



☆ 附出國會議心得報告

# 行政院國家科學委員會專題研究計畫成果報告

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## 摘要

在本計劃支助下，我們完成下列工作：

1. 在外場下帶電粒子之準精確可解性的研究。  
已完成兩篇論文。一篇已發表在  
*Physical Review A* 63 (2001) 062105；另一篇則已被  
*J. Math. Phys.* 接受，將於年底發表。

2. 強磁場下核子及電子氣之化學平衡  
(將發表在 *中華物理學刊 Chin. J. Phys.* 上)。

關鍵詞：

## ABSTRACT

~~We~~ We have completed the following works:

1. Quasi-exactly solvability of charged particles in external fields. One paper has appeared in Phys. Rev. A63 (2001) 062105, and the other is to be published in the J. Math. Phys. (Dec).
2. Chemical equilibrium of a degenerate gas of nucleons and electrons in a strong magnetic field.  
(to be published in the Chin. J. Phys. (Dec))

Key words: \_\_\_\_\_

# Charged particles in external fields as physical examples of quasi-exactly-solvable models: A unified treatment

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We present a unified treatment of three cases of quasi-exactly-solvable problems, namely, a charged particle moving in Coulomb and magnetic fields for both the Schrödinger and the Klein-Gordon case, and the relative motion of two charged particles in an external oscillator potential. We show that all these cases are reducible to the same basic equation, which is quasiexactly solvable owing to the existence of a hidden  $sl_2$  algebraic structure. A systematic and unified algebraic solution to the basic equation using the method of factorization is given. Analytical expressions of the energies and the allowed frequencies for the three cases are given in terms of roots of one and the same set of Bethe ansatz equations.

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## I. INTRODUCTION

It is well known that exact solutions are hard to come by in physics (in fact, in all sciences). Many exactly solvable examples presented in textbooks of physics are only exceptions. More often than not they serve only as paradigms to illustrate the fundamental principles in their respective fields. For real problems, approximation methods are indispensable.

Recently, it was found that for certain quantum-mechanical problems analytical solutions are possible, but only for parts of the energy spectra and for particular values of the fundamental parameters. First it was realized that the problem of two electrons moving in an external oscillator potential belongs to this class of problems [1,2]. Later, it was discovered that the two-dimensional Schrödinger equation of an electron moving in an attractive/repulsive Coulomb field and a homogeneous magnetic field also share similar characteristics [3–5]. More recently, the latter problems were extended to the two-dimensional Klein-Gordon [6] and the Dirac equation [7].

The essential features shared by all these above examples are as follows. The differential (Schrödinger, Klein-Gordon, and Dirac) equations are solved according to the standard procedure. After separating out the asymptotic behaviors of the system, one obtains an equation for the part that can be expanded as a power series of the basic variable. It is at this point that deviation from the standard exactly solvable cases appears: instead of the two-step recursion relations for the coefficients of power series so often encountered in exactly-solvable problems, one gets three-step recursion relations. The complexity of the recursion relations does not allow one to do anything to guarantee normalizability of the eigenfunctions. However, one can impose a sufficient condition for normalizability by terminating the series at a certain order of the power of the variable, i.e., by choosing a polynomial. By doing so one could obtain exact solutions to the original problem, but only for certain energies and for specific values of the parameters of the problem. These parameters are the frequency of the oscillator potential and the external magnetic fields.

It was soon realized [8,7] that the above quantum-mechanical problems are just examples of the so-called quasi-exactly-solvable models, recently discovered by physicists and mathematicians [9–16]. This is a special class of quantum-mechanical problems for which several eigenstates can be found explicitly. The reason for such quasiexact solvability is usually the existence of a hidden Lie-algebraic structure [10–14]. More precisely, a quasi-exactly-solvable Hamiltonian can be reduced to a quadratic combination of the generators of a Lie group with finite-dimensional representations.

In this paper we would like to show that three of the four problems mentioned in the second paragraph, namely, (a) charged particle moving in Coulomb and magnetic fields (the Schrödinger case), (b) charged particle in Coulomb and magnetic fields (the Klein-Gordon case), and (c) relative motion of two charged particles in an external oscillator potential, can be given a unified treatment. We shall show that all these cases are simply variations of the same basic equation [Eq. (10) below], which is quasiexactly solvable owing to the existence of a hidden  $sl_2$  algebraic structure. This algebraic structure was first realized by Turbiner for the case of two electrons in an oscillator potential [8]. We shall give a systematic and unified algebraic solution to the basic equation using the method of factorization presented in [7]. Our method allows one to find the analytic expressions of the energies, and the allowed frequencies once and for all in terms of the roots of a set of Bethe ansatz equations. This is in sharp contrast to the method of solving recursion relations, which must be performed for each and every order of the polynomial part in order to get these expressions.

We will define the three problems in Sec. II. In Sec. III the basic equation is solved by the method of factorization. The Lie-algebraic structure underlying the basic equation is discussed in Sec. IV. Section V then concludes the paper.

## II. BRIEF DESCRIPTION OF THE THREE PROBLEMS

In this section we shall give a brief description of the three cases of charged particles moving in external fields, which we will consider in the rest of the paper. Following

the previous works, we adopt the atomic units  $\hbar = m = e = 1$  in the cgs system.

#### A. Electron in Coulomb and magnetic fields: The Schrödinger case

This general case was considered in [3-5,7]. The Hamiltonian of a planar electron in a Coulomb field and a constant magnetic field  $\mathbf{B} = B\hat{z}$  ( $B > 0$ ) along the  $z$  direction is

$$H = \frac{1}{2} \left( \mathbf{p} + \frac{1}{c} \mathbf{A} \right)^2 - \frac{Z}{r}, \quad (1)$$

where  $c$  is the speed of light,  $Z$  (positive or negative) is the charge of the source of the Coulomb field, and the vector potential  $\mathbf{A}$  is  $\mathbf{A} = \frac{1}{2} \mathbf{B} \times \mathbf{r}$  in the symmetric gauge.

An ansatz of the eigenfunction in the polar coordinates  $(r, \theta)$  is

$$\Psi(r, \theta) = \frac{u(r)}{\sqrt{r}} \exp(im\theta - iEt), \quad m = 0, \pm 1, \pm 2, \dots \quad (2)$$

Here  $m$  is the angular momentum quantum number and  $E$  is the energy. The radial wave function  $u(r)$  satisfies the radial Schrödinger equation

$$\left[ \frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{2} \left( m^2 - \frac{1}{4} \right) \frac{1}{r^2} - \frac{1}{2} \omega_L^2 r^2 + \frac{Z}{r} + E - m\omega_L \right] u(r) = 0, \quad (3)$$

where  $\omega_L = B/2c$  is the Larmor frequency.

#### B. Electron in Coulomb and magnetic fields: The Klein-Gordon case

In [6] the above problem is extended to the Klein-Gordon case, assuming the same ansatz of the wave function as in Eq. (2). Now the radial wave function  $u(r)$  obeys the following equation:

$$\left[ \frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{2} \left( m^2 - \frac{Z^2}{c^2} - \frac{1}{4} \right) \frac{1}{r^2} - \frac{1}{2} \omega_L^2 r^2 + \frac{EZ}{c^2 r} + \frac{E^2}{2c^2} - \frac{c^2}{2} - m\omega_L \right] u(r) = 0. \quad (4)$$

But now, as noted in [6], the quantum number  $m$  must satisfy the relation

$$m^2 - \frac{Z^2}{c^2} > 0 \quad (5)$$

in order for the solutions to make sense. This relation forbids the existence of the  $s$  states ( $m = 0$ ).

#### C. Relative motion of two electrons in an external oscillator potential

In [2] the author considered the problem of a three-dimensional Schrödinger equation for two electrons (interacting with Coulomb potential) moving in an external harmonic-oscillator potential characterized by frequency  $\omega_{ext}$ . The Hamiltonian is

$$H = -\frac{1}{2} \nabla_1^2 + \frac{1}{2} \omega_{ext}^2 \mathbf{r}_1^2 - \frac{1}{2} \nabla_2^2 + \frac{1}{2} \omega_{ext}^2 \mathbf{r}_2^2 + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}. \quad (6)$$

The total wave function is factorizable into three parts that depend, respectively, only on the center of mass, the relative coordinates, and the spins of the electrons. The wave function of the center-of-mass coordinates satisfies the Schrödinger equation of a three-dimensional oscillator, the solution of which is well known. The spin part dictates the parity of the wave function of the relative motion. The Schrödinger equation for the relative motion is

$$\left[ -\frac{1}{2} \nabla_r^2 + \frac{1}{2} \omega_r^2 r^2 + \frac{1}{2r} \right] \phi(r) = \epsilon' \phi(r), \quad (7)$$

where  $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$ ,  $\omega_r = \omega_{ext}/2$ , and  $\epsilon'$  is one-half of the eigenenergy of the relative motion (in the notation of [2]). By assuming an ansatz of the wave function in the spherical coordinates of the form

$$\phi(r) = \frac{u(r)}{r} Y_{lm}(\hat{\mathbf{r}}), \quad (8)$$

where  $Y_{lm}$  are the spherical harmonics, we get from Eq. (7) the following equation

$$\left[ \frac{1}{2} \frac{d^2}{dr^2} - \frac{l(l+1)}{2} \frac{1}{r^2} - \frac{1}{2} \omega_r^2 r^2 - \frac{1}{2r} + \epsilon' \right] u(r) = 0. \quad (9)$$

We note here that if we change the sign of the  $1/r$  term in the last equation, we get an equation that describes the relative motion in the oscillator potential of an electron and a positron. This case will be included in our discussions.

#### III. THE BASIC EQUATION AND THE METHOD OF FACTORIZATION

After making some appropriate changes of the parameters, we can recast Eqs. (3), (4), and (9) into the same basic form, namely,

$$\left[ \frac{1}{2} \frac{d^2}{dr^2} - \frac{\gamma(\gamma-1)}{2} \frac{1}{r^2} - \frac{1}{2} \omega^2 r^2 + \frac{\beta}{r} + \alpha \right] u(r) = 0. \quad (10)$$

Here  $\beta$ ,  $\gamma$ , and  $\omega$  ( $\gamma, \omega > 0$ ) are real parameters, and  $\alpha$  is the eigenvalue of Eq. (10). Explicit expressions of these parameters for the three cases will be given in the next section. That this equation is quasireactly solvable means that, given

a fixed value of the parameter  $\gamma$  and  $\beta$  (or  $\omega$ ), the equation can be solved exactly only for a particular set of parameter  $\omega$  (or  $\beta$ ) and eigenvalue  $\alpha$ .

Now we make the following change of variables:  $x \equiv \sqrt{2\omega}r$  and  $b \equiv \sqrt{2\omega}\beta$ . Then Eq. (10) becomes

$$\left[ \frac{d^2}{dx^2} - \frac{\gamma(\gamma-1)}{x^2} - \frac{x^2}{4} + \frac{b}{x} + \frac{\alpha}{\omega} \right] u(x) = 0. \quad (11)$$

The values of  $\alpha$  and  $b$  in Eq. (11) may be found by means of a method closely resembling the method of factorization in nonrelativistic quantum mechanics [7]. We shall discuss this method briefly below. Let us assume

$$u(x) = x^\gamma \exp(-x^2/4) Q(x), \quad (12)$$

where  $Q$  is a polynomial. As mentioned in the Introduction, the assumption that  $Q$  be a polynomial is only a sufficient condition for normalizability of the eigenfunction  $u(x)$ . Substituting Eq. (12) into Eq. (11), we have

$$\left[ \frac{d^2}{dx^2} + \left( \frac{2\gamma}{x} - x \right) \frac{d}{dx} + \left( \epsilon + \frac{b}{x} \right) \right] Q(x) = 0, \quad (13)$$

where  $\epsilon = \alpha/\omega - (\gamma + 1/2)$ .

