Energy level of an electron in a saddle-potential quantum dot under a uniform magnetic field obtained by the invariant eigenoperator method*

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We show that the recently proposed invariant eigenoperator method can be successfully applied to solving the energy levels of an electron in a saddle-potential quantum dot under a uniform magnetic field. The Landau diamagnetism decreases with the value $\omega_y^2 - \omega_x^2$ due to the existence of the saddle potential.

Keywords: saddle-potential quantum dot, energy level of electron, invariant eigenoperator method

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1. Introduction

In recent years, a quantum dot in an external potential and under a magnetic field has been used in quantum control and quantum computation. In this paper we shall consider the energy level of an electron in a saddle-potential quantum dot under a uniform magnetic field (UMF). Usually in quantum mechanics people derive energy levels by choosing diagonalized representation for the concerned Hamiltonians. However, due to the complicacy arising from the coupling of multiple modes, the diagonalization method in many cases does not work effciently or seems tough. By combining the Schrödinger operator[1] and the Heisenberg equation of motion[2], we have proposed the "invariant eigenoperator" (IEO) method[3] to explore the energy-level gap of dynamic Hamiltonians, which can solve the energy-levels for many Hamiltonians in solid state physics, molecular physics, and quantum optics with convenience and directness.[4−11] In this paper, we continue to use this method to study the energy-level of a Hamiltonian describing an electron in a saddle-potential quantum dot under the UMF. To our knowledge, such an energy level has not been reported in the literature before. The physical background of this problem could be the case for two-dimensional quantum point contact in semiconductor devices modeled in terms of a saddle potential under a uniform magnetic field. This paper is organized as follows: In Section 2, we outline the main points of the IEO method to derive the energy-gap of the dynamic system. In Section 3, we briefly review the energy gap of the Hamiltonian describing an electron under a UMF and that with an Isotropic Harmonic Oscillator Potential. In Section 4, we discuss the energy gap of the electron in a UMF when a saddle-potential quantum dot also exists, it will be derived for the first time. Then in Section 5, we calculate the magnetization caused by a saddle potential and the variation of Landau diamagnetism. Our calculation results in the conclusion that the IEO method provides a concise and direct approach for deriving the energy level for this system.

2. The IEO method

We trace back to the original idea of Schrödinger's quantization scheme: he took the identification $\mathrm{i}\,\mathrm{d}/\mathrm{d}t \leftrightarrow \hat{H}, \hbar = 1$, so $\mathrm{i}\,\mathrm{d}/\mathrm{d}t$ is named the Schrödinger operator in many references. Similarly, we have $(\mathrm{i}\,\mathrm{d}/\mathrm{d}t)^n \leftrightarrow \hat{H}^n$, now we set up an equation for operator $\hat{O}_e$,

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \hat{O}_e = \lambda \hat{O}_e, \tag{1}$$

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when $n = 1$, it looks like $\mathrm{i}(\mathrm{d}/\mathrm{d}t)\Psi = \hat{H}\Psi$. Thus we call Eq. (1) the n-order invariant eigenoperator equation, and call λ the n-order eigenvlaue. Successively using the Heisenberg equation

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_e = \left[\hat{O}_e, \hat{H}\right], \tag{2}$$

n-times, we can write Eq. (1) as

$$\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^n \hat{O}_e = \left[\ldots\left[\left[\hat{O}_e, \hat{H}\right], \ldots, \hat{H}\right]\right] = \lambda\hat{O}_e. \tag{3}$$

In this equation, we relate the n-power of the Schrödinger operator to the n-Heisenberg commutators, i.e. repeatedly employing the Heisenberg equations and looking for the resulting equation to close. To our knowledge, such an equation has not been reported in the literature before. When $n = 1$, equation (1) reduces to

$$\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\hat{O}_e = \left[\hat{O}_e, \hat{H}\right] = \lambda\hat{O}_e, \tag{4}$$

which is a first-order IEO equation and is an extension of the Heisenberg equation with "$= \lambda\hat{O}_e$" supplemented. Since we have endowed $(\mathrm{i}\mathrm{d}/\mathrm{d}t)^n$ with n-power of energy gap, if we can find such an $\hat{O}_e$ that satisfies Eq. (1) then we are able to say that $\sqrt[n]{\lambda}$ is the energy-level gap. This is the physical meaning of Eq. (1). To put it in the opposite way, if we did not notice that $(\mathrm{i}\mathrm{d}/\mathrm{d}t)^n$ corresponds to $\hat{H}^n$, we would not have known the physical meaning of λ.

