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Semiclassical quantum theory and its applications in two dimensions by conformal mapping

Hyo Suk Yi, Hyeong Rag Lee, and Ki Soo Sohn
Department of Physics, Kyungpook National University, Taegu, 702-701, Korea

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The semiclassical quantum theory is investigated with conformal mapping to analyze the energy levels for a central force potential in two dimensions. The conformal mapping produces a modification in the effective potential which provides the correct phase for the WKB wave function. With this modification in the effective potential the semiclassical quantum theory, the so-called WKB approximation, yields the exact energy spectrum for a central force potential in two dimensions, such as the parabolic potential, the attractive Coulomb potential, and the donor impurity states under a plane magnetic field in a two-dimensional system. Among these, the result for the last one is compared with experimental results and other numerical results.

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I. INTRODUCTION

The recent advances in crystal-growth techniques, such as molecular-beam epitaxy (MBE) [1] and metal-organic chemical vapor deposition (MOCVD) [2], have made possible the growth of semiconductors with controlled changes of composition and doping on a very fine scale. With these increasingly sophisticated microelectronic fabrication techniques the electronic properties in reduced dimensions are studied widely in many areas. Two-dimensional electrons can be found in the vicinity of junctions between insulators and semiconductors, between layers of different semiconductors, and between a vacuum and liquid helium [3]. A wide variety of works in two dimensions have been reviewed by Ando, Fowler, and Stern [4]. Since the integral [5] and the fractional [6] quantum Hall effects were discovered in two-dimensional electron systems under a high magnetic field, the two dimensions have been the subject of intense investigation in quantum solid state physics as well as in quantum field theory [7]. The theoretical methods for the explanation of these new phenonomena might be beyond three-dimensional quantum physics.

After quantum theory was developed in 1926, the Schrödinger wave equation was published for free particles [8] in one dimension. However, the exact solution for the Schrödinger equation can be given only for some special forms of the potential. Therefore, the approximate values of the energy levels are obtained by using the perturbation theory or the variational method in many cases. The WKB method provides the exact energy levels for many cases in one dimension. For the spherical symmetric potential in two or three dimensions, the Schrödinger equation is transformed into the effective one-dimensional representation by the radial wave equation. But this method provides an undefined boundary condition at $r=0$ which causes the direct application of the WKB method to be difficult. In three dimensions, several papers [9,10] reported the necessity for the modification in an effective potential by replacing the number $l(l+1)$ by $(l+\frac{1}{2})^2$.

In this paper, we study the WKB method to get the exact energy levels confined in a spherical symmetric potential in two dimensions. The semiclassical quantum theory in one dimension is reviewed in Sec. II. In Sec. III, we present the correct quantization rule by conformal mapping in two-dimensional (2D) polar coordinates. In Sec IV, we apply this method to the various 2D electron systems such as 2D electrons under an external magnetic field, 2D hydrogenic impurity states, and 2D impurity states under an external magnetic field. Section V summarizes the present work and suggests the future direction of our studies.

II. THE QUANTIZATION RULE IN ONE DIMENSION

The Schrödinger equation in one dimension can be written as

$$\frac{d^2\Psi(x)}{dx^2}+\frac{1}{\hbar^2}p(x)^2\Psi(x)=0 \tag{1}$$

with

$$p(x)=\{2m[E-V(x)]\}^{1/2} .$$

We might try a solution of the form $\Psi(x)=e^{iu(x)}$ for the slowly varying potential $V(x)$ in the above differential equation. A well-known WKB method for obtaining the approximate solution consists of substituting an expansion of $u(x)$ in powers of $\hbar$ into the differential equation. Retaining only of the first term of the series one finds

$$\Psi(x)=A\frac{1}{\sqrt{k(x)}}\exp\left[\pm i\int_{x_0}^{x}k(x)dx\right] \quad \text{for } V(x)<E \tag{2}$$

