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WKB Approximation in Three Dimensions

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An extension to three dimensions of the WKB approximation method for the quasiclassical wave function is discussed. The extended method is applicable to problems which possess an axis of symmetry, but for which the potential need not be a separable function of the coordinates. The essential difference from the one-dimensional WKB approximation lies in the effect of the curvature of the wave fronts, which plays a central role in the three-dimensional case, and which has a direct physical interpretation. Formulas are derived for the wave function on the axis in both the allowed and the forbidden zones, as well as for the three-dimensional connection formulas. Application of the new method is made to the case of a pure Coulomb wave function and to the case of a particular nonseparable potential which is of interest in the theory of nuclear reaction rates at high density.

I. INTRODUCTION

IF the characteristic dimensions of a quantum-mechanical system are large compared with typical de Broglie wavelengths, the wave function of the system can be obtained through a semiclassical approximation scheme. For one-dimensional problems such a scheme is the well-known WKB method, which provides simple approximations for the wave function in both the classically forbidden and allowed regions, as well as connection formulas relating the behavior of the approximate wave functions on opposite sides of the turning point. Some general considerations have also been given in the multidimensional case,[1,2] but these are not always directly applicable to practical problems.

In this paper we discuss an explicit semiclassical approximation for the wave function of a single particle moving in a nonseparable potential in three dimensions. We assume that the potential field possesses an axis of symmetry, and we shall consider the wave function only on or near this axis. The relation of our approximation to the work of Van Vleck and of Schiller in the multi-dimensional case is discussed in Appendix A.

In Sec. II we derive our approximation scheme for the general three-dimensional case. The lowest-order equation of the resulting hierarchy is simply the eikonal equation of geometrical optics. The behavior of the wave function can therefore be interpreted in terms of wave fronts and ray paths (or particle trajectories), and for this reason we freely borrow the nomenclature of geometrical optics throughout. In Sec. III we derive the equation for the curvature coefficient of the wave fronts, and we show that an explicit solution requiring at most the evaluation of one-dimensional integrals is then possible. The three-dimensional connection formulas which permit the continuation of the wave function across the turning surface are derived in Sec. IV, and in Sec. V we discuss the case of scattering in a pure Coulomb potential as an illustration of the method.

A practical problem requiring the application of our approximation scheme occurs in the evaluation of "pycnonuclear" reaction rates.[3,4] Under conditions which may prevail in the degenerate cores of highly condensed stars, the electrostatic interaction potential is no longer a separable function of the coordinates, and the wave function therefore cannot be calculated by conventional methods. Accordingly in Sec. VI we reduce the problem (approximately) to one involving only the three-dimensional relative coordinate of a pair of neighboring nuclei and then apply the work of Secs. II through IV to calculate the "tail" of the ground-state wave function, where the nuclei come very close together.

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[1] J. H. Van Vleck, Proc. Natl. Acad. Sci. U.S. 14, 178 (1928).
[2] R. Schiller, Phys. Rev. 125, 1109 (1962).
[3] A. G. W. Cameron, Astrophys. J. 130, 916 (1959).
[4] R. A. Wolf, Phys. Rev. 137, B1634 (1965).

II. DERIVATION OF THE THREE-DIMENSIONAL WKB APPROXIMATION

The Schrödinger equation for the wave function ψ of a particle with energy E moving in a potential $V(\mathbf{r})$ may be written as

$$\nabla^2\psi(\mathbf{r})+k^2(\mathbf{r})\psi(\mathbf{r})=0, \quad (1)$$

where

$$k^2(\mathbf{r})=(2\mu/\hbar^2)[E-V(\mathbf{r})], \quad (2)$$

and μ is the reduced mass. In terms of the logarithm S of the wave function,

$$\psi(\mathbf{r})=\exp[iS(\mathbf{r})], \quad (3)$$

we have

$$i\nabla^2S-\nabla S\cdot\nabla S+k^2=0. \quad (4)$$

In the quasiclassical limit the change in the wavelength is small over an interval of a single wavelength, and the first term in Eq. (4) is therefore negligible in comparison with the second. The function S can then be determined by an iteration scheme:

$$S=S_0+S_1+\cdots,$$

where S_0 is the solution of the "eikonal" equation,

$$\nabla S_0\cdot\nabla S_0=k^2(\mathbf{r}), \quad (5)$$

S_1 is the solution of

$$2\nabla S_1\cdot\nabla S_0=i\nabla^2S_0, \quad (6)$$

and so on. These equations contain the essential features of the quasiclassical approximation. As is usual in the one-dimensional case, we shall carry only the first two terms of the perturbation series (S_0+S_1).

It is convenient to rewrite Eq. (5) in the form

$$\nabla S_0=k(\mathbf{r})\mathbf{e}, \quad \mathbf{e}\cdot\mathbf{e}=1, \quad (7)$$

where k is the positive square root of Eq. (2). In general S_0 and $\mathbf{e}$ may be complex, and Eq. (7) does not necessarily make $\mathbf{e}$ a vector of unit absolute magnitude. By analogy with geometrical optics we refer to the (complex) surfaces $S_0=$constant as "wave fronts," the unit normals $\mathbf{e}$ to these surfaces as "ray vectors" or "propagation vectors," and a curve whose tangents are the vectors $\mathbf{e}$ as a "ray path" of the system. These curves and surfaces are defined in a complex, six-dimensional space, but we shall of course derive expressions for S in real space.

