

# 1 Quantum analysis

## 1.1 Determining the energies directly

Set

$$|\psi\rangle = \sum_{j=0}^N \alpha_j |N-j, j\rangle, \quad |N-j, j\rangle = \left(b_1^\dagger\right)^{N-j} \left(b_2^\dagger\right)^j |0\rangle$$

Now

$$\begin{aligned} H|\psi\rangle &= \frac{k}{8} \sum_{j=0}^N (N-2j)^2 \alpha_j |N-j, j\rangle - \frac{\mu}{2} \sum_{j=0}^N (N-2j) \alpha_j |N-j, j\rangle \\ &\quad - \frac{\mathcal{E}}{2} \sum_{j=0}^N j \alpha_j |N-j+1, j-1\rangle - \frac{\mathcal{E}}{2} \sum_{j=0}^N (N-j) \alpha_j |N-j-1, j+1\rangle \end{aligned}$$

We want to determine  $\{\alpha_j\}$  such that  $H|\psi\rangle = E|\psi\rangle$ .

For  $|\psi\rangle$  to be an eigenstate the following recursion relation must be satisfied

$$\frac{k}{8}(N - 2j)^2\alpha_j - \frac{\mu}{2}(N - 2j)\alpha_j - \frac{\mathcal{E}}{2}(j + 1)\alpha_{j+1} - \frac{\mathcal{E}}{2}(N + 1 - j)\alpha_{j-1} = E\alpha_j$$

with the constraint that

$$\begin{aligned}\alpha_{-1} &= 0, \\ \alpha_{N+1} &= 0.\end{aligned}\tag{1}$$

Choosing  $\alpha_0 = 1$ , which determines the magnitude of the state, we see from the explicit form of the recursion relation that  $\alpha_j$  is a polynomial in  $E$  of order  $j$ ; e.g.

$$\begin{aligned}\alpha_1 &= \frac{kN^2}{4\mathcal{E}} - \frac{\mu N}{\mathcal{E}} - \frac{2E}{\mathcal{E}} \\ \alpha_2 &= \left( \frac{k(N-2)^2}{8\mathcal{E}} - \frac{\mu(N-2)}{2\mathcal{E}} - \frac{E}{\mathcal{E}} \right) \left( \frac{kN^2}{4\mathcal{E}} - \frac{\mu N}{\mathcal{E}} - \frac{2E}{\mathcal{E}} \right) - \frac{N}{2}\end{aligned}$$

Hence equation (1) is a polynomial equation of order  $N + 1$ , the roots of which are precisely the energy eigenvalues.

