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1992 J. Phys. A: Math. Gen. 25 65

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J. Phys. A: Math. Gen. 25 (1992) 65–72. Printed in the UK

Exact solution of the Coulomb problem on a lattice

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Received 26 June 1991

Abstract. We study the difference Schrödinger equation with the Coulomb potential on the uniform one-dimensional lattice. Exact formulae for the eigenfunctions of both the bound state and scattering problem are obtained in terms of the Gauss hypergeometric function. Some characteristics of the bound states and the scattering phase shift are calculated. Limit relations between lattice and continuum Coulomb problems are established.

1. Introduction

The Schrödinger equation for a particle 'hopping' on a discrete lattice ('Wannier particle') provides a problem which has as much mathematical interest as importance due to applications in exciton physics (see [1] and references therein) and in lattice gauge theories [2]. Exactly solvable models have a special place in the field; they are rare and very desirable.

To our knowledge, the only known instances up to now where the Schrödinger equation on a lattice admits a complete analytical solution were those of the linear potential on the uniform one-dimensional lattice [3] and the harmonic oscillator on the multi-dimensional cubic lattice [4]. In these models the eigenfunctions of the discrete spectrum are expressed through known special functions (Bessel and Mathieu functions).

It is natural to expect that the Coulomb potential on a lattice might be another 'privileged' model for which the discrete Schrödinger equation is solved exactly. Indeed, in [5] the eigenvalue spectrum of the Coulomb Hamiltonian on the Bethe lattice was obtained analytically by means of a continuous fraction expansion of the Green function [6]. Being a powerful tool for deriving the eigenvalues, the method, however, fails to provide any information whatever about the eigenfunctions. But the very existence of analytical expressions for the eigenvalues is evidence that there can also exist closed-form formulae for the eigenfunctions.

In this paper we show that this is the case for the uniform one-dimensional lattice (the simplest version of the Bethe lattice of coordination 2). More precisely, we derive analytically the solutions to the difference Schrödinger equation

$$\Psi(x+1) - 2\Psi(x) + \Psi(x-1) + \left(E - \frac{q}{x}\right)\Psi(x) = 0 \tag{1}$$

$$\Psi(0) = 0 \qquad x \in Z_+ = \{0, 1, 2, \ldots\}$$

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0305-4470/92/010065+08$03.50 © 1992 IOP Publishing Ltd

with arbitrary energy E. They are expressed in terms of the Gauss hypergeometric function ${}_2F_1$. The condition of the norm boundness of Ψ yields the quantization rule for the eigenvalues obtained in [5]. The discrete spectrum eigenfunctions are given in terms of Meixner polynomials (a particular set of the classical orthogonal polynomials of a discrete variable [7]). This enables us to calculate exactly various characteristics of the bound states.

In addition, we study the scattering problem related to the Hamiltonian (1) and derive an exact formula for the corresponding phase shift. Somewhat surprisingly, it is about the same as for the continuum Coulomb Hamiltonian. Aside from the models with zero-range interaction potentials, we believe that this is the first time that a non-trivial scattering problem on a lattice is solved exactly.

2. Bound states

2.1. General solution

Note that the problem (1) should be supplemented with one more condition, say $\Psi(1) = 1$, which fixes a normalization constant and is of no importance.

It is convenient to introduce the momentum k related to the energy by the standard lattice dispersion rule [1]

$$E = E(k) = 2(1 - \cos k). \tag{2}$$

Following the analogy with the continuum Coulomb problem [8], we seek the solution to equation (1) in the form

$$\Psi(x) = x\, L(x) \mathrm{e}^{\mathrm{i}kx}.$$

Substituting this ansatz into (1) leads to an equation for L:

$$(x+1)L(x+1) - \mathrm{e}^{-\mathrm{i}k}(2x \cos k + q)\, L(x) + (x-1)\mathrm{e}^{-2\mathrm{i}k} L(x-1) = 0. \tag{3}$$