It is seen that the problem of finding the spectrum of Eq. (13) is equivalent to determining the eigenvalues of the operator

$$H = -\frac{d^2}{dx^2} - \left( \frac{2\gamma}{x} - x \right) \frac{d}{dx} - \frac{b}{x}. \quad (14)$$

We want to factorize the operator (14) in the form

$$H = a^\dagger a + \epsilon. \quad (15)$$

The eigenfunctions of the operator  $H$  at  $\epsilon=0$  must satisfy the equation

$$a\psi = 0. \quad (16)$$

Suppose polynomial solutions exist for Eq. (13), say  $Q = \prod_{k=1}^n (x - x_k)$ , where  $x_k$  are the zeros of  $Q$  and  $n$  is the degree of  $Q$  (we mention here that the order  $n$  in this paper is equal to  $(n-1)$  in [2-6] where  $x^{n-1}$  is the highest order term in  $Q$ ). Then the operator  $a$  must have the form

$$a = \frac{\partial}{\partial x} - \sum_{k=1}^n \frac{1}{x - x_k}, \quad (17)$$

and the operator  $a^\dagger$  has the form

$$a^\dagger = -\frac{\partial}{\partial x} - \frac{2\gamma}{x} + x - \sum_{k=1}^n \frac{1}{x - x_k}. \quad (18)$$

Substituting Eqs. (17) and (18) into Eq. (15) and then comparing the result with Eq. (14), we obtain the following set of equations for the zeros  $x_k$  (the so-called Bethe ansatz equations [13]):

$$\frac{2\gamma}{x_k} - x_k - 2 \sum_{j \neq k}^n \frac{1}{x_j - x_k} = 0, \quad k=1, \dots, n \quad (19)$$

as well as the two relations,

$$b = 2\gamma \sum_{k=1}^n x_k^{-1}, \quad \epsilon = n. \quad (20)$$

Summing all the  $n$  equations in Eq. (19) enables us to rewrite the first relation in Eq. (20) as

$$b = \sum_{k=1}^n x_k. \quad (21)$$

From the second relation in Eq. (20), one gets

$$\epsilon = n = \alpha/\omega - \left( \gamma + \frac{1}{2} \right). \quad (22)$$

For  $n=1,2$  the zeros  $x_k$  and the values of the parameter  $b$  for which solutions in terms of the polynomial of the corresponding degrees exist can easily be found from Eqs. (19) and (21) in the form

$$\begin{aligned} n=1, \quad x_1 &= \pm \sqrt{2\gamma}, \quad b = \pm \sqrt{2\gamma}; \\ n=2, \quad x_1 &= -x_2 = \sqrt{2\gamma+1}, \quad b=0, \\ x_1 &= 2\gamma/x_2, \quad x_2 &= \pm (1 + \sqrt{4\gamma+1})/\sqrt{2}, \\ b &= \pm \sqrt{2(4\gamma+1)}. \end{aligned} \quad (23)$$

For general values of  $n$  it is difficult to solve for the  $x_k$ 's from Eq. (19) and one must resort to numerical methods. But some properties of the solutions are known. First, from Eq. (19) we see that if  $\{x_k\}$  is a set of solutions to Eq. (19), then so is  $\{-x_k\}$ . This means, by Eq. (21), that for every possible value of  $b$ , there is a corresponding negative value  $-b$ . Second, as we shall see later in Sec. IV, the number of values of  $b$  for a fixed order  $n$  is  $n+1$ .

We now apply the above results to the three cases mentioned previously. The essential step is to solve the Bethe ansatz equations (19) for the roots  $x_k$ 's for each order  $n$ . Then from Eqs. (21) and (22) we obtain the values of the allowed pair of frequency and energy. Here we will give only the general expressions. The reader can easily reproduce the expressions for the two simplest orders (i.e.,  $n=1$  and 2) given in [2-6] by substituting Eq. (23) into the general expressions.

#### A. Electron in Coulomb and magnetic fields: The Schrödinger case

In this case,  $\gamma = |m| + 1/2$ ,  $\omega = \omega_L$ ,  $\beta = Z = \pm |Z|$ , and  $\alpha = E - m\omega_L$ . The upper (lower) sign in  $\beta$  corresponds to the case of attractive (repulsive) Coulomb interaction. We have

$$\omega_L = \frac{2Z^2}{b^2}, \quad E = \omega_L(n + m + |m| + 1). \quad (24)$$

These are the general expressions for the frequency (and hence the magnetic field) and the energy in terms of the values of  $b$ . They reproduce the results in [3–5].

#### B. Electron in Coulomb and magnetic fields: The Klein-Gordon case

For definiteness, we consider positive-energy solutions for the attractive Coulomb potential ( $Z > 0$ ). This is the case considered in [6]. Negative-energy solutions and the case for repulsive Coulomb field can be treated in exactly the same way. In this case,  $\gamma = \sqrt{m^2 - Z^2/c^2} + 1/2$ ,  $\omega = \omega_L$ ,  $\beta = ZE/c^2$ , and  $\alpha = E^2/2c^2 - c^2/2 - m\omega_L$ . In order for the wave function to make sense,  $\gamma$  has to be real. This implies that  $m^2 - Z^2/c^2 > 0$ , which forbids the existence of the  $m = 0$  states (the  $s$  states) in the Klein-Gordon case, as noted in [6].

Using  $\omega_L = 2\beta^2/b^2$  we get the allowed magnetic field as

$$B = 2c\omega_L = \frac{4Z^2E^2}{b^2c^3} \quad (25)$$

and from Eq. (22) we obtain the corresponding energy  $E$ ,

$$E^2 = c^4 \left[ 1 - \frac{4Z^2}{b^2c^2} (n+1+m+\sqrt{m^2-Z^2/c^2}) \right]^{-1}. \quad (26)$$

These are the most general expressions for the energy and the frequency.

For negative-energy solutions, the energy is given by the negative roots of Eq. (26). The only difference is that the roots of the Bethe ansatz equations have opposite signs in view of Eq. (21). This only changes the nodal structure of the wave functions. From the expression  $\beta = ZE/c^2$ , we note the equivalence between the positive- (negative-) energy solutions in the attractive Coulomb case and the negative- (positive-) energy solutions in the repulsive Coulomb case.

Let us mention here that for the cases in Secs. III A and III B, we may consider a dual situation of the original problem: we may consider the magnetic field  $B$  (and thus  $\omega_L$ ) as a fixed quantity, and the Bethe ansatz equations instead give the allowed values of the energy and the Coulomb charge  $Z$ .

#### C. Relative motion of two electrons in an external oscillator potential

In this case,  $\gamma = l + 1/2$ ,  $\omega = \omega_r$ ,  $\beta = -1/2$ , and  $\alpha = \epsilon'$ . We have the following general solutions:

$$\omega_r = \frac{1}{2b^2}, \quad \epsilon' = \omega_r \left( n + l + \frac{3}{2} \right). \quad (27)$$

They are also the solutions for the case of an electron and a positron in the oscillator potential ( $\beta = +1/2$ ).

#### IV. HIDDEN LIE-ALGEBRAIC STRUCTURE OF THE BASIC EQUATION

The basic equation (10), or its equivalent form (13), possesses an underlying Lie-algebraic structure that is responsible for its quasiexact solvability. In fact, Turbiner has identified an  $sl_2$  structure for the case of two charged particles in an oscillator potential [8]. In view of the fact that all the previous cases considered in this paper are related by the same basic equation (10), one expects the same hidden structure to be present in all these cases. This is indeed the case and it is sufficient to show that an  $sl_2$  algebra is in fact the underlying structure possessed by Eqs. (10) or (13). In this section we shall carry out Turbiner's analysis to Eq. (13), with only slight modifications in the parameters to suit the general situation. Only the main ideas are given here, and we refer the reader to [8] for details.

Let us construct three generators in the following manner:

$$\begin{aligned} J_n^+ &= r^2 \frac{d}{dr} - nr, \\ J_n^0 &= r \frac{d}{dr} - \frac{n}{2}, \\ J_n^- &= \frac{d}{dr}. \end{aligned} \quad (28)$$

These generators realize the  $sl_2$  algebra,

$$[J_n^+, J_n^-] = -2J_n^0, \quad [J_n^0, J_n^\pm] = \pm J_n^\pm \quad (29)$$

for any value of the parameter  $n$ . If  $n$  is a non-negative integer, then there exists for the  $sl_2$  algebra a  $(n+1)$ -dimensional irreducible representation  $\mathcal{P}_{n+1}(r) = \langle 1, r, r^2, \dots, r^n \rangle$ . From this it is clear that any differential operator formed by taking the polynomial of the generators (28) will have the space  $\mathcal{P}_{n+1}$  as the finite-dimensional invariant subspace. This is the main idea underlying the quasi-exactly-solvable operators [8–14].

Now consider the quasi-exactly-solvable operator that is quadratic in the  $J_n$ 's,

$$T_2 = -J_n^0 J_n^- + 2\omega J_n^+ - \left( \frac{n}{2} + 2\gamma \right) J_n^-. \quad (30)$$

This operator belongs to the class VIII according to the classification given in [10]. In terms of  $r$ ,  $T_2$  becomes

$$T_2 = -r \frac{d^2}{dr^2} + 2(\omega r^2 - \gamma) \frac{d}{dr} - 2\omega nr. \quad (31)$$

Let us now consider the eigenvalue problem

$$T_2 Q(r) = 2\beta(n) Q(r). \quad (32)$$

This eigenvalue problem possesses  $n+1$  eigenvalues  $\beta(n)$ , and the corresponding eigenfunctions are in the form of a polynomial of the  $n$ th power, while other eigenfunctions are nonpolynomial, which in general cannot be found in closed

analytic form [8]. Let us first substitute the form (31) into Eq. (32), then divide the resulting equation by  $2\omega r$  and change the variable  $r$  to  $x \equiv \sqrt{2}\omega r$ . This leads to the following equation

$$\left[ \frac{d^2}{dx^2} + \left( \frac{2\gamma}{x} - x \right) \frac{d}{dx} + \left\{ n + \sqrt{\frac{2}{\omega}} \beta(n) \frac{1}{x} \right\} \right] Q(x) = 0. \quad (33)$$

This is exactly Eq. (13), provided that  $\epsilon = n$  and  $b = \sqrt{2/\omega} \beta(n)$ . This means that Eq. (13) is quasiexactly solvable if  $\epsilon = n$ , which is exactly our relation in Eq. (22), and that there are only  $n+1$  allowed values of  $b = \sqrt{2/\omega} \beta$  in Eq. (13) [cf. Eq. (23)].

Translating back to the original three cases considered in this paper, these results imply the following. In Sec. III C,  $\beta$  is a fixed parameter ( $\beta = \pm 1/2$ ), hence the finite number ( $= n+1$ ) of the values of  $b$  implies the same number of the allowed frequency  $\omega_{ext}$  of the external oscillator potential and the corresponding energy. This is the case found in [2] and presented here again from a new light. For the cases in Secs. III A ( $\beta = Z$ ) and III B ( $\beta = ZE/c^2$ ), the above results mean that, at a fixed order  $n$ , there are exactly  $n+1$  allowed values of the pair of energy and magnetic field for a fixed Coulomb charge, or of the pair of energy and Coulomb charge for a fixed magnetic field.