To clarify this point of view, for example we take $n = 2$ in Eq. (1), and assuming that $|\Psi_a\rangle$ and $|\Psi_b\rangle$ are two adjacent stationary eigenstates of Hamiltonian $\hat{H}$ with eigenvalues E_a and E_b, respectively, we have

$$\begin{aligned}\langle\Psi_a|\left(\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}t}\right)^2\hat{O}_e|\Psi_b\rangle &= \langle\Psi_a|\left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right]|\Psi_b\rangle \\ &= (E_b - E_a)^2\langle\Psi_a|\hat{O}_e|\Psi_b\rangle \\ &= \lambda\langle\Psi_a|\hat{O}_e|\Psi_b\rangle. \end{aligned}\tag{5}$$

Since $\langle\Psi_a|\hat{O}_e|\Psi_b\rangle$ is a nonzero matrix element, the energy gap between $|\Psi_a\rangle$ and $|\Psi_b\rangle$ is $E_b - E_a = \sqrt{\lambda}$. We name Eq. (1) as the IEO equation.

3. Brief review of an electron moving in the UMF and an isotropic harmonic oscillator potential

We briefly review the movement of an electron in a UMF. This quantum motion was first investigated by Landau.[12,13] The electron (with mass m) in the presence of a UMF is described by the Hamiltonian (in the units of $\hbar = c = 1, \hbar$ is the Planck constant, c is the light velocity)

$$\begin{aligned}H_0 &= \frac{1}{2m}\left(\Pi_x^2 + \Pi_y^2\right) = \left(\Pi_+\Pi_- + \frac{1}{2}\right), \\ \Pi_\pm &= \frac{1}{\sqrt{2m\omega_\mathrm{c}}}\left(\Pi_y \mp \mathrm{i}\Pi_x\right), \end{aligned}\tag{6}$$

where the kinetic momenta $\Pi_j = p_j + eA_j$ $(j = x, y)$, the vector potential is $\boldsymbol{A} = (-By/2, Bx/2, 0)$ in the symmetric gauge, B is the intensity of the UMF along the z axis, $\omega_\mathrm{c} = eB/m$ is the cyclotron frequency, m is the mass of electron, the kinetic momenta obey the commutative relation

$$[\Pi_x, \Pi_y] = -\mathrm{i}m\omega_\mathrm{c}, \quad [\Pi_-, \Pi_+] = 1, \tag{7}$$

H_0 can be expressed as

$$\begin{aligned}H_0 = &\frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{\omega_\mathrm{c}}{2}\left(xp_y - yp_x\right) \\ &+ \frac{1}{8}m\omega_\mathrm{c}^2\left(x^2 + y^2\right). \end{aligned}\tag{8}$$

When there is an additional isotropic harmonic potential descried in Fig. 1,

$$H' = \frac{1}{2}m\omega_0^2\left(x^2 + y^2\right), \tag{9}$$

the Hamiltonian becomes

$$H_1 = H_0 + \frac{1}{2}m\omega_0^2\left(x^2 + y^2\right). \tag{10}$$

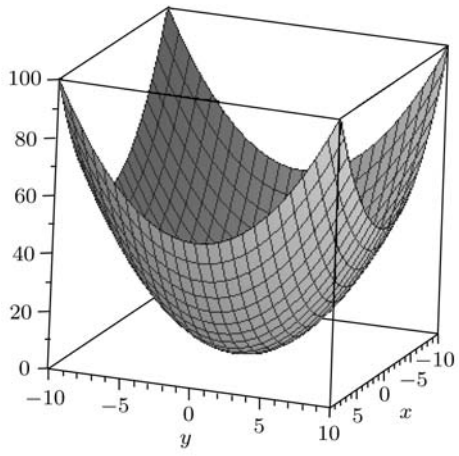


Fig. 1. The isotropic harmonic potential.

