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MAGNETO-CONTROLLING QUANTUM STATES OF A SINGLE PARTICLE INTERACTING WITH A SQUARE BARRIER

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We obtain the exact solutions of a single particle magneto-confined in a one-dimensional (1D) quantum wire with a single square barrier. Theoretical analysis and numerical computation show that for a set of fixed barrier height and width, the quantum levels and states of the system depend on the displacement d of the magnetic trap, and for a fixed d value the system occupies only one or two lower quantum levels of $n \leq 20$ of a free harmonic oscillator. In the barrier region, the finite-sized effect implies that only for some discrete barrier parameters and d values, the system has the Hermitian polynomial solutions, otherwise it has the infinite series solutions. Therefore, one can manipulate the external motional states of the system and prepare some required lower energy states by adjusting the displacement of the magnetic trap experimentally.

Keywords: Quantum wire; square barrier; magneto-controlling; quantum motional state.

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1. Introduction

It is well-known that for a free harmonic oscillator with infinite boundary coordinates, the boundary conditions of quantum-mechanical wavefunctions lead to n possible quantum eigenstates and eigenenergies for $n = 0, 1, 2, \ldots$. From this result, we think that if one considers a system which obeys the same Schrödinger equation of the free harmonic oscillator but satisfies more boundary conditions, the eigenstates and eigenenergies should be limited further, namely some of the n possible eigenstates will be forbidden. Such a system can be realized by a single particle harmonically confined in a one-dimensional (1D) quantum wire with a single square barrier.

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The advances in modern semiconductor processing techniques has enabled us to construct the microscopically bounded installations such as the quantum wells, quantum wires and quantum dots, as well as their fabrications that allow the artificial confinement of only a few particles. Due to the discontinuity of the band edges at the semiconductor interfaces[1] or the dipole potential of a far detuned laser beam,[2] a single square barrier potential or an array of square barriers can be produced in the 1D quantum wire.[3−12] The systems including square barriers provide so much convenience for us to study quantum tunneling and preparing quantum states, that they have attracted considerable interest of researchers.[13−24] The transfer matrices technique,[3] Floquent scatter theory,[5−12] path integral method[13−15] and the Wigner function for the square barrier[21] were applied to these studies. In the case of a square barrier and a bounded well, an interesting result is that the matter wave packet[16–18] behaves like a quantum chaos without classical counterpart.[16] The finite-size effects of the spatially bounded quantum systems have widely been investigated,[25–28] and can lead to new forms of quantum states and levels.[1,29–31] Particularly, the parabolic potential can be generated and applied to the atomic system,[32] and the center site of the potential may be controlled by a magnetic field.[33] Therefore, the magneto-confined particle in the quantum wire with a square barrier is an interesting quantum system whose external states and levels can be manipulated by adjusting the magnetic field.

In the present paper, we use the above system to reveal that given the height and width of the potential barrier, the external quantum levels and states of the system depend on the experimentally controllable center sites of the magnetic trap. For a given center site, the system can occupy only one or two lower quantum levels of $n \leq 20$ of a free harmonic oscillator. In the square barrier region, the finite-sized effect implies that the wavefunction can be a Hermitian polynomial or a superposition of two infinite series solutions of the same eigenenergy,[30,31] depending on the potential barrier parameters and displacements of the magnetic trap. The results show that we can manipulate the external quantum states by adjusting the magnetic trap and can apply the system to perform the quantum logic operations by laser-coupling the external motional states with the internal electronic states.[34,35] Although this system is simple, the results are very interesting and useful, and can be experimentally tested.