From Eq. (7) one can derive the relation

$$(\mathbf{e}\cdot\nabla)\mathbf{e}=k^{-1}[\nabla k-(\mathbf{e}\cdot\nabla k)\mathbf{e}]. \quad (8)$$

We shall only consider cases in which some field line of the potential is a straight line, and one ray path (with $\mathbf{e}$ real) coincides with this line, which is one solution of Eq. (8). We shall see that the wave function in the vicinity of this line is given simply in terms of properties *along* the line, including curvature coefficients. We shall use this line as the z axis of a polar-coordinate system.

Equation (6) can be rewritten as

$$\nabla S_1\cdot\mathbf{e}=\tfrac{1}{2}i[k^{-1}\mathbf{e}\cdot\nabla k+\text{div }\mathbf{e}],$$

and this expression as well as Eq. (5) can be easily integrated. There are two solutions, depending upon the sign of $\mathbf{e}$ along the axis, which we shall call the "incoming" and the "outgoing" wave. Correct to first order in our expansion, we have

$$i[S^{\pm}(z_2)-S^{\pm}(z_1)]$$

$$=\pm i\int_{z_1}^{z_2} k\,dz-\tfrac{1}{2}\ln\frac{k(z_2)}{k(z_1)}\mp\int_{z_1}^{z_2}H^{\pm}dz, \quad (9)$$

where $H(\mathbf{r})=\tfrac{1}{2}\text{div }\mathbf{e}$, and the upper sign denotes the incoming wave.

If S_0 is real, the function H is the coefficient of mean curvature of the wave front,[5] and we shall call it the "curvature coefficient" even when it is complex. In Sec. III we shall derive an expression for $H(z)$ (in terms of a boundary value) and shall see that H^- is *not* necessarily $-H^+$: Although $\mathbf{e}^-=-\mathbf{e}^+$, the ingoing and outgoing rays off the axis traverse different regions, and the curvatures are different.

Equation (9) constitutes our desired generalization of the WKB approximation. It provides a unique value for the quasiclassical wave function at any point along the ray path in terms of the boundary conditions on S and ∇S (or equivalently, S and H) at the initial point z_1. The difference between Eq. (9) and the one-dimensional case is essentially contained in the last term involving H. In fact, if the surfaces of constant S_0 happen to coincide with the planes $z=$constant, then H vanishes, and Eq. (9) reduces exactly to the one-dimensional approximation. The significance of this term is also clear in the three-dimensional case. If H is real in the allowed region, then $H\,dz$ is the fractional increase in the width of the wave front, which must be accompanied by an equal fractional decrease in the amplitude.

III. THE CURVATURE COEFFICIENT

From the eikonal equation and the definition of the ray vector $\mathbf{e}$ as given in Eq. (7), together with the fact that on the axis both ∇k and ∇S_0 have only a z component, it is not difficult to show that the quasiclassical wave function near the axis must possess cylindrical symmetry.[6] For this reason we shall find it convenient to work in a system of cylindrical polar coordinates (ρ,ϕ,z) with the z axis parallel to the line of symmetry. Because of the local symmetry, the curvature coefficient at the axis assumes the simple form

$$H^{\pm}(z)=\frac{\partial(e^{\pm}{}_\rho)}{\partial\rho}\bigg|_{\rho=0}=k^{-1}\frac{\partial^2 S_0{}^{\pm}}{\partial\rho^2}\bigg|_{\rho=0}, \quad (10)$$

[5] M. Kline, Commun. Pure Appl. Math. **14**, 473 (1961).

[6] It must be emphasized, however, that the wave function is only locally axially symmetric, and that this has nothing whatever to do with the long-range symmetry at points far from the axis.

where e_ρ is the component of **e** in the ρ direction. Since H is explicitly the (nonvanishing) derivative of a function which goes to zero at the axis, this equation shows that H^+ can be quite different from H^- even though the vectors $\mathbf{e}^\pm$ on the symmetry line are identical except for sign. Equation (10) also demonstrates the dependence of the quasiclassical wave function along the symmetry axis upon the potential at neighboring points of space: For points slightly off the axis the wave function is given by

$$S(z,\rho) \approx S(z,0) + \frac{1}{2!} kH\rho^2. \tag{11}$$

The function H satisfies a first-order differential equation which can be derived from the definition (7) of the ray vector. Since the curl of a gradient is identically zero, the curl of Eq. (7) provides an equation involving only the propagation vector **e** and the magnitude k of the reciprocal wavelength. If we now take the curl of the resulting equation and make use of the local symmetry and of the relation (10) between the curvature coefficient and the transverse derivative of the ray vector, we obtain

$$\pm \frac{dH^\pm}{dz} \pm \frac{d\ln k}{dz} H^\pm + (H^\pm)^2 = \frac{\partial^2 \ln k}{\partial \rho^2}\bigg|_{\rho=0}, \tag{12}$$

which is the desired result. Equation (12) is a Ricatti equation, which is a well-studied type of nonlinear differential equation that can even be solved analytically[7] for sufficiently simple functional forms for $k(z)$. The solution of the equation involves one arbitrary constant of integration, which is determined by the boundary conditions.