Furthermore, it has been shown [8] that there exist  $[(n+1)/2]$  positive eigenvalues and the same number of negative eigenvalues of  $b$  (here  $[a]$  represents the integral part of  $a$ ). In the general situation considered in this paper, positive (negative) values of  $b$  correspond to the attractive (repulsive)

Coulomb field for positive-energy solutions. For negative-energy solutions, the sign of  $b$  is reversed for the two kinds of Coulomb field. Hence, our unified treatment together with the Lie-algebraic analysis of these cases give a very simple explanation as to why the number of the positive-energy levels for a fixed order  $n$  considered in [2–6] are all equal to  $[(n+1)/2]$ .

## V. CONCLUSIONS

In this paper we have presented a unified treatment of three cases of quasi-exactly-solvable problems, namely, a charged particle moving in Coulomb and magnetic fields for both the Schrödinger and the Klein-Gordon case, and the relative motion of two charged particles in an external oscillator potential. We show that all these cases are reducible to the same basic equation [Eq. (10)], which is quasiexactly solvable owing to the existence of a hidden  $sl_2$  algebraic structure. A systematic and unified algebraic solution to the basic equation using the method of factorization is given. Our method allows one to express the analytic expressions of the energies and the allowed frequencies once and for all in terms of the roots of a set of Bethe ansatz equations. Our treatment also reveals that the eigenenergies and the allowed frequencies in these cases are all given by the roots of the same set of Bethe ansatz equations.

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# Planar Dirac Electron in Coulomb and Magnetic Fields: a Bethe ansatz approach

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## Abstract

The Dirac equation for an electron in two spatial dimensions in the Coulomb and homogeneous magnetic fields is an example of the so-called quasi-exactly solvable models. The solvable parts of its spectrum was previously solved from the recursion relations. In this work we present a purely algebraic solution based on the Bethe ansatz equations. It is realised that, unlike the corresponding problems in the Schrödinger and the Klein-Gordon case, here the unknown parameters to be solved for in the Bethe ansatz equations include not only the roots of wave function assumed, but also a parameter from the relevant operator. We also show that the quasi-exactly solvable differential equation does not belong to the classes based on the algebra  $sl_2$ .

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1. Recently a new type of spectral problem, so-called quasi-exactly solvable model (QESM), was discovered by physicists and mathematicians [[1]-[8]]. This is a special class of quantum-mechanical problems for which analytical solutions are possible only for parts of the energy spectra and for particular values of the fundamental parameters. The reason for such quasi-exactly solvability is usually the existence of a hidden Lie-algebraic structure [[2]-[6]]. More precisely, quasi-exactly solvable (QES) Hamiltonian can be reduced to a quadratic combination of the generators of a Lie group with finite-dimensional representations.

The first physical example of QESM in atomic physics is the system of two electrons moving in an external oscillator potential discussed in [9, 10]. The authors of these works apparently were unaware of the mathematical development in QESM. Later, several physical QESM were discovered, which include the two-dimensional Schrödinger [11], the Klein-Gordon [12], and the Dirac equations [13] of an electron moving in an attractive/repulsive Coulomb field and a homogeneous magnetic field. The essential features shared by all these above examples are as follows. The differential equations are solved according to the standard procedure. After separating out the asymptotic behaviors of the system, one obtains an equation for the part which can be expanded as a power series of the basic variable. But instead of the two-step recursion relations for the coefficients of power series so often encountered in exactly solvable problems, one gets three-step recursion relations. The complexity of the recursion relations does not allow one to determine the energy spectrum exactly from the normalisability of the eigenfunctions. However, one can impose a sufficient condition for normalisability by terminating the series at a certain order of power of the variable; *i.e.* by choosing a polynomial. By doing so one could obtain exact solutions to the original problem, but only for certain energies and for specific values of the parameters of the problem. These parameters, namely, are the frequency of the oscillator potential and the external magnetic fields.

In [14] a systematic and unified algebraic treatment was given to the above-mentioned systems, with the exception of the Dirac case. This was made possible by realising that these systems are governed essentially by the same basic equation, which is quasi-exactly

solvable owing to the existence of a hidden  $sl_2$  algebraic structure. This algebraic structure was first realised by Turbiner for the case of two electrons in an oscillator potential [15]. In this algebraic approach, analytic expressions of the solvable parts of the energy spectrum and the allowed parameters were expressible in terms of the roots of a set of Bethe ansatz equations.

In this paper we would like to extend the method of [14] to the planar Dirac equation of an electron in the Coulomb and magnetic fields. It turns out that a set of Bethe ansatz equation can also be set up in this case. However, unlike the systems considered in [14], here the unknown variables in the Bethe ansatz equations involved not only the roots of the wave functions assumed, but also a parameter from the relevant operator. We also demonstrate that the Bethe ansatz approach yields the same spectrum as that obtained by solving recursion relations. Finally, we show that the quasi-exactly solvability of this system is not related to the  $sl_2$  algebra.

## 2. In 2+1 dimensions the Dirac algebra

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu}, \quad g^{\mu\nu} = \text{diag}(1, -1, -1) \quad (1)$$

may be represented in terms of the Pauli matrices as  $\gamma^0 = \sigma_3$ ,  $\gamma^k = i\sigma_k$ , or equivalently, the matrices  $(\alpha_1, \alpha_2) = \gamma^0(\gamma^1, \gamma^2) = (-\sigma_2, \sigma_1)$  and  $\beta = \gamma^0$ . Then the Dirac equation for an electron minimally coupled to an external electromagnetic field has the form (we set  $c = \hbar = 1$ )

$$(i\partial_t - H_D)\Psi(t, \mathbf{r}) = 0, \quad (2)$$

where

$$H_D = \alpha\mathbf{P} + \beta m - eA^0 \equiv \sigma_1 P_2 - \sigma_2 P_1 + \sigma_3 m - eA^0 \quad (3)$$

is the Dirac Hamiltonian,  $P_k = -i\partial_k + eA_k$  is the operator of generalized momentum of the electron,  $A_\mu$  the vector potential of the external electromagnetic field,  $m$  the rest mass of the electron, and  $-e$  ( $e > 0$ ) is its electric charge. The Dirac wave function  $\Psi(t, \mathbf{r})$

is a two-component function. In an external Coulomb field and a constant homogeneous magnetic field  $B > 0$  along the  $z$  direction, the potential  $A_\mu$  assume the following forms in the symmetric gauge

$$A^0(r) = Ze/r \ (e > 0), \quad A_x = -By/2, \quad A_y = Bx/2. \quad (4)$$

We assume the wave functions to have the form

$$\Psi(t, \mathbf{x}) = \frac{1}{\sqrt{r}} \exp(-iEt) \psi_l(r, \varphi), \quad (5)$$

where  $E$  is the energy of the electron, and

$$\psi_l(r, \varphi) = \begin{pmatrix} F(r)e^{il\varphi} \\ G(r)e^{i(l+1)\varphi} \end{pmatrix} \quad (6)$$

with integral number  $l$ . The function  $\psi_l(r, \varphi)$  is an eigenfunction of the conserved total angular momentum  $J_z = L_z + S_z = -i\partial/\partial\varphi + \sigma_3/2$  with eigenvalue  $j = l + 1/2$ . It should be reminded that  $l$  is not a good quantum number. Only the eigenvalues  $j$  of the conserved total angular momentum  $J_z$  are physically meaningful.

By putting Eq.(5) and (6) into (2), and taking into account of the equations

$$P_x \pm iP_y = -ie^{\pm i\varphi} \left( \frac{\partial}{\partial r} \pm \left( \frac{i}{r} \frac{\partial}{\partial \varphi} - \frac{eBr}{2} \right) \right), \quad (7)$$

we obtain

$$\frac{dF}{dr} - \left( \frac{l + \frac{1}{2}}{r} + \frac{eBr}{2} \right) F + \left( E + m + \frac{Z\alpha}{r} \right) G = 0, \quad (8)$$

$$\frac{dG}{dr} + \left( \frac{l + \frac{1}{2}}{r} + \frac{eBr}{2} \right) G - \left( E - m + \frac{Z\alpha}{r} \right) F = 0, \quad (9)$$

where  $\alpha \equiv e^2 = 1/137$  is the fine structure constant. In a strong magnetic field the asymptotic solutions of  $F(r)$  and  $G(r)$  have the forms  $\exp(-eBr^2/4)$  at large  $r$ , and  $r^\gamma$  with  $\gamma = \sqrt{(l + 1/2)^2 - (Z\alpha)^2}$  for small  $r$ . One must have  $Z\alpha < 1/2$ , otherwise the wave function will oscillate as  $r \rightarrow 0$  when  $l = 0$  and  $l = -1$ .

Let us assume

$$F(r) = r^\gamma \exp(-eBr^2/4) Q(r), \quad G(r) = r^\gamma \exp(-eBr^2/4) P(r). \quad (10)$$

In [13] we showed that parts of the spectrum could be analytically solved for by imposing the sufficient condition that  $Q(r)$  and  $P(r)$  be polynomials, thus showing that the system belongs to the QESM. The spectrum was solved in [13] from the recursion relations for the coefficients in the series expansion in  $Q$  and  $P$ . In this paper, we will show that the same spectrum can also be obtained in a purely algebraic way. This is achieved by the method of factorisation which leads to a set of Bethe ansatz equations [13, 14].

Substituting Eq.(10) into Eq.(8) and (9) and eliminating  $P(r)$  from the coupled equations, we have

$$\left\{ \frac{d^2}{dr^2} + \left[ \frac{2\gamma}{r} - eBr + \frac{Z\alpha/r^2}{E+m+Z\alpha/r} \right] \frac{d}{dr} + E^2 - m^2 \right. \\ \left. + \frac{2EZ\alpha}{r} + \frac{l+\frac{1}{2}}{r^2} - \frac{\gamma}{r^2} - eB(\Gamma+1) \right. \\ \left. + \frac{Z\alpha/r^2}{E+m+Z\alpha/r} \left[ \frac{\gamma}{r} - eBr - \frac{l+1/2}{r} \right] \right\} Q(r) = 0, \quad (11)$$

where  $\Gamma = l + 1/2 + \gamma$ . Once  $Q(r)$  is solved, the form of  $P(r)$  is obtainable from Eqs.(8) and (10). If we let  $x = r/l_B$ ,  $l_B = 1/\sqrt{eB}$ , Eq.(11) becomes

$$\left\{ \frac{d^2}{dx^2} + \left[ \frac{2\gamma}{x} - x + \frac{Z\alpha}{x((E+m)l_Bx + Z\alpha)} \right] \frac{d}{dx} \right. \\ \left. + (E^2 - m^2)l_B^2 + \frac{2EZl_B\alpha}{x} + \frac{(l+1/2-\gamma)}{x^2} - (\Gamma+1) \right. \\ \left. - \frac{Z\alpha(l+1/2-\gamma)}{x^2[(E+m)l_Bx + Z\alpha]} - \frac{Z\alpha}{(E+m)l_Bx + Z\alpha} \right\} Q(x) = 0. \quad (12)$$

Eq.(12) can be rewritten as

$$\left\{ \frac{d^2}{dx^2} + \left[ \frac{2\beta}{x} - x - \frac{1}{x+x_0} \right] \frac{d}{dx} + \epsilon + \frac{b}{x} - \frac{c}{x+x_0} \right\} Q(x) = 0. \quad (13)$$

Here  $\beta = \gamma + 1/2$ ,  $x_0 = Z\alpha/[(E+m)l_B]$ ,  $\epsilon = (E^2 - m^2)l_B^2 - (\Gamma+1)$ ,  $b = b_0 + L/x_0$ ,  $b_0 = 2EZ\alpha l_B$ ,  $L = (l+1/2-\gamma)$ , and  $c = x_0 + L/x_0$ . On expressing  $l_B$  in the expression of  $\epsilon$  in terms of  $x_0$ , we get

$$\epsilon = \frac{E-m}{E+m} \left( \frac{Z\alpha}{x_0} \right)^2 - (\Gamma+1). \quad (14)$$

It is obvious that the energy  $E$  is determined once we know the values of  $\epsilon$  and  $x_0$ . The corresponding value of the magnetic field  $B$  is then obtainable from the expression  $l_B = Z\alpha/[(E+m)x_0]$ . Solution of  $x_0$  is achieved below by means of the Bethe ansatz equations.

