Exact solution of a lattice band problem related to an exactly soluble many-body problem: The missing-states problem

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We introduce and solve a lattice version of an easily soluble one-dimensional continuum quantum system with a periodic potential. The relationship of the one problem to the other is identical to the relationship of the one-dimensional quantum many-body lattice gas recently introduced by Shastry [Phys. Rev. Lett. **60**, 639 (1988)] and by Haldane [Phys. Rev. Lett. **60**, 635 (1988)] to the one-dimensional quantum many-body continuum gas earlier solved by Sutherland. Thus it is hoped that by understanding the "missing" states in this simple case, we might better understand the missing states in the more complicated many-body case, which in many instances comprise all the states. The results are not encouraging.

I. INTRODUCTION

In two recent and extremely interesting papers—one by Shastry[1] and the other by Haldane[2]—a very clever method was introduced that can produce from certain exact solutions of continuum quantum many-body problems, the exact solutions to corresponding lattice quantum many-body problems. The method simply consists in finding a corresponding one-body hopping operator J_i that has exactly the same effect on the lattice functions as the one-body kinetic energy operator $-\nabla_i^2$ on the continuum functions. Then in the continuum Hamiltonian, we replace the kinetic energy by a sum over J_i's. The solutions to the lattice problem will be given by the solutions to the continuum problem evaluated at the lattice points.

However, as we remarked, one can only find such a J—and hence use the trick—for certain functions. The requirement is that if we take a continuum function of m variable x_j and expand it in a Fourier expansion, then the function must *only* contain Fourier components in the first Brillouin zone, i.e., $-\pi < k_j \leq \pi$, for all $j=1,\ldots,M$. This is a great restriction, as is the condition that we can find *exact* solutions to the continuum problem in the first place. We shall refer to all states that cannot be obtained by the trick—because the corresponding continuum states extend beyond the first Brillouin zone—as missing states.

This trick was applied by Shastry and by Haldane to a one-dimensional continuum many-body problem first solved by Sutherland[3]—a system of M particles interacting by a two-body pair potential

$$v(x)=\frac{2\lambda(\lambda-1)(\pi/N)^2}{\sin^2(\pi x/N)}.$$

The continuum problem can be solved for all states and all coupling constants; for instance, the ground state is given by

$$\psi(x_1,\ldots,x_M)=\prod_{j=1}^{M-1}\prod_{k=j+1}^{M}|\sin[\pi(x_k-x_j)/N]|^{\lambda}.$$

Assuming $\lambda=2n$, $n=1,2,\ldots$, then the maximum Fourier component has $k=2n\pi(M-1)/N$. Thus the trick only works for $N\geq 2n(M-1)$. In particular, only for $n=1$ can we find the ground state of the lattice gas at a particle density of $\frac{1}{2}$, and then we cannot find any finite fraction of the excited states by using the trick.

We would like to find out where the missing states are, and to this end we begin with a much simpler one-body continuum problem, and then use the same trick to construct a related lattice or discrete problem.

II. ONE-DIMENSIONAL LATTICE

We consider a particle on a one-dimensional lattice with sites labeled by an index x: $\ldots,-1,0,1,2,\ldots$. Let $|x\rangle$ be the state with the particle at site x. Then J is a translationally invariant hopping operator defined by

$$J|x\rangle=\sum_r J(r)|x+r\rangle.$$

Thus if we define the wave function $\psi(x)$ of the state $|\psi\rangle$ by

$$|\psi\rangle=\sum_x \psi(x)|x\rangle,$$

then

$$\begin{aligned}J|\psi\rangle&=\sum_x\sum_r \psi(x)J(r)|x+r\rangle\\&=\sum_{x'}\sum_r \psi(x'-r)J(r)|x'\rangle\\&=\sum_x \psi'(x)|x\rangle,\end{aligned}$$

where

$$\psi'(x)=\sum_r J(x-r)\psi(r)=J\psi$$

gives the matrix representation of J acting on the wave function. This is the representation we shall use in the rest of the paper.

Defining the discrete Fourier transform by

$$\psi(x)=\int_{-\pi}^{\pi}dk\,e^{ikx}\psi_F(k),$$

then since J acts on ψ as a convolution,

$$\psi_F'(k)=2\pi J_F(k)\psi_F(k).$$

We now select the operator J so that it mimics $-d^2/dx^2$ on continuous functions. What this means is the following: Use the formula for the discrete Fourier transform, with the true Fourier transform $\psi_F(k)$, to define a new function $\psi_c(x)$ of a continuous variable x. Then the action of $-d^2/dx^2$ on $\psi_c(x)$ is given by

$$\frac{-d^2}{dx^2}\psi_c(x) = \int_{-\pi}^{\pi} dk(-d^2/dx^2)e^{ikx}\psi_F(k)$$
$$= \int_{-\pi}^{\pi} dk\, k^2 e^{ikx}\psi_F(k).$$

Thus, we are to choose $2\pi J_F(k) = -k^2$.