The key point is that this equation is quite similar to one of the fifteen Gauss relations [9] between the contiguous hypergeometric functions:

$$a(\xi - 1)\, F(a+1) + [2a - c - (a-b)\,\xi]\, F(a) + (c-a)\, F(a-1) = 0 \tag{4}$$

where $F(a)$ stands for ${}_2F_1(a, b; c; \xi)$. Namely, the coefficients of equation (3) are linear in x whereas those of equation (4) are linear in a. This suggests the following functional form for $L(x)$:

$$L(x) = {}_2F_1(-x+\beta,\, b;\, c;\, \xi\,) \tag{5}$$

where β, b, c and ξ do not depend on x and may be functions of the momentum k. Upon writing down the relation (4) for the hypergeometric function (5) and comparing the result with equation (3), one gets a set of equations for the parameters of the ansatz (5):

$$(\beta - x)(\xi - 1) = \gamma(x-1)\,\mathrm{e}^{-2\mathrm{i}k}$$

$$c + x - \beta = \gamma(x+1)$$

$$-\,2x + 2\beta - c + (x - \beta + b)\,\xi = -2\gamma\,\mathrm{e}^{-\mathrm{i}k}(x \cos k + q/2)$$

where γ is an arbitrary factor by which one can multiply equation (3). These equations are to be satisfied for any x with the other parameters fixed, so that the first two equations yield

$$\gamma = 1 \qquad \beta = 1 \qquad c = 2 \qquad \xi = 1 - e^{-2ik}.$$

The third equation fixes the last parameter of the ansatz (5):

$$b = 1 + i\eta(k) \qquad \eta(k) = \frac{q}{2\sin k}. \tag{6}$$

Thus, the function

$$\Psi(x) = x\, e^{ikx}\, {}_2F_1(-x+1,\, 1+i\eta(k);\, 2;\, 1-e^{-2ik}) \tag{7}$$

solves the difference Schrödinger equation (1) with arbitrary energy E.

2.2. Eigenfunctions

We now proceed to study the discrete spectrum of the problem. For a bound state, the wavefunction (7) should decrease fast enough as $x \to \infty$ in order to provide the norm boundness

$$\sum_{x \in Z_+} |\Psi(x)|^2 \leqslant \infty. \tag{8}$$

As follows from the known asymptotics of the hypergeometric function [9] (see also the next section), equation (8) holds true provided the exponent of equation (7) decreases as $x \to \infty$ and the hypergeometric function is a finite polynomial in x. This yelds the quantization rule for the momentum:

$$k_n = i\kappa_n \qquad \kappa_n \geqslant 0$$

$$1 + i\eta(i\kappa_n) = -n \qquad n = 0, 1, 2, \ldots \tag{9}$$

so that

$$\sinh \kappa_n = -\frac{q}{2(n+1)}. \tag{10}$$

Therefore, in the case of the attractive Coulomb potential ($q < 0$) we get the eigenvalue spectrum

$$E_n = 2\,[1 - \cos(i\kappa_n)] = -2\left[\left(1 + \frac{q^2}{4(n+1)^2}\right)^{1/2} - 1\right] \tag{11}$$

which coincides with the result of [5] for the trivial Bethe lattice with coordination $c = 2$.

Of course, there are no bound states if the Coulomb potential is repulsive ($q > 0$). As we shall see in the next section, for $q > 0$ equation (11) corresponds to zeros of the S matrix related to the lattice Hamiltonian (1) on the complex plane of the momentum.

According to (7) and (9), the eigenfunctions of the bound states (11) are given by

$$\Psi_n(x) = A_n\, x\, \mu_n^{x/2}\, {}_2F_1(-x+1,\, -n;\, 2;\, 1-\mu_n^{-1}) \tag{12}$$

where $\mu_n = e^{-2\kappa_n}$ and A_n is a normalization constant fixed by

$$\sum_{x\in Z_+} |\Psi_n(x)|^2 = 1. \tag{13}$$

It is worthwile noticing that up to a factor the hypergeometric function of (12) coincides with the Meixner polynomial $m_n^{(2,\mu_n)}(x-1)$, so that

$$\Psi_n(x) = A_n\, x\, \mu_n^{x/2}\, m_n^{(2,\mu_n)}(x-1). \tag{14}$$

The Meixner polynomials

$$m_n^{(\gamma,\mu)}(x) = (\gamma+x)_n\ {}_2F_1(-x,\, -n;\, -\gamma-x-n+1;\, \mu^{-1}) \tag{15}$$

are of the family of the classical orthogonal polynomials of a discrete variable, of which much is known [7]. The following relations proven in [7] are rather useful when dealing with the eigenfunctions (14).

