PHYSICAL REVIEW VOLUME 109, NUMBER 5 MARCH 1, 1958

Variational Principles for the Wave Function in Scattering Theory

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(Received October 18, 1957)

Variational principles are designed for the solution of the Schrödinger equation when a point source is placed in the presence of an inhomogeneous, absorbing medium represented by an arbitrary complex potential function. When the point source is allowed to recede to infinity, these stationary structures reduce to variational principles for the wave function in the standard scattering problem, namely the outgoing solution to the Schrödinger equation for an incident plane wave. Finally in the asymptotic region, the well-known bifunctional variational principles for the transition amplitudes arise automatically from the stationary forms for the wave function describing the standard scattering problem. A few examples leading to variationally improved wave functions are discussed.

INTRODUCTION

THE object of the present report is to draw attention to the fact that variational principles may be constructed for the solution to the point source scattering problem. Then, by allowing the point source to recede to infinity, these stationary structures become variational principles for the wave function describing the general propagation problems defined by a plane wave incident upon an inhomogeneous medium. Furthermore, upon selecting the observation point in the asymptotic region, the variational principles for the wave function reduce, as they should, to the well-known bifunctional variational principles for the transition amplitude.

In Sec. I, two variational principles for the point source problem are discussed while Sec. II develops stationary expressions for the wave function in the ordinary scattering problem. A few simple applications are given in Sec. III. Although these variational principles need not in principle be restricted to single-particle scattering, this study will be limited to potential scattering where the potential may be nonspherical as well as complex.

I. POINT-SOURCE VARIATIONAL PRINCIPLE

The point-source problem is defined by the equation

$$[\nabla^2+k^2-U(\mathbf{r})]\Psi(\mathbf{p},\mathbf{r})=\delta(\mathbf{r}-\mathbf{p}). \tag{1}$$

Upon including the outgoing boundary condition, the integral equation for the symmetric function $\Psi(\mathbf{p},\mathbf{r})$ may be written as

$$\Psi(\mathbf{p},\mathbf{r})=G(\mathbf{r},\mathbf{p})+\int G(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\Psi(\mathbf{p},\mathbf{r}')d\mathbf{r}', \tag{2}$$

where $G(\mathbf{r},\mathbf{r}')$ is the free-wave Green's function

$$G(\mathbf{r},\mathbf{r}')=e^{ik|\mathbf{r}-\mathbf{r}'|}/-4\pi|\mathbf{r}-\mathbf{r}'|. \tag{3}$$

Thus (2) represents the problem of a point source at $\mathbf{p}$ in the presence of the medium described by the complex potential function $U(\mathbf{r})$, and behaves asymptotically like the following outgoing wave:

$$\lim_{r\to\infty}\Psi(\mathbf{p},\mathbf{r})=\frac{e^{ikr}}{-4\pi r}\left[e^{-i\mathbf{k}\cdot\mathbf{p}}+\int\Psi(\mathbf{p},\mathbf{r}')U(\mathbf{r}')e^{-i\mathbf{k}\cdot\mathbf{r}'}d\mathbf{r}'\right]$$
$$=\frac{e^{ikr}}{-4\pi r}\psi(-\mathbf{k}|\mathbf{p}). \tag{4}$$

Here, $\mathbf{k}$ is a vector of magnitude k pointing in the direction $\mathbf{r}$, and $\psi(-\mathbf{k}|\mathbf{p})$ is the wave function evaluated at the source point $\mathbf{p}$ which describes the motion of a plane wave incident in the negative $\mathbf{k}$ direction and scattered by $U(\mathbf{r})$. We note in passing that (4) contains the statement of reciprocity, namely,

$$\left|\lim_{r\to\infty}\frac{\Psi(\mathbf{p},\mathbf{r})}{G(\mathbf{r},\mathbf{p})}\right|=|\psi(-\mathbf{k}|\mathbf{p})|, \tag{5}$$

which states that the relative magnitude of the field due to a point source placed at $\mathbf{p}$ when observed along the $\mathbf{k}$ direction in the far-field region is the same as the magnitude of the field observed at the near-field point $\mathbf{p}$ when a plane wave of unit amplitude is incident upon the scattering center in the $-\mathbf{k}$ direction.