The energy gap for Hamiltonian Eq. (10) can be derived by using the IEO method, which can be seen as the deduction in the following sections (i.e. let $\omega_x^2 = -\omega_0^2, \omega_y^2 = \omega_0^2$ in Eq. (30)), and the results are

$$\Delta E_1 = \frac{|\omega_\mathrm{c} - \omega_\mathrm{c}'|}{2}, \quad \Delta E_2 = \frac{\omega_\mathrm{c} + \omega_\mathrm{c}'}{2} \equiv \Delta E'_\mathrm{iso}, \tag{11}$$

where

$$\omega_{\rm c}' = \sqrt{4\omega_0^2 + \omega_{\rm c}^2}, \tag{12}$$

$\Delta E_1 = |\omega_{\rm c} - \omega_{\rm c}'|/2$ is unphysical, $\Delta E_2 = (\omega_{\rm c} + \omega_{\rm c}')/2$ is the physical energy gap describing an electron in the UMF under an isotropic harmonic potential.

4. The Hamiltonian for a two-dimensional quantum point contact in semiconductor devices under a UMF

We model the quantum point contact as a saddle potential[14,15] whose curvature form is expressed in terms of x and y as

$$V(x,y) = V_0 - \frac{1}{2}m\omega_x^2 x^2 + \frac{1}{2}m\omega_y^2 y^2, \tag{13}$$

where V_0 is the constant potential at the saddle point and $-m\left(\omega_x^2 x^2 - \omega_y^2 y^2\right)/2$ is the saddle potential, described as shown in Fig. 2, $-m\omega_x^2 x^2/2$ represents the

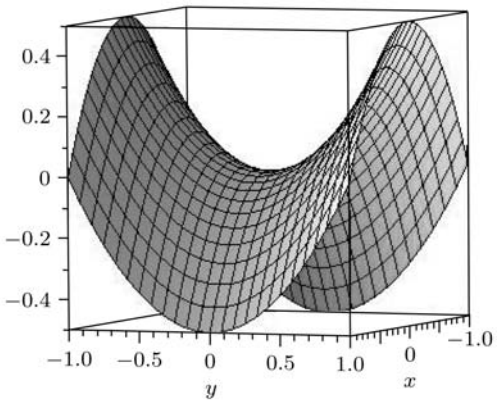


Fig. 2. The saddle potential.

inverted harmonic oscillator potential in x direction, while $m\omega_y^2 y^2/2$ represents the harmonic oscillator potential in the y direction, ω_x and ω_y are the corresponding frequencies respectively. Combined with Eq. (8), the Hamiltonian for an electron in the saddle potential under a UMF is given by

$$\begin{aligned} H =& \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{1}{8}m\omega_{\rm c}^2\left(x^2 + y^2\right) \\ &+ \frac{\omega_{\rm c}}{2}\left(xp_y - yp_x\right) - \frac{1}{2}m\left(\omega_x^2 x^2 - \omega_y^2 y^2\right) \\ &+ V_0. \end{aligned} \tag{14}$$

By introducing

$$\Omega_1^2 = \omega_{\rm c}^2 - 4\omega_x^2, \quad \Omega_2^2 = \omega_{\rm c}^2 + 4\omega_y^2, \tag{15}$$

H becomes

$$\begin{aligned} H =& \frac{1}{2m}\left(p_x^2 + p_y^2\right) + \frac{\omega_{\rm c}}{2}\left(xp_y - yp_x\right) \\ &+ \frac{1}{8}m\Omega_1^2 x^2 + \frac{1}{8}m\Omega_2^2 y^2 + V_0. \end{aligned} \tag{16}$$