2. Quantum-Mechanical Exact Solutions

We consider a single particle loaded into a 1D quantum wire along the x-direction with a square barrier of width $2l$ generated by the discontinuity of the band edges at the semiconductor interfaces,[1] then impose a 1D harmonic trapping potential by using an homogeneous magnetic field. The previous experiment has demonstrated that the center site of the magnetic trap can be controlled to translate a variable distance ranging up to 300 μm, by changing the currents through the coils of the magnetic trap.[33] Given such a system, it is feasible to study the preparation and

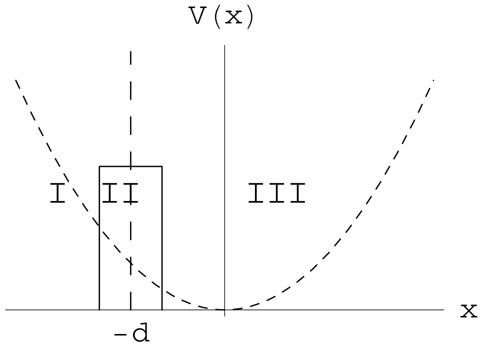

Fig. 1. Potential distribution of the system from Eq. (1) for a positive displacement d of the trap center. The magnetic trapping potential and square barrier are indicated by the dashed curve and solid lines respectively. There are three regions: (I) $x < -l - d$, (II) $-l - d \le x \le l - d$ and (III) $x > l - d$.

controlling of the external quantum states through the manipulation to the magnetic field.

For simplicity, we adopt the reference frame with origin fixed at the center site of magnetic trap and assume the coordinate of barrier center vanishes initially. Let the displacement of the trap center be d which is positive towards the x-direction or negative in the opposite direction. Thus after making a displacement d, the potential function becomes

$$V(x) = \begin{cases} V_0 + \dfrac{1}{2}x^2, & -l - d \le x \le l - d\,, \\ \\ \dfrac{1}{2}x^2, & x < -l - d \quad \text{or} \quad x > l - d\,. \end{cases} \tag{1}$$

Here lengths x, l, d and barrier height V_0 have been normalized by the harmonic oscillator length $l_h = \sqrt{\hbar/(m\omega)} = \sqrt{2c/eB}$ and the level difference $\hbar\omega$ respectively, where m is the effective mass of the particle, $\omega = eB/(2cm)$ is the Larmor cyclotron frequency with B being the intensity of the magnetic field, c is the velocity of light in vacuum and e is the unit charge. The coordinate of the barrier center is $-d$ and the distance between the trap center and barrier center is $|d|$. For $d > 0$, the barrier center lies to the left side of the trap center, as shown in Fig. 1. On the contrary, the barrier center coordinate becomes positive for $d < 0$. We estimate the amplitude of the harmonic oscillator length being $l_h \sim 10$ μm for $B \sim 10$ μT, and $l_h \sim 10^{-9}$ m for $B \sim 30$ T. The dimensionless barrier width $2l$ and the displacement d will be taken in the regions $2l \in (0, 3)$ and $d \in (-3, 3)$ in units of l_h. The experimentally motivated values of the barrier height and width can also be in larger regions[1–3,16] and some of them will be taken in our calculations. We have labeled the barrier region as region II and its left and right sides as region I and III in Fig. 1 respectively.

Quantum motion of the system is governed by the Schrödinger equation

$$\Psi_{xx} + (\lambda - x^2)\Psi = 0\,, \tag{2}$$

where the dimensionless energy λ reads

$$\lambda = \begin{cases} 2(E - V_0), & -l - d \leq x \leq l - d\,, \\ 2E, & x < -l - d \quad \text{or} \quad x > l - d\,. \end{cases} \tag{3}$$

Here Ψ denotes the external motional state of the particle, and E is the eigenenergy in units of $\hbar\omega$. Obviously, in regions I and III, Eqs. (2) and (3) are identified by a free harmonic oscillator equation whose state functions Ψ_n and eigenenergies $E_n = n + \frac{1}{2}$ are well-known. We will investigate how these eigenstates are limited by the boundary conditions at the barrier boundaries. The eigenenergies E_n cannot been changed in region II for the considered eigenstates Ψ_n. From Eq. (3), it is seen that in region II ($-l-d \leq x \leq l-d$), only $\lambda \geq 0$ ($E \geq V_0$) is permitted by classical mechanics, and $\lambda < 0$ is classically inaccessible, where the quantum tunneling may occur.