In the field-free case, where k is everywhere a constant, all ray paths are straight lines. Then H is purely real, and the general solution of Eq. (12) is simply

$$H^\pm(z) = \pm (z - Z^\pm), \tag{13}$$

where we have taken the vector $\mathbf{e}^+$ to lie in the direction of increasing z. The parameter $Z^\pm$ represents a focal point of the ray system, as is evident from the form of the wave function on and near the axis:

$$\psi^\pm(z,\rho) \approx \text{const.} \times \frac{\exp(\pm ikr^\pm)}{r^\pm},$$
$$r^\pm \equiv [\rho^2 + (z - Z^\pm)^2]^{1/2}, \tag{14}$$

where we have used Eqs. (9), (11), and (13). In Eq. (14), $r^\pm$ is the radial distance from the focal point (wave diverging from Z^- or converging onto Z^+).

If we consider a spherically symmetric potential, the radius of a surface of constant k is simply r, the radial distance from the force center. In this case, if the

[7] H. T. Davis, *Introduction to Nonlinear Differential and Integral Equations* (Dover Publications, Inc., New York, 1962), pp. 57–76.

boundary condition on S_0 is such that $H = r^{-1}$ at one point, then the solution of Eq. (12) is $H = r^{-1}$ for all **r**. The last term in Eq. (9) then gives $-\ln(r_2/r_1)$, which means that the function $r\psi$ satisfies a one-dimensional Schrödinger equation.

IV. THE CONNECTION FORMULAS

As is well known, the WKB approximation breaks down near the "turning points," where $k^2 = 0$, and one must make recourse to special "connection formulas" in order to relate the approximate wave functions in the classically allowed and the classically forbidden regions. In three dimensions the allowed and forbidden regions are separated by a "turning surface," defined by the equation $k^2(\mathbf{r}) = 0$. If a ray in the allowed region approaches this surface at some angle other than normal, that component of the real part of the ray vector which is directed perpendicular to the equipotential surfaces will vanish, and the ray will be turned back before reaching the turning surface. Thus the only ray paths which traverse the turning surface do so at normal incidence (in the strict, classical limit), and we shall discuss the connection formulas only for such a ray and its immediate neighborhood.

In the vicinity of the turning surface the potential can be expanded in a Taylor series:

$$V(\mathbf{r}) = E + \nabla V \cdot (\mathbf{r} - \mathbf{r}_0) + \cdots, \tag{15}$$

where $\mathbf{r}_0$ is some point on the surface, and ∇V is evaluated at $\mathbf{r}_0$. If we restrict ourselves to a "linear connection," i.e., if we assume $\nabla V \neq 0$ and neglect higher terms, then the approximate potential given by the first two terms of Eq. (15) has axial symmetry, and it is convenient to work in a system of cylindrical coordinates with the z axis as the axis of symmetry and with origin at the turning point. We shall assume $\partial V/\partial z > 0$, so that the region with $z > 0$ is the forbidden region. The incoming wave in a typical scattering problem thus propagates in the direction of increasing z.

Let us first consider the WKB approximation near the turning point. From Eq. (15) we have

$$k = (-z)^{1/2}, \tag{16}$$

where k and z are expressed in units of γ and γ^{-1}, respectively, and $\gamma = [(\partial V/\partial z)2\mu/\hbar^2]^{1/3}$. With this simple form for k, Eq. (12) can be solved analytically by standard methods[7] to give

$$H^\pm = \frac{\frac{1}{2}C^\pm(\pm z)^{-1/2}}{1 + C^\pm(\pm z)^{1/2}}, \tag{17}$$

where $C^\pm$ is a constant of integration. The integrals required by Eq. (9) can now be done analytically also, and the resulting wave functions are, in the allowed region ($z < 0$),

$$iS^\pm(z) = \mp i\frac{2}{3}(-z)^{3/2} - \frac{1}{4}\ln(-z) - \ln[1 + C_a^\pm(\pm z)^{1/2}], \tag{18a}$$

and in the forbidden region $(z>0)$,

$$iS^{\pm}(z) = \mp\tfrac{2}{3}z^{3/2}-\tfrac{1}{4}\ln z-\ln[1+C_f^{\pm}(\pm z)^{1/2}], \quad (18b)$$

where C_a and C_f are the values of the constant in Eq. (17) appropriate to the allowed and forbidden regions, respectively.

In order to relate a given linear combination of incoming and outgoing waves of the form (18a) in the allowed region to the appropriate corresponding linear combination of waves (18b) in the forbidden region we must consider the connection formulas for our three-dimensional approximation. These formulas can be derived most simply by an extension of the method using analytic continuation developed by Furry[8] in the one-dimensional case. This is outlined in Appendix B and gives the following result:

$$\tfrac{1}{2}|k|^{-1/2}\left\{\exp\left[+i\int_{-|z|}^{0}|k|\,dz+i\eta-i\frac{\pi}{4}-\int_{-|z|}^{0}H^-dz\right]\right.$$

$$\left.+\exp\left[-i\int_{-|z|}^{0}|k|\,dz-i\eta+i\frac{\pi}{4}+\int_{-|z|}^{0}H^+dz\right]\right\}$$

$$\rightleftharpoons |k|^{-1/2}\left\{\sin\eta\,\exp\left[+\int_{0}^{|z|}|k|\,dz+\int_{0}^{|z|}H^-dz\right]\right.$$

$$\left.+\tfrac{1}{2}e^{-i\eta}\exp\left[-\int_{0}^{|z|}|k|\,dz-\int_{0}^{|z|}H^+dz\right]\right\}. \quad (19)$$

This is the direct analog of the familiar one-dimensional formula, and, as there, the lower arrow is to be used only in the event $\eta=0$, corresponding to a purely ingoing (decaying) "wave" in the forbidden region. Because of the difference in curvature of the ingoing and outgoing waves, the left-hand side of this equation no longer has the form of a simple trigonometric function, but now involves both waves explicitly.

