Quantum Phase Crossovers in Finite Systems

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Abstract

- We study quantum phase crossovers for finite systems without taking the thermodynamic limit.
- We utilize a mapping of the spectrum of an integrable model obtained by the *algebraic Bethe ansatz* method into the **quasi-exactly solvable** spectrum of a one-particle Schrödinger operator.
- Investigation of the potential determine critical ground-state couplings.
- Through specific *ground-state correlation functions* these couplings determine the quantum phase crossovers in the integrable system for finite particle number.
- We demonstrate the method used with two examples of bosonic Hamiltonians.

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Introduction

We begin with the Schrödinger operator eigenvalue equation in one dimension

$$-\frac{\partial^2\psi_k}{\partial x^2}+V(x)\psi_k=E_k\psi_k \tag{1}$$

where for the potential $V(x)$ it is assumed there is a bifurcation of the global minimum at x_c such that $V(x)\approx V_0-2V_1(x-x_c)^2+V_2(x-x_c)^4$ with $V_2>0$.

Definition 1 *Consider the Schrodinger operation equation (1) where the potential $V(x)$ smoothly depends on a dimensionless coupling parameter γ. Treating (1) as a classical problem, approximate the ground-state energy as the minimum of the potential via $\tilde{E}_0=\min_{x\in\mathbb{R}}V(x)$. If m is the smallest integer for which $\partial^m\tilde{E}_0/\partial\gamma^m$ is discontinuous at some coupling γ_c, we say there is an mth-order quantum phase crossover of the quantum system at γ_c.*

Of interest to the examples considered below are second-order crossovers.

Let $H=H(\gamma)$ denote the Hamiltonian for some integrable model acting on a finite-dimensional Hilbert space where γ is a dimensionless coupling parameter. Let $|\Psi_j\rangle$ denote the eigenstates of H with energy levels $\mathcal{E}_j$.

Now assume that $\mathcal{E}_j$ can be mapped to energies E_k of a Schrodinger operator such that $\forall j$, $\exists k$ satisfying $\mathcal{E}_j=\chi E_k$ for some *positive* scale factor χ which is independent of γ, j and k.

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

A corollary of the theorem is that the ground state wave-function of the Schrodinger operator has no zeros.

Definition 2 *Suppose the ground state energy $\mathcal{E}_0$ of an integrable model exactly maps to the ground state energy E_0 of a Scrhodinger operator through $\mathcal{E}_j=\chi E_k$ If the Schrodiner operator exhibits a second-order quantum phase crossover at some dimensionless coupling γ_c as in Definition 1, then we say that the integrable model also exhibits a second-order quantum phase crossover at γ_c.*

Atomic-molecular bosonic model

We describe the interconversion of bosonic atomic and di-atomic molecular modes by the Hamiltonian [1]

$$H=\frac{\delta}{2}n_a+\frac{\Omega}{2}(a^\dagger a^\dagger b+b^\dagger aa) \tag{2}$$

where $a^\dagger$ and $b^\dagger$ denote the creation operators for atomic and molecular modes respectively and $n_a=a^\dagger a$, $n_b=b^\dagger b$, $N=n_a+2n_b$.

The exact solution gives the energy levels as $E=\delta M+\Omega\sum_{j=1}^{M}v_j$ where the parameters $\{v_j\}$ are the roots of the Bethe ansatz equations [2]

$$\frac{1}{2v_j}-v_j-\gamma=\sum_{k\neq j}^{M}\frac{2}{v_k-v_j}\qquad j=1,\ldots,M. \tag{3}$$

Above, $\gamma=\delta/\Omega$ is the dimensionless coupling, $N=2M$ with dimension of the Hilbert space $M+1$.

From the ground-state energy, one can use the Hellman–Feynman theorem to compute the ground-state correlations: $\langle n_a\rangle=2\partial\mathcal{E}_0/\partial\delta$, $\theta=-\partial\mathcal{E}_0/\partial\Omega$ where the coherence correlator is $\theta=-\left\langle a^\dagger a^\dagger b+b^\dagger aa\right\rangle/2$.

For a given solution of (3) with corresponding energy, we set

$$\psi(x)=\exp\left(-\frac{\gamma x^2}{8}-\frac{x^4}{64}\right)\prod_{j=1}^{M}\left(\frac{x^2}{4}-v_j\right). \tag{4}$$

Then $\psi(x)$ satisfies (1) with $\chi=\Omega$ and **potential**

$$V(x)=-\frac{\gamma}{4}+\frac{(\gamma^2-3-2N)x^2}{16}+\frac{\gamma x^4}{32}+\frac{x^6}{256}. \tag{5}$$

We find crossover coupling, $\gamma_c=\sqrt{2N+3}$.