We are interested in determining the state functions of region II as follows. It is clear that for a given energy, the linearly ordinary differential equation (2) of the second order has a general solution consisting of the linear superposition between its two linearly independent special solutions.[36,37] One of the special solutions is the usual eigenstate and another is not quadratically integrable for the systems with the infinite boundaries, but both are quadratically integrable in region II with finite boundaries. Therefore, the finite-sized effect enables us to solve Eq. (2) for the general solution in region II. Setting the general solution in the form $\Psi(x) = \exp(-x^2/2)u(x)$ and inserting it into Eq. (2) yields the equation of $u(x)$,

$$u_{xx} - 2xu_x + (\lambda - 1)u = 0\,. \tag{4}$$

It is the well-known Hermite equation, whose two linear independent series solutions may be finite or infinite. We can apply the coordinate transformation $z = x^2$ to make it the confluent hypergeometric equation with two linear independent solutions in terms of the confluent hypergeometric functions as[30]

$$u_1 = F(0.25(1-\lambda), 0.5, x^2), \qquad u_2 = xF(0.25(3-\lambda), 1.5, x^2)\,, \tag{5}$$

where $F(p, q, x^2)$ is the confluent hypergeometric function. When p is zero or negative integers, $F(p, q, x^2)$ is a finite series, namely the Hermitian polynomial, otherwise it is an infinite series.

In regions I and III, when we consider the well-known Hermitian polynomial solution $H_n(x)$ which makes the state satisfy boundary condition $\Psi(\pm\infty) = 0$ at $x = \pm\infty$, the dimensionless energy λ becomes one of the integers $2n+1$ for $n = 0, 1, \ldots$. If n is an even number, u_1 is equal to $H_n(x)$ and u_2 still is an infinite series. For an odd number n, we have $u_2 = H_n(x)$ and u_1 an infinite series. We can take the general solution $\Psi_{II} = \exp(-\frac{x^2}{2})[Bu_1(x) + Cu_2(x)]$ only for region II with finite boundaries. Applying these results to the three regions yields the solution

$$\Psi = \begin{cases} \Psi_I = A\exp\left(-\frac{x^2}{2}\right)H_n(x), & x < -l-d\,, \\ \Psi_{II} = \exp\left(-\frac{x^2}{2}\right)[Bu_1(x) + Cu_2(x)], & -l-d \le x \le l-d\,, \\ \Psi_{III} = D\exp\left(-\frac{x^2}{2}\right)H_n(x), & x > l-d\,. \end{cases} \tag{6}$$

Here $\lambda = 2n + 1 - V_0$ in region II $(-l - d \le x \le l - d)$ of Eq. (3), A, B, C, D are arbitrary constants adjusted by the matching conditions at barrier boundaries and the normalization. The corresponding energies are fixed by Eq. (3) of regions I or III with $\lambda = 2n + 1$ as

$$E_n = n + \frac{1}{2}\,. \tag{7}$$

For a free harmonic oscillator, the quantum number n in Eq. (7) can take arbitrary non-negative integer. However, for the considered system with a square barrier the matching conditions at barrier boundaries and the normalization will confine n to some particular non-negative integers. This is an interesting finite-sized effect. Setting $a = l-d$ and $b = l+d$, the matching conditions at barrier boundaries $x = a$ and $x = -b$ reads

$$\begin{cases} \Psi_I|_{x=-b} = \Psi_{II}|_{x=-b}, & \Psi_{II}|_{x=a} = \Psi_{III}|_{x=a}\,, \\ \left.\frac{d\Psi_I}{dx}\right|_{x=-b} = \left.\frac{d\Psi_{II}}{dx}\right|_{x=-b}, & \left.\frac{d\Psi_{II}}{dx}\right|_{x=a} = \left.\frac{d\Psi_{III}}{dx}\right|_{x=a}; \end{cases} \tag{8}$$

and by the normalization condition, we mean

$$\int_{-\infty}^{-b} |\Psi_I|^2 dx + \int_{-b}^{a} |\Psi_{II}|^2 dx + \int_{a}^{\infty} |\Psi_{III}|^2 dx = 1\,. \tag{9}$$