3. We observe that the problem of finding the spectrum for Eq.(13) is equivalent to determining the eigenvalues of the operator

$$D = -\frac{d^2}{dx^2} - \left( \frac{2\beta}{x} - x - \frac{1}{x+x_0} \right) \frac{d}{dx} - \frac{b}{x} + \frac{c}{x+x_0}. \quad (15)$$

We want to factorise the operator (15) in the form

$$D = a^+ a + \epsilon. \quad (16)$$

The eigenfunctions of the operator  $H$  at  $\epsilon = 0$  must satisfy the equation

$$aQ(x) = 0. \quad (17)$$

Suppose polynomial solution exist for Eq.(13), say  $Q$  equals a non-vanishing constant, or  $Q = \prod_{k=1}^n (x - x_k)$ , where  $x_k$  are the zeros of  $Q$ , and  $n$  is the degree of  $Q$ . In the case where  $Q$  is a constant (which may be viewed as corresponding to  $n = 0$ ), the operators  $a$  and  $a^+$  have the form

$$a = \frac{d}{dx}, \quad a^+ = -\frac{d}{dx} - \left( \frac{2\beta}{x} - x - \frac{1}{x+x_0} \right). \quad (18)$$

If  $Q = \prod_{k=1}^n (x - x_k)$ ,  $a$  and  $a^+$  will assume the form

$$a = \frac{d}{dx} - \sum_{k=1}^n \frac{1}{x - x_k} \quad (19)$$

and

$$a^+ = -\frac{d}{dx} - \left( \frac{2\beta}{x} - x - \frac{1}{x+x_0} \right) - \sum_{k=1}^n \frac{1}{x - x_k}. \quad (20)$$

We now substitute the forms of  $a$  and  $a^+$  into Eq.(16) and compare the result with Eq.(15). This leads to conditions that must be satisfied by the various parameters and the roots  $x_k$ 's. For constant  $Q$  ( $n = 0$ ), one has

$$\epsilon = b = c = 0. \quad (21)$$

The fact that  $c = 0$  implies

$$x_0^2 = -L. \quad (22)$$

For  $n \geq 1$ , one gets

$$b_0 + \frac{L}{x_0} = 2\beta \sum_{k=1}^n \frac{1}{x_k}, \quad \epsilon = n, \quad (23)$$

$$x_0 + \frac{L}{x_0} = \sum_{k=1}^n \frac{1}{x_k + x_0}, \quad (24)$$

$$\frac{2\beta}{x_k} - x_k - \frac{1}{x_k + x_0} - 2 \sum_{j \neq k}^n \frac{1}{x_j - x_k} = 0, \quad k = 1, \dots, n. \quad (25)$$

Eqs.(22), (24) and (25) constitute the set of  $n + 1$  Bethe ansatz equations relevant to this Dirac system, which involve  $n + 1$  unknown parameters  $\{x_0, x_1, \dots, x_n\}$ . It is worthwhile to note that, unlike the corresponding equations in the Schrödinger and the Klein-Gordon case discussed in [14], this set of Bethe ansatz equations involved not only the roots  $x_k$ 's, but also a parameter  $x_0$  from  $H$ . Summing Eq.(25) over  $k$  leads to the expression  $b_0 = x_0 + \sum_{k=1}^n x_k$ , i.e.  $b_0$  is simply the sum of all the roots of the Bethe ansatz equations. From the second equation in Eq.(23) we get

$$E^2 - m^2 = \frac{1}{J_B^2} (\Gamma + n + 1). \quad (26)$$

Since  $-1/2 \leq \Gamma \leq 0$  for  $Z\alpha < 1/2$  [13], we see from Eq.(26) that the solvable parts of the spectrum must satisfy  $|E| \geq m$ .

So we see that the solution of the solvable parts of the spectrum  $E$  boils down to solving the Bethe ansatz equations for  $x_0$  in the differential operator, and the roots  $x_k$  ( $k = 1, \dots, n$ ) of  $Q(x)$ . Once the value of  $x_0$  for each order  $n = \epsilon$  is known, the energy  $E$  is given by Eq.(14). The corresponding magnetic field  $B$  is then determined from the definition of  $b_0$ , or from Eq.(26). The Bethe ansatz equations thus provides a systematic solutions of the QES spectrum. Of course, as the order of the degree of  $Q$  increases, analytical solutions of the Bethe ansatz equations becomes difficult, and one must resort to numerical methods.

4. In what follows we shall show the consistency of the solutions by the Bethe ansatz approach and that by the recursion relations presented in [13] for the first three lowest orders ( $n = 0, 1, 2$ ) in  $Q$ . Instead of solving for  $x_0$ , our strategy is to eliminate it in Eq.(14) by means of the equations (22)-(25) so as to obtain an equation obeyed by  $E$  for each order

of  $Q$ . This equation is then compared with the corresponding equation obtained from the recursion relations as presented in [13].

From Eq.(21) and (22) we have  $x_0^2 = -L$  and  $\epsilon = 0$  when  $Q$  is a constant. Substitute these values of  $x_0$  and  $\epsilon$  into Eq.(14), and using the fact that  $\Gamma L = (Z\alpha)^2$ , we obtain the corresponding value of  $E$  as

$$E = -\frac{m}{2(l + \gamma + 1)} . \quad (27)$$

This is the result presented in [13]. The corresponding allowed value of the magnetic field  $B$  is then obtained from Eq.(26) and (27). The fact that  $x_0$  be real leads to  $L < 0$ , which in turn implies that the energy levels given by Eq.(27) are only possible for  $l < 0$ . This is consistent with the conclusion obtained in by the method of recursion relations [13].

For  $n = 1$ , we find from Eqs.(14), (23), (24) and (25) that

$$\Gamma + 2 = \frac{E - m (Z\alpha)^2}{E + m x_0^2} , \quad (28)$$

$$b_0 + \frac{L}{x_0} = \frac{2\beta}{x_1} , \quad (29)$$

$$\frac{1}{x_1 + x_0} = x_0 + \frac{L}{x_0} , \quad (30)$$

$$\frac{2\beta}{x_1} - x_1 - \frac{1}{x_1 + x_0} = 0 . \quad (31)$$

Eq.(29), (30), and (31) imply  $x_1 = b_0 - x_0$ . Substituting  $x_1$  into Eq.(30), we obtain

$$x_0^2 = L \left[ \frac{E + m}{2E(Z\alpha)^2} - 1 \right]^{-1} . \quad (32)$$

Then from Eq.(32) and Eq.(28), we get

$$\left[ 4(\Gamma + 1) - \frac{\Gamma}{z^2 \alpha^2} \right] E^2 + 4Em + \frac{\Gamma}{(Z\alpha)^2} m^2 = 0 . \quad (33)$$

The energy  $E$  can be solved from Eq.(33) by the standard formula, after which the magnetic field is determined from Eq.(26). Eq.(33) does not resemble the one obtained from recursion relation in [13]. However, on multiplying Eq.(33) by  $\Gamma + 1$  and making use of the fact that  $(Z\alpha)^2 = \Gamma(\Gamma - 2\gamma)$ , we can show, after some algebra, that Eq.(33) is equivalent to the corresponding equation given in [13].



Finally we consider the case for  $n = 2$ . We have Eq.(14) with  $\epsilon = 2$ , together with Eqs.(23), (24) and (25) in the forms

$$\Gamma + 3 = \frac{E - m (Z\alpha)^2}{E + m \frac{x_0^2}{x_0^2}}, \quad (34)$$

$$b_0 + \frac{L}{x_0} = \frac{2\beta}{x_1} + \frac{2\beta}{x_2}, \quad (35)$$

$$\frac{1}{x_1 + x_0} + \frac{1}{x_2 + x_0} = x_0 + \frac{L}{x_0}, \quad (36)$$

$$\frac{2\beta}{x_1} - x_1 - \frac{1}{x_1 + x_0} - \frac{2}{x_2 - x_1} = 0, \quad (37)$$

$$\frac{2\beta}{x_2} - x_2 - \frac{1}{x_2 + x_0} - \frac{2}{x_1 - x_2} = 0. \quad (38)$$

From these equations we find  $x_1 + x_2 = b_0 - x_0$  and  $x_1 x_2 = 2\beta x_0 (b_0 - x_0) / (b_0 x_0 + L)$ . Putting these expressions into Eq.(36) and using the fact that  $\Gamma = 2\beta + L - 1$ , we arrive at

$$(b_0^2 - 2\beta) x_0^2 + b_0 \Gamma x_0 + [b_0^2 (L - 1) - L (2\beta + 1)] + \frac{b_0 \Gamma L}{x_0} = 0. \quad (39)$$

Now multiplying Eq.(39) by  $\Gamma$ , using  $\Gamma L = (Z\alpha)^2$ , and expressing  $b_0$ ,  $l_B$ , and  $1/x_0^2$  in terms of  $E$ , we get finally

$$\begin{aligned} & \left\{ 4(2\Gamma + 3) - \frac{1}{(Z\alpha)^2} \left[ 6\Gamma + 2(\gamma + 1) + \frac{(2\gamma + 1)\Gamma}{\Gamma + 3} \right] \right\} E^3 \\ & + \left\{ 12 - \frac{1}{(Z\alpha)^2} \left[ 2(\gamma + 1) - \frac{(2\gamma + 1)\Gamma}{\Gamma + 3} \right] \right\} E^2 m \\ & + \frac{1}{(Z\alpha)^2} \left[ 6\Gamma + 2(\gamma + 1) + \frac{(2\gamma + 1)\Gamma}{\Gamma + 3} \right] E m^2 \\ & + \frac{1}{(Z\alpha)^2} \left[ 2(\gamma + 1) - \frac{(2\gamma + 1)\Gamma}{\Gamma + 3} \right] m^3 = 0. \end{aligned} \quad (40)$$

Again, this equation does not look the same as that obtained from the recursion relations. But we can show they are in fact equivalent as they differ only by a multiplicative factor  $(\Gamma + 1)(\Gamma + 2)$ .

5. One may as well solve the QES energy spectrum of the problem from the differential equation of  $P(x)$  instead of  $Q(x)$ . The analysis proceeds in exactly the same way as we did for  $Q(x)$ . We shall only give the outline below in order to show the similarity and differences between the two sets of Bethe ansatz equations.