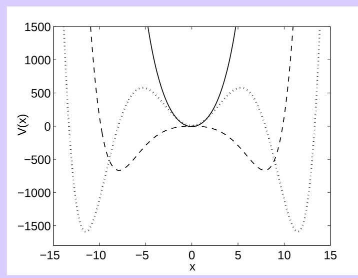

Fig.1: Generic behaviour of the sextic potential (5), where the critical coupling is given by γ_c. Here we take $N=100$. For $\gamma>\gamma_c$ (solid line: $\gamma=30$), $-\gamma_c<\gamma<\gamma_c$ (dash line: $\gamma=-10$) or $\gamma<-\gamma_c$ (dot line: $\gamma=-30$).

For this potential there is a second-order quantum phase crossover of the same universality class as the Landau (or mean-field) theory and the interacting boson model. The classical critical behaviour of the correlation functions is: $\theta-\theta_c\sim\gamma-\gamma_c$, $\gamma\to(\gamma_c)_-$, $\theta-\theta_c\sim 0$, $\gamma\to(\gamma_c)_+$, with $\theta_c=0$. Similar results hold for $\langle n_a\rangle$, consistent with the following figure.

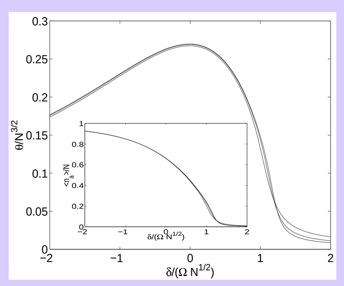

Fig.2: Coherence correlator for the ground state of (2) for $N=20,30,40$. The inset shows $\langle n_a\rangle/N$, the average fractional occupation of unbound atoms in the ground state.

Attractive two-site Bose–Hubbard model

Quantum tunneling of bosons, based on a two-mode approximation, is described by the Bose-Hubbard Hamiltonian [3]:

$$H=-\frac{k}{8}(n_1-n_2)^2+\frac{\mathcal{E}}{2}(b_1^\dagger b_2+b_2^\dagger b_1) \tag{6}$$

where $b_j^\dagger$, $j=1,2$ denote the single-particle creation operators associated with two bosonic modes and $n_1=b_1^\dagger b_1$, $n_2=b_2^\dagger b_2$ are the corresponding number operators.

The total particle number $N=n_1+n_2$ is even. We consider the attractive case: $k>0$ and take $\mathcal{E}>0$.

A Bethe ansatz solution of (6) has been described in [4]. The eigenvalues of the Hamiltonian are given by $E=\mathcal{E}\sum_{l=1}^{M}v_l-kN^2/8$, while those of the number operator are $N=2M+4\kappa-1$, where the v_l are solutions of the Bethe ansatz equations

$$-\gamma+\frac{2\kappa v_j}{v_j^2-1}=\sum_{l\neq j}^{M}\frac{1}{v_l-v_j},\qquad j=1,\ldots,M. \tag{7}$$

$\gamma=\mathcal{E}/k$ is the dimensionless coupling and we restrict to $\kappa=1/4$.

We exactly map the spectrum of (6) into that of the Schrodinger operator equation (1). Setting

$$\psi(x)=\exp(-\gamma\cosh(x))\prod_{j=1}^{M}(\cosh(x)+v_j)$$

then $\psi(x)$ satisfies (1) with the **potential**

$$V(x)=\gamma^2\sinh^2(x)-(N+1)\gamma\cosh(x) \tag{8}$$

and $\chi=k/2$. This mapping is faithful for the ground-state energies. This is a double Morse (QES) potential with crossover coupling $\gamma_c=(N+1)/2$, in the same universality class as (2), agrees to leading order in N with the results of [4].

The coherence correlator $\theta=-\langle b_1^\dagger b_2+b_2^\dagger b_1\rangle/2$, displays the same classical critical behaviour as previous case with $\theta_c=k\gamma_c$.

Conclusion

We have developed a technique for determining quantum phase crossovers in finite integrable models, and applied it to the Hamiltonians (2,6).

In both cases a crossover dimensionless coupling γ_c is N-dependent, highlighting problems studying quantum phase crossovers in the thermodynamic limit.

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