and

$$\Psi(x)=B\frac{1}{\sqrt{\kappa(x)}}\exp\left[\pm\int_{x_0}^{x}\kappa(x)dx\right] \quad \text{for } V(x)>E \tag{3}$$

where

$$k(x)=\left\{\frac{2m}{\hbar^2}[E-V(x)]\right\}^{1/2}, \quad V(x)<E$$

$$\kappa(x)=\left\{\frac{2m}{\hbar^2}[V(x)-E]\right\}^{1/2}, \quad V(x)>E$$

and x_0 represents the turning point. Apparently the above procedures break down near the turning point of the classical motion, where $k(x)$ and $\kappa(x)$ are zero. Since each of the wave functions obtained in different regions becomes infinite at any point where $k^2(x)$ is zero, neither form can be retained during the transit from one to another region. The so-called connection formula [11,12] allows one to infer either of the wave functions that are valid in intervals on opposite sides of the turning point. Near the turning point x_1 of the slowly varying potential, we may write

$$V(x)-E(x)=c(x-x_1), \quad c=\text{const}. \tag{4}$$

When the turning point is to the right of the classical region, the appropriate WKB solution to the Schrödinger equation is

$$\frac{2}{\sqrt{k}}\cos\left[\int_x^{x_1}k\,dx-\frac{1}{4}\pi\right]\leftrightarrow\frac{1}{\sqrt{\kappa}}\exp\left[-\int_{x_1}^{x}\kappa\,dx\right]. \tag{5}$$

Meanwhile when the turning point, x_2 is to the left of the classical region, the appropriate WKB solution to the Schrödinger equation is

$$\frac{1}{\sqrt{\kappa}}\exp\left[-\int_x^{x_2}\kappa\,dx\right]\leftrightarrow\frac{2}{\sqrt{k}}\cos\left[\int_{x_2}^{x}k\,dx-\frac{1}{4}\pi\right]. \tag{6}$$

For the well-shaped potential with two classical turning points the connection formula provides the condition

$$\int_{x_2}^{x_1}k(x)dx=(N+\tfrac{1}{2})\pi, \tag{7}$$

where $N=0,1,2,\ldots,$. Therefore, the quantization rule for bound states in a one-dimensional continuous potential can be expressed by the phase integral

$$\oint k(x)dx=\frac{1}{\hbar}\oint\sqrt{2m[E-V(x)]}dx=(2N+1)\pi \tag{8}$$

and provides the discrete values of E. Here, the integral is taken over the full period of the coordinate x. At this moment, the connection formula yields a half wavelength change due to the boundary condition of the continuous potential. In one dimension, the WKB approximation provides the correct energy levels in many cases such as the parabolic potential well, etc [13,14]. This can also be applied in three-dimensional polar coordinates by using an effective potential.

III. THE QUANTIZATION RULE IN TWO DIMENSIONS

The kinetic energy is usually replaced by the differential operator in the expansion of the Hamiltonian. The operator can be expanded in polar coordinates if the potential has a circular symmetry. In two dimensions the radial distance and angle are given by

$$r=\sqrt{x^2+y^2}, \quad \theta=\tan^{-1}\left[\frac{y}{x}\right], \tag{9}$$

where $x=r\cos(\theta)$ and $y=r\sin(\theta)$. Evidently the radial distance r cannot be negative. The corresponding two-dimensional Laplacian can be written as

$$\begin{aligned}\nabla^2&=\frac{1}{r}\frac{\partial}{\partial r}\left[r\frac{\partial}{\partial r}\right]+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\\&=\frac{1}{\sqrt{r}}\frac{\partial^2}{\partial r^2}\sqrt{r}+\frac{1}{4r^2}+\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}.\end{aligned} \tag{10}$$