Once the parameters l, V_0 of the potential barrier and the trap displacement d are given, we can substitute Eq. (6) into Eqs. (8) and (9) to obtain the undetermined constants A, B, C, D and the admissible quantum numbers in the dimensionless energy $\lambda = 2n + 1 - V_0$. After eliminating constants A, B, C, D, the admissible quantum number n is determined by the algebraic equation

$$M(1,a)M(2,-b) - M(1,-b)M(2,a) = 0\,, \tag{10}$$

where $M(k,c) = u_k(c)\frac{d}{dx}H_n|_{x=c} - H_n(c)\frac{d}{dx}u_k|_{x=c}$ for $k = 1, 2$ and $c = a, b$. Noticing $a = l-d,\ b = l+d$ and $\lambda = 2n+1-V_0$, for a given parameter set l, V_0, d it is possible that this equation does not have the solutions of some integers n. By continuously varying d values, we solve Eq. (10) for $n = 0, 1, \ldots, 20$ respectively, finding that only for some discrete d values a few lower quantum numbers are allowable.

Table 1. Quantum levels n for different d and fixed barrier parameters $V_0 = 4$, $l = 0.5682$.

d	0	±0.1053	±0.1828	±0.5454	±0.8694	±1.0816	±1.3696
n	0	3	1	2	2	3	3
d	±1.5258	±1.7784	±1.9148	±2.1299	±2.1300	±2.2647	±2.2674
n	4	4	5	5	0	1	6
d	±2.4397	±2.4447	±2.5975	±2.7064	±2.7143		
n	6	2	7	3	7		

It is worth noting that in region II if the barrier height obeys $\lambda = 2(E_n - V_0) = 2n' + 1$ for $n' = 0, 1, \ldots$, Eqs. (2) and (3) imply that the solution Ψ_{II} is in the form of a Hermitian polynomial. Combining this equation with Eq. (7) gives the quantized barrier height $V_0 = n - n'$. However, u_1 and u_2 cannot be the Hermitian polynomial simultaneously, which implies $B = 0$ or $C = 0$ in the general solution of Eq. (6). In two such cases, Eq. (10) is simplified as

$$\begin{cases} C = 0, \quad M(1, a) = 0, \quad M(1, -b) = 0\,; \\ B = 0, \quad M(2, a) = 0, \quad M(2, -b) = 0\,. \end{cases} \tag{11}$$

It is clear that Eqs. (10) and (11) are the existence conditions of the exact solutions (6). The comparison between Eqs. (10) and (11) shows that Eq. (11) is two special cases of Eq. (10). The parameter set $\{V_0, l, d, n\}$ which satisfies Eq. (11) can obey Eq. (10), but not the contrary. An obvious condition of the case (11) is $n = V_0 + n' \geq V_0$. Similarly, for a given parameter set l, V_0, d only a few lower quantum numbers are allowed by Eq. (11).

When the parameters $l, V_0, d, \lambda(n)$ are given by Eqs. (10) or (11), the constants A, B, C, D in Eq. (6) can be easily obtained by inserting Eq. (6) into Eqs. (8) and (9). Thus the quantum-mechanical solution of the system is determined completely.