The following expression defines a variational principle for the point-source problem:

$$S_1(\mathbf{r},\mathbf{p})=2\Psi(\mathbf{r},\mathbf{p})-\int\Psi(\mathbf{r}',\mathbf{p})[\nabla'^2+k^2-U(\mathbf{r}')]\Psi(\mathbf{r}',\mathbf{r})d\mathbf{r}'. \tag{6}$$

For exact, $\Psi(\mathbf{r},\mathbf{r}')$, S_1 reduces to $\Psi(\mathbf{r},\mathbf{p})$, while for arbitrary variation $\delta\Psi(\mathbf{r},\mathbf{p})$,

$$\delta S_1(\mathbf{r},\mathbf{p})=2\delta\Psi(\mathbf{r},\mathbf{p})-\int\delta\Psi(\mathbf{r}',\mathbf{p})[\nabla'^2+k^2-U(\mathbf{r}')]\times\Psi(\mathbf{r}',\mathbf{r})d\mathbf{r}'-\int\Psi(\mathbf{r}',\mathbf{p})\times[\nabla'^2+k^2-U(\mathbf{r}')]\delta\Psi(\mathbf{r}',\mathbf{r})d\mathbf{r}' \tag{7}$$
$$=\lim_{r'\to\infty}\left\{-\int_{S'}\left[\Psi(\mathbf{r}',\mathbf{p})\frac{\partial}{\partial r'}\delta\Psi(\mathbf{r}',\mathbf{r})-\delta\Psi(\mathbf{r}',\mathbf{r})\frac{\partial}{\partial r'}\Psi(\mathbf{r}',\mathbf{p})\right]dS'\right\}$$
$$=0.$$

The surface term vanishes in virtue of the outgoing radiation condition upon $\Psi(\mathbf{r}',\mathbf{p})$, a condition which is also imposed upon the trial functions.

A second variational principle for $\Psi(\mathbf{r},\mathbf{p})$ is given by

$$S_2(\mathbf{r},\mathbf{p})=\Psi(\mathbf{r},\mathbf{p})\times\exp\left\{1-\int\frac{\Psi(\mathbf{r}',\mathbf{p})[\nabla'^2+k^2-U(\mathbf{r}')]\Psi(\mathbf{r}',\mathbf{r})d\mathbf{r}'}{\Psi(\mathbf{r},\mathbf{p})}\right\}. \quad (8)$$

Again, $S_2=\Psi(\mathbf{r},\mathbf{p})$ for exact $\Psi(\mathbf{r}',\mathbf{r})$ and the stationary character of S_2 may be easily demonstrated by taking arbitrary variations about the true solution.

II. VARIATION PRINCIPLES FOR THE WAVE FUNCTION IN THE STANDARD SCATTERING PROBLEM

The standard scattering problem is defined as the outgoing solution of the Schrödinger equation for an incident plane wave. Let us imagine that the plane wave moves from left to right in the direction fixed by the wave number vector $\mathbf{k}_0$. If the source point $\mathbf{p}$ in (2) is now allowed to recede to the left into the direction $-\mathbf{k}_0$, then (2) becomes

$$\lim_{\mathbf{p}\to\infty}\Psi(\mathbf{r},\mathbf{p})\to\frac{e^{ikr_p}}{-4\pi r_p}e^{i\mathbf{k}_0\cdot\mathbf{r}}+\int G(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\times\Psi(\mathbf{r}',\mathbf{p})d\mathbf{r}'=N\psi(\mathbf{k}_0|\mathbf{r}), \quad (9)$$

where $\psi(\mathbf{k}_0|\mathbf{r})$ is the wave function for the standard scattering problem and N is an uninteresting amplitude factor $(-4\pi r_p)^{-1}\exp(ikr_p)$.