For the central force potential, the time-independent Schrödinger equation is given by

$$-\frac{\hbar^2}{2\mu}\nabla^2\Psi(\mathbf{r})+V(r)\Psi(\mathbf{r})=E\Psi(\mathbf{r}) \tag{11}$$

with

$$\Psi(\mathbf{r})=R(r)\Theta(\theta).$$

Apparently the angular momentum corresponding to the coordinate θ in an isotropic medium is quantized by the condition

$$\oint p_\theta d\theta=mh. \tag{12}$$

The θ direction can be assumed by the plane wave, $\Theta(\theta)=c\exp^{im\theta}$. Therefore

$$p_\theta^2\Theta(\theta)=-\frac{\hbar^2}{r^2}\frac{\partial^2}{\partial\theta^2}\Theta(\theta)=\frac{m^2\hbar^2}{r^2}\Theta(\theta). \tag{13}$$

Using Eqs. (11) and (13), the effective one-dimensional Schrödinger equation is given by

$$-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2}\chi(r)-\frac{\frac{1}{4}\hbar^2}{2\mu r^2}\chi(r)+\frac{m^2\hbar^2}{2\mu r^2}\chi(r)+V(r)\chi(r)=E\chi(r), \tag{14}$$

where $\chi(r)=\sqrt{r}R(r)$. Equation (14) might be written in the form

$$\frac{d^2}{dr^2}\chi(r)+\frac{1}{\hbar^2}q(r)^2\chi(r)=0 \tag{15}$$

with

$$q(r)=\{2\mu[E-V_{\rm eff}(r)]\}^{1/2},$$

where the effective potential is expressed by

$$V_{\rm eff}(r)=V(r)+\frac{\hbar^2}{2\mu r^2}(m^2-\tfrac{1}{4}).$$

Structurally, Eq. (15) has the same form as that of Eq. (1). And the quantization condition for the r coordinate can be expressed by

$$\frac{2}{\hbar}\int_{r_1}^{r_2}\sqrt{2\mu[E-V_{\rm eff}(r)]}dr=(2N+1)\pi \quad (N=0,1,2,\ldots,). \tag{16}$$

But the condition is not completely solved because of the undefined boundary condition at $r=0$.

Let us consider the attractive Coulomb potential, $V(r)=-Ze^2/r$. The left turning point at which p_r^2 vanishes is found to be

$$r_1=\frac{(m-\frac{1}{2})(m+\frac{1}{2})\hbar^2}{\mu Ze^2\left[1+\left[1+\frac{2E(m-\frac{1}{2})(m+\frac{1}{2})\hbar^2}{\mu Z^2e^4}\right]^{1/2}\right]} \quad \text{if } Z>0,\ m\neq 0 . \tag{17}$$

In the case of $m=0$, the left turning point is found to be negative, but the radial distance r is bounded from zero. This result explicitly shows the failure of the application of the WKB approximation to the two-dimensional polar coordinate systems. Furthermore the direct application is incorrect because of the undefined boundary condition at $r=0$. More subtle points are discussed in Refs. [12,13,14] relating to the connection formula near $r=0$ in three-dimensional polar coordinates. This difficulty can be avoided by the use of a logarithmic variable which is the conformal mapping of the two-dimensional rectangular coordinates. For this transformation, we put

$$re^{i\phi}=e^{(u+iv)} , \tag{18}$$

where $r=e^u$ and $\phi=v$. In this representation the Schrödinger equation for the coordinate u is found to be

$$\frac{d^2}{du^2}U(u)+\frac{1}{\hbar^2}q(u)^2U(u)=0 \tag{19}$$

with

$$q(u)=\{2\mu e^{2u}[E-V(u)]-m^2\hbar^2\}^{1/2}$$

and

$$U(u)=R(r) .$$

Clearly this equation has the form of (1) and is well defined in the whole range of $-\infty<u<\infty$. Then the quantization rule for u coordinate is given by

$$\frac{2}{\hbar}\int_{u_1}^{u_2}q(u)du=(2N+1)\pi \quad (N=0,1,2,\ldots,) \tag{20}$$

