Supersymmetric semiclassical approach to confined quantum problems

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It is suggested that the supersymmetric WKB (SWKB) method may be useful in studying the deviation of the energy levels of a quantum system due to the presence of a spherically confining boundary. For illustration, we present the explicit results for the Coulomb and three-dimensional harmonic-oscillator potentials. It is observed that the confining geometry removes the angular-momentum degeneracy of the electronic energy levels of a free atom. Our predicted energy eigenvalues are in agreement with the exact ones obtained numerically.

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The study of confined quantum systems has recently received renewed attention due to a variety of related physical problems. The model of an atom or a molecule confined to a box has proved to be a useful model for simulating the effect of neighboring atoms in many physical situations. Such a model was first proposed by Michels, de Boer, and Bijl [1], who considered a hydrogen atom enclosed in a sphere of finite radius and calculated the change in polarizability and increase in kinetic energy for this system. Over the course of years this confined-atom (or -molecule) model has been used to calculate a variety of physical properties. The interested reader may refer to Fröman, Yngve, and Fröman [2], who give a list of 64 references on allied topics. The fabrication of quantum dots in semiconductor physics [3] has given an added impetus to this field [4].

In recent years, a variety of techniques have been used to study such confined atomic and molecular systems [5–13]. The main difficulty in these studies arises due to nonavailability of an accurate method of solving the corresponding Schrödinger equation under nonstandard boundary conditions on the wave functions. Accurate results are obtainable at the expense of extensive mathematical and numerical manipulations, thus hindering the physical analysis of the corresponding system. The methods employed for dealing with confined quantum systems fall broadly in the following categories. In the first, a direct numerical solution of the Schrödinger equation is sought imposing the boundary condition that the wave function becomes zero at the surface of the enclosing boundary [10]. The second type of calculations are based on perturbative approaches [7,11,12]. The method based on the variational techniques [8,9] is found to be quite effective. A semiclassical approach to these problems leads to simple analytic results. Recently Fröman, Yngve, and Fröman [2] and Yngve [5] have shown that the energy shift of a confined single-particle system can be obtained using the semiclassical quantization formula of Dennison and Uhlenbeck (DU) [14] for the symmetric double-well oscillator.

The purpose of this note is to demonstrate that the supersymmetry-inspired WKB (SWKB) method [15–17] can be an alternative approach for computing the energy levels of confined quantum systems with reasonable accuracy. During the last decade, the new SWKB quantization procedure based on supersymmetric quantum mechanics (SUSYQM) [18,19] has been found to be very useful in analyzing bound-state spectra. It is now well established that the leading-order SWKB quantization rule not only yields exact bound-state spectra for all shape-invariant potentials [16], but also frequently gives better results than the usual WKB method for the non-shape-invariant potentials [20,21]. However, the application of the SWKB method has so far been confined to studying the energy spectra of a single-particle system under standard boundary conditions on the wave functions. To the best of our knowledge, the feasibility of application of the same to confined quantum systems has not been tested earlier, and in this respect such an attempt will be interesting.

For obtaining the SWKB expression for the energy shift of the bound electron of a compressed atom, we shall follow the idea of Yngve [5]. Using the fact that due to the tunneling effect each single-well level is split into two, the DU quantization condition [14] is given by

$$\int_{x_1}^{x_2}\{2m[E_n-V(x)]\}^{1/2}dx \pm \hbar\tan^{-1}(\tfrac{1}{2}e^{-2K}) = (n+\tfrac{1}{2})\pi\hbar\ , \quad (1)$$

where $n=0,1,2,3,\ldots$ with

$$K=\frac{1}{\hbar}\int_0^{x_1}\{2m[V(x)-E_n]\}^{1/2}dx\ , \quad (2)$$

where the plus and minus signs in (1) correspond to the even-parity and odd-parity states, respectively, and x_1 and x_2 are the classical turning points, x_1 being nearer to the origin.