In the language of solid-state physics, the functions $\psi_c(x) = e^{ikx}$ are the Bloch functions, chosen from the first band corresponding to the Brillouin zone $-\pi < k \leq \pi$. The functions $\psi_c(x)$ made from linear combinations of Bloch functions from the first band form a vector space; such functions we call functions from the first band. Then, taking as an example $\psi_F(k) = e^{-ikj}$,

$$\psi_c(x) = \int_{-\pi}^{\pi} dk\, e^{ik(x-j)},$$

which are the Wannier functions, equal to $2\pi\delta_{xj}$ when x is restricted to be an integer. However, as emphasized by several authors, if we multiply two functions from the first band, the product is not necessarily a function from the first band. Since J acts as $-d^2/dx^2$ only on functions from the first band, the Leibniz rule for differentiating products will not hold.

III. FINITE-DIMENSIONAL VECTOR SPACE

Let us consider a particular set of wave functions

$$\phi_m(x) = [2\sin(\pi x/N)]^{2m}$$
$$= [\phi_1(x)]^m$$
$$= \{2[1-\cos(2\pi x/N)]\}^m$$
$$= (1-e^{2\pi ix/N})^m(1-e^{-2\pi ix/N})^m$$

with $m = 1,2,\ldots$.

These functions, and any linear combination of such functions $\phi(x)$, form a vector space I of functions with the following properties:

$$\phi(x+N) = \phi(x), \quad \phi(0) = 0, \quad \phi(-x) = \phi(x).$$

This is a finite-dimensional vector space, and there are only M-independent functions, where $M = N/2$, for N even or $M = (N-1)/2$, for N odd. This can easily be seen by considering the functions

$$\sum_k (\delta_{x,j+kN} + \delta_{x,-j+kN}), \quad j = 1,2,\ldots,M.$$

We will take as our independent basis functions for the vector space I the functions

$$\phi_m(x) = [\phi_1(x)]^m, \quad m = 1,2,\ldots,M.$$

On occasion, we will use the symbol ϕ to represent the change of variable from integer x to $\phi = \phi_1(x)$ taking discrete values $\phi_j = [2\sin(\pi j/N)]^2$, $j = 1,2,\ldots,M$, on the lattice. Also, when formulas do not generalize in the obvious way for N even, we will assume N to be odd and $M = (N-1)/2$.

We have called these functions of type I because we interpret the periodic potential as leading to a discrete band problem. The band edges are determined by functions of the four types:

$$\phi(x+N) = \pm\phi(x), \quad \phi(0) = 0, \quad \phi(-x) = \pm\phi(x).$$

Thus our states give exactly one-quarter of the band edges. The other band-edge states can be determined by similar methods. However, each of the four types of band-edge states has its own distinct set of special values of the coupling constant.

IV. ACTION OF J ON THE VECTOR SPACE

Let us now consider the action of J on the vector space I by considering the action of J on the basis set $\phi_m(x) = [\phi_1(x)]^m$, $m = 1,2,\ldots,M$. By construction,

$$J\phi_m(x) = \frac{-d^2}{dx^2}\phi_m(x)$$
$$= \frac{-d^2}{dx^2}[2\sin(\pi x/N)]^{2m}.$$

Simple differentiation gives

$$J\phi_m(x) = \alpha_m\phi_m(x) - \beta_m\phi_{m-1}(x)$$
$$= [\alpha_m - \beta_m v(x)]\phi_m(x),$$

where

$$\alpha_m = (2\pi m/N)^2,$$

$$\beta_m = 2m(2m-1)(2\pi/N)^2,$$

$$v(x) = 1/\phi_1(x).$$

The interpretation is that $v(x)$ is a potential with strength β_m, and $\phi_m(x)$ is the corresponding ground-state wave function with ground-state energy α_m. We also see why we need to restrict ourselves to functions which vanish for $x = 0$, in order to interpet $v(x)$ as a potential for which $v(x)\phi_1(x) = 1$.