where u_1 and u_2 are two classical turning points. Converting the coordinate u into the original coordinate r, we get the correct quantization rule in two dimensions. That is, the quantization rule in the r representation is

$$\frac{2}{\hbar}\int_{r_1}^{r_2}\sqrt{2\mu[E-V'(r)]}dr=(2N+1)\pi \quad (N=0,1,2,\ldots,) \tag{21}$$

where $V'(r)=V(r)+(m^2\hbar^2)/(2\mu r^2)$ and r_1, r_2 are turning points in the representation of the polar coordinates. Here, the effective potential in the radial direction can be written in the form

$$V'(r)=V_{\text{eff}}(r)+\frac{\frac{1}{4}\hbar^2}{2\mu r^2} \tag{22}$$

with

$$V_{\text{eff}}(r)=V(r)+\frac{m^2\hbar^2}{2\mu r^2}-\frac{\frac{1}{4}\hbar^2}{2\mu r^2} . \tag{23}$$

The last term in Eq. (23) is originated from the kinetic energy as explained earlier. Exactly the same amount of the potential is raised by the conformal mapping and cancels it. For the attractive hydrogenic potential, we obtain

$$q(r)=\left\{2\mu\left[E+\frac{Ze^2}{r}-\frac{m^2\hbar^2}{2\mu r^2}\right]\right\}^{1/2} \tag{24}$$

and the left turning point is found to be

$$r_1=\frac{m^2\hbar^2}{\mu Ze^2\left[1+\left[1+\frac{2Em^2\hbar^2}{\mu Z^2e^4}\right]^{1/2}\right]} \quad \text{if } Z>0 . \tag{25}$$

Compared with Eq. (17), the number $(m^2-\frac{1}{4})$ is replaced by m^2 in this result, which is the modification due to conformal mapping.

IV. APPLICATIONS

Using the quantization rule which is provided in Eq. (21), we can calculate energy levels of various systems in two dimensions. In this section, we consider three cases: (1) The two-dimensional electron under an external magnetic field (parabolic potential), (2) the hydrogenic impurity states (Coulomb potential) in two dimensions, and (3) the hydrogenic impurity states under an external magnetic field which is a combined system of the previous two cases.

A. Two-dimensional electron under an external magnetic field

Consider the two-dimensional electrons confined in the x-y plane subjected to the magnetic field perpendicular to the plane. The uniform external magnetic field $\mathbf{B}=(0,0,B_0)$ can be described by a vector potential $\mathbf{A}=(B_0/2)(-y,x,0)$. Then, the two-dimensional Schrödinger equation is given by

$$\frac{1}{2\mu}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]\Psi(\mathbf{r})=E\Psi(\mathbf{r}) . \tag{26}$$

Since the symmetric gauge yields the harmonic potential in the radial direction, the wave function can be written as $\Psi(\mathbf{r})=R(r)\Theta(\theta)$ as before. With the quantization rule in the θ direction, we obtain the effective one-dimensional Schrödinger equation,

$$\left[-\frac{1}{2\mu\sqrt{r}}\frac{\partial^2}{\partial r^2}\sqrt{r}-\frac{\frac{1}{4}\hbar^2}{2\mu r^2}+\frac{m^2\hbar^2}{2\mu r^2}\right]R(r)+\frac{1}{2}\mu r^2\omega^2R(r)=E'R(r) \tag{27}$$

where $r=\sqrt{x^2+y^2}$, $E'=E+m\hbar\omega$, and $\omega=eB_0/2\mu c$ is the cyclotron frequency. We identify the effective potential as

$$V'(r)=\frac{1}{2}\mu r^2\omega^2+\frac{m^2\hbar^2}{2\mu r^2} , \tag{28}$$

in which the radial motions of the electrons are confined. By the application of Eq. (21), we can obtain the quantization rule for the radial motion,

$$2\int_{r_1}^{r_2}\frac{\sqrt{2\mu[E'-\frac{1}{2}\mu\omega^2r^2-m^2\hbar^2/(2\mu r^2)]}}{\hbar}dr-\pi$$
$$=2N\pi \quad (N=0,1,2,\ldots,)\ . \tag{29}$$

The left-hand side can be integrated with ease and produces the discrete energy levels

$$E_n=2(n+\tfrac{1}{2})\hbar\omega \tag{30}$$

with

$$n=N+|m|/2+m/2=0,1,2,\ldots\ .$$

The result represents the correct Landau levels in the presence of a transverse magnetic field.