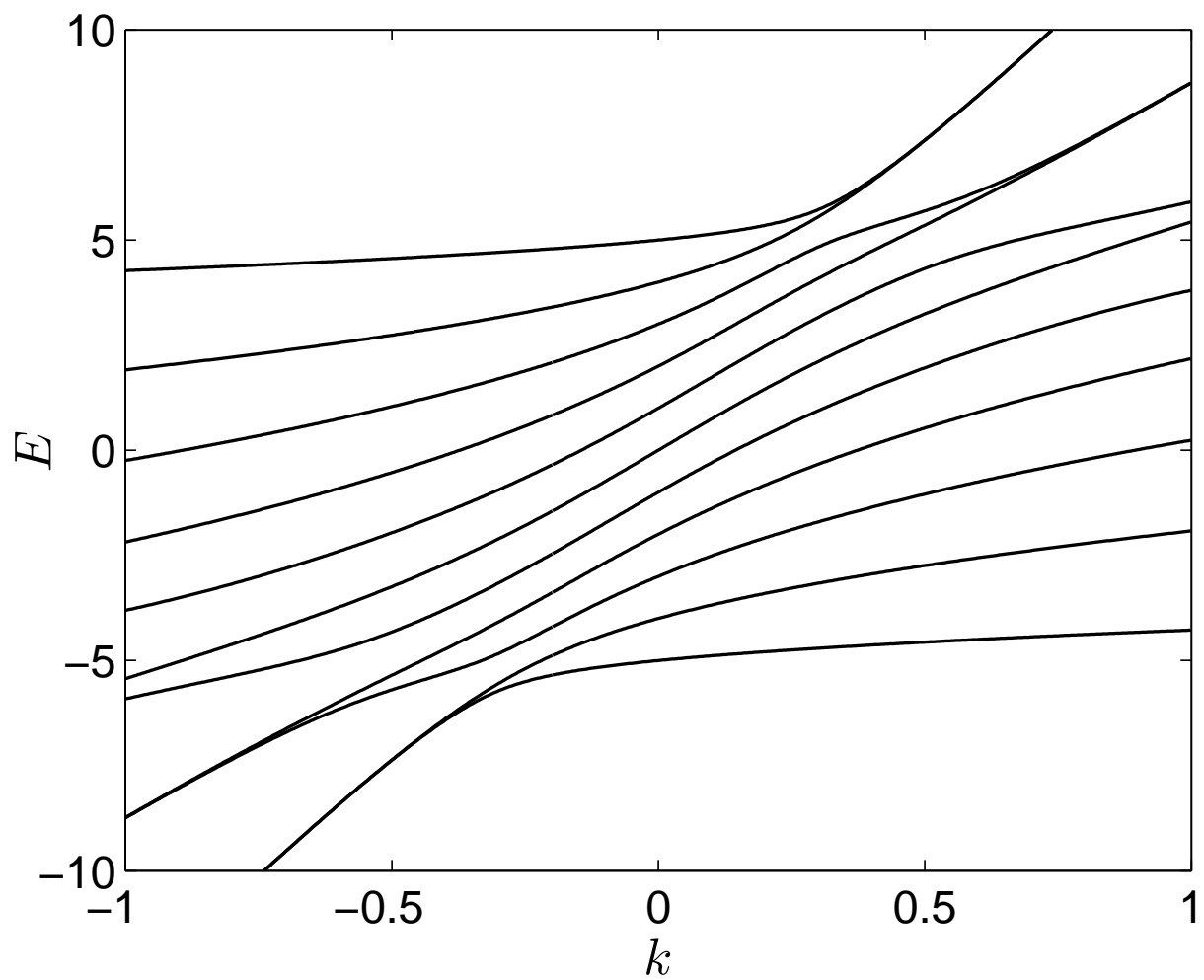


Figure 1: Energy levels versus coupling  $k$  for  $N = 10$ ,  $\mu = 0$  and  $\mathcal{E} = 1$ .

## 1.2 Quantum dynamics

Recall the time evolution of any state is determined by

$$|\phi(t)\rangle = U(t)|\phi_0\rangle,$$

where  $U(t)$  is the temporal evolution operator given by

$$U(t) = \exp(-iHt) = \sum_{j=0}^M |\Psi_j\rangle\langle\Psi_j| \exp(-iE_j t),$$

$|\Psi_j\rangle$  is an eigenstate with energy  $E_j$  and  $|\phi_0\rangle$  represents the initial state. Using these expressions we can compute the time evolution for expectation value of the imbalance

$$\langle(N_1 - N_2)(t)\rangle = \langle\psi(t)|N_1 - N_2|\psi(t)\rangle. \quad (2)$$

From the semi-classical analysis we found the transition between localised and delocalised oscillations occurs at  $k/\mathcal{E} = 4/N$ .

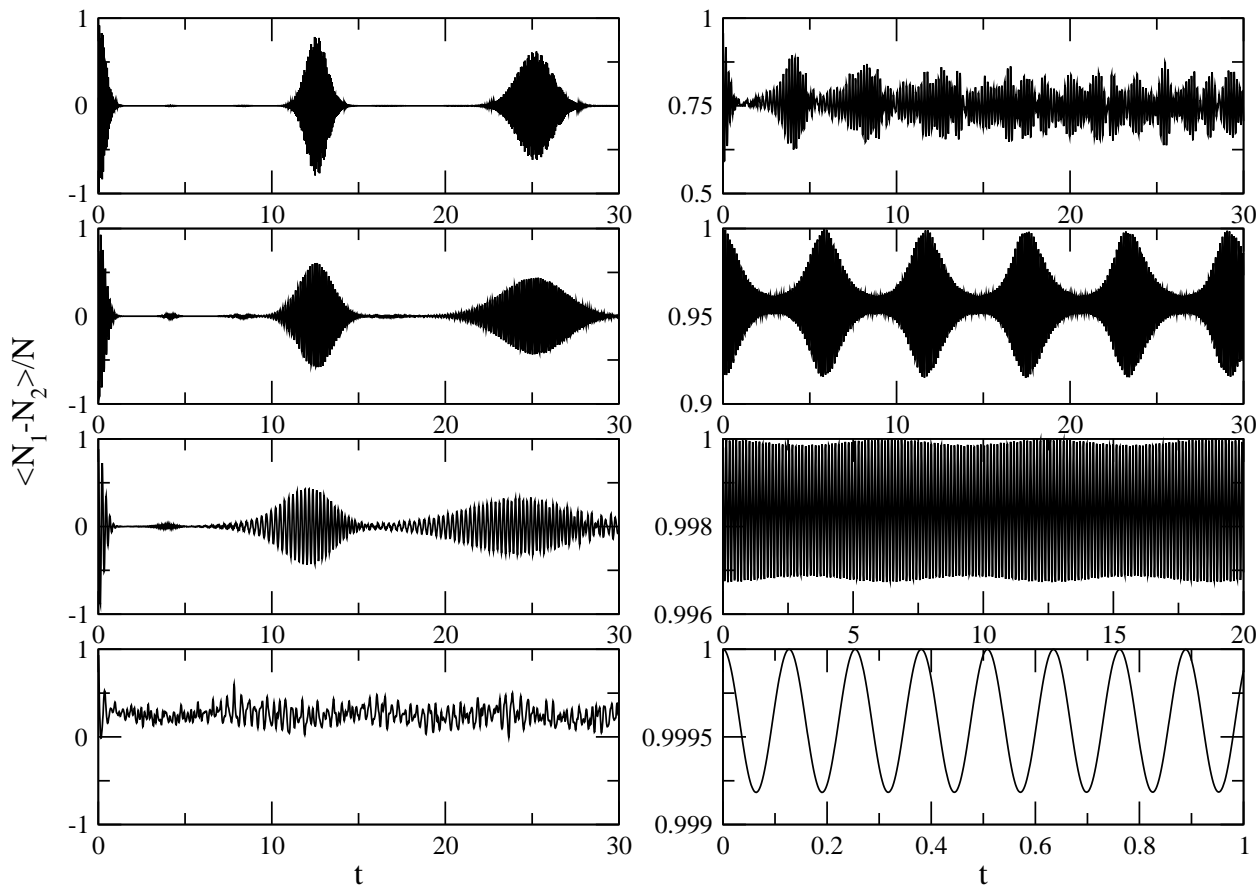


Figure 2: Time evolution of the expectation value between  $k/\mathcal{E} = 1/N$  and  $k/\mathcal{E} = 1$ . On the left, from the top to the bottom  $k/\mathcal{E} = 1/N, 2/N, 3/N, 4/N$  and on the right, from the top to the bottom  $k/\mathcal{E} = 5/N, 10/N, 50/N, 1$ , where  $N = 100$  and the initial state is  $|N, 0\rangle$ .