For a free atom, the radial wave function satisfying the Schrödinger equation

$$\frac{d^2\chi}{dr^2}+\frac{2m}{\hbar^2}[E-V_{\text{eff}}(r)]\chi(r)=0 \tag{3}$$

with

$$V_{\text{eff}}(r)=V(r)+l(l+1)\hbar^2/2mr^2 \tag{4}$$

obeys the boundary conditions

$$\chi(0)=0\ ,\quad \chi(\infty)=0\ . \tag{5}$$

When such an atom is confined in a sphere of radius a with an impenetrable wall, the second boundary condition in (5) is changed by requiring

$$\chi(a)=0\ . \tag{6}$$

To obtain an approximate solution of Eq. (3) with the modified boundary condition (6), one may consider an effective double-well potential symmetric around $r=a$ [5], because the odd-parity solution of this problem in the interval $0<r<a$ fulfills the boundary condition (6). Hence the DU quantization condition (1) with the lower sign chosen and $V(x)$ replaced by $V_{\text{eff}}(r)$ should give the energy levels $E_n(a)$ for the confined atom. In SUSYQM, the role of $V_{\text{eff}}(r)$ is played by the partner potential

$$V_-(r)=W^2(r)-\frac{\hbar}{\sqrt{2m}}W'(r)\ , \tag{7}$$

in which $W(r)$ is the superpotential. The corresponding energy eigenvalue is denoted by $E_n^{(-)}$. For unbroken supersymmetry,

$$\begin{aligned} V_-(r)&=V_{\text{eff}}(r)-E_0=V(r)+\frac{l(l+1)\hbar^2}{2mr^2}-E_0\ ,\\ E_n^{(-)}&=E_n-E_0\ , \end{aligned} \tag{8}$$

where E_0 is the ground-state ($n_r=0$) energy for the potential $V(r)$. Using (7) in (1) we expand the integrand in powers of $\hbar$. Retaining terms up to order $\hbar$ and integrating we get

$$\begin{aligned} &\frac{\sqrt{2m}}{\hbar}\int_{r_1(a)}^{r_2(a)}[E_n^{(-)}(a)-W^2]^{1/2}dr\\ &=\frac{\sqrt{2m}}{\hbar}\int_{r_1}^{r_2}[E_n^{(-)}-W^2]^{1/2}dr+\tan^{-1}\left[\frac{\{W(a)+[W^2(a)-E_n^{(-)}]^{1/2}\}}{2\sqrt{E_n^{(-)}}}\exp\left[\left(-2\sqrt{2m}\ \right)/\hbar\right]\int_{r_2}^{a}[W^2-E_n^{(-)}]^{1/2}dr\right] \end{aligned} \tag{9}$$

in which the limits of the first two integrals correspond to the roots of the equation obtained from the zeros of the respective integrands.

Equation (9) is our working formula to study the shift of the energy levels due to the finite boundary. The integrals can be evaluated in closed form for potentials for which the superpotentials are simple. For illustration, we shall now present the explicit results for the compressed hydrogen atom and for the harmonic-oscillator potential.

(a) For the effective Coulomb potential

$$V(r)=-\frac{e^2}{r}+l(l+1)\hbar^2/2mr^2 \tag{10}$$

the superpotential is

$$W(r)=\sqrt{m/2}\frac{e^2}{(l+1)\hbar}-\frac{(l+1)\hbar}{\sqrt{2m}\,r}\ . \tag{11}$$

It is clear that even for $l=0$ the term W^2 contains a residual repulsive piece which is essential for the creation of the double-well structure in this formulation. Using (11) in (9) and evaluating the standard integrals [22], we obtain finally

$$\begin{aligned} &\int_{r_1(a)}^{r_2(a)}\{2m[E_n^{(-)}(a)-W^2]\}^{1/2}dr\\ &\qquad=\pi\left[\left[\frac{me^2}{\sqrt{-2mE_n(a)}}\right]-(l+1)\hbar\right], \end{aligned} \tag{12a}$$

$$\begin{aligned} &\int_{r_1}^{r_2}[2m(E_n^{(-)}-W^2)]^{1/2}dr\\ &\qquad=\pi\left[\left[\frac{me^2}{\sqrt{-2mE_n}}\right]-(l+1)\hbar\right]. \end{aligned} \tag{12b}$$