The equation for  $P(x)$  can be cast into the following form

$$\left\{ \frac{d^2}{dx^2} + \left[ \frac{2\beta}{x} - x - \frac{1}{x+x'_0} \right] \frac{d}{dx} + \epsilon' + \frac{b'}{x} - \frac{c'}{x+x'_0} \right\} P(x) = 0. \quad (41)$$

Here  $x'_0 = Z\alpha/[(E-m)l_B]$ ,  $\epsilon' = (E^2 - m^2)l_B^2 - \Gamma$ ,  $b' = b_0 + c'$ , and  $c' = -\Gamma/x'_0$ . Other parameters are as defined previously. Instead of Eq.(14) we now have

$$\epsilon' = \frac{E+m}{E-m} \left( \frac{Z\alpha}{x'_0} \right)^2 - \Gamma. \quad (42)$$

We note here the sign difference before the mass terms in Eq.(14) and (42). It is obvious that Eq.(41) is in the same form as Eq.(13), and hence is also quasi-exactly solvable. Suppose  $P(x)$  has the factorized form  $P(x) = \prod_{k=1}^{n'} (x - x'_k)$ , then the set of Bethe ansatz equations for the parameters  $\{x'_0, x'_1, \dots, x'_{n'}\}$  is given by

$$-\frac{\Gamma}{x'_0} = \sum_{k=1}^{n'} \frac{1}{x'_k + x'_0}, \quad (43)$$

$$\frac{2\beta}{x'_k} - x'_k - \frac{1}{x'_k + x'_0} - 2 \sum_{j \neq k}^{n'} \frac{1}{x'_j - x'_k} = 0, \quad k = 1, \dots, n'. \quad (44)$$

In place of Eq.(23) we have

$$\begin{aligned} b_0 - \frac{\Gamma}{x'_0} &= 2\beta \sum_{k=1}^{n'} \frac{1}{x'_k}, \\ \epsilon' &= n', \quad n' = 1, 2, \dots \end{aligned} \quad (45)$$

Summing Eq.(44) over  $k$  gives  $b_0 = \sum_{k=1}^{n'} x'_k$ . For any given integral value of  $\epsilon' = n'$  the QES part of the energy  $E$  is determined from Eq.(42) once the values of  $x'_0$  is obtained from the Bethe ansatz equations. The corresponding value of the magnetic field  $B$  is then obtainable from the expression  $l_B = Z\alpha/[(E-m)x'_0]$ .

We note here that since the two sets of Bethe ansatz equations Eq.(22), (24)-(25) and Eq.(43)-(44) give the same spectrum of the QES energy  $E$  and the corresponding  $B$ , we have, from the values of  $\epsilon$ ,  $\epsilon'$  and  $b_0$ , the following necessary conditions:

$$n' = n + 1, \quad (46)$$

$$\begin{aligned} b_0 &= x_0 + \sum_{k=1}^n x_k \\ &= \sum_{k=1}^{n+1} x'_k. \end{aligned} \quad (47)$$

Conversely, one can easily show that Eq.(46) and (47) are also the sufficient conditions for the two sets of Bethe ansatz equations to give the same QES energy spectrum and magnetic field. The condition (46) implies that the degree of the polynomial  $P(x)$  is of one order higher than that of  $Q(x)$ , which is in complete agreement with the result obtained in [13].

6. We now demonstrate that the QES equations (13) and (41) cannot be represented as bilinear combination of the generators of the  $sl_2$  algebra. The question of whether there exists non- $sl_2$ -based one-dimensional QESM was first posed in [2] in which all  $sl_2$ -based QESM are classified. The first example of such a kind was given in [16], which presents a potential arising in the context of the stability analysis around the kink solution for  $\phi^4$ -type field theory in  $1+1$  dimensions.

We shall show that Eq.(13) is not generated by the  $sl_2$  algebra. The same conclusion applies immediately to Eq.(41), since both equations have the same form. Let us rewrite Eq.(13) as

$$\left\{ - (x^2 + x_0 x) \frac{d^2}{dx^2} + [x^3 + x_0 x^2 + (1 - 2\beta)x - 2\beta x_0] \frac{d}{dx} - \epsilon x^2 + (c - b - \epsilon x_0)x - b x_0 \right\} Q(x) = 0. \quad (48)$$

Turbiner [2] has shown that all  $sl_2$ -based second order QES differential equations can be cast into the form

$$-P_4(x) \frac{d^2 Q}{dx^2} + P_3(x) \frac{dQ}{dx} + (P_2(x) - \lambda) Q = 0, \quad (49)$$

where

$$\begin{aligned} P_4(x) &= a_{++}x^4 + a_{+0}x^3 + (a_{+-} + a_{00})x^2 + a_{0-}x + a_{--}, \\ P_3(x) &= 2(2j-1)a_{++}x^3 + [(3j-1)a_{+0} + b_+]x^2 \\ &\quad + [2j(a_{+-} + a_{00}) + a_{00} + b_0]x + ja_{0-} + b_-, \\ P_2(x) &= 2j(2j-1)a_{++}x^2 + 2j(ja_{+0} + b_+)x + a_{00}j^2 + b_0j. \end{aligned} \quad (50)$$

Here  $a_{kl}$ 's and  $b_k$ 's ( $k, l = +, 0, -$ ) are constants, and  $j$  is a non-negative integer or half-

integer. Eq.(49) corresponds to the eigenvalue problem

$$HQ = \lambda Q, \quad H = - \sum_{\substack{k,l=+,0,- \\ k \geq l}} a_{kl} J^k J^l + \sum_{k=+,0,-} b_k J^k, \quad (51)$$

which has a polynomial solution of power  $2j$  in  $x$ . Here  $J^k$ 's are the generators of  $sl_2$ :

$$J^+ = x^2 \frac{d}{dx} - 2jx, \quad J^0 = x \frac{d}{dx} - j, \quad J^- = \frac{d}{dx}. \quad (52)$$

Comparing Eqs.(48) and (49) we find that the two equations are inconsistent with each other. For instance, the coefficient of  $x^4$  in  $P_4$  requires  $a_{++} = 0$ , whereas the coefficient of  $x^3$  in  $P_3$  implies  $2(2j-1)a_{++} = 1$ , which gives a non-vanishing  $a_{++}$  for positive integral and half-integral values of  $j$ . This shows that Eq.(13) is not  $sl_2$ -based.

7. In conclusion, we have given an algebraic solution to the planar Dirac equation of an electron in the Coulomb and magnetic fields. The relevant Bethe ansatz equations are presented. Unlike the corresponding equations in the Schrödinger and the Klein-Gordon case discussed in [14], the unknown variables in this set of Bethe ansatz equations include not only the roots of the polynomial assumed, but also a parameter from the QES differential operator. Equivalence between this approach and that by the recursion relations is demonstrated. Finally, we show that the QES equation for this problem does not belong to any of the classes based on the  $sl_2$  algebra.

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# Chemical Equilibrium of a Degenerate Gas of Nucleons and Electrons in a Strong Magnetic Field

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## Abstract

The equations that define the equilibrium of a homogeneous relativistic gas of neutrons, protons and electrons in a constant magnetic field are obtained. We compute the relative densities of the particles at equilibrium as function of the density of neutrons and the magnetic field. It is found that, when only the first Landau level is being filled, the proton density is enhanced as compared to the case without the magnetic field. For an ultrastrong field there exists the possibility that the proton density is greater than the neutron density. However, when higher Landau levels are being filled, the values of the particle density at equilibrium quickly converge to those obtained without the magnetic field.

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The discovery of giant magnetic fields at the surface of neutron stars has greatly stimulated recent interest in the behavior of relativistic electrons in a constant strong magnetic field [1, 2, 3]. Observations of hard X-rays from pulsar Hercules X-1 allowed one to estimate the magnetic field at the pulsar surface to be of the order of  $10^{13}$  G. Such a magnetic field "frozen" in a neutron star must become stronger and stronger, reaching the ultrastrong value of the order of  $10^{18}$  G in the central part of the neutron star [4]. It is also believed that a new class of gamma-ray bursters, so-called soft gamma repeaters [5], are newly born neutron stars that have very large surface magnetic fields of the order up to  $10^{15}$  G. These extremely magnetized neutron stars have been named the magnetars [6]. Furthermore, fields of the order of  $10^{23}$  G [7] and even possibly  $10^{33}$  G [8] may exist at the electroweak phase transition. It is worthwhile noting that the magnetic field in a neutron star may be considered as a macroscopically uniform field with respect to the characteristic scales, such as the Compton wavelengths, of constituent particles of the neutron star. However, the field is extremely nonuniform at the electroweak phase transition. In any case, such a strong field will affect in an essential way the behaviors of charged particles in the star.

Inspired by these developments, we shall consider in this paper the effects of strong constant magnetic fields on the chemical equilibrium of a degenerate ideal gas of neutrons (n), protons (p), and electrons (e). We assume in what follows that the gas is spatially homogeneous due to the homogeneity of the magnetic field.

The first physical quantity which we must define is the chemical potential  $\mu_i$  ( $i = e, p, n$ ), or the Fermi energy (if the gas temperature is equal to zero), of the relativistic charged and neutral particles as a function of magnetic field.

Without any magnetic field ( $B = 0$ ) and at zero temperature ( $\theta = 0$ ), the chemical potential  $\mu_i$  of an ideal gas of particles of type  $i$  and mass  $m_i$  is related to the particle

density  $n_i$  by [9]

$$(\bar{\mu}_i^2 - 1)^{3/2} = n_i/n_{0i}, \quad n_{0i} = m_i^3 c^3 / 3\pi^2 \hbar^3. \quad (1)$$

In the presence of a magnetic field  $\mathbf{B} = (0, 0, B)$ , the chemical potential and density of the neutron gas are still given by eq.(1). But now the number density and chemical potential of the charged particles are related by

$$n_i = \frac{eB}{4\pi^2 \hbar^2 c} \sum_n (2 - \delta_{0n}) \int_{-\infty}^{\infty} \frac{dp}{\exp((E_n - \mu_i)/\theta) + 1}, \quad i = e, p, \quad (2)$$

where  $e > 0$  is the magnitude of the elementary charge,  $E_n = (p^2 c^2 + m_i^2 c^4 + 2eB\hbar cn)^{1/2}$  is the energy spectrum of a relativistic charged particle,  $n = 0, 1, 2, \dots$  enumerates the Landau levels,  $p$  is the momentum component parallel to  $\mathbf{B}$ , and  $\theta$  is the temperature. In what follows we shall express values of  $\mu_i$  in dimensionless units:  $\bar{\mu}_i = \mu_i/mc^2$ . Eq. (2) may be considered as a relation between  $n_i$ ,  $\mu_i$  and  $\theta$  at a given  $B$ . By integrating with respect to  $p$  in (2), making allowance for  $E_{\max} = \mu_i$  at  $\theta = 0$ , it is easy to obtain:

$$\frac{\sqrt{2}n_i}{3n_{0i}} \left( \frac{B_{0i}}{B} \right)^{3/2} = \left( (\bar{\mu}_i^2 - 1) \frac{B_{0i}}{2B} \right)^{1/2} + 2 \sum_{n=1}^{n_{mi}} \left( (\bar{\mu}_i^2 - 1) \frac{B_{0i}}{2B} - n \right)^{1/2}. \quad (3)$$

Here the critical field  $B_{0i} = m_i^2 c^3 / e\hbar$ , and the value  $n_{mi}$  is given by  $n_{mi} = [(\bar{\mu}_i^2 - 1)B_{0i}/2B]$ , where  $[x]$  is the integral part of  $x$ . We note here that  $B_{0e} \approx 4.41 \cdot 10^{13}$  G and  $B_{0p} = 3.4 \cdot 10^6 B_{0e}$ .

Let us now consider the conditions for chemical equilibrium of a degenerate gas of protons, neutrons and electrons in the presence of large magnetic fields. We also suppose that the temperature  $\theta$  is equal to zero, since for a typical 100-year old neutron star, its temperature is estimated to be  $10^8$  K (about 10 keV), which can be considered cold as compared to the Fermi energy (about 1000 MeV) of the degenerate relativistic neutrons [10].