B. Hydrogenic impurity states in two dimensions

Let us consider the attractive hydrogenic potential in two dimensions,

$$V(r)=-\frac{Ze^2}{r}\ . \tag{31}$$

As discussed in the previous section, the conformal mapping in two dimensions modifies the effective potential represented by the radial distance r in the Schrödinger equation as

$$V'(r)=V(r)+\frac{m^2\hbar^2}{2\mu r^2}\ . \tag{32}$$

Equation (21) yields the quantization rule for the coordinate r,

$$\begin{aligned}\oint\frac{\sqrt{2\mu[E-V'(r)]}}{\hbar}dr&=2\int_{r_1}^{r_2}\frac{\sqrt{2\mu|E|+2\mu Ze^2r-m^2\hbar^2}}{\hbar r}dr-\pi\\&=\frac{2}{\hbar}\left[0+\frac{-m^2\hbar^2}{\sqrt{m^2\hbar^2}}\pi+\frac{2\mu Ze^2(-1)}{2\sqrt{2\mu|E|}}(-\pi)\right]-\pi\\&=\frac{2}{\hbar}\left[-|m|\hbar+\frac{Ze^2}{2\sqrt{2\mu|E|}}\right]\pi-\pi=2N\pi \quad (N=0,1,2,\ldots,)\end{aligned} \tag{33}$$

and $l=|m|$ in a two-dimensional system. Therefore, the energy levels bounded in an attractive hydrogenic potential in two dimensions are

$$E=\frac{1}{2}\frac{Z^2e^4\mu}{\hbar^2(N+l+1/2)^2} \quad (N=0,1,2,\ldots,)\ , \tag{34}$$

i.e.,

$$E=E_n=\frac{1}{2}\frac{Z^2e^4\mu}{\hbar^2(n-\frac{1}{2})^2} \quad (n=N+l+1=1,2,\ldots,) \tag{35}$$

and those agree with the exact results.

C. Impurity states in an arbitrary external magnetic field

In this section, we consider a two-dimensional hydrogenic impurity under a transverse magnetic field $\mathbf{B}=(0,0,B_0)$. We write the Schrödinger equation as

$$H\Psi(r,\phi)=E\Psi(r,\phi)\ . \tag{36}$$

Since the electron is confined by the combined potentials due to the impurity and the magnetic field, the system is described by the Hamiltonian,

$$H=\frac{1}{2\mu}\left[\mathbf{p}-\frac{e}{c}\mathbf{A}\right]^2-\frac{e^2}{\epsilon r}\ , \tag{37}$$

where $\mathbf{A}$ is the vector potential of the field and μ and ϵ are the effective mass and the dielectric constant, respectively. We choose the same vector potential $\mathbf{A}=(B_0/2)(-y,x,0)$ as before. Using one dimensionless atomic units [energy in units of an effective Rydberg $\mathcal{R}^*=\mu e^4/(2\hbar^2\epsilon^2)$, length in units of an effective Bohr radius $1\ a_B^*=\hbar^2\epsilon/(\mu e^2)$], we obtain

$$H=H_0-\frac{2}{r} \tag{38}$$

with

$$H_0=-\nabla^2+i\gamma\frac{\partial}{\partial\phi}+\frac{\gamma^2r^2}{4}\ , \tag{39}$$