(i) The polynomials $m_n^{(2,\mu)}$ are orthogonal in $l_2\left(Z_+\right)$ with the weight function

$$\rho(x,\mu) = \mu^x\,(1+x)$$

so that

$$\sum_{x\in Z_+} \rho(x,\mu)\, m_n^{(2,\mu)}(x)\, m_k^{(2,\mu)}(x) = \delta_{nk}\, d_n^2 \tag{16}$$

$$d_n^2 = \mu^{-n}\,(1-\mu)^{-2}\, n!\,(n+1)!.$$

(ii) Recurrence relation:

$$x\, m_n(x) = \alpha\, m_{n+1}(x) + \beta_n\, m_n(x) + \gamma_n\, m_{n-1}(x) \tag{17}$$

where $m_n(x) \equiv m_n^{(2,\mu)}(x)$ and

$$\alpha = \frac{\mu}{\mu-1} \qquad \beta_n = \frac{n+\mu(n+2)}{1-\mu} \qquad \gamma_n = \frac{n(n+1)}{\mu-1}. \tag{18}$$

Now we proceed to evaluate some characteristics of the bound states.

2.3. Normalization constant, mean radius and average potential energy

Hereafter we set $\mu = \mu_n = e^{-2\kappa_n}$, where κ_n is defined by (10).

Let us begin with calculation of the normalization constant A_n from (14). Substituting (14) into equation (13) yields

$$A_n^2 \sum_{x \in Z_+} x^2 \mu^x [m_n^{(2,\mu)}(x-1)]^2 = 1.$$

Upon shifting the sum argument $x \to x+1$ one gets

$$1 = \mu A_n^2 \{d_n^2 + S_n^{(1)}\} \tag{19}$$

where use has been made of equation (16) and where we have introduced the notation

$$S_n^{(l)} = \sum_{x \in Z_+} x^l \rho(x,\mu)[m_n^{(2,\mu)}]^2 \qquad l = 1, 2, \ldots. \tag{20}$$

The sum $S_n^{(1)}$ is evaluated by means of the recurrence relation (17):

$$S_n^{(1)} = \frac{1}{1-\mu}[n + \mu(n+2)]\, d_n^2 \tag{21}$$

and from equation (19) one gets the normalization constant:

$$A_n = \frac{2}{(n+1)!}\exp[-(n+1)\kappa_n] \sinh\kappa_n \sqrt{\tanh\kappa_n}.$$

Next, let us calculate the mean radius of a bound state

$$r_n = \sum_{x \in Z_+} x\, \Psi_n^2(x).$$

Upon using (14) and making the transform $x \to x+1$ in the resulting sum, we have

$$r_n = \mu A_n^2 (d_n^2 + S_n^{(1)} + S_n^{(2)}) \tag{22}$$

where $S_n^{(l)}$ is defined by (20). To evaluate the sum $S_n^{(2)}$, we again use the recurrence relation (17) which follows ($m_n(x) \equiv m_n^{(2,\mu)}$)

$$[x\, m_n(x)]^2 = (\alpha^2 m_{n+1}^2 + \beta_n^2 m_n^2 + \gamma_n^2 m_{n-1}^2 + \ldots)$$

where ... stands for a sum of products of two Meixner polynomials with different indices. Such terms do not contribute in (20) due to the orthogonality (16), so that we have

$$S_n^{(2)} = \alpha^2 d_{n+1}^2 + \beta_n^2 d_n^2 + \gamma_n^2 d_{n-1}^2 \tag{23}$$

with the coefficients from (18). Equations (21)–(23) yield the following value for the mean radius:

$$r_n = \frac{n+1}{\sinh 2\kappa_n}(2 + \cosh 2\kappa_n) = \frac{(n+1)\left[6(n+1)^2 + q^2\right]}{|q|[4(n+1)^2 + q^2]^{1/2}}. \tag{24}$$

Finally, consider the average Coulomb potential energy of a bound state:

$$U_n = \sum_{x \in Z_+} \frac{q}{x} \Psi_n^2(x).$$

From (14) and (16) one gets

$$U_n = q\mu A_n^2 d_n^2 = -2e^{-2\kappa_n} \sinh\kappa_n \tanh\kappa_n.$$

Apparently, this shows failure of the virial theorem which is a specific feature of the Schrödinger dynamics on a lattice.