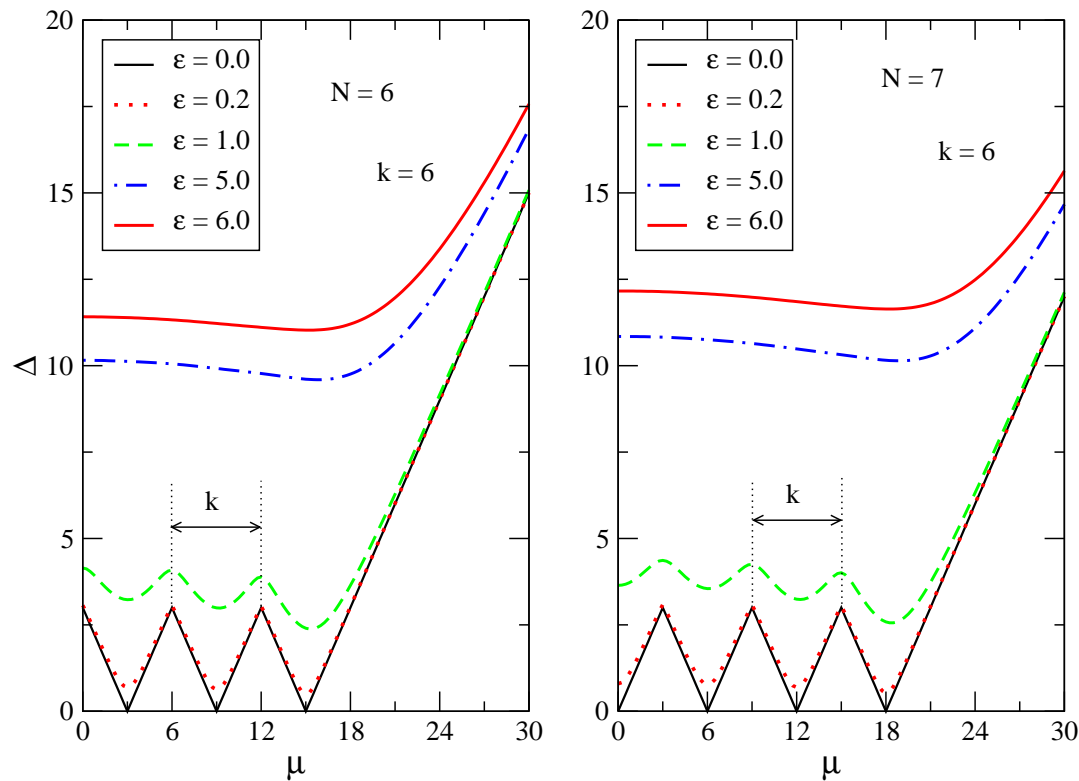


Figure 3: Energy gap  $\Delta$  versus the external potential  $\mu$  for different choices of the coupling parameter  $\mathcal{E} = 0, 0.2, 1, 5, 6$ . On the left,  $N = 6$ , and on the right,  $N = 7$ . In the extreme regime  $\mathcal{E} = 0$  the minima and maxima represent the level crossings as depicted in Fig. ???. For small values of  $\mathcal{E}$  the difference between two consecutive minima or maxima is constant and equal to  $k$ . As  $\mathcal{E}$  increases just one minimum survives.