V. ASSOCIATED CONTINUUM PROBLEM

Before we continue in our solution of the lattice problem, let us look at the associated continuum problem

$$\frac{-d^2\psi}{dx^2} + gv(x)\psi = E\psi.$$

We try as a solution for the ground state,

$$\psi_1(x) = |2\sin(\pi x/N)|^{\lambda},$$

and after differentiation find

$$E_1 = (\pi\lambda/N)^2,$$

$$g = \lambda(\lambda-1)(2\pi/N)^2.$$

For the excited states, we write the Hamiltonian in a basis of states $\phi_m(x)$, where now

$$\phi_m(x) = \psi_1(x)[2\sin(\pi x/N)]^{2(m-1)} = |2\sin(\pi x/N)|^{\lambda+2(m-1)}.$$

Once again, we have

$$\frac{-d^2}{dx^2}\phi_m(x) = \alpha_m\phi_m(x) - \beta_m\phi_{m-1}(x) = [\alpha_m - \beta_m v(x)]\phi_m(x),$$

where now

$$\alpha_m = [\pi(2m+\lambda-2)/N]^2,$$

$$\beta_m = (2m+\lambda-2)(2m+\lambda-3)(2\pi/N)^2.$$

Again,

$$v(x) = 1/\phi_1(x).$$

VI. DISCRETE CASE

For either the continuum or the discrete case, the general eigenvalue equation we wish to solve is

$$J\psi + gv(x)\psi = E\psi.$$

Expanding $\psi(x)$ in the basis functions as

$$\psi(x) = \sum_m \psi_m\phi_m(x),$$

we find for the eigenvalue equation the simple result

$$\sum_m \psi_m[(\alpha_m - E)\phi_m(x) + (g-\beta_m)\phi_{m-1}(x)] = 0.$$

For either the continuum or the lattice problem, the appropriate coefficients α_m and β_m must be used.

In this expression, however, for the lattice problem, $\phi_0(x)$ must be interpreted as 1 for $x \neq kN$, where k is an integer. [For the continuum problem, the coefficient $(g-\beta_1)$ of $\phi_0(x)$ vanishes, so we need not worry about $\phi_0(x)$ at all.] But since we are in the vector space **I**, when extended to all integer x, we must have

$$\phi_0(x) = 1 - \sum_k \delta_{x,kN} = 1 - \Delta(x).$$

Since the M functions

$$\phi_m(x) = [\phi_1(x)]^m, \quad m = 1,2,\ldots,M,$$

are a complete set of basis functions for the vector space **I**, it is possible to express $\phi_0(x)$ in terms of these basis functions.

Alternatively, define the variable $\phi = \phi_1(x)$. Then, since $\phi_m = \phi^m$, we seek for $\Delta(x) = \Delta[\phi]$ a polynomial in ϕ of degree M, which vanishes for

$$\phi = \phi_j = [2\sin(\pi j/N)]^2, \quad j = 1,2,\ldots,M,$$

and is equal to 1 for $\phi = 0$. Such a polynomial is unique, and is given by

$$\Delta[\phi] = \prod_{j=1}^{M}(\phi_j - \phi)/\phi_j = \prod_{j=1}^{M}\{1 - [\sin(\pi x/N)/\sin(\pi j/N)]^2\} = \sin(\pi x)/[N\sin(\pi x/N)] = \sum_{k=0}^{M}(-\phi)^k(M+k-1)!/[(M-k-1)!(2k+1)!].$$

In evaluating this expression, we have used two standard formulas, which can be found for instance in Gradshteyn and Ryzhik[4] as GR(1.391.3) and GR(1.332.2). The formula for N even is slightly different.

Finally, this gives us the expansion for $\phi_0(x)$ as

$$\phi_0(x) = \sum_{k=1}^{M}\phi_k(x)(-1)^{k-1}(M+k-1)! \times [(M-k-1)!(2k+1)!]^{-1} = \sum_{k=1}^{M}\phi_k(x)\gamma_k,$$

with

$$\gamma_k = (-1)^{k-1}(M+k-1)!/[(M-k-1)!(2k+1)!].$$

Returning to the eigenvalue equation, after substituting this expression for $\phi_0(x)$ and collecting coefficients of $\phi_m(x)$, we find the following equations:

$$0 = (\alpha_m - E)\psi_m + (g-\beta_{m+1})\psi_{m+1} + (g-\beta_1)\gamma_m\psi_1, \quad m = 1,\ldots,M.$$

In this expression, we are to interpret ψ_{M+1} as 0.

We see why the particular value $g = \beta_1$ for the coupling constant is privileged, for then the last term in all the equations vanishes. This happens for the continuum case for all λ. However, for these situations, we have that $E_m = \alpha_m$ for all $m = 1,\ldots,M$. The continuum case corresponds to M infinite.

VII. CONSISTENCY RELATION

These equations can be iterated starting from

$$\psi_M = (\beta_1 - g)\gamma_M\psi_1/(\alpha_M - E),$$

and using

$$\psi_m = [(\beta_{m+1}-g)\psi_{m+1} + (\beta_1 - g)\gamma_m\psi_1]/(\alpha_m - E),$$

until we arrive at ψ_1, and the consistency condition

$$1 = \sum_{k=1}^{M}\gamma_k\prod_{j=1}^{k}(\beta_j - g)/(\alpha_j - E),$$

or equivalently

$$0 = \sum_{k=0}^{M}\prod_{j=1}^{k}(\beta_j - g)\gamma_k\prod_{j=k+1}^{M}(\alpha_j - E),$$

with the understanding that $\beta_0 - g = 1$, $\gamma_0 = -1$, and the empty product is 1.