We are interested in reactions in which the total density of baryons  $n_b = n_p + n_n$  is conserved and the charge neutrality condition of a gas  $n_p = n_e$  is satisfied. These processes are called the direct URCA processes [11, 9, 10]. Our purpose here is to determine the



density of protons as a function of the density of neutrons from the condition of chemical equilibrium, namely,  $\mu_n = \mu_p + \mu_e$ , and the neutrality condition. A similar problem but in the context of the equation of state, *i.e.* pressure of the gas as a function of the particle density, was considered in [12] for magnetic fields much smaller than  $B_{0p}$ , namely, for  $B$  up to only  $100B_{0e} \approx 10^{-4}B_{0p}$ . For ultrastrong magnetic fields ( $B > B_{0p}$ ), the problem was first considered in [13]. In [13], however, the problem was only partially solved by restricting to the lowest Landau level of electrons and/or protons only. Also, for  $B < B_{0p}$  the chemical potential of the protons was approximated by the expression obtained in the absence of the magnetic field. Here we shall determine the density of protons numerically without making any approximation.

An essential observation which we employed in our numerical solution is that, under the charge neutrality condition  $n_p = n_e$ , the chemical potentials  $\mu_p$  and  $\mu_e$  in the presence of a magnetic field, as given by eq.(3), are related by

$$\bar{\mu}_p = \left[ 1 + (\bar{\mu}_e^2 - 1) \left( \frac{m_e}{m_p} \right)^2 \right]^{1/2}, \quad (4)$$

which is exactly the relation satisfied by  $\bar{\mu}_p$  and  $\bar{\mu}_e$  without a magnetic field. In the absence of a magnetic field, eq.(4) is easily proved from eq.(1). To show that eq.(4) is also satisfied by the chemical potentials when  $B \neq 0$ , we substitute  $n_p = n_e$ ,  $B_{0p}/B_{0e} = (m_p/m_e)^2$  and  $n_{0p}/n_{0e} = (m_p/m_e)^3$  into eq.(3) for the proton ( $i = p$ ), we get

$$\frac{\sqrt{2}n_e}{3n_{0e}} \left( \frac{B_{0e}}{B} \right)^{3/2} = \left[ (\bar{\mu}_p^2 - 1) (m_p/m_e)^2 \frac{B_{0e}}{2B} \right]^{1/2} + 2 \sum_{n=1}^{n_{mp}} \left( (\bar{\mu}_p^2 - 1) (m_p/m_e)^2 \frac{B_{0e}}{2B} - n \right)^{1/2}. \quad (5)$$

The left hand side of eq.(5) exactly equals the left hand side of eq.(3) for the electron ( $i = e$ ). Since eq.(3) is a monotonic increasing function, we get by equating the right hand side of both eq.(3) and (5) the equality  $n_{mp} = n_{me}$  and

$$(\bar{\mu}_p^2 - 1) (m_p/m_e)^2 = (\bar{\mu}_e^2 - 1). \quad (6)$$

Hence eq.(4) is proved. The equality  $n_{mp} = n_{me}$  implies that the Landau levels of electrons and protons, are populated in the same manner. This is a direct consequence of the equality of the number of electrons and protons assumed here and the fact that the density of states per Landau level is independent of the mass of the charged particles.

Our numerical results are presented in Fig. 1 and 2 for strong ( $B < B_{0p}$ ) and ultrastrong ( $B > B_{0p}$ ) magnetic fields, respectively. These curves represent the normalized proton density number  $n_p/n_{0n}$  as a function of the normalized neutron density number  $n_n/n_{0n}$  at various values of magnetic field. The dotted curve gives the corresponding values in the absence of the magnetic field. In the presence of the magnetic field, the density of protons is a piecewise continuous and monotonic increasing function of the neutron density. The values of the proton density at which the first derivatives do not exist are the values at which a Landau level is being completely filled. It turns out that, for  $B < B_{0p}$ , the approximation made in [13] by treating the protons as if no magnetic field were present is a very good one.

From the figures one observes the following distinctive effects that a strong magnetic field has on the chemical equilibrium of the degenerate gas of nucleons and electrons: (a) when only the first Landau level is populated, the values of  $n_p/n_{0n}$  in the presence of finite  $B$ 's are for the most part higher than the corresponding value when the field is absent; (b) in the presence of an ultrastrong magnetic field, there appear values of densities (populating only the first Landau level) for which  $n_p > n_n$ ; and (c) when higher Landau levels are being filled, the curves corresponding to finite magnetic fields all converge to the one without magnetic field.

Features (a) and (b) had been noted previously in [13]. Such behavior may be understood as follows. When the neutron density at a fixed magnetic field is low enough (or equivalently, when the magnetic field at a fixed neutron density is high enough) that only the first Landau level is filled by the electrons and protons, the chemical potentials of the electrons and protons

are given by (from eq.(1) and (3)):

$$\begin{aligned}\mu_n &= m_n c^2 \left[ 1 + (n_n/n_{0n})^{2/3} \right]^{1/2}, \\ \mu_i &= m_i c^2 \left[ 1 + (2n_i B_{0i})^2 / (3n_{0i} B)^2 \right]^{1/2}, \quad i = e, p.\end{aligned}\quad (7)$$

Eq. (7) shows that a higher magnetic field  $B$  tends to lower the chemical potential of the electron when  $B > B_{0e}$  (and the chemical potential of the proton as well when  $B > B_{0p}$ ). To maintain chemical equilibrium among the particles at a fixed value of  $n_n/n_{0n}$ , the chemical potentials of the electrons and protons have to be raised so that the equilibrium condition  $\mu_n = \mu_p + \mu_e$  is still satisfied. This is achieved through the increase in the density of electrons, and hence the density of protons by the neutrality condition assumed here. For a given value of  $n_n/n_{0n}$ , the value of  $n_p/n_{0n}$  in the presence of finite  $B$ 's are, for the most part, higher than the corresponding value when the field is absent, until the proton density reaches a value  $(n_p/n_{0n})_{\text{cross}} \approx (3B/2B_0)^{3/2} (m/m_n)^3$ , which is the point of intersection between the curves with  $B \neq 0$  and  $B = 0$ . When  $B > B_{0p}$ , there exist values of the densities for which  $n_p > n_n$ . This gives the possibility of stars with proton-rich matter. These ranges of particle densities are of great interest, since in zero magnetic field the ratio  $n_p/n_n$  is always less than unity, with a maximum equal to  $1/8$  [9]. The fact that the density of proton is raised under these conditions has the important implication that the direct URCA reaction is enhanced, leading to a more efficient neutron star cooling through neutrino emission.

However, as soon as the higher Landau levels are being filled, the behaviour of the system under the magnetic field does not deviate much from that without the magnetic field. In fact, for large  $n$  they are nearly identical. This can be proved as follows. For large  $n$  we have  $n_{mi} \approx (\bar{\mu}_i^2 - 1)B_{0i}/2B$ . Then eq.(3) can be approximated by

$$\begin{aligned}\frac{\sqrt{2}n_i}{3n_{0i}} \left( \frac{B_{0i}}{B} \right)^{3/2} &\approx 2 \int_0^{n_{mi}} (n_{mi} - n)^{1/2} dn \\ &= \frac{4}{3} (\bar{\mu}_i^2 - 1)^{3/2} \left( \frac{B_{0i}}{2B} \right)^{3/2}.\end{aligned}\quad (8)$$

This leads to  $n_i/n_{0i} = (\bar{\mu}_i^2 - 1)^{3/2}$ , which is exactly the result, namely eq.(1), when  $B = 0$ .

To conclude, we have discussed the effects of strong constant magnetic fields on the chemical equilibrium of a degenerate gas of neutrons, protons, and electrons. The equations for chemical equilibrium under the condition of charge neutrality are numerically solved for different values of the magnetic field and the neutron density. The effect of higher Landau levels were considered, which was left out in previous work [13]. It is found that the chemical potentials of the electrons and the protons are related in the same way, namely, through eq.(4), regardless of whether there is a magnetic field or not. When only the first Landau level is being filled, the proton density is enhanced, as compared to the case without the magnetic field. For an ultrastrong field there exists the possibility that the proton density is greater than the neutron density, giving a proton-rich matter. However, when higher Landau levels are being filled, the values of the particle density at equilibrium quickly converge to those obtained without the magnetic field. The latter result indicates that, when the density of the particles are very high, the influence of the magnetic field is negligible.

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### Figures Captions

**Fig. 1.** Plot of  $\log(n_p/n_{0n})$  verses  $\log(n_n/n_{0n})$  (continuous curves) for values of  $B/B_{0e}$  at (from bottom to top):  $10^2$ ,  $10^3$ ,  $10^4$  and  $10^5$ . The dotted line corresponds to the curve with  $B = 0$ .

**Fig. 2.** Same as in Fig. 1, but for values of  $B/B_{0e}$  at (from bottom to top):  $10^7$ ,  $10^9$ ,  $10^{11}$  and  $10^{13}$ .



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## 出席國際學術會議心得報告

何俊麟

1. 會議名稱: 7th International Conference on squeezed states and Uncertainty Relations
2. 日期、地點: 90年6月4日至6月8日於美國波士頓大學。
3. 心得:

本會是每年舉行之有關相干態之理論、實驗及應用之國際大會。從事量子光學及量子力學之學者，大多會在此會上發表其最新研究成果。更重要的是，多位當代大師會在此綜評各個相關領域的重要進展及未來的方向。

此次大會與會人數估計近三四百人。本人在會中發表了一篇應用相干態之工作（題目為：Simple variational approach to the quantum Frenkel-Kontorova model）。

會議期間，本人出席聆聽多位大師的演講，近而對當前的重要成果及方向有更深入的了解。在會議期間也認識了多位研究領域相近的外國學者，並交換研究心得，得益匪淺。

何俊麟

90.10.18

# Simple variational approach to the quantum Frenkel-Kontorova model

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## Abstract

In this work a mean field approach to the Quantum Frenkel-Kontorova model is presented. Our approach is based on Dirac's time-dependent variational principle together with the Jackiw-Kerman (JK) function as the single particle state. The JK wavefunction can be viewed as the  $q$ -representation of the squeeze state. We showed that our approach reproduces the essential features observed in a previous quantum Monte Carlo studies.

## I. INTRODUCTION

The Frenkel-Kontorova (FK) model [1] is a simple one-dimensional model used to study incommensurate structures appearing in many condensed-matter systems, such as charge-density waves, magnetic spirals, and adsorbed monolayers. These modulated structures arise as a result of the competition between two or more length scales. The FK model describes a chain of atoms connected by harmonic springs subjected to an external sinusoidal potential. In an important development in the study of the classical FK model, Aubry [2] first made use of the connection between the FK model, the so-called "standard map", and the Kolmogorov-Arnold-Moser (KAM) theorem to reveal many interesting features of the FK model. Particularly, he showed that when the mean distance (also called the winding number) between two successive atoms is rational, the system is always pinned. But when the winding number is irrational, there exists a critical external field strength below (above) which the system is unpinned (pinned). This transition is called by Aubry a "transition by breaking of analyticity", and is closely connected with the breakup of a KAM torus. It is very analogous to a phase transition, and various critical exponents and questions of universality have been extensively studied in the past.

