Scattering phase approach for energy spectrum in quantum dots

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Abstract

We present a semiclassical approach to evaluate quantum energy levels in asymmetrical quantum dots and wells, where analytical solutions for Schrödinger equation are not possible. In spatial regions where the potential profile is steep, the wave function is locally solved and gives rise to a momentum-dependent phase correction $\phi_s(k)$ as shown in the figure. For smooth profiles, the usual WKB approximation works. Combining scattering phases accumulated in both steep and smooth regions, we arrive at a generalized EBK quantization rule that can be solved algebraically to obtain the energy levels. We present several examples in which this semiclassical approximation works very well, even for the low-lying excitations.

Key words: Semiclassical Approximation; EBK Quantization; Quantum Dots; Quantum Wells

1. Introduction

The energy spectrum of a confined system can be obtained by solving the Schrödinger equation directly. But, if the potential profile is smooth at the length scale of the particle wavelength, the energy spectrum can be obtained by the much easier semiclassical WKB approximation.[1,2] However, in quantum dot systems, we often encounter sharp confining potential at sample edges, leading to the breakdown of the conventional semiclassical approximation. In this paper, we develop a more general semiclassical approach which holds even at the presence of sharp confining potentials. Our approach leads to the modified Einstein-Brillouin-Keller (EBK) quantization integral,[3,2]

$$\oint \sqrt{2m[E-V(x)]}dx = 2n\pi + \phi_s(E), \qquad (1)$$

where $\phi_s(E)$ is the energy-dependent scattering phase[4] due to collision with sharp confining potential at the boundaries. The WKB approximation is the special case where the scattering phase becomes an energy-independent constant $\phi_s(E) = \pi$. In the next section, we show how to evaluate the scattering phase for general confining potentials.

2. Scattering Phase due to Potential

Consider a particle moving under the influence of a smooth potential $V(x)$ and a sharp confining potential $V_c(x)$ on the left-hand side,

$$V_c(x) = \Theta(-x)[V_0 + V_1|x|], \qquad (2)$$

where $V_0 = k_0^2/2m$ is the potential height and $V_1 = k_1^3/2m$ is the slope. The scattering due to $V_c(x)$ can be solved exactly and the eigenstates are

$$|\psi\rangle = |k\rangle + e^{-i\phi_s(k)}|-k\rangle. \qquad (3)$$

The scattering phase $\phi_s(k)$ is apparently energy-dependent as shown in Figure 1. For the hard-wall potential ($k/k_0 = k/k_1 = 0$), the scattering phase is π, while for smooth potential ($k/k_0 \ll 1, k/k_1 \gg 1$)the phase becomes $\pi/2$ as in the WKB approximation.

The confining potential can be viewed as depletion of Hilbert space and the completeness of the eigenstates in Eq. 3 implies that

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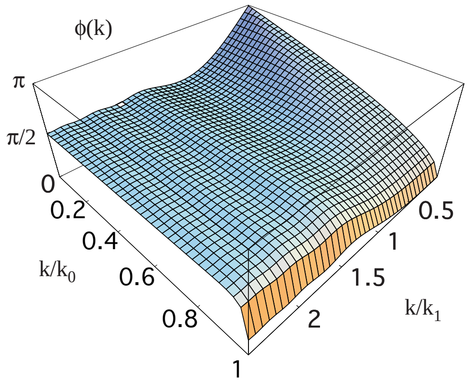

Fig. 1. Scattering phase for different potential height $V_0 = k_0^2/2m$ and slop $V_1 = k_1^3/2m$.

$$\sum_{\phi=0,\phi_s(k)} \int \frac{dk}{2\pi} e^{i\phi} |k\rangle\langle e^{i\phi} k| = \mathbf{1}. \tag{4}$$

Following the standard derivation of the path-integral formalism, the modified completeness identity in Eq. 4 changes the single-particle Green's function. In the semiclassical limit, it is described by the modified Van Vleck's formula[5,6]

$$G(r, r'; t) \simeq \frac{1}{\sqrt{2\pi i}} \sum_t \sqrt{C_t} \exp[iA_t - i\phi_t], \tag{5}$$

where the summation is over all possible classical trajectories with end points $r(t) = r$ and $r(0) = r'$. The action along the trajectory is A_t with quadratic fluctuations C_t. The scattering phase $\phi_t = 0$ if the classical trajectory is not reflected by $V_c(x)$ while $\phi_t = \pi_s(k)$ if the trajectory is reflected.

The most powerful use of Van Vleck's formula is that it leads to the EBK quantization rule in the semiclassical limit. By setting $r = r'$ in the Green's function and integrating over all possible r, we obtain the quantum partition function $Z(t) = \sum_n \exp[-iE_n t]$. The energy levels are then identified as singularities of $Z(\omega)$ in the frequency space. Within the stationary phase approximation, it can be shown[3] that the total Berry phase, $\oint pdq - \phi_s$, is quantized in units of 2π that leads to the modified quantization rule in Eq. 1. It is interesting that the sharp confining potential $V_c(x)$only gives rise to an energy-dependent scattering phase and the semiclassical approximation still works as long as the potential $V(x)$ between turning points is smooth.

3. Simple Applications

We apply the modified EBK quantization rule to a finite potential well of length L and with height $V_0 = k_0^2/2m$. After some algebra, the scattering phase is shown to be $\phi(k) = 2\cos^{-1}[(k/k_0)^2 - 1]$. The quantized energy $E_n = k_n^2/2m$ satisfies

$$2k_n L = 2n\pi + \phi(k_n). \tag{6}$$

Quite surprisingly, the spectrum obtained by the semiclassical approach is identical to the exact solution.

Another example is the three-dimensional hemispherical quantum dot. After separation of variable, the system can be described by an effective one-dimensional potential $V(r) = l(l+1)/2mr^2$ for $r < a$ and $V(r) = \infty$ for $r > a$. The scattering phase approach gives the approximate spectrum

$$E_{n,l} = \frac{\pi^2}{2ma^2} \left(n + \frac{l'}{2} + \frac{3}{4} \right)^2, \tag{7}$$

where $l' = \sqrt{l(l+1)}$. This result is in excellent agreement with the exact solution $j_l(\sqrt{2mE_n}a) = 0$ and becomes identical in the large n limit as expected.

The semiclassical approach developed here can be readily applied to higher dimensions or more complicated systems such as Andreev reflection in superconducting junctions. The excellent agreement with the exact solutions in previous examples shows that the sharp confining potential does not kill the semiclassical approach, but only gives rise to a nontrivial scattering phase correction.

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