5. The energy gap derived by the IEO method

Enlightened by the commutative relations

$$\begin{aligned} [x, H] &= \frac{{\rm i}p_x}{m} - \frac{{\rm i}\omega_{\rm c}}{2}y, \\ [y, H] &= \frac{{\rm i}p_y}{m} + \frac{{\rm i}\omega_{\rm c}}{2}x, \end{aligned} \tag{17}$$

$$\begin{aligned} [\,p_x, H] &= -\frac{{\rm i}\omega_{\rm c}}{2}p_y - \frac{\rm i}{4}m\Omega_1^2 x - {\rm i}eE, \\ [\,p_y, H] &= \frac{{\rm i}\omega_{\rm c}}{2}p_x - \frac{\rm i}{4}m\Omega_2^2 y, \end{aligned} \tag{18}$$

we guess that the IEO is

$$O_e = x + fy + gp_x - hp_y, \tag{19}$$

where f, g, and h are parameters to be determined. Now from Eqs. (17) and (18) we calculate

$$\begin{aligned} &[O_e, H] \\ =& \left(f\frac{{\rm i}\omega_{\rm c}}{2} - \frac{\rm i}{4}gm\Omega_1^2\right)x + \left(-\frac{{\rm i}\omega_{\rm c}}{2} + \frac{\rm i}{4}hm\Omega_2^2\right)y \\ &+ \left(\frac{\rm i}{m} - \frac{{\rm i}\omega_{\rm c}}{2}h\right)p_x + \left(\frac{{\rm i}f}{m} - \frac{{\rm i}g\omega_{\rm c}}{2}\right)p_y. \end{aligned} \tag{20}$$

It then follows

$$\begin{aligned} &\left({\rm i}\frac{\partial}{\partial t}\right)^2 O_e \\ =& \left[\left[O_e, H\right], H\right] \\ =& \left[\frac{\omega_{\rm c}^2 + \Omega_1^2}{4} - \frac{m\omega_{\rm c}}{8}h\left(\Omega_2^2 + \Omega_1^2\right)\right]x \\ &+ \left[f\frac{\left(\omega_{\rm c}^2 + \Omega_2^2\right)}{4} - \frac{gm\omega_{\rm c}}{8}\left(\Omega_1^2 + \Omega_2^2\right)\right]y \\ &+ \left[-\frac{f\omega_{\rm c}}{m} + \frac{g\left(\Omega_1^2 + \omega_{\rm c}^2\right)}{4}\right]p_x \\ &+ \left[\frac{\omega_{\rm c}}{m} - \frac{h\left(\Omega_2^2 + \omega_{\rm c}^2\right)}{4}\right]p_y. \end{aligned} \tag{21}$$

Comparing the right-hand side of Eq. (21) with O_e in Eq. (19), we see that when the following proportional relation holds:

$$\begin{aligned} &1 : f : g : (-h) \\ =& \left[\frac{\omega_{\rm c}^2 + \Omega_1^2}{4} - \frac{m\omega_{\rm c}}{8}h\left(\Omega_2^2 + \Omega_1^2\right)\right] \\ &: \left[f\frac{\left(\omega_{\rm c}^2 + \Omega_2^2\right)}{4} - \frac{gm\omega_{\rm c}}{8}\left(\Omega_1^2 + \Omega_2^2\right)\right] \end{aligned}$$

$$: \left[-\frac{f\omega_{\rm c}}{m}+\frac{g\left(\Omega_1^2+\omega_{\rm c}^2\right)}{4}\right]$$
$$: \left[\frac{\omega_{\rm c}}{m}-\frac{h\left(\Omega_2^2+\omega_{\rm c}^2\right)}{4}\right], \tag{22}$$

then equation (21) can be recast into

$$\begin{aligned}&\left(\mathrm{i}\frac{\partial}{\partial t}\right)^2 O_e\\ &=\left[\frac{\omega_{\rm c}^2+\Omega_1^2}{4}-\frac{m\omega_{\rm c}}{8}h\left(\Omega_2^2+\Omega_1^2\right)\right]\\ &\quad\times\left(x+fy+gp_x-hp_y\right)\\ &=\left[\frac{\omega_{\rm c}^2+\Omega_1^2}{4}-\frac{m\omega_{\rm c}}{8}h\left(\Omega_2^2+\Omega_1^2\right)\right]O_e. \end{aligned}\tag{23}$$