Needless to say, quantum effects are very important in the FK model. However, unlike the classical case, study of quantum FK models is rather scanty. It was first considered in a quantum Monte Carlo (QMC) analysis in [3]. Their main observation is that the map



appropriate to describe the quantum case is no longer the standard map, but rather a map with a sawtooth shape. Theoretical explanation of this phenomenon was later attempted in [4]. In this work the authors first showed that the sawtooth map could not be explained in the naive mean field approximation (MFA), *i.e.* the Hartree's independent-particle approximation, which they used. It was then argued that to get the sawtooth map one must go beyond the MFA by including the contributions from the so-called quasidegenerate states. These states are inhomogeneous configurations corresponding to excited states in the MFA which are nearly degenerate in energy with the naive MFA ground state. They contribute substantially to the actual quantum ground state through quantum tunneling. The sawtooth map emerged after the mixing of these quasidegenerate states were taken into account in [4].

More recently, a different approach was proposed in [5] which uses a generalized squeezed state many-body wavefunction to demonstrate that the sawtooth behavior is simply the result of quantum fluctuations. Similar to [4], this work also adopted an approximation that goes beyond the MFA. In our opinion, the approach of [5] is very appealing in principle. However, the variational method applied there is problematic, and some difficulties in this work need be overcome before it could be considered satisfactory.

In [6] we showed that all the essential features observed in the QMC studies can in fact be obtained from an independent-particle picture of the many-body ground state, *i.e.* in the MFA. In the independent-particle picture the many-body trial wavefunction is factorizable into single-particle states. One can assume the single-particle state to have the form of a squeeze state. For the quantum FK model, a simpler and, in our view, more elegant approach is to adopt Dirac's time-dependent variational principle together with the Jackiw-Kerman (JK) function [7] as the single particle state. The JK wavefunction can be viewed as the  $Q$ -representation of the squeeze state [8]. We shall show that our simple independent-particle approach produces an effective classical Hamiltonian which is bounded below, admits simple numerical solution of the ground state without recourse to QMC analysis, and reproduces the essential features observed in QMC studies.

## II. EFFECTIVE HAMILTONIAN

The Hamiltonian of the quantum FK model is given by

$$\mathcal{H} = \sum_i \left[ \frac{\hat{p}_i^2}{2m} + \frac{\gamma}{2} (\hat{q}_{i+1} - \hat{q}_i)^2 - V \cos(l_0 \hat{q}_i) \right]. \quad (1)$$

Here  $\hat{q}_i$  and  $\hat{p}_i$  are the position and momentum operators, respectively, of the  $i$ th atom,  $\gamma$  the elastic constant of the spring,  $V$  and  $2\pi/l_0$  are the strength and the period of the external potential. As in [4], it is convenient to use the dimensionless variables  $\hat{Q}_i = l_0 \hat{q}_i$ ,  $\hat{P}_i = l_0 \hat{p}_i / \sqrt{m\gamma}$ , and  $K = V l_0^2 / \gamma$ . With these new variables, we obtain the following dimensionless Hamiltonian  $H$

$$H = \sum_i \left[ \frac{\hat{P}_i^2}{2} + \frac{1}{2} (\hat{Q}_{i+1} - \hat{Q}_i)^2 - K \cos(\hat{Q}_i) \right]. \quad (2)$$

We have  $\mathcal{H} = \gamma H/l_0^2$ . The effective Planck constant is  $\tilde{\hbar} = \hbar l_0^2/\sqrt{m\gamma}$ . For the classical FK model, the Aubry transition occurs at the critical value  $K_c = 0.971635 \dots$ .

To study the ground state properties of the quantum FK model in (2), we adopt here the time-dependent variational principle pioneered by Dirac. In this approach, one first constructs the effective action  $\Gamma = \int dt \langle \Psi, t | i\hbar \partial_t - H | \Psi, t \rangle$  for a given system described by  $H$  and  $|\Psi, t\rangle$ . Variation of  $\Gamma$  is then the quantum analogue of the Hamilton's principle. The time-dependent Hartree-Fock approximation emerges when a specific ansatz is made for the state  $|\Psi, t\rangle$ . We now assume the trial wavefunction of the ground state of our quantum FK system to have the Hartree form  $|\Psi, t\rangle = \prod_i |\psi_i, t\rangle$ , where the normalized single-particle state  $|\psi_i, t\rangle$  is taken to be the JK wavefunction [7]:

$$\langle Q_i | \psi_i, t \rangle = \frac{1}{(2\pi\tilde{\hbar}G_i)^{1/4}} \times \exp \left\{ -\frac{1}{2\tilde{\hbar}} (Q_i - x_i)^2 \left[ \frac{1}{2}G_i^{-1} - 2i\Pi_i \right] + \frac{i}{\tilde{\hbar}} p_i (Q_i - x_i) \right\}. \quad (3)$$

The real quantities  $x_i(t)$ ,  $p_i(t)$ ,  $G_i(t)$  and  $\Pi_i(t)$  are variational parameters the variations of which at  $t = \pm\infty$  are assumed to vanish. Squeezed state function in the form of the JK wavefunction has the advantage that the physical meanings of the variational parameters contained in the JK wavefunction are most transparent, as we shall show below. Furthermore, the JK form is in the general Gaussian form so that integrations are most easily performed.

It is not hard to check that  $x_i$  and  $p_i$  are the expectation values of the operators  $\hat{Q}_i$  and  $\hat{P}_i$ :  $x_i = \langle \Psi | \hat{Q}_i | \Psi \rangle$ ,  $p_i = \langle \Psi | \hat{P}_i | \Psi \rangle$ . Also, one has  $\langle \Psi | (\hat{Q}_i - x_i)^2 | \Psi \rangle = \tilde{\hbar}G_i$ , and  $\langle \Psi | i\hbar \partial_t | \Psi \rangle = \sum_i (p_i \dot{x}_i - \tilde{\hbar}G_i \dot{\Pi}_i)$ , where the dot represents derivative with respect to (w.r.t.) time  $t$ . It is now clear that  $\tilde{\hbar}G_i$  is the mean fluctuation of the position of the  $i$ -th atom, and that  $G_i > 0$ . From the form of the effective action one sees that that  $p_i$  and  $\Pi_i$  are the canonical conjugates of  $x_i$  and  $G_i$ , respectively. The Dirac variational principle leads to the following effective Hamiltonian

$$\begin{aligned} H_{eff} &= \langle \Psi | H | \Psi \rangle \\ &= \sum_i \frac{1}{2} \left[ p_i^2 + \tilde{\hbar} \left( \frac{1}{4}G_i^{-1} + 4\Pi_i^2 G_i \right) \right] \\ &\quad + \sum_i \frac{1}{2} (x_{i+1} - x_i)^2 \\ &\quad + \sum_i \frac{\tilde{\hbar}}{2} (G_{i+1} + G_i) \\ &\quad - \sum_i K \exp \left( -\frac{\tilde{\hbar}}{2} G_i \right) \cos x_i. \end{aligned} \quad (4)$$

The last term in (4) can be very easily obtained from  $\langle \Psi | F(Q_i) | \Psi \rangle = \sum_{m=0}^{\infty} F^{(2m)}(x_i) (\tilde{\hbar}G_i)^m / (2m)!!$ , where  $F^{(n)}(x) = \partial^n F(x) / \partial x^n$ , and  $n!! \equiv n(n-2)(n-4) \dots 1$ . Eq. (4) is bounded from below.

We can obtain the equations for the equilibrium states in the Hartree-Fock approximation by directly varying the effective Hamiltonian  $H_{eff}$  w.r.t. the variables. Varying  $H_{eff}$  w.r.t.  $p_i$ ,  $\Pi_i$ ,  $x_i$  and  $G_i$  give, respectively,

$$p_i = 0, \quad 4\Pi_i G_i = 0, \quad (5)$$

$$x_{i+1} - 2x_i + x_{i-1} = K \exp\left(-\frac{\tilde{h}}{2} G_i\right) \sin x_i, \quad (6)$$

$$\frac{1}{4} G_i^{-2} - K \exp\left(-\frac{\tilde{h}}{2} G_i\right) \cos x_i - 2 = 4\Pi_i^2. \quad (7)$$

The second equation in (5) implies  $\Pi_i = 0$  as  $G_i > 0$ . This in turn means that the right hand side of eq.(7) is equal to zero:

$$\frac{1}{4} G_i^{-2} - K \exp\left(-\frac{\tilde{h}}{2} G_i\right) \cos(x_i) - 2 = 0. \quad (8)$$

In the limit  $\hbar = 0$ , eq.(6) is equivalent to the standard map.

### III. NUMERICAL RESULTS

We numerically solve for the set of variables  $x_i$  and  $G_i$  which characterize the ground state using the Newton method. In all our numerical computations the winding number  $P/Q = 610/987$ , which is an approximation of the golden mean winding number  $(\sqrt{5}-1)/2$ , is used with the periodic boundary condition  $x_{i+Q} = x_i + 2\pi P$ . This winding number is much more accurate than those used in previous works to approximate the golden mean number, thus giving us better accuracy in the computations of physical quantities related to the ground state. We emphasize that all values of  $x_i$  and  $G_i$  are determined by the same numerical method consistently. In particular, we do not have to input the values of  $G_i$  from quantum Monte Carlo results in order to solve for the  $x_i$ , as was done in [5].

Having obtained the values of  $x_i$  which give the mean positions of the quantum atoms in the chain, we can compare the results with the classical configuration, following [3], in two ways: (1) by the quantum hull function, which is the plot of  $x_i \pmod{2\pi}$  of the atoms against their unperturbed positions  $2\pi iP/Q \pmod{2\pi}$ ; (2) by the so-called  $g$ -function, defined by

$$g_i \equiv K^{-1} (x_{i+1} - 2x_i + x_{i-1}) \quad (9)$$

versus the actual atomic positions  $x_i$ . From (6), we also have

$$g_i = \exp\left(-\frac{\tilde{h}}{2} G_i\right) \sin x_i. \quad (10)$$

Here  $G_i$  is related to  $x_i$  by eq.(8). We see from this equation that quantum fluctuations  $G_i$  will modify the shape of the classical *sine*-map. In addition to these two types of graphs, we also plot the graph of  $G_i$  against the unperturbed and the actual positions. The formal graph was first introduced in [3] to show the strong correlation of the fluctuations of atoms' positions with their unperturbed positions. We introduce the latter type of graphs here since we think that such graphs provide better picture about how the quantum fluctuations of the atoms are related to their actual positions.

In Fig. 1 we show the four graphs mentioned above with different values of  $\tilde{\hbar}$  for the supercritical case  $K = 5$ . Fig. 1(a) shows the quantum hull functions. For small values of  $\tilde{\hbar}$  the quantum hull function consists of a countable set of steps discontinuities, just as in the classical case: the atoms are in a pinning phase. In fact, the atoms are more likely to be located near the valley of the external potential well, namely, near  $x_i = 0 \pmod{2\pi}$ . As the quantum effect increases, i.e., for increasing values of  $\tilde{\hbar}$ , the quantum hull function gradually changes into a monotonic analytic function, signifying that the system is entering the depinning phase. There exists a critical value, approximately  $\tilde{\hbar}_c = 6.58$  for  $K = 5$ , above which the quantum hull function changes from a nonanalytic function to an analytic one. This is a quantum analogue of the Aubry transition in the classical case, and can therefore be called the quantum Aubry transition.