The second form of the consistency relation is useful,

for we see that if g is equal to β_n, then the consistency relation simplifies to

$$0=\sum_{k=0}^{n-1}\prod_{j=0}^{k}(\beta_j-g)\gamma_k\prod_{j=k+1}^{M+1}(\alpha_j-E)$$

or

$$0=\prod_{j=n}^{M+1}(\alpha_j-E)\left[\sum_{k=0}^{n-1}\prod_{j=0}^{k}(\beta_j-g)\gamma_k\prod_{j=k+1}^{n-1}(\alpha_j-E)\right].$$

Therefore we immediately have the $M-n+1$ eigenvalues

$$E_{j-n+1}=\alpha_j\,,\quad j=n,\ldots,M\ \text{ for } g=\beta_n\,.$$

The other eigenvalues we refer to as the missing eigenvalues, in reference to the continuum problem. They are $n-1$ in number and are given by the abbreviated consistency relation

$$0=\sum_{k=0}^{n-1}\prod_{j=0}^{k}(\beta_j-g)\gamma_k\prod_{j=k+1}^{n-1}(\alpha_j-E)\,.$$

The simplest nontrivial case is $n=2$, with a single missing state E_1 given by

$$\alpha_1-E_M=\gamma_1(\beta_1-g)=\gamma_1(\beta_1-\beta_2)$$

or

$$E_M=\alpha_1+\gamma_1(\beta_2-\beta_1)=(2\pi/N)^2[1+5M(M-1)/3]\,.$$

We compare this with the largest of the other energy levels, E_{M-1}:

$$E_{M-1}=\alpha_M=(2\pi M/N)^2\,,$$

and see that $E_M>E_{M-1}$, as expected.

VIII. ABBREVIATED CONSISTENCY RELATION

Let us again suppose that $g=\beta_n$ and so $E_{j-n+1}=\alpha_j$ for $j=n,\ldots,M$. We shall examine the abbreviated consistency relation for the case when M becomes very large, and the energy is scaled by $E=(2\pi M/N)^2\varepsilon$. Then α_j is small compared to E for $j<n$, and

$$\gamma_k\rightarrow(-1)^{k-1}M^{2k}/(2k+1)!\,.$$

Substitution into the expression for the abbreviated consistency relation from the preceding section gives

$$0=\sum_{k=0}^{n-1}(-1/\varepsilon)^k(2k+2n)!\times[(2k+1)!(n-k-1)!(k+n)!]^{-1}\,.$$

The values of ε for the missing states are easily evaluated numerically as the $n-1$ zeros of this polynomial.

IX. CONCLUSION

We now close our discussion with a brief summary and a few remarks. Although we have constructed a lattice Hamiltonian which faithfully mimics the continuum Hamiltonian on functions in the first Brillouin zone, this is not even sufficient to insure that we recover the continuum model as the continuum limit of the lattice model. This happens only at the special values of the coupling constant $g=\beta_m$, when the wave function is analytic at the origin.

We see that the missing states behave independently of the "simple" states with $E=\alpha_m$, and seem to interact among each other just like any other complicated system. Thus the more missing states we have, the more difficult is the problem of determining these states and their energies. The only simplification we have is an explicit evaluation of the secular equation—of great use for the numerical evaluation of this particular one-body problem— but unlikely to be of much use for the many-body problem of Shastry and Haldane. This leads us to be rather pessimistic about the possibility of a complete solution of the lattice model—as was done for the continuum model.

There is one further possibility for progress, and that is to define a new lattice model which has exactly the properties we want—namely, all the wave functions are given by the lattice version of the lowest-energy continuum wave functions. Thus, we define the lattice Hamiltonian by its action on the basis functions $\phi_m(x)$ as before:

$$\begin{aligned}(H-E)\phi_m(x)&=(\alpha_m-E)\phi_m(x)+(g-\beta_m)\phi_{m-1}(x)\\&=[(\alpha_m-E)+(g-\beta_m)v(x)]\phi_m(x)\,.\end{aligned}$$

However, now α_m and β_m are given by the continuum expressions, depending on a parameter λ, which is then adjusted so that $g=\beta_1$. Then all energies are given by $E=\alpha_m$, $m=1,\ldots,M$. However, one is a bit vague about what the functions $\phi_m(x)$ are. Should they be the continuum expressions, or the original discrete expressions? They almost certainly are not orthogonal, and thus H is not Hermitian. Finally, one realizes that if one plays this new game, there is too much freedom, and unless H has a direct and appealing interpretation— as is the case of the original lattice Hamiltonian as introduced by Shastry and Haldane in the spin language—one is simply giving the solutions.

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