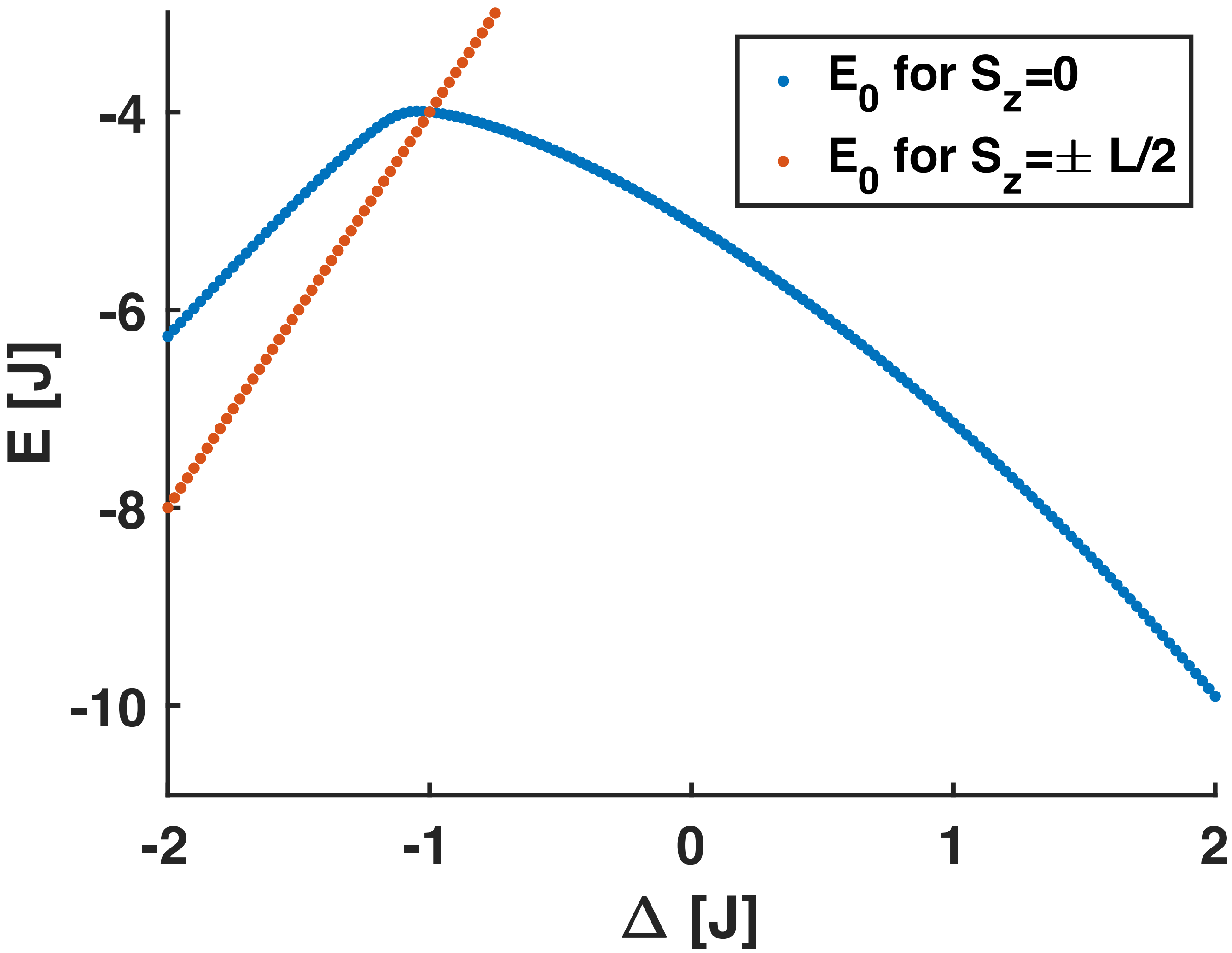


Figure 1: Lowest energy eigenvalue for the $S_z = 0$ magnetization sector (blue data) and the $S_z = \pm\frac{L}{2}$ sector (orange data) as a function of $\Delta \in [-2, 2]$. As $\Delta < -1$ the ground-state changes from being in the $S_z = 0$ sector to being in the $S_z = \pm\frac{L}{2}$ sector. This hints to the fact that for $\Delta < -1$ the system tends to a Ising ferromagnetic order in the ground-state, as suggested by studying the limit $\Delta \to -\infty$.