where

$$\gamma=\frac{\mu_B^*B_0}{\mathcal{R}^*}=\frac{\hbar\omega_0^*}{2\mathcal{R}^*}=\frac{\epsilon^2\hbar^3B_0}{(\mu)^2e^3c}$$

and

$$r=(x^2+y^2)^{1/2}\ .$$

Inserting Eqs. (10) and (39) into Eq. (38), we can obtain the Hamiltonian in dimensionless units as,

$$H=\left[\frac{1}{\sqrt{r}}\frac{\partial^2}{\partial r^2}\sqrt{r}-\frac{1}{4r^2}-\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2}\right]+i\gamma\frac{\partial}{\partial\theta}-\frac{2}{r}\ . \tag{40}$$

Writing the wave function as $\Psi(r,\theta)=e^{im\theta}R(r)$, and inserting into Eq. (36), we obtain the Schrödinger equation

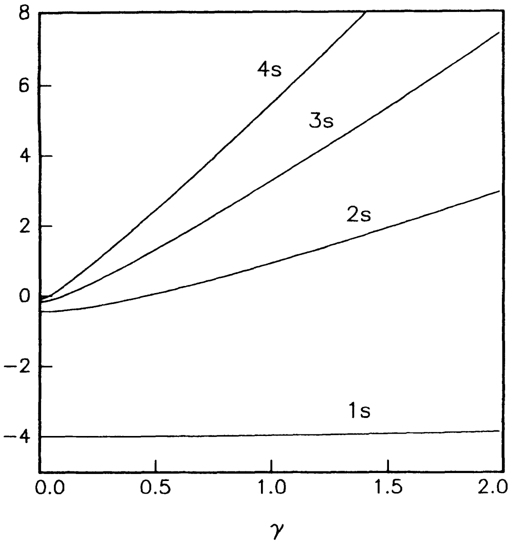

FIG. 1. The 2D donor energy levels in effective Rydberg units are shown as a function of γ for the 1s, 2s, 3s, and 4s states.

for the radial motion,

$$p_r^2 R(r) + \frac{R(r)}{4r^2} + \left[\frac{2}{r} - \frac{m^2}{r^2} - m\gamma - \tfrac{1}{4}\gamma^2 r^2 + E \right] R(r) = 0 \ . \tag{41}$$

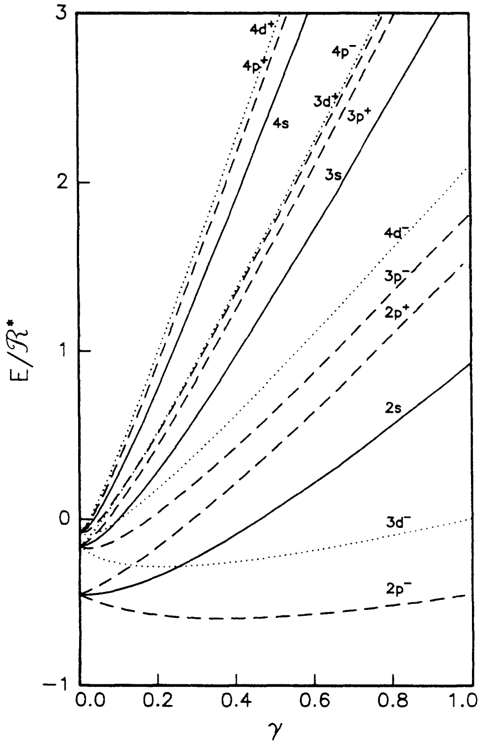

FIG. 2. The 2D donor energy levels in effective Rydberg units are shown as a function of γ ranging from 0 to 1 for $2p^-$, $3d^-$, $2s$, $2p^+$, $3p^-$, $4d^-$, $3s$, $3p^+$, $4p^-$, $3d^+$, $4s$, $4p^+$, and $4d^+$ states.