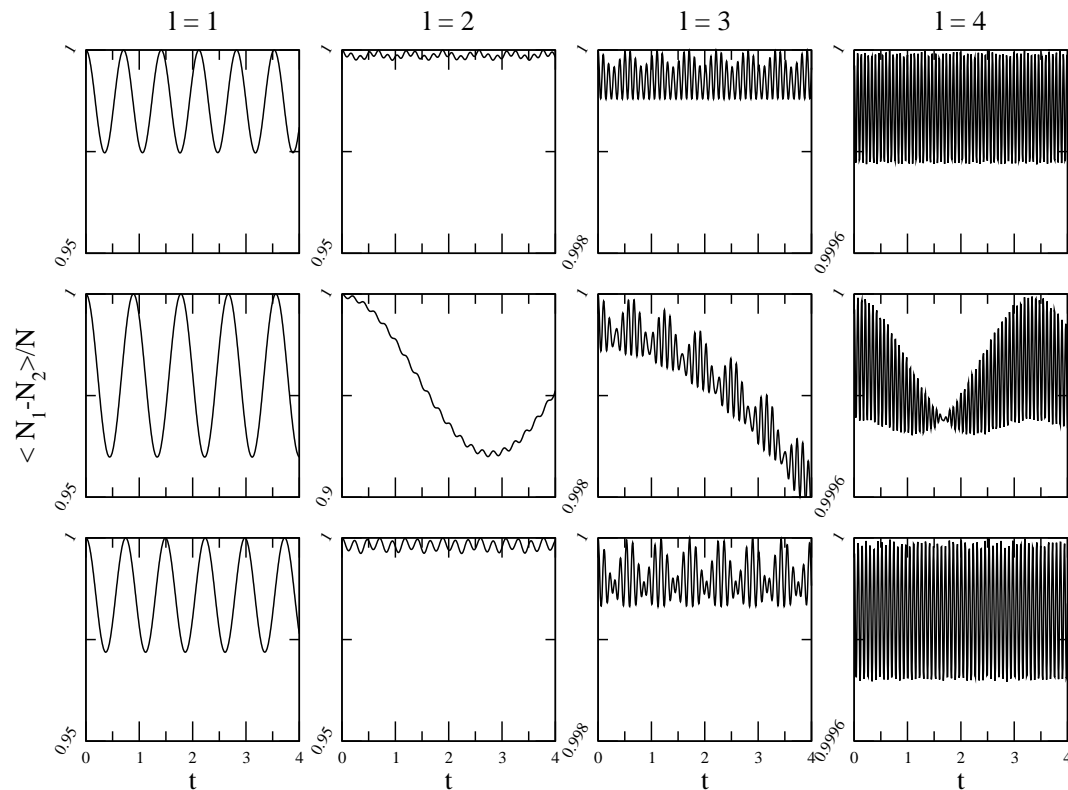


Figure 4: Dynamics of the expectation value of the relative number of particles for  $N = 50$ ,  $k/\mathcal{E} = 60$  and with the initial state  $|N, 0\rangle$ . The central graph, at each column, represents the point where the energy gap is minimal ( $l = 1, 3$ ) or maximal ( $l = 2, 4$ ), occurring at  $\mu_c/\mathcal{E} = 1470, 1440, 1410, 1380$  (from left to right). In each case the graphs above and below show dynamics of points around the minimum or maximum, chosen as  $\mu/\mathcal{E} = \mu_c/\mathcal{E} \mp 5$ . It is clear that each minimum and maximum is associated with a change in the dynamical behaviour.

### 1.3 Bethe ansatz solution

Recall the Jordan-Schwinger realisation of the  $su(2)$  algebra :

$$S^+ = b_1^\dagger b_2, \quad S^- = b_2^\dagger b_1, \quad S^z = \frac{1}{2}(N_1 - N_2)$$

which is  $(N+1)$ -dimensional when the constraint of fixed particle number  $N = N_1 + N_2$  is imposed. In terms of this realisation the Hamiltonian is

$$H = \frac{k}{2}(S^z)^2 - \mu S^z - \frac{\mathcal{E}}{2}(S^+ + S^-). \quad (3)$$

The same  $(N + 1)$ -dimensional representation of  $su(2)$  is given by the mapping to differential operators

$$S^z = u \frac{d}{du} - \frac{N}{2}, \quad S^+ = Nu - u^2 \frac{d}{du}, \quad S^- = \frac{d}{du}$$

acting on the  $(N + 1)$ -dimensional space of polynomials functions with basis  $\{1, u, u^2, \dots, u^N\}$ .

We can then equivalently represent (3) as the second-order differential operator

$$\begin{aligned}
 H &= \frac{k}{2} \left( u^2 \frac{d^2}{du^2} + (1 - N)u \frac{d}{du} + \frac{N^2}{4} \right) - \mu \left( u \frac{d}{du} - \frac{N}{2} \right) \\
 &\quad - \frac{\mathcal{E}}{2} \left( Nu + (1 - u^2) \frac{d}{du} \right) \\
 &= \frac{ku^2}{2} \frac{d^2}{du^2} + \frac{1}{2} \left( (k(1 - N) - 2\mu)u + \mathcal{E}(u^2 - 1) \right) \frac{d}{du} \\
 &\quad + \frac{kN^2}{8} + \frac{\mu N}{2} - \frac{\mathcal{E}Nu}{2}.
 \end{aligned}$$

Solving for the spectrum of the Hamiltonian (??) is then equivalent to solving the eigenvalue equation

$$HQ = EQ \tag{4}$$

where  $Q(u)$  is a polynomial function of  $u$  of order  $N$ .

A Bethe ansatz solution is now straightforward to derive. First express  $Q(u)$  in terms of its roots  $\{v_j\}$ :

$$Q(u) = \prod_{j=1}^N (u - v_j).$$

Evaluating  $HQ = EQ$  at  $u = v_k$  for each  $k$  leads to the set of Bethe ansatz equations

$$\frac{\mathcal{E}v_k^2 + (k(1 - N) - 2\mu)v_k - \mathcal{E}}{kv_k^2} = \sum_{j \neq k}^N \frac{2}{v_j - v_k}, \quad k = 1, \dots, N. \quad (5)$$

Writing the asymptotic expansion  $Q(u) \sim u^N - u^{N-1} \sum_{j=1}^N v_j$  and by considering the terms of order  $N$  in (4), the energy eigenvalues are found to be

$$E = \frac{kN^2}{8} - \frac{\mu N}{2} + \frac{\mathcal{E}}{2} \sum_{j=1}^N v_j. \quad (6)$$