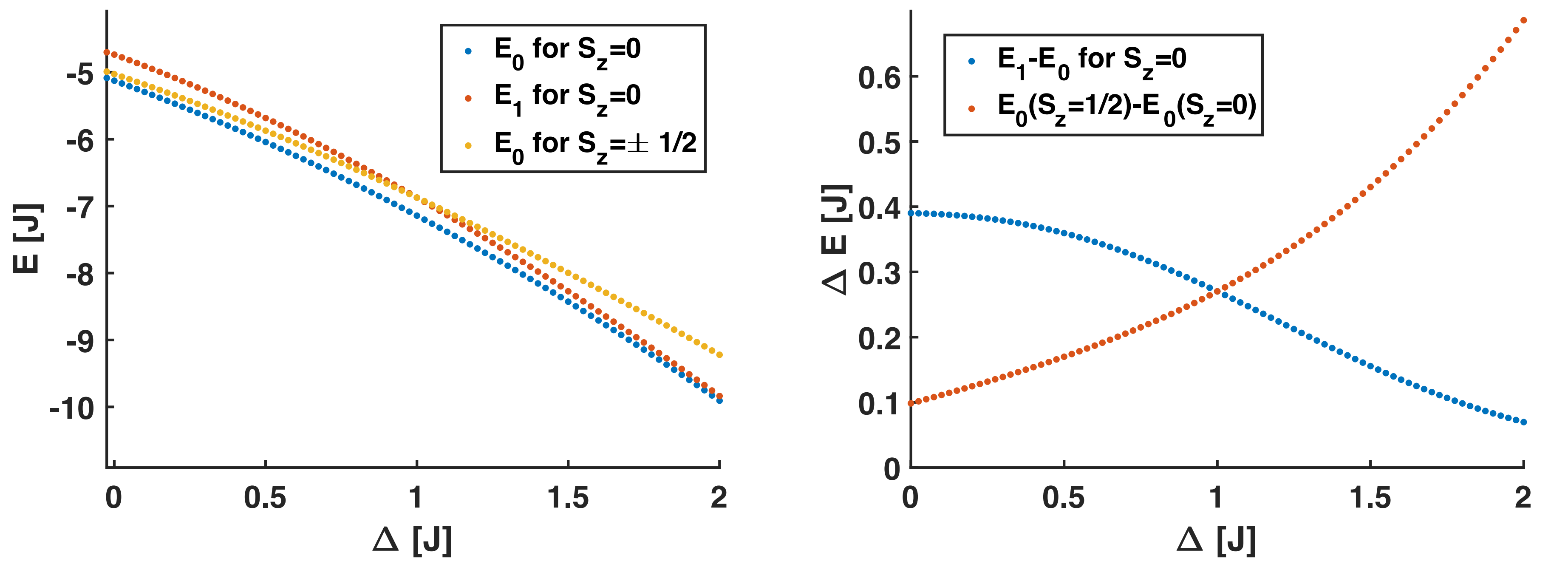


Figure 2: Left panel: Lowest energy eigenvalue for the $S_z = 0$ magnetization sector ($E_0(S_z = 0)$, blue data) and for the $S_z = \pm\frac{1}{2}$ sector ($E_0(S_z = \pm 1/2)$, yellow data), and first excited state energy for the $S_z = 0$ magnetization sector ($E_1(S_z = 0)$, orange data), as a function of $\Delta \in [0, 2]$. For $\Delta = 1$ the two energy levels $E_1(S_z = 0)$ and $E_0(S_z = \pm 1/2)$ cross. This is a signature of the transition to an anti-ferromagnetic regime present for $\Delta > 1$. This is more apparent in the right panel, where the $S_z = 0$ excitation gap $\Delta E(S_z = 0) = E_1(S_z = 0) - E_0(S_z = 0)$ (blue data) and the single-particle gap $\Delta E_{1p} = E_0(S_z = \pm 1/2) - E_0(S_z = 0)$ (orange data), are plotted vs. $\Delta \in [0, 2]$. This level crossing can be qualitatively understood from the fact that in the Ising anti-ferromagnet limit $\Delta \to \infty$ there are two doubly degenerate ground states $|\uparrow\downarrow\uparrow .. \downarrow\rangle$ and $|\downarrow\uparrow\downarrow .. \uparrow\rangle$, both with $S_z = 0$, therefore $\Delta E(S_z = 0)$ decays to 0 for $\Delta \to \infty$. On the other hand, in the anti-ferromagnetic limit there is a finite energy cost scaling with Δ for adding a spin $\uparrow$ or $\downarrow$ excitation. On the other hand, the fact that $\Delta E_{1p} < \Delta E(S_z = 0)$ for $\Delta < 1$ can be understood in the limit $\Delta = 0$, where in the limit $L \to \infty$ with PBC there is an energy cost $\propto dk = \frac{2\pi}{L}$ for adding/removing a particle (corresponding to a spin $\uparrow$ excitation) on top of the ground-state Slater determinant, whereas the cost for moving a particle from an occupied to an empty low-lying single-particle state costs double the energy (removing a state with energy $\propto -dk$ and adding one with energy $\propto dk$).