3. Scattering states

For the continuous spectrum of the Hamiltonian (1) the momentum k is real and runs over the band $[0, \pi]$. Equation (7) yields the wavefunction of the continuous spectrum which is subjected to the regular boundary condition at the origin.

The exact expression for the wavefunction enables us to calculate the phase shift in the Coulomb scattering problem on the lattice, being provided with the asymptotics of the hypergeometrical function of (7) at $x \to \infty$. Its leading term is of the form

$$ {}_2F_1(-x,\, 1+\mathrm{i}\eta;\, 2;\, 1-\mathrm{e}^{-2\mathrm{i}k}) \sim B(k)\,\frac{\mathrm{e}^{-\mathrm{i}kx}}{x}\,\sin[\mathrm{i}k(x+1) - \mathrm{i}\eta\ln(2x\sin k) + \mathrm{i}\delta_{\mathrm{c}}(k)] \qquad (25) $$

where

$$ \delta_{\mathrm{c}}(k) = \arg\Gamma(1+\mathrm{i}\eta) \qquad (26) $$

and

$$ B(k) = \frac{\exp(\pi\eta/2 - k\eta)}{|\Gamma(1+\mathrm{i}\eta)|\sin k}. $$

As follows from equations (7) and (25), the scattering wavefunction defined as

$$ \Psi(x,k) = B^{-1}(k)\, x\, \mathrm{e}^{\mathrm{i}kx}\ {}_2F_1(-x+1,\, 1+\mathrm{i}\eta(k);\, 2;\, 1-\mathrm{e}^{-2\mathrm{i}k}) \qquad (27) $$

has the asymptotics

$$ \Psi(x,k) \sim \sin\{\mathrm{i}kx - \mathrm{i}\eta\ln(2x\sin k) + \mathrm{i}\delta_{\mathrm{c}}(k)\}\left[1 + \mathrm{O}\left(\frac{1}{x}\right)\right] \qquad x \to \infty. \qquad (28) $$

Recall that energy is related to the momentum k by the dispersion rule (2) and the Coulomb parameter η is defined by equation (6).

It is easy to check that if the Coulomb potential is set to be zero ($\eta = 0$), equation (27) gives the trivial wavefunction of the free difference Hamiltonian on the lattice:

$$ \Psi(x,k)_{|\eta=0} = \sin kx. $$

Comparing this with the asymptotics (28) shows that the phase $\delta_{\mathrm{c}}(k)$ may be interpreted as the phase shift for the Coulomb scattering problem on the lattice.

Remarkably, the asymptotics (28) is very similar to its continuum analogue [8] in the Coulomb scattering problem on the half line $[0, \infty)$. Aside from normalization factors, the only difference is in the form of the momentum dependence of the logarithmic phase of (28) and that of the Coulomb parameter (6): in our case momentum is involved through $\sin k$ to be compared to k in the continuum limit.

Defining the S matrix through the phase shift in the standard way

$$ S(k) = \mathrm{e}^{2\mathrm{i}\delta_{\mathrm{c}}(k)} = \frac{\Gamma(1+\mathrm{i}\eta)}{\Gamma(1-\mathrm{i}\eta)} \qquad (29) $$

allows one to interpret the bound states (11) as poles of the S matrix on the upper half plane of the complex momentum k. In the case of the repulsive Coulomb potential equation (11) with $\sinh\kappa_n = q/2(n+1)$ describes the zeros of the S matrix (29) (resonances) with the 'eigenfunctions' exponentially increasing as $x \to \infty$.

We did not find in the literature a suitable asymptotic representation for the hypergeometric function which follows equation (25). This is why we outline the proof of the asymptotics (25).