## 1.4 Mapping to a Schrödinger equation

Hereafter we set  $\hbar^2/2m = 1$  so the one-dimensional Schrödinger equation is of the form

$$-\frac{d^2\Psi}{dx^2} + V(x)\Psi = E\Psi. \quad (7)$$

Set

$$Q(u) = \prod_{j=1}^M (u - v_j) \quad (8)$$

and look for solutions of the form

$$\Psi = e^{v(x)} Q(u(x)). \quad (9)$$

Now

$$\begin{aligned} \frac{d^2\Psi}{dx^2} &= \left( \frac{d^2v}{dx^2} + \left( \frac{dv}{dx} \right)^2 \right) e^v Q + \left( 2 \frac{du}{dx} \cdot \frac{dv}{dx} + \frac{d^2u}{dx^2} \right) e^v \frac{dQ}{du} \\ &\quad + \left( \frac{du}{dx} \right)^2 e^v \frac{d^2Q}{du^2}. \end{aligned}$$

Hence a solution of the following differential equation

$$-\left(\frac{du}{dx}\right)^2 \frac{d^2 Q}{du^2} - \left(\frac{d^2 u}{dx^2} + 2\frac{du}{dx} \cdot \frac{dv}{dx}\right) \frac{dQ}{du} + \left(V - \frac{d^2 v}{dx^2} - \left(\frac{dv}{dx}\right)^2\right) Q = EQ$$

where  $Q$  is a polynomial in  $u$  is equivalent to (partially) solving the Schrödinger equation. For the differential operator form of the Hamiltonian with  $\mu = 0$

$$H = \frac{ku^2}{2} \frac{d^2}{du^2} + \frac{1}{2} (k(1-N)u + \mathcal{E}(u^2 - 1)) \frac{d}{du} + \frac{kN^2}{8} - \frac{\mathcal{E}Nu}{2}$$

we find

$$\begin{aligned} u &= \exp\left(\sqrt{\frac{-k}{2}}x\right) \\ v &= \frac{\mathcal{E}}{k} \cosh\left(\sqrt{\frac{-k}{2}}x\right) - \sqrt{\frac{-kN^2}{8}}x \\ V &= \frac{\mathcal{E}^2}{k^2} \sinh^2\left(\sqrt{\frac{-k}{2}}x\right) + \frac{(N+1)\mathcal{E}}{k} \cosh\left(\sqrt{\frac{-k}{2}}x\right) \end{aligned}$$

The wavefunctions are of the form

$$\Psi = \exp\left(\frac{\mathcal{E}}{k} \cosh\left(\sqrt{\frac{-k}{2}}x\right) - \sqrt{\frac{-kN^2}{8}}x\right) \prod_{j=1}^N \left(\exp\left(\sqrt{\frac{-k}{2}}x\right) - v_j\right)$$

such that

$$\frac{\mathcal{E}v_k^2 + k(1-N)v_k - \mathcal{E}}{kv_k^2} = \sum_{j \neq k}^N \frac{2}{v_j - v_k}, \quad k = 1, \dots, N.$$

**Theorem 1** *Consider a Schrödinger equation with locally bounded potential  $V(x)$  satisfying  $V(x) \rightarrow \infty$  as  $|x| \rightarrow \infty$ . Let  $|\psi_j\rangle$ ,  $j = 0, 1, \dots, \infty$  denote the eigenfunctions of the Schrödinger equation with eigenvalues  $E_j$  respectively, ordered such that  $E_j < E_k$  whenever  $j < k$ . Then  $|\psi_j\rangle$  has precisely  $j$  (real) zeroes.*

It follows from the theorem that the  $N+1$  eigenstates of the Hamiltonian are in one-to-one correspondence with the lowest  $N+1$  eigenstates of the Schrödinger equation. In particular the ground state of the Hamiltonian maps to the ground-state wavefunction of the Schrödinger equation.