Next in Fig. 1(b) we show the graphs of the  $g$ -function. The curve defined by (10) with  $G_i$  satisfying (8) are shown here as dashed curves for different  $\tilde{\hbar}$ . In the classical limit ( $\tilde{\hbar} = 0$ ) this curve is simply the standard map (*sine-curve*). As  $\tilde{\hbar}$  increases, the amplitude of the curve decreases. For sufficiently large  $\tilde{\hbar}$ , the curve resembles more closely a "sawtooth" shape. This is first noted in QMC study in [3]. Here we see that it comes out very naturally from the equation of motion (8) and (10). We have therefore demonstrated that the sawtooth map could be recovered in the MFA. In the supercritical case ( $K = 5$ ), when  $\tilde{\hbar} < \tilde{\hbar}_c$ , the positions  $x_i$  of the atoms cover only a subset of the  $g$ -curves. This is in accord with the fact that the atoms are in the pinning phase [cf. Fig. 1(a)]. As  $\tilde{\hbar}$  increases, the points begin to spread along the  $g$ -curve. When  $\tilde{\hbar} > \tilde{\hbar}_c$ , the  $g$ -graph is completely covered as the system has entered the depinning phase.

Fig. 1(c) shows the quantum fluctuations  $G_i$  plotted against the actual atomic positions  $x_i$ . The dashed curves represent the curves of eq.(8) for different  $\tilde{\hbar}$ . For small  $\tilde{\hbar}$ , the atoms are located near  $x_i = 0 \pmod{2\pi}$  with small values of  $G_i$  which means, from (3), that the wavefunctions are highly peaked at these positions. As the quantum effect increases, the external potential is so modified that now the atoms could be found at other positions, but with atoms at  $x_i = \pi \pmod{2\pi}$  having the largest value of  $G_i$ . This indicates that wavefunctions of the atoms near the top of the potential are more extended with smaller amplitudes. Again, when  $\tilde{\hbar} > \tilde{\hbar}_c$ , the curves of (8) are completely covered by the solutions  $x_i$ . To compare with the results in [3], we plot the values of  $G_i$  against the unperturbed positions in Fig. 1(d). One sees that the values of  $G_i$  are strongly correlated with the unperturbed positions, as first noted in [3]. For  $\tilde{\hbar} < \tilde{\hbar}_c$  the graphs consists of steps discontinuities, and for  $\tilde{\hbar} > \tilde{\hbar}_c$  the graphs are continuous. This is correlated with the graphs of the quantum hull function in Fig. 1(a), since from (8) any fixed value of  $x_i$  correspond to a fixed value of  $G_i$ .

Next we show in Fig. 2 the corresponding graphs for the case  $K = 1.5$ . This represents the situation which is slightly over the critical classical case. The general trends of the behavior of the graphs are the same as those in Fig. 1. As expected, quantum Aubry transition takes place at a smaller  $\tilde{\hbar}_c = 1.17$ . We note here that the shape of the  $g$ -function at large  $\tilde{\hbar}$  in this case is intermediate between a *sine* and a sawtooth map.

We have also checked the subcritical cases with  $K < K_c$ . The classical system is already in the depinning phase in this regime. Quantum fluctuations only enhance the trend of depinning. The  $g$ -function is found to be closer to a *sine*-shape with smaller amplitude for

higher  $\tilde{\hbar}$ . This is consistent with the QMC results [3].

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## Figures captions

**Fig. 1** Structure of the quantum ground state for  $K = 5$  and winding number  $P/Q = 610/987$  at  $\tilde{\hbar} = 2$  (black dots), 6 (white dots) and 7 (black curve). (a) quantum hull function plotted against unperturbed atomic positions; (b)  $g$ -function plotted against actual atomic positions (the dashed curves represent eq.(10) with  $G_i$  satisfying (8)); (c) and (d) quantum fluctuations  $G_i$  plotted against the actual and unperturbed positions, respectively. The dashed curves in (c) represent the curves of eq.(8) for different  $\tilde{\hbar}$ .

**Fig. 2** Same as Fig. 1 for  $K = 1.5$  and  $\tilde{\hbar} = 0.5$  (black dots), 1.0 (white dots) and 2 (black curve).

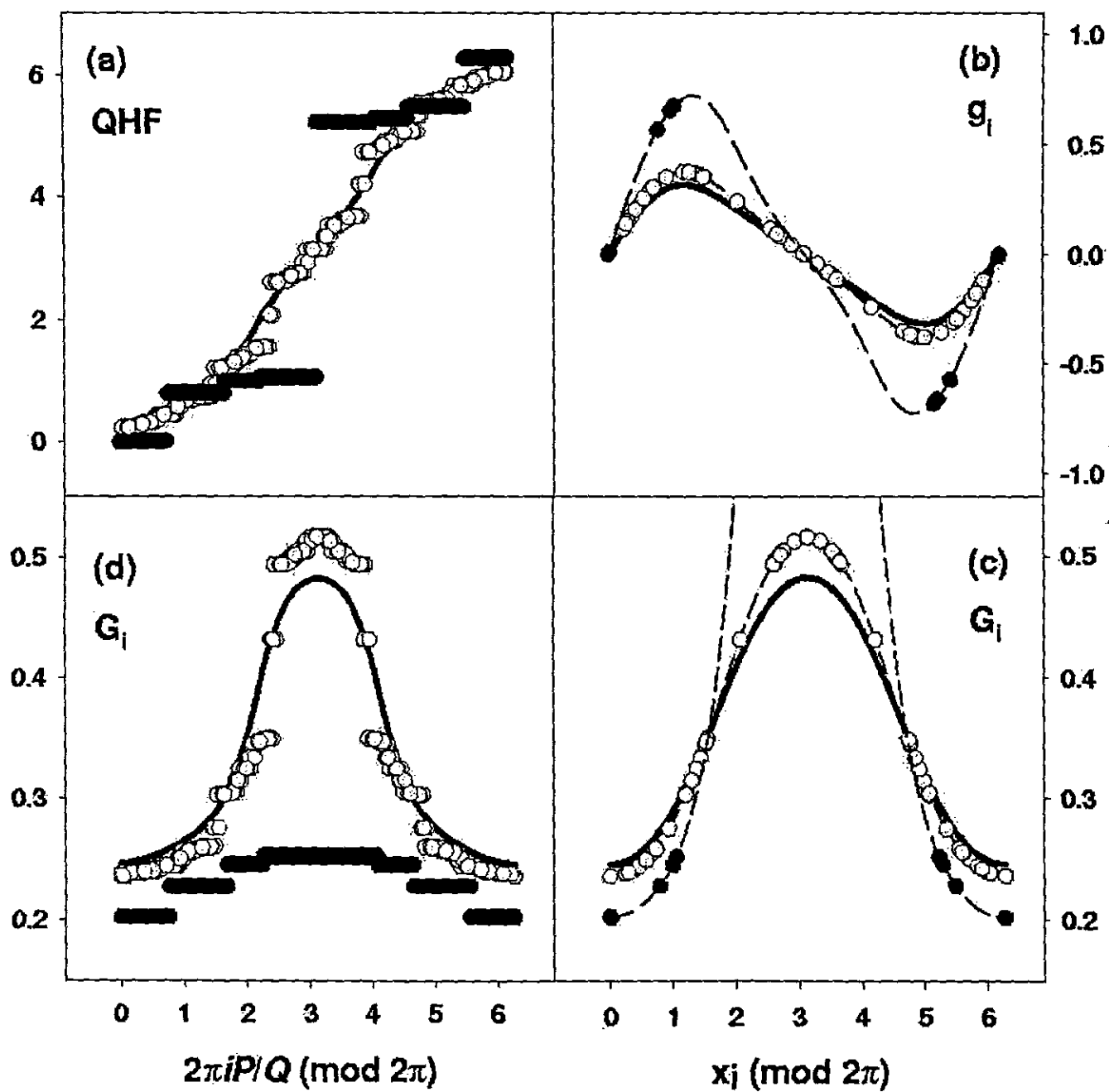


Fig. 1.

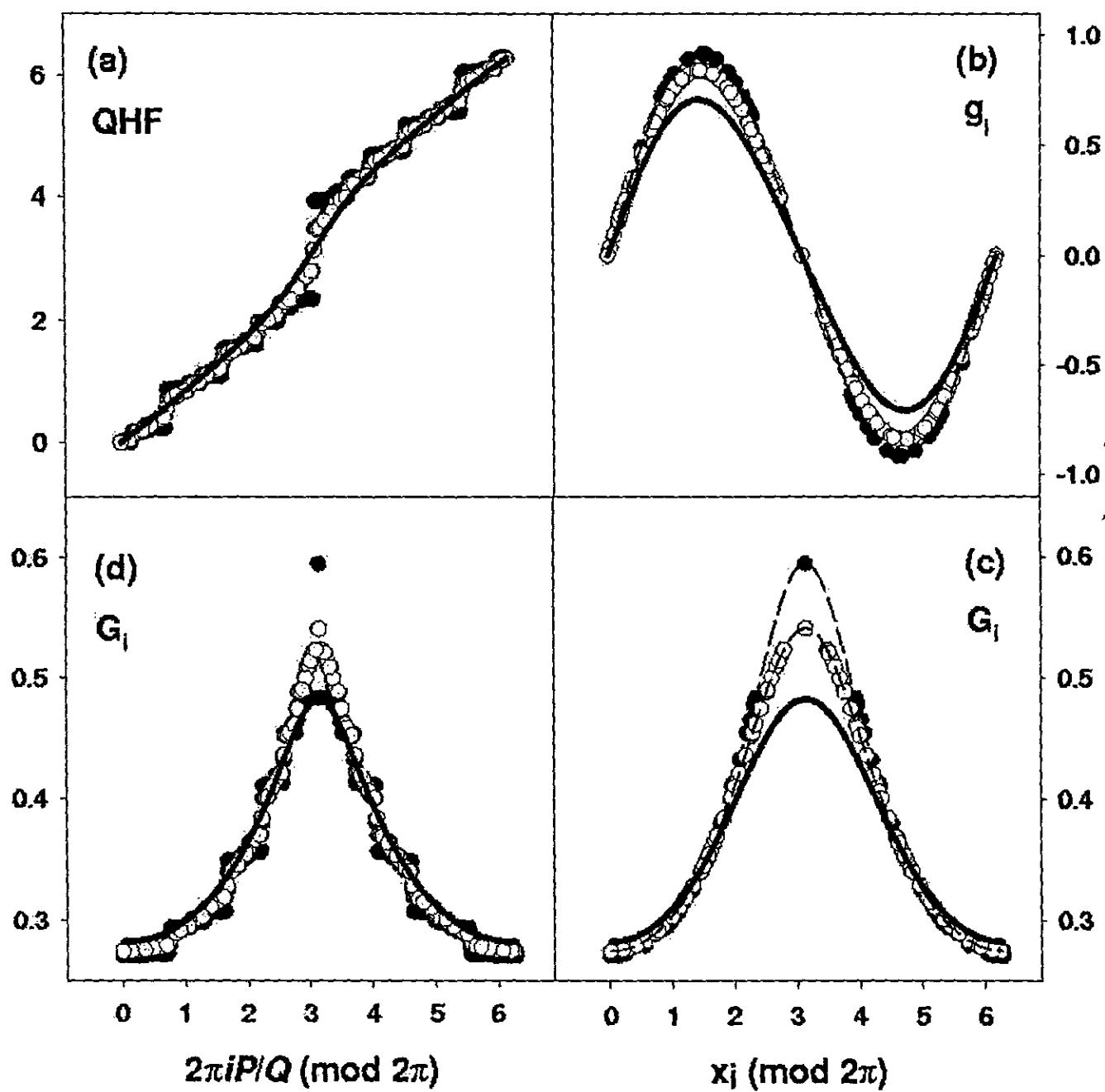


Fig. 2.