Thus the square of the energy gap for an electron in the saddle potential under a UMF is

$$(\Delta E)^2=\frac{\omega_{\rm c}^2+\Omega_1^2}{4}-\frac{m\omega_{\rm c}}{8}h\left(\Omega_2^2+\Omega_1^2\right). \tag{24}$$

Now we determine h, from $1:(-h)$ in Eq. (22) we can determine

$$h_{\pm}=\frac{\Omega_1^2-\Omega_2^2\pm\sqrt{\left(\Omega_1^2-\Omega_2^2\right)^2+8\omega_{\rm c}^2\left(\Omega_2^2+\Omega_1^2\right)}}{m\omega_{\rm c}\left(\Omega_2^2+\Omega_1^2\right)}. \tag{25}$$

Substituting Eq. (25) into Eq. (24) we see that the energy gap for h_+ is

$$\begin{aligned}(\Delta E_1)^2&=\frac{\omega_{\rm c}^2+\Omega_1^2}{4}-\frac{m\omega_{\rm c}}{8}h\left(\Omega_2^2+\Omega_1^2\right)\\ &=\frac{2\omega_{\rm c}^2+\Omega_1^2+\Omega_2^2}{8}\\ &\quad-\frac{1}{8}\sqrt{\left(\Omega_2^2-\Omega_1^2\right)^2+8\omega_{\rm c}^2\left(\Omega_1^2+\Omega_2^2\right)}\\ &=\frac{\omega_{\rm c}^2+A}{2}-\frac{1}{2}\sqrt{\left(\omega_{\rm c}^2+A\right)^2+4\omega_x^2\omega_y^2}, \end{aligned}\tag{26}$$

where we have defined

$$A\equiv\omega_y^2-\omega_x^2, \tag{27}$$

while the energy gap for h_- is

$$(\Delta E_2)^2=\frac{\omega_{\rm c}^2+A}{2}+\frac{1}{2}\sqrt{\left(\omega_{\rm c}^2+A\right)^2+4\omega_x^2\omega_y^2}. \tag{28}$$

Since $(\Delta E_1)^2<0$, equation (26) for the energy gap ΔE_1 is unphysical, we neglect it. Thus the energy gap for an electron in the saddle potential under a UMF is

$$\begin{aligned}&\Delta E\\ &=\Delta E_2\\ &=\sqrt{\frac{\omega_{\rm c}^2+A}{2}+\frac{1}{2}\sqrt{\left(\omega_{\rm c}^2+A\right)^2+4\omega_x^2\omega_y^2}}\\ &=\sqrt{\frac{\omega_{\rm c}^2+\omega_y^2-\omega_x^2}{2}+\frac{1}{2}\sqrt{\left(\omega_{\rm c}^2+\omega_y^2-\omega_x^2\right)^2+4\omega_x^2\omega_y^2}}. \end{aligned}\tag{29}$$

This is the main result of this work. In order to see the convenience of the IEO method, and to give some contrast, using the same method as discussed above, we also calculate the physical energy gap for the Hamilton describing an electron in a two anisotropic inverted harmonic oscillator potential under a UMF (as described in Fig. 3.)

$$\begin{aligned}&H_2\\ &=\frac{1}{2m}\left(p_x^2+p_y^2\right)+\frac{1}{8}m\omega_{\rm c}^2\left(x^2+y^2\right)\\ &\quad+\frac{\omega_{\rm c}}{2}\left(xp_y-yp_x\right)-\frac{1}{2}m\left(\omega_x^2x^2+\omega_y^2y^2\right), \end{aligned}\tag{30}$$

and obtain

$$(\Delta E'')^2=\frac{\omega_{\rm c}^2-B}{2}\pm\frac{1}{2}\sqrt{\left(\omega_{\rm c}^2-B\right)^2-4\omega_x^2\omega_y^2}, \tag{31}$$

where

$$B=\omega_x^2+\omega_y^2, \tag{32}$$

we can see for Hamilton H_2, when $\omega_{\rm c}<(\omega_x+\omega_y)$, in Eq. (31) $\left(\omega_{\rm c}^2-B\right)^2-4\omega_x^2\omega_y^2<0$, the energy gap becomes unphysical, while for H_1 it has no such confinment.