4. (Bonus) Exact diagonalization with translation invariance

(i) Follow Lecture 11 to build the list of representatives $\hat{\Sigma}_R$, and their orbit lengths $\hat{Q}_R$.

↳ The "lexicographically" ordered list $\hat{\Sigma}_R$ plays the role of the lookup table $\hat{I}[J]$, $J = 0, \dots, (\#\text{ representatives at given } k) - 1$.

(ii) Use a map data structure for $\hat{J}[I]$ table (or simply binary search) to infer the index of a given representative $\tilde{\sigma}_R$ in the array $\hat{\Sigma}_R$.

(Extra cost $\mathcal{O}(\log(\dim \mathcal{H})) \sim \mathcal{O}(10)$).

(iii) Construct sparse matrix Hamiltonian as described in Lecture 11.

(iv) Use Lanczos algorithm to find low-lying energy levels in all momentum blocks.

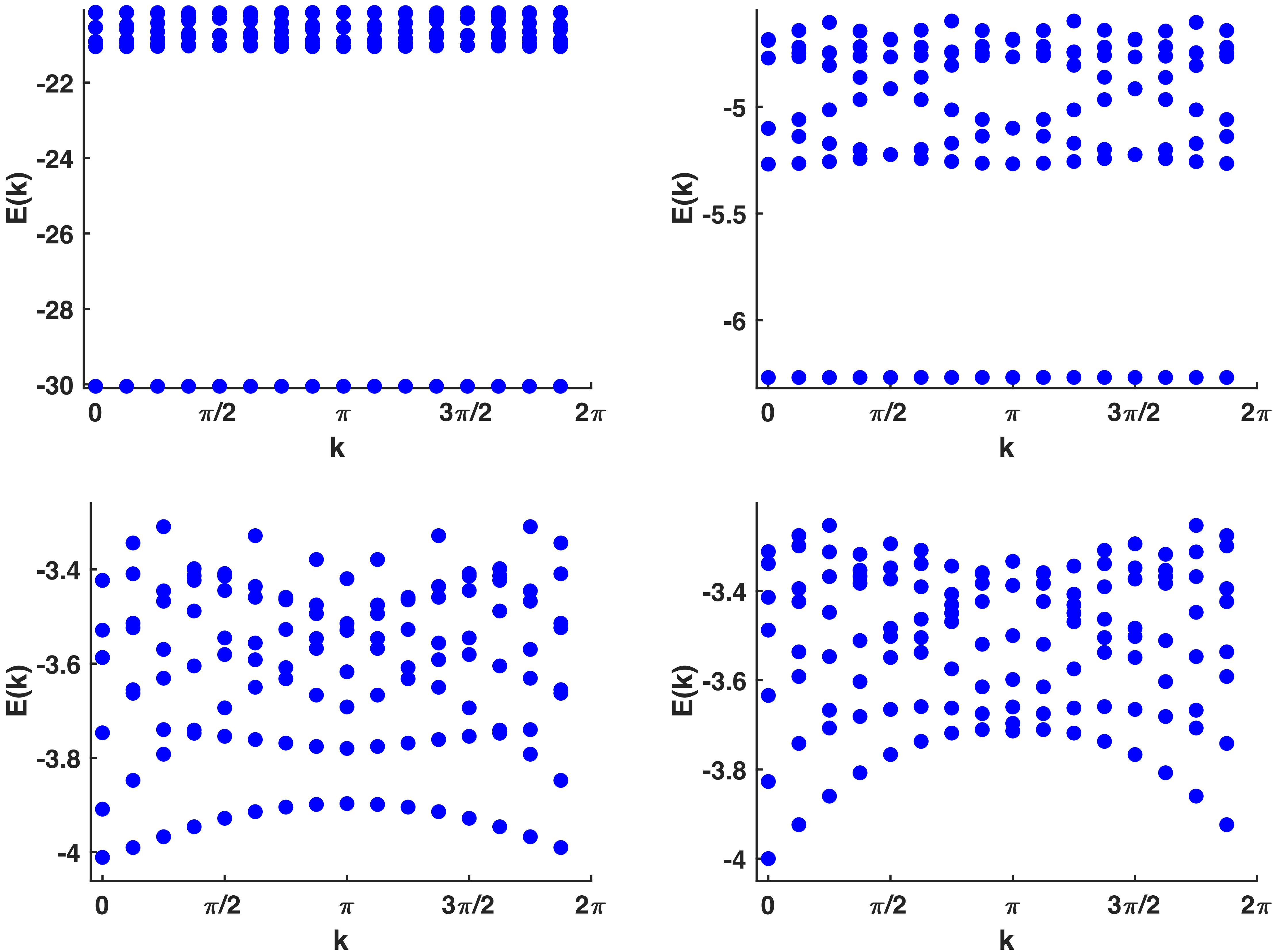


Figure 3: Up left: $\Delta = -10$. *Up right:* $\Delta = -2$. *Down left:* $\Delta = -1.1$. *Down right:* $\Delta = -1$.