By making use of the standard integral representation [9] we write the hypergeometric function as

$$
{}_2F_1(-x,\ 1+\mathrm{i}\eta;\ 2;\ 1-\xi) = [\Gamma(1+\mathrm{i}\eta)\Gamma(1-\mathrm{i}\eta)]^{-1}\ I
$$

$$
I = \int_0^1 \mathrm{d}t\, t^{\mathrm{i}\eta}\,(1-t)^{-\mathrm{i}\eta}\,[1-t(1-\xi)]^{x} \tag{30}
$$

where $\xi = \mathrm{e}^{-2\mathrm{i}k}$. Clearly, $|1-t(1-\xi)| < 1$ for $t \in (0,1)$ and $|1-t(1-\xi)| = 1$ at $t = 0, 1$. Therefore, the large-x asymptotics of (30) is generated by the endpoints $t = 0, 1$ of the integral. Upon taking into account only the leading terms of the integrand near these points, the integral can be evaluated in terms of the gamma function to obtain

$$
I = I_0 + I_1
$$

$$
I_0 \sim (1-\xi)^{-1-\mathrm{i}\eta}\, x^{-1-\mathrm{i}\eta}\, \Gamma(1+\mathrm{i}\eta)
$$

$$
I_1 \sim (1-\xi^{-1})^{-1+\mathrm{i}\eta}\, x^{-1+\mathrm{i}\eta}\, \xi^{x}\, \Gamma(1-\mathrm{i}\eta)
$$

where I_0 and I_1 represent the contributions of the points $t = 0, 1$. A straightforward calculation now leads to the asymptotics (25).

4. Continuum limit

So far we have considered a lattice with a unit step between sites. One can easily generalize the treatment for a lattice of arbitrary step h which corresponds to the Schrödinger equation

$$
h^{-2}\{\Psi(x+h) - 2x\Psi(x) + \Psi(x-h)\} + \left(E - \frac{q}{x}\right)\Psi(x) = 0 \tag{31}
$$

$$
\Psi(0) = 0 \qquad x = 0, h, 2h, \ldots.
$$

Namely, the solutions to the equations (1) and (31) are related by the scaling transforms

$$
x \to \frac{x}{h} \qquad q \to qh \qquad E \to Eh^2 \qquad k \to kh \tag{32}
$$

to be performed in all formulae above.

It is natural to expect that when $h \to 0$ the properly normalized wavefunctions of the difference operator (31) will converge to those of the continuum Coulomb Hamiltonian. This limit can be established by making use of the known relation for the hypergeometric function [9]:

$$
\lim_{a\to\infty}\ {}_2F_1(a,\ b;\ c;\ x/a) = \ {}_1F_1(b;\ c;\ x) \tag{33}
$$

where ${}_1F_1$ stands for the confluent hypergeometric function [9].

Consider the discrete spectrum eigenfunctions (14). Due to the definition (15) and (33), in the continuum limit the Meixner polynomials converge to the Laguerre polynomials [7],

$$\lim_{\Delta\to\infty} \frac{1}{n!} m_n^{(\gamma,1-\Delta)}(x/\Delta) = L_n^{\gamma-1}(x).$$

Upon taking into account the scaling transforms (32), this results in the following limit relation for the wavefunctions of the bound states:

$$\lim_{h\to 0} h^{-1/2}\,\Psi(x/h) = C_n\, r\mathrm{e}^{-r/2}\, L_n^1(r) \tag{34}$$

where

$$r = \frac{|q|x}{n+1} \qquad C_n^2 = \frac{|q|}{2}(n+1)^{-3}\,.$$

The RHS of (34) coincides with the eigenfunction of the continuum s-wave Coulomb Hamiltonian on the half line [8]. Also, it is clearly seen that the eigenvalues (11) and the mean radii (24) tend to the corresponding continuum values as $h \to 0$:

$$E_n(h) = \frac{q^2}{4(n+1)^2} + \mathrm{O}(h^2)$$

$$r_n(h) = \frac{3}{|q|}(n+1)^2 + \mathrm{O}(h^2).$$

For the scattering states (27) according to (32) and (33) we have

$$\lim_{h\to 0} \Psi(x/h,\, kh) = \mathrm{e}^{-\pi\eta_c/2}|\Gamma(1+\mathrm{i}\eta_c)|\, kx\mathrm{e}^{\mathrm{i}kx}\ {}_1F_1(1+\mathrm{i}\eta_c;\, 2;\, -2\mathrm{i}kx)$$

where $\eta_c = q/2k$. This limit coincides with the well-known solution of the Coulomb scattering problem on the half line [8]. Of course, the Coulomb phase shift (26) converges to its continuum value $\arg\Gamma(1+\mathrm{i}\eta_c)$.

Acknowledgments

I am grateful to C Gignoux and B Vignon for hospitality at ISN.

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