In the three-dimensional case, Eq. (19) by itself is not sufficient to determine the connection of the wave function across the turning point, as one must also have an additional connection formula for the curvature coefficient. This is also discussed in Appendix B and may be stated in the form

$$H^{\pm}\xrightarrow[|z|\to 0]{}\frac{\tfrac{1}{2}iCz^{-1/2}}{1\pm iCz^{1/2}}, \quad (20)$$

where C has the same value in both the allowed and the forbidden regions, and is to be determined from the boundary conditions.

In the allowed region, the wave fronts are real surfaces in three-space, and thus the curvature coefficient and the constant C in Eq. (20) must both be real. In the forbidden region, however, this condition leads to a complex curvature coefficient, which simply reflects the

fact that the surfaces $S_0=$constant are now defined in a complex space of six dimensions.[9] The physical reason for the complex curvature coefficient can be understood by considering an arbitrary, oscillatory wave impinging upon the turning surface. This wave can be resolved into two components, propagating, respectively, perpendicular and parallel to the turning surface. Clearly the perpendicular component will be strongly damped as it propagates into the forbidden region, and this is reflected in the exponential variation of the zero-order WKB approximation. On the other hand, the transverse part of the wave is affected quite differently. Near the turning surface, this component is essentially unchanged from the allowed region, so that the variation of the wave function in the ρ direction is mainly oscillatory, which shows up in the fact that H is almost purely imaginary near the turning surface. Deep in the forbidden region, however, H is almost purely real, with the sign such that the wave function decreases away from the axis along the ρ direction. This is associated with the fact that the surface of constant amplitude which passes through point (ρ,ϕ,z) intersects the symmetry axis at a distance δz farther into the forbidden zone than the surface which intersects the axis at z, and hence the former surface is one of smaller amplitude.

V. COULOMB SCATTERING

As an illustrative example we consider scattering in a pure repulsive Coulomb potential.[10] We shall express lengths and inverse wave numbers k^{-1} in units of the "Bohr radius" r^* defined as

$$r^*=\hbar^2/\mu Z_1 Z_2 e^2, \quad (21)$$

where μ is the reduced mass, and Z_1, Z_2 are the atomic charges of the two particles. The reduced wave vector for the relative motion is given by

$$k^{-1}\equiv n=Z_1 Z_2 e^2/\hbar v, \quad (22)$$

where v is the relative velocity. Throughout this section we shall consider only large values of n, corresponding to "low"-energy scattering.

An exact, normalized wave function for two particles approaching each other from minus infinity is given by[11]

$$v^{1/2}\psi(z,r)\equiv e^{iS^+}=\Gamma(1+in)e^{-n\pi/2}e^{ikz}F(-in,\,1,\,ik(r-z)),$$
$$(23)$$

where F is a confluent hypergeometric function, and r is the radial distance from the force center. This wave function already includes both the incident and the

[8] W. H. Furry, Phys. Rev. **71**, 360 (1947).

[9] A similar situation occurs in the theory of inhomogeneous wave propagation in the optics of metals, as discussed by M. Born and E. Wolf, *Principles of Optics* (The Macmillan Company, New York, 1964), Chap. XIII.

[10] See also M. Rosen and D. R. Yennie, J. Math. Phys. **5**, 1505 (1964).

[11] L. I. Schiff, *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1955), p. 184.

scattered wave, although in the asymptotic limit of $z \to -\infty$ only the incident wave is present. For negative values of z with $|kz|$ large compared with both unity and n^2, the asymptotic expansion[12] of the Coulomb wave function gives

$$iS^+ \sim i[kz + n \ln k(r-z)], \quad H^+ \sim \tfrac{1}{2} n^2/|z|^2, \quad (24)$$

where H^+ is expressed in units of $(r^*)^{-1}$. In this region the wave function contains only the incident Coulomb-distorted plane wave. As Eq. (24) (or a classical calculation) shows, the curvature introduced by the long-range Coulomb force on an incident plane wave is only of order $|kz|^{-2}$, and not $|z|^{-1}$, as $z \to -\infty$.

For negative values of z but with $1 \ll |z| \ll n$ (i.e., in the classically forbidden region) one can reduce F to an expansion[13] involving the Bessel function $I_\nu(x)$ of purely imaginary argument:

$$F \approx I_0[(4(r-z))^{1/2}] + \cdots . \quad (25)$$

With the help of Stirling's formula for $\ln\Gamma(1+in)$ and the asymptotic expansion for the Bessel function, we find

$$iS^+ \approx [4(r-z)]^{1/2} - \tfrac{1}{4}\ln[4(r-z)] - n\pi$$
$$+ \tfrac{1}{2}\ln n + i(n \ln n - n) + i\tfrac{1}{4}\pi,$$
$$H^+ \approx -\tfrac{1}{2}|z|^{-1}. \quad (26)$$

For a pure Coulomb potential, only the pure ingoing wave is present in the forbidden region.