The integral in the exponential on the right-hand side (RHS) of (9) is also evaluated. For simplification, we use the units $\hbar=m=e^2=1$ and finally obtain

$$E_n(a)=-\frac{1}{2}\Big/\left[n+\frac{1}{\pi}\tan^{-1}\left(\tfrac{1}{2}e^{-2K(a)}\right)\right]^2, \tag{13}$$

where

$$e^{-2K(a)}=F\left[\frac{a-n^2+nQ_\alpha}{a-n^2-nQ_\alpha}\right]^n e^{-2Q_\alpha} \tag{14}$$

with

$$\begin{aligned} Q_\alpha&=\left[\frac{a^2}{n^2}-2a+(l+1)^2\right]^{1/2},\\ F&=\left[\frac{1}{(l+1)}-\frac{(l+1)}{a}+\left[\frac{(l+1)^2}{a^2}-\frac{2}{a}+\frac{1}{n^2}\right]^{1/2}\right]\Big/\left[\frac{1}{(l+1)^2}-\frac{1}{n^2}\right]^{1/2},\\ n&=n_r+l+1\ . \end{aligned} \tag{15}$$

Since F becomes singular for the $n_r=0$ state, it will not be possible to compute $E_n^{(-)}(a)$ for this state. One may check easily that for the uncompressed atom (i.e., $a\rightarrow\infty$), (13) leads to the standard result $E_n=-1/2n^2$.

(b) For the harmonic oscillator in three dimensions, the effective potential and the energy eigenvalues are

$$V_{\text{eff}}(r)=\tfrac{1}{2}m\omega^2r^2+\frac{l(l+1)\hbar^2}{2mr^2}\ , \tag{16a}$$

$$E_n\equiv\hbar\omega(2n_r+l+\tfrac{3}{2})\ . \tag{16b}$$

The corresponding superpotential is

$$W(r)=\left[\frac{m}{2}\right]^{1/2}\omega r-\frac{l(l+1)\hbar}{\sqrt{2m}\,r}\ . \tag{17}$$

Using (17) in (9) and evaluating the integrals one obtains after simplification

$$E_n(a)=E_n+\frac{2}{\pi}\hbar\omega\tan^{-1}[\tfrac{1}{2}Ge^{-2K(a)}] \tag{18}$$

with

$$e^{-2K(a)}=\left[\frac{m\tilde{E}_n^2a^2-(l+1)^2\hbar^2-(l+1)\hbar Q_\alpha}{m\tilde{E}_na^2-(l+1)^2\hbar^2+(l+1)\hbar Q_\alpha}\right]^{(l+1)/2}\left[\frac{m\omega^2a^2-\tilde{E}_n+\omega Q_\alpha}{m\omega^2a^2-\tilde{E}_n-\omega Q_\alpha}\right]^{(1/2)(\tilde{E}_n/\hbar\omega)}e^{-(Q_\alpha/\hbar)}\ ,$$

$$Q_\alpha=\sqrt{m^2\omega^2a^4-2m\tilde{E}_na^2+(l+1)^2\hbar^2}\ ,$$

$$\tilde{E}_n=\hbar\omega(2n_r+l+1)\ ,$$

$$G=\left[\left[\frac{m}{2}\right]^{1/2}\omega a-\frac{(l+1)\hbar}{\sqrt{2m}\,a}+\left[\tfrac{1}{2}m\omega^2a^2+\frac{(l+1)^2\hbar^2}{2ma^2}-\tilde{E}_n\right]^{1/2}\right]\Big/\sqrt{\tilde{E}_n-\hbar\omega(l+1)}\ . \tag{19}$$

Again, the energy eigenvalues of the confined harmonic oscillator in SWKB theory cannot be evaluated for the $n_r=0$ state as G becomes singular.