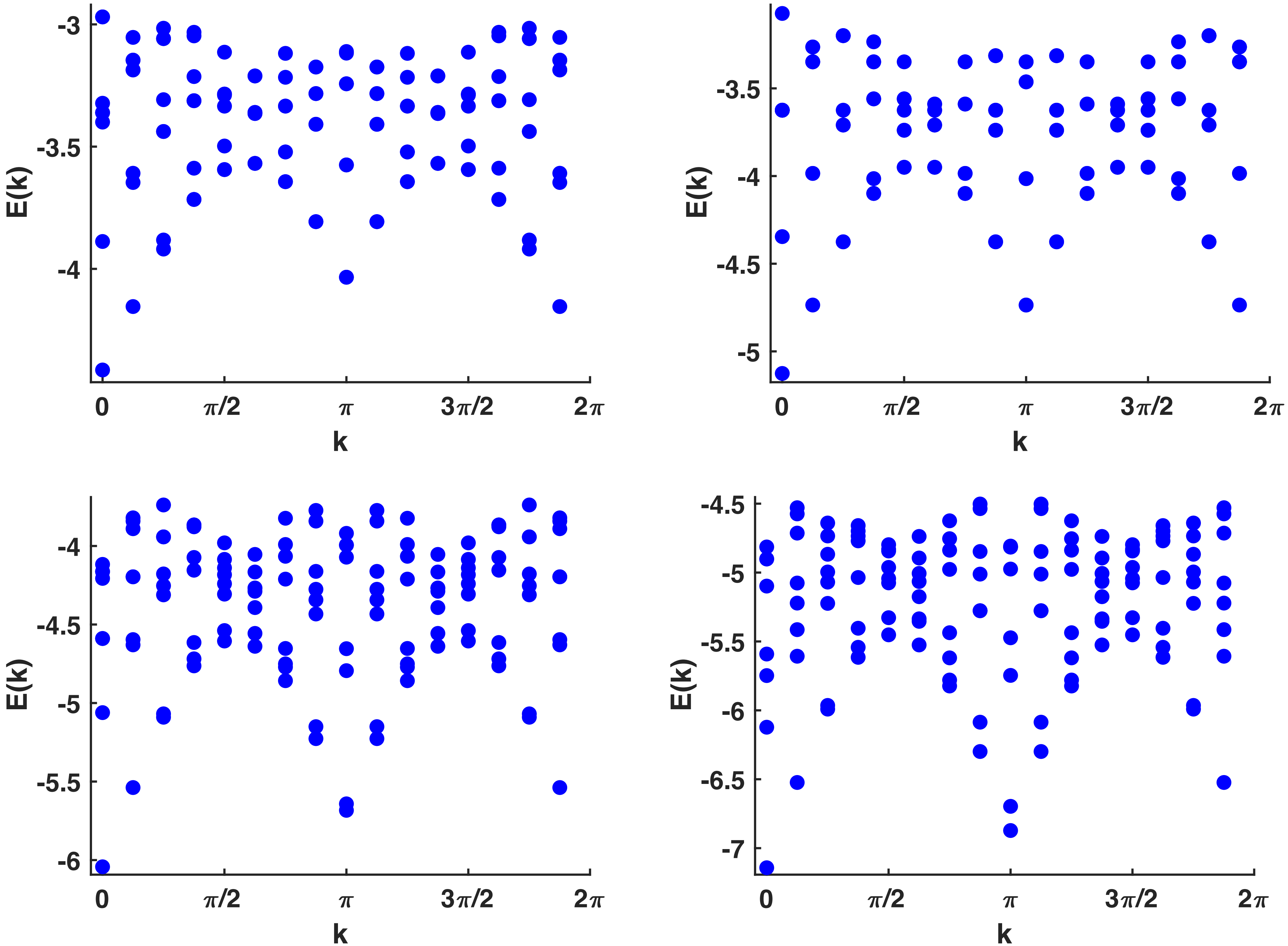


Figure 4: Up left: $\Delta = -0.5$. *Up right:* $\Delta = 0$. *Down left:* $\Delta = 