We now turn to our WKB approximation. In our units and with $\rho \ll |z|$ we have

$$k^2(\mathbf{r}) = \frac{1}{n^2} - \frac{2}{r} \approx \frac{1}{n^2} - \frac{2}{|z|} + \frac{\rho^2}{|z|^3}. \quad (27)$$

The turning point on the negative z axis thus occurs at $z = -2n^2$. Equation (12) for the curvature coefficient H in this case has the general solution

$$H^\pm = \pm \frac{1}{z}\left\{ 2 + \left[|z|\left(\frac{1}{n^2} - \frac{2}{|z|}\right) \right.\right.$$
$$\left.\left. + C^\pm |z|\left(\frac{1}{n^2} - \frac{2}{|z|}\right)^{1/2} \right]^{-1} \right\}, \quad (28)$$

where the constant $C^\pm$ is the constant of integration appropriate to the incoming or outgoing wave, respectively. In order to represent the incident, Coulomb-distorted plane wave, we need $C^+ = -1/n$, by comparison of Eq. (24) with the asymptotic limit of Eq. (28).

In the allowed region, the WKB wave functions thus

[12] Reference 11, p. 116.
[13] F. L. Yost, J. A. Wheeler, and G. Breit, Phys. Rev. **49**, 174 (1936).

become, for $\rho \ll |z|$,

$$iS^\pm(z,\rho) = \mp i2n\left\{ \left(\frac{|z|}{2n^2}\right)^{1/2}\left(\frac{|z|}{2n^2} - 1\right)^{1/2} \right.$$
$$\left. - \ln\left[\left(\frac{|z|}{2n^2}\right)^{1/2} + \left(\frac{|z|}{2n^2} - 1\right)^{1/2} \right] \right\}$$
$$- \tfrac{1}{4}\ln\left(\frac{1}{n^2} - \frac{2}{|z|}\right) - \ln\frac{|z|}{2n^2}$$
$$- \ln\left[1 + \left(\frac{1}{n^2} - \frac{2}{|z|}\right)^{1/2} \Big/ C^\pm \right]$$
$$+ \tfrac{1}{2}ik(z)H^\pm(z)\rho^2 + \ln N(n), \quad (29)$$

where $N(n)$ is a normalizing constant. We set

$$N(n) = \tfrac{1}{2}n^{-1/2}e^{i(n\ln n - n)} \quad (30)$$

and with this choice the asymptotic limit of Eq. (29) for $-z \gg 2n^2$ reduces to Eq. (24).

Near the turning point, the curvature coefficient (28) assumes the form

$$H^\pm \approx \frac{\mp\tfrac{1}{2}i[1/(2n^2)^{1/2}nC^\pm](2n^2 - |z|)^{-1/2}}{1 + i[(1 - 2(nC^\pm)^2)/(2n^2)^{1/2}nC^\pm](2n^2 - |z|)^{1/2}}. \quad (31)$$

This expression, together with the connection formula (20) and the fact that $C^+ = -1/n$, leads immediately to the result $C^- = +1/n$. These constants are the same in both the allowed and the forbidden regions, for the reasons discussed in the preceding section. With this result, the connection formula (19) leads to the prediction of a reflected wave in addition to the incoming wave in the allowed region. For a pure Coulomb potential we need only the function which is regular at the origin, i.e., we take $\eta = 0$ in Eq. (19). With $N(n)$ given by Eq. (30), the reflected wave in the allowed region has the asymptotic form (for $z \ll -2n^2$ and $n \gg 1$)

$$iS^-(z,\rho) \sim +i[k|z| - n \ln 2k|z|] + \ln\frac{n}{2k|z|}$$
$$+ 2i(n \ln n - n) - i\frac{\pi}{2} + i\frac{\rho^2}{2n|z|}, \quad (32)$$

which agrees with the asymptotic form of the exact wave function.[12]

Finally, in the forbidden region, the WKB exponents are

$$iS^\pm(z,\rho)$$
$$= \pm 2n\left[\left(\frac{|z|}{2n^2}\right)^{1/2}\left(1 - \frac{|z|}{2n^2}\right)^{1/2} + \sin^{-1}\left(\frac{|z|}{2n^2}\right)^{1/2} - \frac{\pi}{2} \right]$$
$$- \tfrac{1}{4}\ln\left(\frac{2}{|z|} - \frac{1}{n^2}\right) - \ln\frac{|z|}{2n^2} - \ln\left[1 \mp \left(1 - \frac{2n^2}{|z|}\right)^{1/2} \right]$$
$$+ \tfrac{1}{2}ik(z)H^\pm(z)\rho^2 + i(n \ln n - n) - \tfrac{1}{2}\ln(4n) - i\tfrac{1}{4}\pi, \quad (33)$$

For $1\ll|z|\ll n$, S^+ reduces to the expression in Eq. (26).

