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COMMENT

Comment on 'Semiclassical approximation of the radial equation with two-dimensional potentials'

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Abstract. It is shown that a subtle variation of the Zwaan–Stueckelberg technique, based on semi-classical JWKB phase integrals and their analytic continuation in the complex plane yields the result of Berry and Ozorio de Almeida, concerning the semi-classical phase-shift and energy eigenvalue appropriate to the radial equation for two-dimensional potentials in the case of s waves.

1. Introduction

Recently, Berry and Ozorio de Almeida (1973, to be referred to as I) have considered the delicate situation concerning the semi-classical JWKB approximation for the radial equation in the case of two-dimensional potentials. Basically they found that for s waves, Jeffreys' connexion formula could not be applied since the classical turning point coincided with the origin. This difficulty was resolved using a comparison-equation method based on the zero-order Bessel function. They found that the s wave phase-shift and bound-state energy eigenvalues were simply analytic continuations of the general non-zero l wave formulae.

We simply wish in this comment to derive their results using the more fundamental and direct Zwaan–Stueckelberg phase-integral technique of Crothers (1971, to be referred to as II).

2. Derivation

Firstly, we greatly simplify their approach in I, § 2 concerning the free particle and the associated inner boundary condition in the case of s waves. Using their notation,

$$\nabla^2 \ln R = 0 \qquad (R \neq 0). \tag{1}$$

On the other hand, applying the theorem of Gauss to a cylinder of unit length, we obtain in cylindrical coordinates

$$\int \nabla^2 \ln R \, d\tau = \int \operatorname{grad}(\ln R) \, . \, d\boldsymbol{S} = \int \frac{1}{R} \boldsymbol{R} \, . \, d\boldsymbol{S} = \int_0^{2\pi} d\theta = 2\pi \tag{2}$$

where $d\tau$ is a volume element, $d\boldsymbol{S}$ is a curved surface element directed outwards and the contributions from the cylinder end sections cancel out. It follows that

$$\nabla^2 \ln R = 2\pi\delta(\boldsymbol{R}) \tag{3}$$

where $\delta(\boldsymbol{R})$ is the delta function. Equation (3) means therefore that $\ln R$ is not a solution of the Schrödinger equation I(1) at $R=0$. Therefore, given that Y_0 and K_0 behave logarithmically at the origin, $\psi_0(R)$ of I(5) is only a solution of I(1) if $B=0$ and $D=0$, a conclusion reached in I by somewhat different reasoning. However, our reasoning is more direct and points to a method for fitting the inner boundary condition at the origin. Quite simply, $\ln R$ is not an analytic function and therefore we can apply the Zwann–Stueckelberg technique, which has two advantages. Firstly, we do not extrapolate the semi-classical phase integrals to the origin, where they become invalid, but merely trace their analytic, valid behaviour along a curve in the complex R plane, which circumvents the origin. Secondly, we force analyticity, which therefore automatically excludes the $\ln R$ type solutions and so automatically satisfies the inner boundary condition.

We wish to solve semi-classically the equation

$$\left(\frac{1}{R}\frac{d}{dR}R\frac{d}{dR}+E-V(R)\right)\chi=0. \tag{4}$$

Restricting ourselves to scattering, that is, $E>0$, the semi-classical JWKB solution is given by

$$\chi\approx\frac{\{A\exp[i\int_0^R(E-V(R))^{1/2}\,dR]+B\exp[-i\int_0^R(E-V(R))^{1/2}\,dR]\}}{R^{1/2}(E-V(R))^{1/4}} \tag{5}$$

where A and B are arbitrary constants. However, for R sufficiently large, we can ignore $V(R)$ so that

$$\chi\sim\frac{(A\,e^{iRE^{1/2}}+B\,e^{-iRE^{1/2}})}{R^{1/2}E^{1/4}}. \tag{6}$$

Then $R=0$ is a transition point and the Stokes lines emitting from it are given by $\arg R=\pm\pi/2$. Assuming the principal branch of $R^{1/2}$ and tracing χ in the positive sense, along a semi-circle of large radius in the complex plane, yields, on the negative R axis:

$$\chi\sim-i|R|^{-1/2}[(A+\alpha B)\,e^{iRE^{1/2}}+B\,e^{-iRE^{1/2}}] \tag{7}$$

where α is the Stokes constant associated with the $\pi/2$ line. But χ is required to be an even analytic function. Therefore it follows that

$$-i(A+\alpha B)=B \tag{8}$$

$$-iB=A \tag{9}$$

so that the Stokes constant is 2i. Substitution in (5) with $c=A\exp(i\pi/4)$ yields

$$\psi_0=\chi R^{1/2}\approx c\frac{\sin[\int_0^R(E-V(R))^{1/2}\,dR+\frac{1}{4}\pi]}{(E-V(R))^{1/4}} \tag{10}$$

which agrees with I(41). Similar considerations apply to the case of $E<0$.

In retrospect, we may question the validity of expression (5) as the JWKB solution of equation (4). Why not apply the JWKB approximation to ψ_0, as against χ? This would, after all, merely have the effect of subtracting $1/4R^2$ from the potential $V(R)$ in the zero- and first-order action integrals inherent in the JWKB approximation. In truth, this would not do, for the purely pragmatic reason that the pole at $R=0$ would then cause the zero-order-action integral $\int_0^R [E-V(R)+(1/4R^2)]^{1/2}\,dR$ to be improperly defined. However, there is an associated but more fundamental reason. Analyticity could not be forced and therefore such an approximate solution would not be acceptable. This is most clearly seen by noting that

$$\oint^{(0+)}\left(E+\frac{1}{4R^2}\right)^{1/2} dR=\pi i \tag{11}$$

no matter how distant the closed contour is from the origin. To see this, we may take the branch-cut to join $\pm i/2E^{1/2}$, and we may use Cauchy principal values or map R to $1/\mu$ and apply Cauchy's residue theorem. In short, analyticity breaks down because the pole at $R=0$ manifests itself in the form of $e^{\pm\pi}$ factors, following a positive circuit of the pole. It may be observed that we have neglected $V(R)$ in these latter arguments. However, normally we require $\lim_{R\to 0} RV(R)$ to exist. This means that the effect of any singularity of $V(R)$, such as the weak singularity of the $a\ln R$ potential of I, is sufficiently localized† that our analyticity arguments and our basic statement, contained in the sentence embracing equation (6), remain true; we should, of course, bear in mind that the behaviour of a logarithmic potential, as $R\to\infty$, is non-physical, in that we require $\lim_{R\to\infty} RV(R)$ to exist.

In conclusion, we have derived the result of I by adopting the more general Zwaan–Stueckelberg phase integral technique rather than a specific comparison-equation method. The technique is essentially a reiteration of that used in II to derive the asymptotic behaviour of $P_l(\cos\theta)$.

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References

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† Taking principal values,

$$\exp\left(\pm i\oint_{|R|=1}^{(0+)} (E-a\ln R)^{1/2}\,dR\right)\sim\exp(\mp\pi a/E^{1/2})$$

which are semiclassically negligible.