3. Lower Quantum Levels and States

Now we take a set of barrier parameters as an example from Eqs. (10) and (11) to calculate the admissible quantum levels with lower energies. For the sake of convenience we assume barrier parameters $V_0 = 4$, $l = 0.5682$ and let n run from 0 to 20 to find the allowable displacement d for each n respectively. The results corresponding to $|d| < 3$ are listed in Table 1. In this table, we show that for a fixed $|d|$ value and for the given barrier parameters only one lower quantum number of $n < 20$ is admissible, namely the system has only one lower energy state, which can be called the ground state of the considered system. However, it is possible that two different $|d|$ values correspond with a same quantum level, which may be the ground state level $n = 0$ of a free harmonic oscillator. Note that for most of $|d|$ values of region $d \in (-3, 3)$ the system does not have lower energy state, and the possible states may be the higher energy states of $n > 20$. In the case of lower energy levels of Table 1, of course, some higher energy states of $n > 20$ also may exist. On

Table 2. Quantum levels n for different d and fixed barrier parameters $V_0 = 2$, $l = 0.7071$.

d	-2.5838	-2.3361	0	2.3361	2.5838
n	1	0	$0, 1$	0	1

the other hand, we can see from Table 1 that for $|d| < 3$, the admissible quantum numbers obey $n < 8$ and the largest n value of region $n < 20$ increases with the increase of $|d|$ values. These results mean that we can adjust the displacement of the magnetic trap to manipulate the quantum states of the system and to prepare some required lower energy states.

It is interesting that when the barrier parameters are supposed to $V_0 = 2$, $l = 0.7071$, the similar calculations show an external two-level system with $d = 0$, as in Table 2. That is, when the trap center coincides with the barrier center, two lower quantum numbers $n = 0, 1$ become allowable simultaneously for the given barrier parameters. Thus we can prepare an external two-level system with longer lifetime compared to that of the free harmonic oscillator, because of the large energy gap between the levels $n = 1$ and $n > 20$. The previous studies revealed that for a trapped-ion system by laser-coupling two or three internal electronic states with two external phonon states, one can perform the controlled phase-flip gate[34] or the other quantum gates.[35] The above external two-level system will be useful for such quantum logic operations, because of the similarity between the considered system and the trapped-ion system. The longer lifetimes of our two external states imply the higher stability of the system.

Given the parameter set n, V_0, l, d from Eqs. (10) or (11), we can combine Eq. (6) with Eqs. (8) and (9) to calculate the undetermined constants A, B, C, D in Eq. (6). In fact, substituting Eq. (6) into Eq. (8) gives four linear equations of A, B, C, D and solving them leads A, B, C to be the functions of D. Then we apply the results to Eq. (9), yielding the value of D and the consequent A, B, C values. The system parameters n, V_0, l, d and constants A, B, C, D determine the quantum-mechanical solution of the system completely. We take eight sets of parameters n, V_0, l, d from Eqs. (6), (8) and (9) to derive constants A, B, C, D, and then apply them to solutions (6). The results are listed as in Table 3, where any one of $\Psi_{II} = [Bu_1(x) + Cu_2(x)] \exp(-x^2/2)$ is an infinite series for the cases $n = 0, 1, 2$ or the Hermitian polynomial for the case $n = 5$. The well-known wavefunctions Ψ_I and Ψ_{III} are not shown here. From Eq. (6), we know that Ψ_I and Ψ_{III} depend on constants A and D. Table 3 shows that when the symmetric potentials with $d = 0$ are selected, we have the symmetric wavefunctions with $A = D$, and in other cases, the solutions may be asymmetric.

According to the probability interpretation of quantum mechanics, norm $|\Psi|^2(x)$ of the wavefunction denotes the probability density of the particle. We take four sets of parameters in Table 3 as examples and insert them into Eq. (6) to illustrate the probability distributions of the trapped particle as the solid curves in Fig. 2.