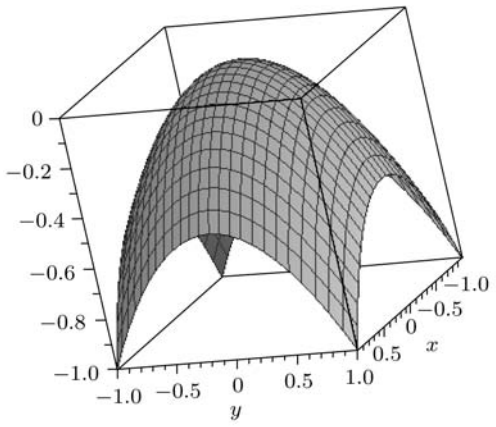


Fig. 3. The two anisotropic inverted harmonic oscillator potential.

6. The variation of Landau diamagnetism

Further, supposing that the difference between the two energy gaps (one is for the saddle potential Eq. (29), the other is for the isotropic potential Eq. (11)) is just the difference between the energies of the two ground states under the two potentials, then

we find that the ground state of the electron in the saddle potential under a UMF is

$$\begin{aligned} & E_0 \\ &= \Delta E - \Delta E'_{\rm iso} + \frac{\sqrt{\omega_{\rm c}^2 + 4\omega_0^2}}{2} \\ &= \sqrt{\frac{\omega_{\rm c}^2 + A}{2} + \frac{1}{2}\sqrt{\left(\omega_{\rm c}^2 + A\right)^2 + 4\omega_x^2\omega_y^2}} - \frac{\omega_{\rm c}}{2}. \quad (33) \end{aligned}$$

When $\omega_{\rm c}$ is large enough

$$E_0 = \sqrt{(\omega_{\rm c}^2 + A) + \frac{\omega_x^2\omega_y^2}{(\omega_{\rm c}^2 + A)}} - \frac{\omega_{\rm c}}{2}. \quad (34)$$

The corresponding magnetization affected by the saddle harmonic potential characterized by ω_x and ω_y is calculated by

$$\begin{aligned} -\frac{\partial E_0}{\partial B} &= -\frac{e}{m}\frac{\partial E_0}{\partial \omega_{\rm c}} \\ &\cong -\frac{e}{2m}\left(\frac{2\omega_{\rm c}}{\sqrt{\left(\omega_{\rm c}^2 + \omega_y^2 - \omega_x^2\right)}} - 1\right), \quad (35) \end{aligned}$$

thus we see that the Landau diamagnetism decreases with the increase in the difference between ω_y^2 and ω_x^2, i.e. the value of $\omega_y^2 - \omega_x^2$. Similarly, the corresponding magnetization affected by the two anisotropic inverted harmonic oscillator potential characterized by ω_x and ω_y is calculated by

$$\begin{aligned} -\frac{\partial E_0''}{\partial B} &= -\frac{e}{m}\frac{\partial E_0''}{\partial \omega_{\rm c}} \\ &\cong -\frac{e}{2m}\left(\frac{2\omega_{\rm c}}{\sqrt{\left(\omega_{\rm c}^2 - \omega_y^2 - \omega_x^2\right)}} - 1\right), \quad (36) \end{aligned}$$

and in this case the Landau diamagnetism increases with the increase of anisotropic harmonic potential.

In summary, by virtue of the IEO method, we have successfully derived the energy gap of the Hamiltonian describing an electron in a saddle potential quantum dot under a uniform magnetic field.

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