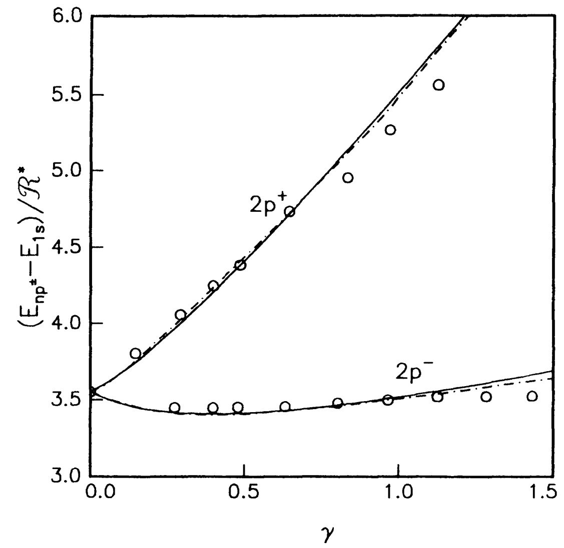

FIG. 3. The transition energy, $E_{2p\pm} - E_{1s}$, for two-dimensional hydrogen, in units of $\mathcal{R}^*$ as a function of magnetic field γ. The circles represent the experimental points of Jarosik *et al.* (Ref. [17]) for impurities in a GaAs well. The dashed line represents the theoretical results of MacDonald and Ritchie (Ref. [16]). The solid line represents our results.

Now applying the quantization rule for the radial motion which is given in Eq. (21), we can obtain the correct condition of energy levels E in dimensionless atomic units,

$$2\int_{r_2}^{r_1} \sqrt{[E - V'(r)]}\,dr = 2(N+1)\pi \quad (N = 0, 1, 2, \ldots,) \tag{42}$$

where

$$V'(r) = -\frac{2}{r} + \frac{m^2}{r^2} + m\gamma + \tfrac{1}{4}\gamma^2 r^2 \ .$$

The results are shown in Figs. 1, 2, and 3 as a function of the magnetic field. In Fig. 1, we present the energy levels (1s, 2s, 3s, and 4s) without the Zeeman term $m\gamma (m = 0)$. For comparison with the exact numerical results by Zhu, Cheng, and Xiong [15], the energy levels with the Zeeman term are shown in Fig. 2. Our results agree exactly with their results so that the differences cannot be seen in the figure. In Fig. 3, we compare our results with the numerical results which are based on the two-point Padé approximation by MacDonald and Ritchie [16] and the experimental results which are obtained with GaAs by Jarosik *et al.* [17].

V. SUMMARY AND DISCUSSION

By replacing the number $(m^2 - \frac{1}{4})$ by m^2 of effective potential in two dimensions, the semiclassical quantum theory yields the correct energy levels for the central field potential in two dimensions. The modification in the effective potential for the two-dimensional polar coordinates can be valid by the conformal mapping of the two-dimensional rectangular coordinates. This is the same as the logarithmic variable change of the radius in three dimensions, which results in the replacement of $l(l+1)$ by $(l+\frac{1}{2})^2$ for the application of semiclassical quantum theory [9].

In the applications, the energy levels calculated by the phase integral method for the electron under an external magnetic field or in the attractive Coulomb potential agree with the exact results solved directly from the Schrödinger equation. We also obtained the correct condition of energy levels for impurity states under an arbitrary magnetic field in a two-dimensional system. Our results for impurity states under an arbitrary magnetic field in a two-dimensional system agree with the numerical results of the two-point Padé approximations by MacDonald and Ritchie [16], the numerical exact solutions by Jhu, Cheng, and Xiong [15], and the experimental results by Jarosik *et al.* [17]. This semiclassical method can be applied to the two-dimensional bound states in any continuous potential. This method can be used extensively to calculate the exact eigenvalues for the two-dimensional systems such as the impurity states, the exciton states, and the two electron states in a quantum well and circular quantum dot under an arbitrary magnetic field, etc. [18,19].

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