Table 3. Quantum states and levels for different system parameters.

n	V_0	$2l$	d	B	C	A	D	$Bu_1(x) + Cu_2(x)$
0	4	1.1364	0	0	1.0371	0.9891	0.9891	$CxF(2.5, 1.5, x^2)$
1	4	1.1364	0.1828	0.2311	0.4668	0.7352	0.0923	$BF(1.5, 0.5, x^2) + CxF(2, 1.5, x^2)$
2	4	1.1364	0.5454	−0.158	0.0287	0.0787	0.4123	$BF(1, 0.5, x^2) + CxF(1.5, 1.5, x^2)$
0	2	1.4142	0	0	0.9599	1.1191	1.1191	$CxF(1.5, 1.5, x^2)$
1	2	1.4142	0	0.4245	0	0.4948	0.4948	$BF(0.5, 0.5, x^2)$
5	3	2.8545	0	0.4161	0	0.0123	0.0123	$BF(-1, 0.5, x^2) = -\frac{1}{2}BH_2(x)$
5	2	1.6975	0.2598	0	1.229	0.0079	0.0138	$CxF(-1, 1.5, x^2) = -\frac{1}{12}CH_3(x)$
5	2	2.2171	0	0	1.5785	0.0101	0.0101	$CxF(-1, 1.5, x^2) = -\frac{1}{12}CH_3(x)$

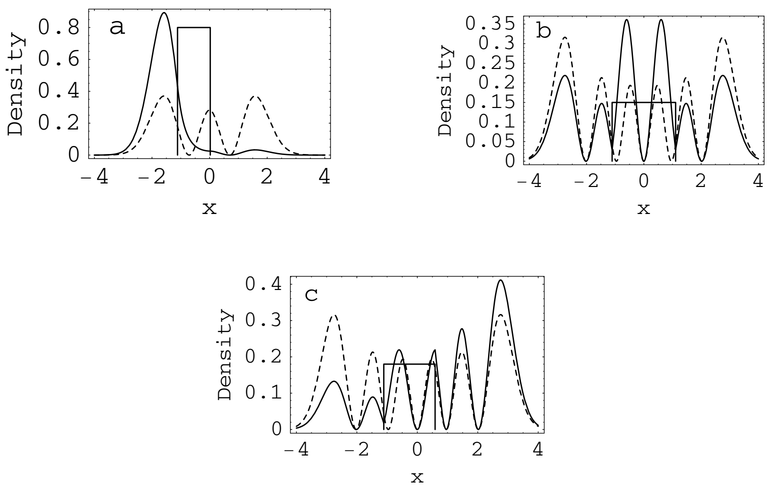

Fig. 2. Plots of the probability distributions $|\Psi(x)|^2$ illustrated by the solid curves from Eq. (6) for the parameters: (a) $n = 2$, $V_0 = 4$, $2l = 1.1364$, $d = 0.5454$, $A = 0.0787$, $B = -0.158$, $C = 0.0287$, $D = 0.4123$. (b) $n = 5$, $V_0 = 2$, $2l = 2.1711$, $d = 0$, $A = 0.0101 = D$, $B = 0$, $C = 1.5785$. (c) $n = 5$, $V_0 = 2$, $2l = 1.6975$, $d = 0.2598$, $A = 0.0079$, $B = 0$, $C = 1.229$, $D = 0.0138$. The corresponding probability densities of a free harmonic oscillator with the same energies are plotted as the dashed curves, and the rectangles denote the square barriers. The spatial coordinate has been normalized by the harmonic oscillator length.

To compare the barrier-trap system with the harmonically trapped particle, the probability densities of a 1D free harmonic oscillator for the same energy levels are exhibited by the dashed curves. In Fig. 2(b), we display that for $d = 0$ the density distribution is spatially symmetric, like that of the free harmonic oscillator. However, when the coordinate $-d$ of barrier center deviates the origin, $-d = -0.5454$ in Fig. 2(a) and $-d = -0.2598$ in Fig. 2(c), the symmetry is broken down. From Figs. 2(a) and 2(c) we see that the maximums of the probability densities may