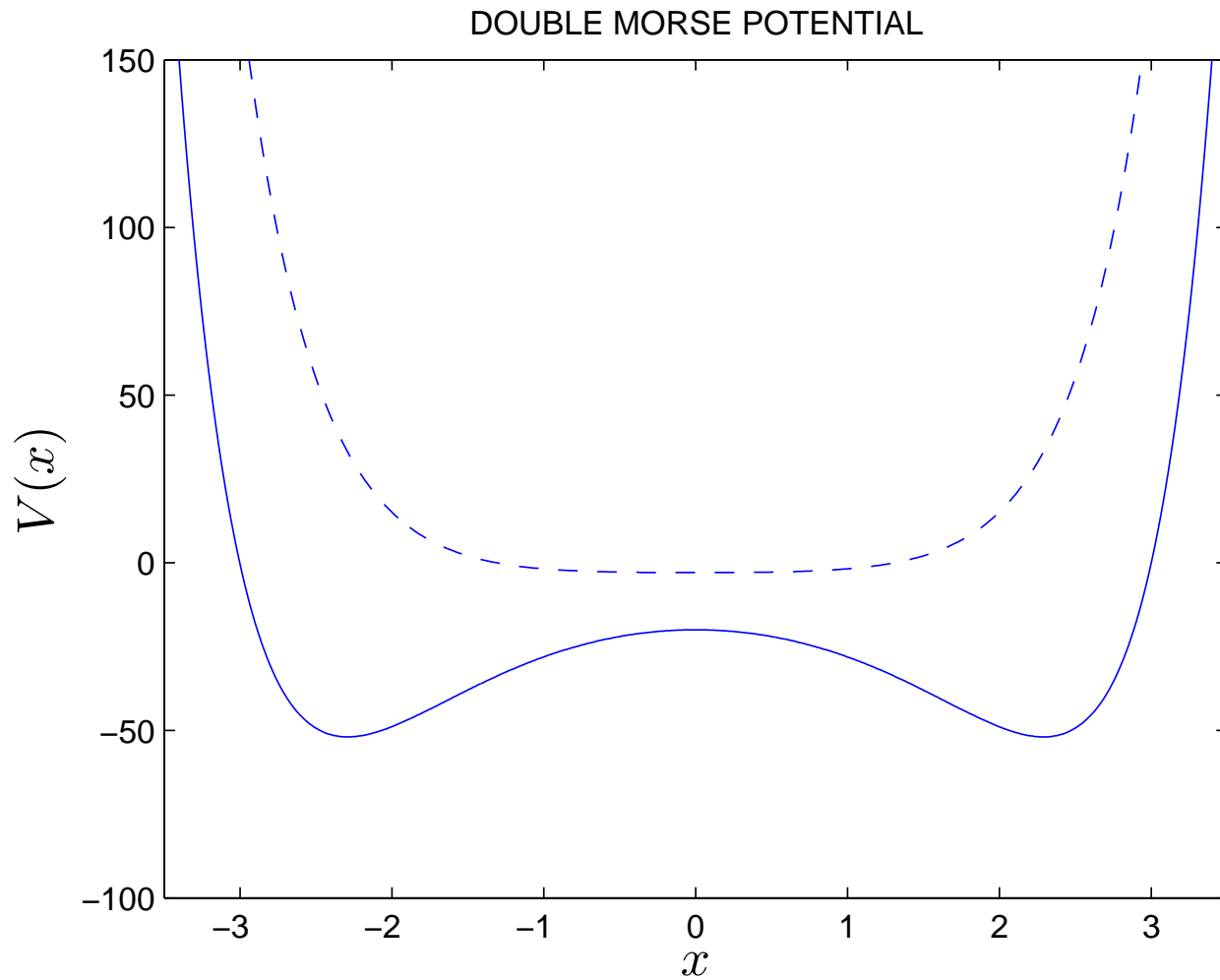


Figure 5: The double Morse potential  $V(x) = A \sinh^2(x) - B \cosh(x)$  for the values  $A = 2, B = 20$  (solid line) and  $A = 2, B = 3$  (dashed line).

$$H = \frac{k}{8}(N_1 - N_2)^2 - \frac{\mathcal{E}}{2}(b_1^\dagger b_2 + b_2^\dagger b_1)$$

The Hellmann–Feynman theorem tells us that

$$\langle \Psi_0 | (N_1 - N_2)^2 | \Psi_0 \rangle = 8 \frac{\partial E_0}{\partial k}.$$

Alternatively

$$\frac{\partial E_0}{\partial k} = \langle \psi_0 | \frac{\partial V}{\partial k} | \psi_0 \rangle$$

where the Schrödinger equation potential is

$$V = \frac{\mathcal{E}^2}{k^2} \sinh^2 \left( \sqrt{\frac{-k}{2}} x \right) + \frac{(N+1)\mathcal{E}}{k} \cosh \left( \sqrt{\frac{-k}{2}} x \right).$$