We compute the energy levels for the ground state as well as for the first few excited states for different values of the size of the boundary, i.e., a for the Coulomb and harmonic-oscillator potentials. Our predicted results for these two cases are presented in Tables I and II, respectively. These results have been compared with the exact ones obtained numerically by solving the Schrödinger equation (3) using appropriate potentials. As seen from Tables I and II, all the energy levels are raised relative to the free-atom values. The extent by which a level is raised increases as a decreases. In the case of the Coulomb problem, for a given a and the principal quantum number, the energy levels split in such a way that the sublevel with the largest l has the lowest energy. It is known, of course, that the splitting of the degeneracy of

TABLE I. Exact and SWKB eigenenergies for the confined hydrogen atom for 2s, 3s, and 3p states as a function of the radius of the spherical box.

State	a	Exact	SWKB	Percent error
2s	8	−0.1695	−0.2154	27.08
	9	−0.2057	−0.2216	7.73
	10	−0.2256	−0.2299	1.91
	11	−0.2367	−0.2371	0.17
	12	−0.2428	−0.2424	−0.16
	13	−0.2462	−0.2458	−0.16
	14	−0.2480	−0.2478	−0.08
	15	−0.2490	−0.2489	−0.04
	16	−0.2495	−0.2494	−0.04
	20	−0.2500	−0.2500	0.00
3s	20	−0.0998	−0.1030	3.21
	25	−0.1092	−0.1091	−0.09
	30	−0.1109	−0.1108	−0.09
	35	−0.1111	−0.1111	0.00
	40	−0.1111	−0.1111	0.00
3p	20	−0.1032	−0.1044	1.16
	25	−0.1098	−0.1097	−0.09
	30	−0.1109	−0.1109	0.00
	35	−0.1111	−0.1111	0.00
	40	−0.1111	−0.1111	0.00

TABLE II. Exact and SWKB eigenenergies for the confined harmonic oscillator for four states as a function of the radius of the spherical box.

n_r	l	a	Exact	SWKB	Percent error
1	0	2.5	4.1842	3.8610	−7.72
		3.0	3.6642	3.6789	0.40
		3.5	3.5233	3.5276	0.12
		4.0	3.5017	3.5019	0.01
		4.5	3.5001	3.5001	0.00
		5.0	3.5000	3.5000	0.00
1	1	3.0	4.9138	4.8337	−1.63
		3.5	4.5808	4.5956	0.32
		4.0	4.5083	4.5098	0.03
		4.5	4.5004	4.5005	0.00
		5.0	4.5000	4.5000	0.00
2	0	3.5	5.7586	5.7483	−0.18
		4.0	5.5394	5.5454	0.11
		4.5	5.5029	5.5032	0.01
		5.0	5.5001	5.5001	0.00
1	2	3.0	6.3074	5.7952	−8.12
		3.5	5.7019	5.7166	0.26
		4.0	5.5287	5.5345	0.10
		4.5	5.5020	5.5023	0.01
		5.0	5.5001	5.5001	0.00

the angular-momentum sublevel is the consequence of a hard wall at $r=a$. As regards the accuracy of our predicted results, a few comments may be made. The agreement of our predicted energy eigenvalues with the exact ones is reasonable only when a is not small. When the confining wall is very close to the origin, it has been observed that very accurate results are obtainable in variational approaches [8,9]. However, in that case one does not get the flavor of the simplicity of an analytic calculation as is done here.

From the above examples we conclude that the use of the lowest-order SWKB method as proposed in this work is a useful alternative means to study confined quantum systems with impenetrable walls. A major advantage of this method over other sophisticated treatments such as the perturbative and variational techniques is its simplicity and reasonable accuracy once the superpotential is constructed according to (7). We believe that it will be worthwhile in future to apply our method to more realistic physical problems. Ballester and Dunlap [23] suggested recently an analytic functional form for a radial potential having a positive curve at the origin for describing the behavior of an atom trapped inside C_{60}. This potential function has similarity with the Morse potential for which the superpotential is known [18]. The application of our SWKB method to study radial vibrations of an atom confined within C_{60} is presently under investigation.

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