0.5$. *Down right:* $\Delta = 1$.

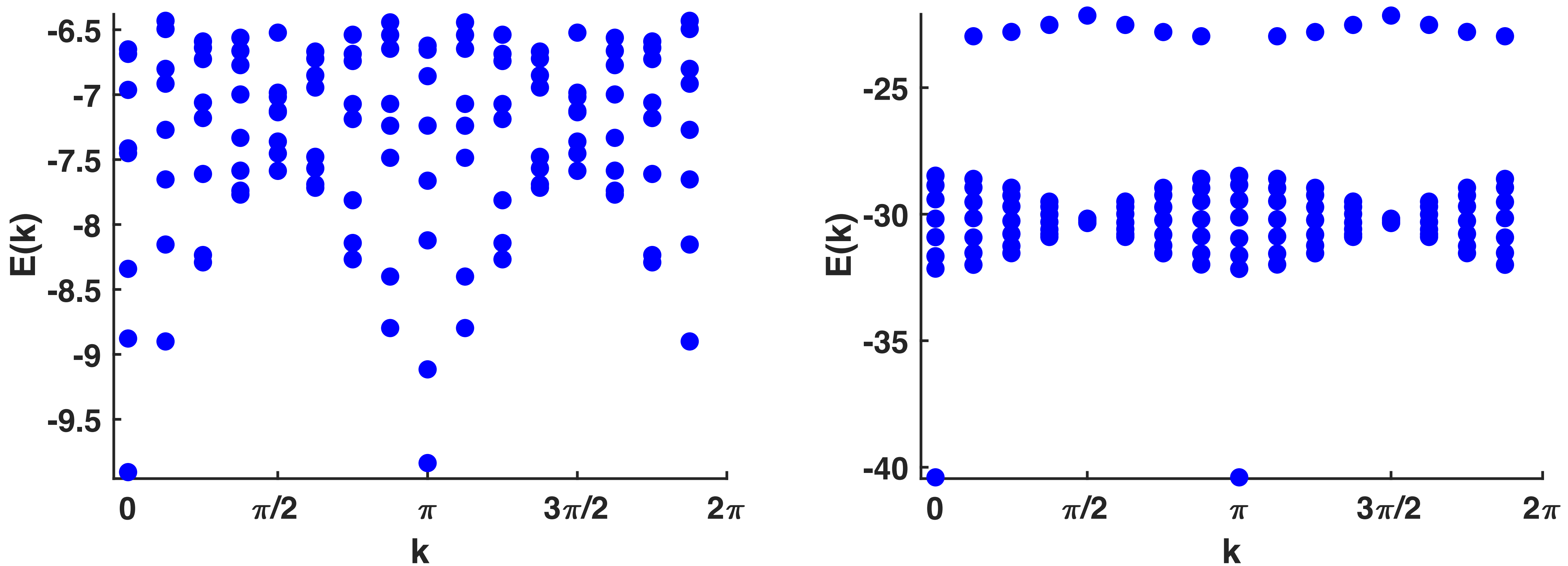


Figure 5: Left: $\Delta = 2$. *Right:* $\Delta = 10$.