For this potential there is a bifurcation of the minimum when

$$\frac{k(N+1)}{\mathcal{E}} = -2.$$

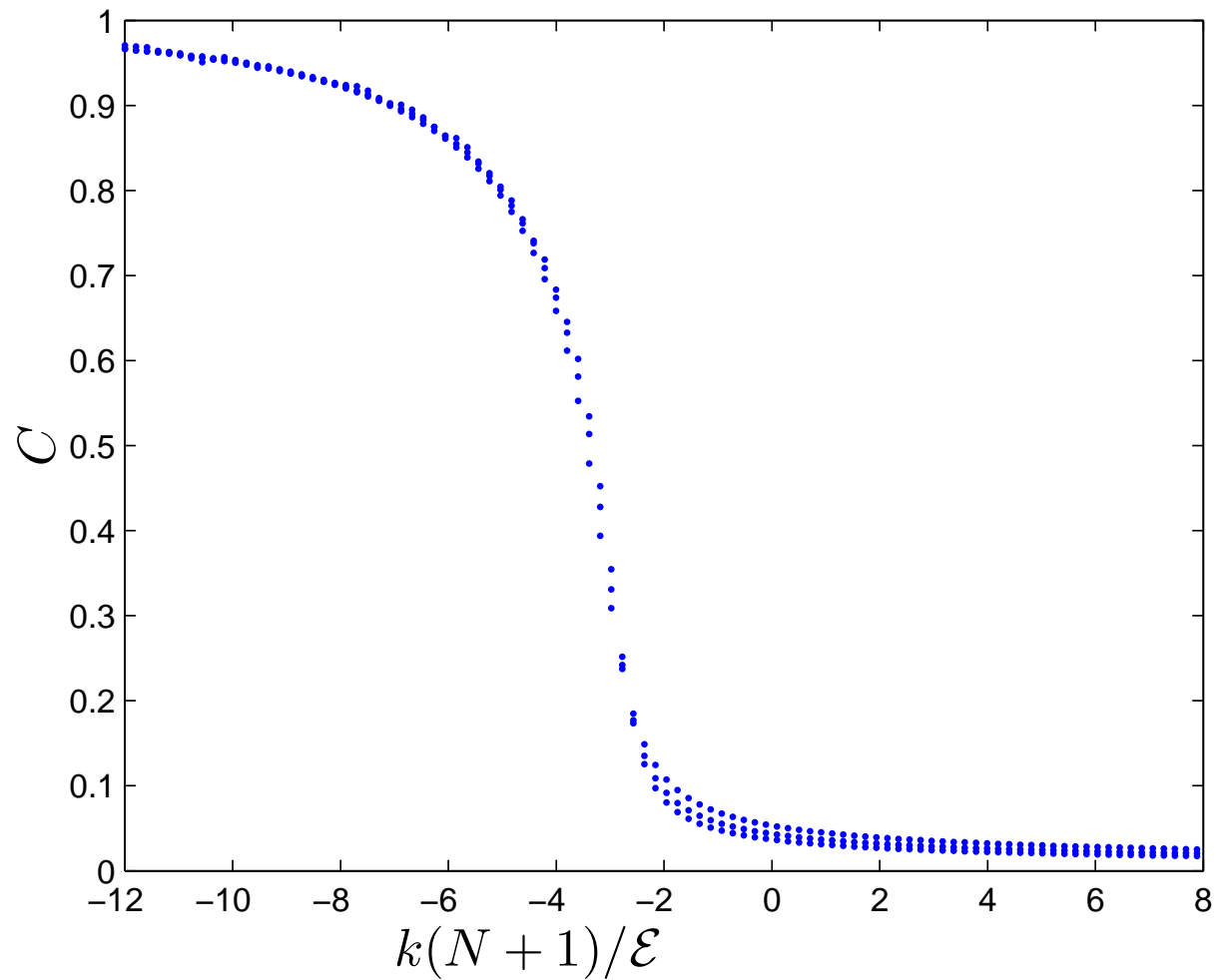


Figure 6: Scaled ground-state imbalance fluctuations for  $N = 18, 22, 26$  where  $C = \frac{1}{N^2} \langle \Psi_0 | (N_1 - N_2)^2 | \Psi_0 \rangle$ .

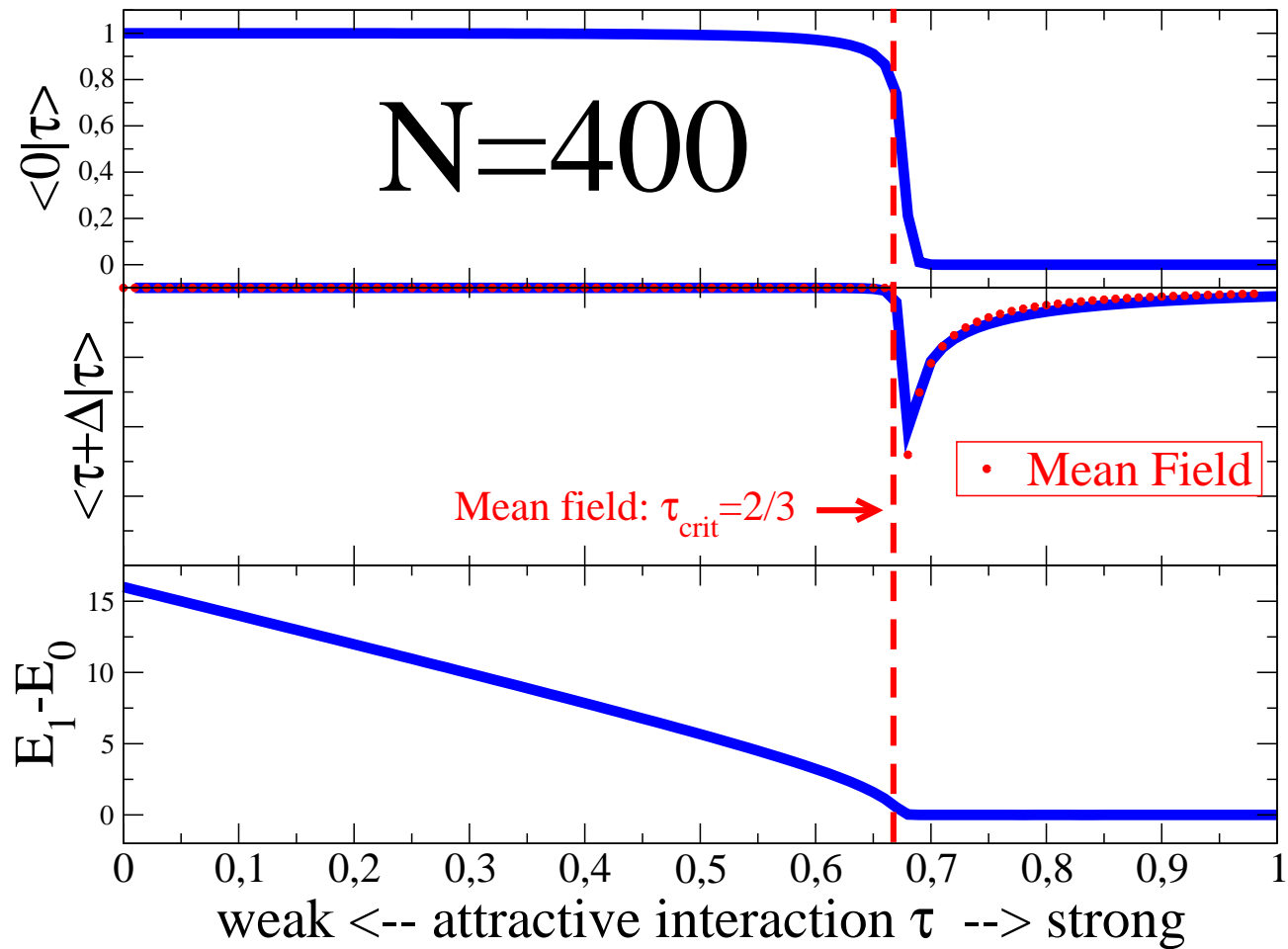


Figure 7: Indicators of phase changes in the ground state for the attractive case. The scaled coupling is  $\tau = \frac{kN}{kN - \mathcal{E}}$  and  $\Delta = 10^{-2}$ .