VI. PYCNONUCLEAR REACTIONS

In very late stages of stellar evolution high densities can be reached at relatively low temperatures. Under these circumstances the electrons form a degenerate Fermi gas at almost uniform density, while the nuclei form a "Coulomb lattice," i.e., a body-centered cubic lattice with the two-body potential being simply the Coulomb potential. We define

$$r^* = \hbar^2/M(Ze)^2 = 28.8A^{-1}Z^{-2} \text{ F}, \quad \lambda \equiv r^*/a \quad (34)$$

where r^* is the "Bohr radius" for a pair of nuclei, and a is the lattice constant. For sufficiently small λ and sufficiently low temperature the amplitude of vibration about the lattice sites is small. The rate of nuclear reactions is then small but not zero, since the zero-point vibrations prevent the nuclei from becoming too strongly localized about the lattice sites, and there is still a small probability of two nearest-neighbor nuclei coming close together. To a fairly good approximation one can reduce this many-body problem to a three-dimensional Schrödinger equation for the relative vector coordinate $\mathbf{r}$ between the two nuclei, while keeping the center of mass of the pair as well as all the other nuclei fixed at their respective equilibrium positions. We shall apply our WKB approximation to this three-dimensional problem to calculate the small "tail" of the ground-state wave function for small r.

Let $\mathbf{R}_{ij}$ be the relative vector coordinate between nucleus i and j at their equilibrium positions. Because of the contribution of the other nuclei the potential $V(\mathbf{r})$ is nonseparable but has a symmetry line along the direction of $\mathbf{R}_{12}$ (and a minimum value when $\mathbf{r} = \mathbf{R}_{12}$). If we express $\mathbf{r}$ in a cylindrical polar system with $\mathbf{R}_{12}$ as z axis and with distances in units of a and energies in units of $(Ze)^2/a$, we have[14]

$$V(\mathbf{r}) = V_0 + \left(\frac{1}{r} - \frac{1}{R_{12}}\right) + \frac{2\pi}{3}(R_{12} - r)^2$$

$$+ \sum_{i \neq 1,2}\left[\frac{1}{|\mathbf{R}_{i1} + \frac{1}{2}(\mathbf{R}_{12} - \mathbf{r})|} - \frac{1}{R_{i1}}\right]$$

$$+ \sum_{i \neq 1,2}\left[\frac{1}{|\mathbf{R}_{i2} - \frac{1}{2}(\mathbf{R}_{12} - \mathbf{r})|} - \frac{1}{R_{i2}}\right]. \quad (35)$$

Along the z axis the lattice sums were evaluated numerically and V and its derivatives were fitted by the following polynomials (with $r^2 = z^2 + \rho^2$ and $\xi = 1 - |z|/$

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[14] W. J. Carr, Jr., Phys. Rev. **122**, 1437 (1961).

R_{12}):

$$V = V_0 + 1.1547\xi(1 - \xi)^{-1} - 1.1602\xi + 1.0394\xi^2$$
$$- 0.4001\xi^3 + 0.0692\xi^4 \pm 0.0001,$$

$$V_z = 5.3333(2 - \xi)^{-2} - 5.1479\xi + 8.7676\xi^2$$
$$- 20.6702\xi^3 + 19.5412\xi^4 - 9.4842\xi^5 \pm 0.01,$$

$$V_{\rho\rho} = 6.1582(2 - \xi)^{-3} + 4.1888 + 0.9398\xi$$
$$- 6.3698\xi^2 + 9.9108\xi^3 - 8.9930\xi^4 \pm 0.15, \quad (36)$$

where the subscripts indicate partial derivatives, and all quantities are evaluated at the axis. For small values of $|\mathbf{R}_{12} - \mathbf{r}|$ this expression reduces to the oscillator potential

$$V \approx V_0 + \frac{2\pi}{3}(\mathbf{R}_{12} - \mathbf{r})^2$$

$$+ \frac{1}{4}\left\{\frac{3[\mathbf{R}_{12} \cdot (\mathbf{R}_{12} - \mathbf{r})]^2}{R_{12}{}^5} - \frac{(\mathbf{R}_{12} - \mathbf{r})^2}{R_{12}{}^3}\right\}. \quad (37)$$

We now consider only cases with zero temperature and with $\lambda \ll 1$ in Eq. (34). Most of the wave function is then contained in regions where Eq. (37) is a good approximation. For this potential the ground-state energy E_0 and the normalized oscillator wave function ψ_{osc} are given by

$$E_0 = V_0 + 4.3073\lambda^{1/2},$$

$$\psi_{\text{osc}} = 0.553\lambda^{9/8}(r^*)^{-3/2}$$
$$\times \exp\{-\lambda^{-1/2}[0.8462(R_{12} - z)^2 + 0.6545\rho^2]\}. \quad (38)$$

With $\lambda \ll 1$ Eqs. (37) and hence (38) are good approximations well into the forbidden region, where the WKB approximation should be valid also. Equation (38) may then be used to provide the initial conditions on the WKB wave function and the curvature coefficient H at some "fitting point" r_f, and we have for the WKB wave function for all $r < r_f$ on the axis

$$\ln\psi(r) = \ln\psi_{\text{osc}}(r_f)$$

$$+ \int_{r_f}^{r} k\,dz - \frac{1}{2}\ln[k(r)/k(r_f)] - \int_{r_f}^{r} H^+ dz. \quad (39)$$