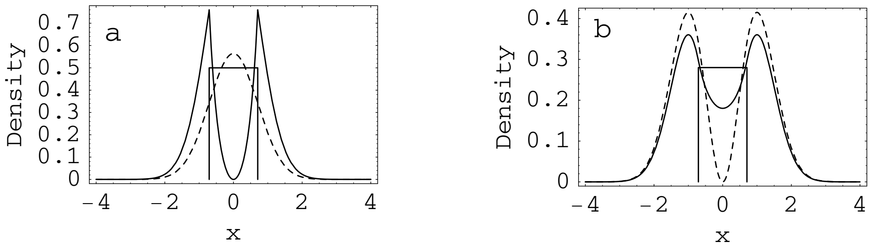

Fig. 3. The probability densities of the external two-level system with parameters $V_0 = 2$, $2l = 1.4142$, $d = 0$ for (a) $n = 0$, and (b) $n = 1$. The rectangles and dashed curves denote the same things with Fig. 2, and the spatial coordinate is in the same units as Fig. 2.

appear at the left side or right side of the barriers. The profiles of the symmetric and asymmetric density distributions are greatly different from those of a free harmonic oscillator, because of the finite-sized effects of the square barrier.

In Table 2, the external two-level system with parameters $V_0 = 2$, $2l = 1.4142$, $d = 0$ is indicated. The corresponding probability densities of the two states are plotted as Fig. 3. Differing from the case of the free harmonic oscillator, here the ground state density vanishes and the probability density of $n = 1$ state does not vanish at the origin. This shows the effects of the square barrier on the probability distributions. It is well-known that the lower quantum states possess higher lifetimes and the probabilities of a ultracold atom occupying higher excitation states of $n > 20$ are very small. In spite of the possible higher excitation states, the above-mentioned lower quantum states will be useful for us to prepare different quantum states by displacing the magnetic trap and to realize some applications of the lower quantum states.

It is worth demonstrating that the above-mentioned results sensitively depend on the forms and parameters of the trapping potential. For example, when the particle is confined between two hard walls and interacting with a square barrier, the time-dependent wavefunction may behave like a quantum chaotic state.[16] On the other hand, for the considered potential form of Eq. (1), if the potential parameters have a small deviation from the existence conditions of the solutions (6), the exact stationary states cannot exist, so the system has to enter the non-stationary states. However, it is impossible for a non-stationary state (e.g. the well-known coherent state of a harmonic oscillator) to strictly satisfy the boundary conditions at the barrier boundaries for every time such that the possible state may become the unpredictable quantum chaotic-like state.

4. Conclusion and Discussions

A single particle magneto-confined in a one-dimensional (1D) quantum wire with a single square barrier potential has been studied. For different potential parameters, several sets of exact solutions which are in the forms of the infinite series or the Hermitian polynomials have been constructed. It is shown theoretically and numerically that for a set of supposed height and width of the potential barrier, the quantum levels and states of the system depend on the displacement d of the magnetic trap, and the latter can be controlled experimentally. The existence conditions Eqs. (10) and (11) of the exact solutions are obtained as the relations among the system parameters and the quantum levels. Fixing a d value, the mutual effect of the magnetic field and the square barrier leads the system to occupy only one or two lower quantum levels of $n \leq 20$ and of a free harmonic oscillator. In the square barrier region, because of the finite-sized effect of the square barrier, only for some discrete barrier parameters and d values does the system have the Hermitian polynomial solutions, otherwise the infinite series solutions. Applying these results, we can adjust the displacement of the magnetic trap to manipulate the external motional states of the system and use laser to couple the external states with the internal states, that is useful for the quantum logic operations. Particularly, only one or two external states of lower energies exist in our system. The large energy gaps between the lower energy states and the possible higher energy states ($n > 20$) imply the longer lifetime of the states and the higher stability of the system compared to that of the free harmonic oscillator.

The above-mentioned results can be easily applied to some similar trapping systems. For example, we can extend the results to the cases of a single magneto-confined particle interacting with the double square barriers or with an array of square barriers. We also can construct a system consisting of above N systems. Although the more barriers there are, the more parameters and matching conditions there are, our method will be useful for solving these problems, and the conclusion will be similar with what we obtain in this paper. With the development of semiconductor processing techniques, the applications of the small-size square barrier system have been continuously increased, and will play more and more important roles.

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