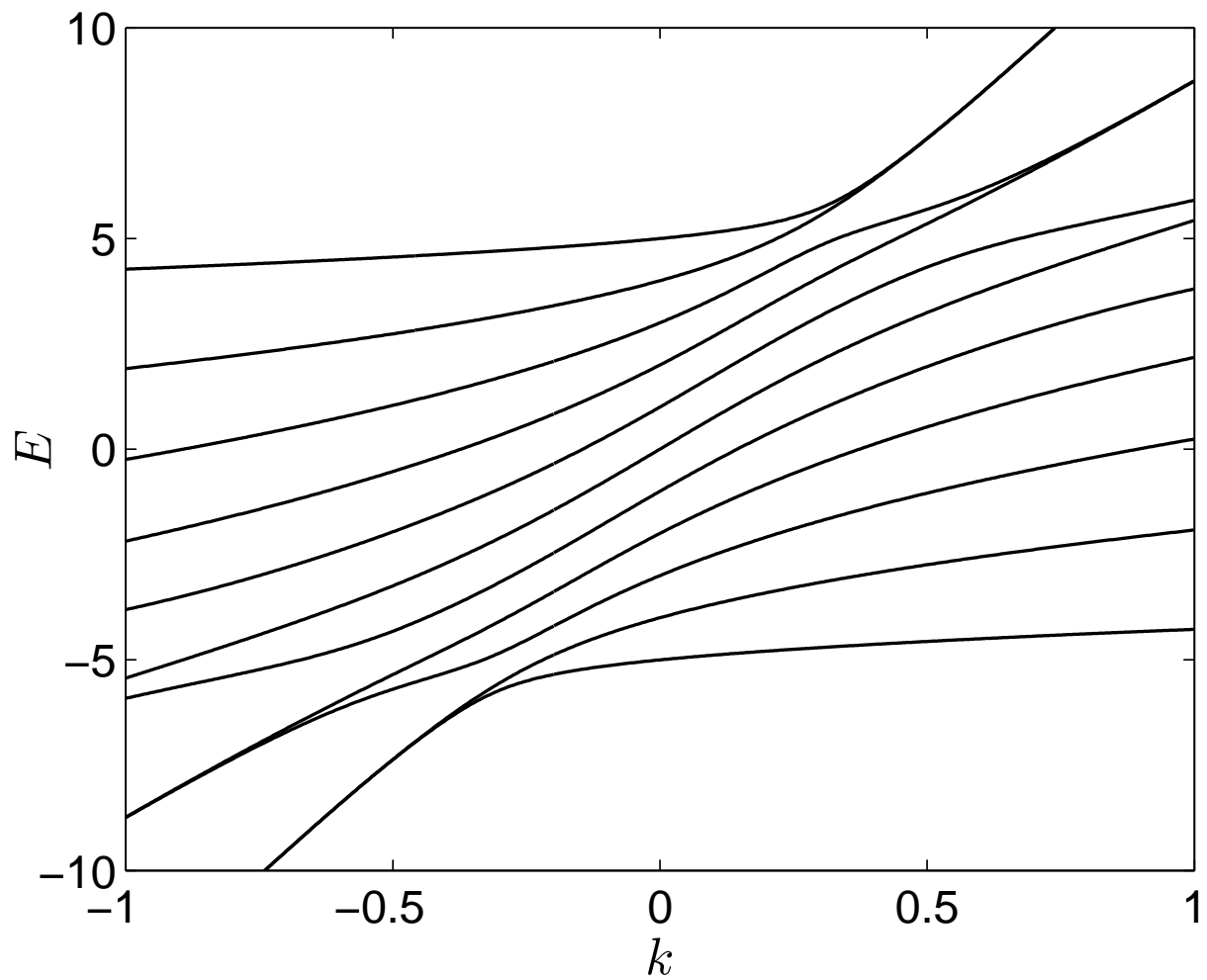


Figure 8: Energy levels versus coupling  $k$  for  $N = 10$ ,  $\mu = 0$  and  $\mathcal{E} = 1$ .

## 2 Conclusions

- Bose–Einstein condensates offer promise in understanding physics at the interface of the microscopic and macroscopic scales, due to controllability of the interactions.
- Mathematical methods which apply for finite system sizes (not the thermodynamic limit) are needed to understand the nature of these systems, as “transitions” are particle number dependent.
- We analysed a simple model which captures the essence of competing linear and non-linear interactions.
- Semi-classical methods provided some insights into the behaviour, but fall short of painting the full picture.
- In the full quantum analysis the qualitative feature of experimentally observed collapse and revival of oscillations was reproduced.
- The model gives insights into the possibility of creating Schrödinger cat states.