Here $k = \lambda^{-1/2}(V - E_0)^{1/2}$, and we have selected the purely decreasing exponential solution in the forbidden region (corresponding to the regular Coulomb function for small r, where the potential is dominated by the Coulomb term). We are mainly interested in $\psi(r)$ for $r \ll 1$, where the screening effects are small. The ratio $\psi(r)/\psi(0)$ may then be approximated by using our WKB expressions (Sec. V) for a pure Coulomb wave function, and by adding and subtracting this result

from Eq. (39), we obtain

$$\psi(r) = 0.553 \frac{\lambda^{7/8}}{(r^*)^{3/2}} \left(\frac{r}{r^*}\right)^{-1/4} \exp\left[\lambda^{-1/2} J(\lambda) + 2\left(\frac{r}{r^*}\right)^{1/2}\right],$$

$$J(\lambda) = -0.8462 (R_{12} - r_f)^2 + \int_{r_f}^{0} (V - E_0)^{1/2} dz \qquad (40)$$

$$-\lambda^{1/2} \left\{ \int_{r_f}^{r} H^+ dz - \tfrac{1}{2} \ln(\lambda r/r^*) - \tfrac{1}{4} \ln[V(r_f) - E_0] \right\}.$$

The dependence of Eq. (40) on the fitting point r_f is spurious, and we chose its numerical value for each value of λ so as to keep the combined errors due to the oscillator potential and the WKB function small. The explicit expression used for r_f was

$$r_f = R_{12} - 1.35 \lambda^{1/6}. \qquad (41)$$

For a number of values of λ in the range $5 \times 10^{-6} < \lambda < 5 \times 10^{-3}$ the Riccati equation for the curvature coefficient H^+ was integrated numerically by the Runge-Kutta technique starting from the fitting point and using Eq. (36). From this, numerical values for $J(\lambda)$ were obtained and used to determine the best coefficients in a series expansion in powers of $\lambda^{1/2}$, namely

$$J(\lambda) = -1.319 + 1.8 \lambda^{1/2} \pm 0.002. \qquad (42)$$

This expression in Eq. (40), together with

$$[V(r_f) - E_0]^{1/4} \approx 1.52 \lambda^{1/12} (1 - 0.068 \lambda^{1/6}),$$

gives the desired wave function.

The use of our wave function for the calculation of pycnonuclear reaction rates and the extension to nonzero temperature will be described elsewhere.

ACKNOWLEDGMENTS

APPENDIX A

We have noted in Sec. II that our Eq. (9) for the quasiclassical wave function differs from the one-dimensional WKB approximation only by the inclusion of the last term involving the curvature coefficient H. We have also shown that this term has a direct physical interpretation. In the general multidimensional case,

Van Vleck,[1] and more recently Schiller,[2] have shown that the quasiclassical wave function may quite generally be written in the form

$$\psi = D^{1/2} \exp(iS/\hbar). \qquad (A1)$$

The function S is the solution of the Hamilton-Jacobi equation, which for the time-independent case in three dimensions may be written as

$$(\nabla S)^2 = 2\mu(V - E). \qquad (A2)$$

This is identical with our Eq. (5) for the zero-order term of the WKB expansion.

The quantity D is the so-called Van Vleck determinant, which is defined by

$$D = \det\left[\frac{\partial^2 S}{\partial q^i \partial \alpha^k}\right], \qquad (A3)$$

where q^i are generalized coordinates and the α^k are constants of the motion. This determinant satisfies a continuity equation, which for a static, three-dimensional potential that is a function only of the coordinates has the form

$$\nabla^2 S + \nabla S \cdot \nabla \ln D = 0. \qquad (A4)$$

This is the same as our Eq. (6), which therefore establishes the equivalence of our version of the WKB approximation with the three-dimensional limit of the general prescription.

APPENDIX B

Furry's derivation[8] of the connection formulas is based upon the analytic continuation of the wave function (18) into the complex z plane and makes explicit use of the fact that the WKB approximation is only asymptotically correct. The argument proceeds as follows. From Eq. (18) it is evident that the leading term of the expansion is purely real along the so-called "Stokes lines," at which $\arg(z e^{-i\pi}) = \theta$ has the value $\pi/3$, π, or $5\pi/3$. These lines are denoted as SI, SII, and SIII, respectively, in Fig. 1. Along a Stokes line, only the coefficient of the increasing exponential term is meaningful, since this alone determines the asymptotic limit, and the coefficient of the decreasing term will in
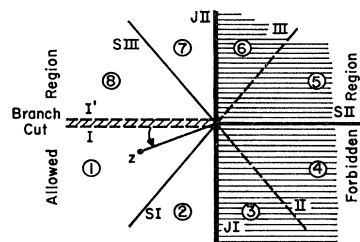

FIG. 1. The complex z plane near a turning point.

general be discontinuous across this line. Equally spaced between the Stokes lines are three "anti-Stokes lines" located at $\theta=0$, $2\pi/3$, $4\pi/3$, and 2π, where the last line is identical with the first except for a branch cut along this axis which is necessary to make the function single-valued. Along these lines the two exponential terms have purely imaginary arguments, and the coefficients of both terms are necessary to give the asymptotic limit. The anti-Stokes lines are indicated by I, II, III, and I' in Fig. 1. Finally, at the lines JI and JII the real part of z changes sign; these lines mark the boundary between the allowed and forbidden regions in the complex plane.

Consider now the analytic continuation of the WKB wave function into the complex plane. The general wave function can be written in the form

$$\psi=(ze^{-i\pi})^{-1/4}\{A[1+iC^{+}(ze^{-i\pi})^{1/2}]^{-1}\exp[-i\tfrac{2}{3}(ze^{-i\pi})^{3/2}]$$
$$+B[1+C^{-}(ze^{-i\pi})^{1/2}]^{-1}\exp[+i\tfrac{2}{3}(ze^{-i\pi})^{3/2}]\}.\quad(B1)$$

We suppose that on line I the coefficients A and B take on the given values A_1 and B_1, respectively, which gives the asymptotic approximation uniquely throughout region 1. As we cross the Stokes line SI into region 2, the coefficient of the dominant exponential term (which in this case is the first term) must remain the same, so that we must have

$$A_2=A_1.\quad(B2a)$$

In general, however, the asymptotic approximation for the wave function in region 2 will be represented by a different linear combination of the two exponentials, so that the "subdominant" solution in region 2 may contain an arbitrary mixture of the increasing and decreasing exponentials. This second solution may be represented by a linear superposition of the dominant and subdominant solutions of region 1, however, and continuity of the subdominant solution for arbitrary values of the coefficients A_1 and B_1 therefore demands

$$[1+C_a^{-}|z|^{1/2}e^{i\pi/6}]^{-1}B_2$$
$$=[1+C_a^{-}|z|^{1/2}e^{i\pi/6}]^{-1}B_1$$
$$+\alpha[1+C_a^{+}|z|^{1/2}e^{i2\pi/3}]^{-1}A_1,\quad(B2b)$$

where C_a is the value of the constant for the allowed region, and α is an undetermined multiplier. In a similar manner, we require the asymptotic approximations to the two independent solutions to be continuous across the boundaries of each of the remaining regions, and

thus arrive at the relations

$$[1+C_f^{+}|z|^{1/2}e^{i3\pi/4}]^{-1}A_3=[1+C_a^{+}|z|^{1/2}e^{i3\pi/4}]^{-1}A_2,$$
$$[1+C_f^{-}|z|^{1/2}e^{i\pi/4}]^{-1}B_3=[1+C_a^{-}|z|^{1/2}e^{i\pi/4}]^{-1}B_2,$$
$$A_4=A_3,$$
$$B_4=B_3,$$
$$[1+C_f^{+}|z|^{1/2}e^{i\pi}]^{-1}A_5=[1+C_f^{+}|z|^{1/2}e^{i\pi}]^{-1}A_4$$
$$+\beta[1+C_f^{-}|z|^{1/2}e^{i\pi/2}]^{-1}B_4,$$
$$B_5=B_4,$$
$$A_6=A_5,$$
$$B_6=B_5,$$
$$[1+C_a^{+}|z|^{1/2}e^{i5\pi/4}]^{-1}A_7=[1+C_f^{+}|z|^{1/2}e^{i5\pi/4}]^{-1}A_6,$$
$$[1+C_a^{-}|z|^{1/2}e^{i3\pi/4}]^{-1}B_7=[1+C_f^{-}|z|^{1/2}e^{i3\pi/4}]^{-1}B_6,$$
$$A_8=A_7,$$
$$[1+C_a^{-}|z|^{1/2}e^{i5\pi/6}]^{-1}B_8=[1+C_a^{-}|z|^{1/2}e^{i5\pi/6}]^{-1}B_7$$
$$+\gamma[1+C_a^{+}|z|^{1/2}e^{i4\pi/3}]^{-1}A_7.\quad(B3)$$

In this equation C_f is the value of the constant appropriate to the forbidden region, and β and γ are the remaining undetermined multipliers.

The analytic continuation expressed by Eqs. (B2) and (B3) finally leads to the following expression for the wave function on the line I':

$$\psi=-i|z|^{-1/4}\{A_8[1+C_a^{+}|z|^{1/2}e^{i3\pi/2}]^{-1}\exp[+i\tfrac{2}{3}|z|^{3/2}]$$
$$+B_8[1+C_a^{-}|z|^{1/2}e^{i\pi}]^{-1}\exp[-i\tfrac{2}{3}|z|^{3/2}]\}.\quad(B4)$$

Since this result must be *identical* with Eq. (B1) with $z\rightarrow|z|e^{i\pi}$ if the wave function is to be single-valued, we thus obtain

$$C_a^{-}=-iC_a^{+}\quad(B5)$$

and

$$-iA_8=B_1,\quad-iB_8=A_1.\quad(B6)$$

The requirement that Eqs. (B2), (B3), (B5), and (B6) be satisfied for arbitrary values of A_1 and B_1 then gives the additional restrictions

$$-iC_f^{+}=C_f^{-}=C_a^{-},\quad(B7)$$

and the desired relation between the coefficients on line I and those on line SII becomes simply

$$A_4=A_1,\quad B_4=B_1+iA_1.\quad(B8)$$

Equations (B5), (B7), and (B8) comprise the desired connection formulas for the wave function and the curvature coefficient, and they lead directly to the relations (19) and (20) given in the text.