When this limiting process is applied to the stationary expression for S_1, the result is

$$\frac{S_1}{N}=2\psi(\mathbf{k}_0|\mathbf{r})-\int\psi(\mathbf{k}_0|\mathbf{r})[\nabla'^2+k^2-U(\mathbf{r}')]\Psi(\mathbf{r}',\mathbf{r})d\mathbf{r}', \quad (10)$$

and by partial integration

$$\frac{S_1}{N}=2\psi(\mathbf{k}_0|\mathbf{r})-\int\Psi(\mathbf{r}',\mathbf{r})[\nabla'^2+k^2-U(\mathbf{r}')]\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'-\int_{S'}\left\{\psi(\mathbf{k}_0|\mathbf{r}')\frac{\partial}{\partial r'}\Psi(\mathbf{r}',\mathbf{r})-\Psi(\mathbf{r}',\mathbf{r})\frac{\partial}{\partial r'}\psi(\mathbf{k}_0|\mathbf{r}')\right\}dS'. \quad (11)$$

But it is shown in Appendix I that the surface integral is exactly $\psi|\mathbf{k}_0|\mathbf{r})$. Therefore,

$$Y_1\equiv\frac{S_1}{N}=\psi(\mathbf{k}_0|\mathbf{r})-\int\Psi(\mathbf{r}',\mathbf{r})[\nabla'^2+k^2-U(\mathbf{r}')]\times\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}' \quad (12)$$

is the variational principle for the wave function $\psi(\mathbf{k}_0|\mathbf{r})$. Now, it is to be noted that the bifunctional character of this new principle has arisen quite naturally from (6). That is, Eq. (12) is stationary for arbitrary, independent variations of two wave functions, namely $\Psi(\mathbf{r}',\mathbf{r})$, the solution to the point source problem with the source point placed at $\mathbf{r}$, and $\psi(\mathbf{k}_0|r)$, which describes the standard scatter problem. Thus, performing variations about the true solutions

$$[\nabla^2+k^2-U(\mathbf{r})]\psi(\mathbf{k}_0|\mathbf{r})=0, \quad (13)$$

and Eq. (1), it follows as in (7) that

$$\delta Y_1=\lim_{r'\to\infty}-\int_{S'}\left\{\Psi(\mathbf{r}',\mathbf{r})\frac{\partial}{\partial r'}\delta\psi(\mathbf{k}_0|\mathbf{r}')-\delta\psi(\mathbf{k}_0|\mathbf{r}')\frac{\partial}{\partial r'}\Psi(\mathbf{r}',\mathbf{r})\right\}dS'=0. \quad (14)$$

The surface term again vanishes as a result of the outgoing radiation condition since

$$\lim_{r'\to\infty}\delta\psi(\mathbf{k}_0|\mathbf{r}')=\delta\left(e^{i\mathbf{k}_0\cdot\mathbf{r}'}+\frac{e^{ikr'}}{r'}f\right)=\frac{e^{ikr'}}{r'}\delta f. \quad (15)$$

A second variational principle for $\psi(\mathbf{k}_0|\mathbf{r})$ follows from (8) by means of the same limiting procedure which led to Y_1 in (12). The result is given by

$$Y_2=\psi(\mathbf{k}_0|\mathbf{r})\exp\left(-\int\Psi(\mathbf{r}',\mathbf{r})[\nabla'^2+k^2-U(\mathbf{r}')]\times\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'\Big/\psi(\mathbf{k}_0|\mathbf{r})\right). \quad (16)$$

Another stationary form for $\psi(\mathbf{k}_0|\mathbf{r})$ follows by eliminating the Schrödinger operator $\nabla^2+k^2-U(\mathbf{r})$. Thus, after replacing $\psi(\mathbf{k}_0|\mathbf{r})$ by its equivalent from the integral equation

$$\psi(\mathbf{k}_0|\mathbf{r})=e^{i\mathbf{k}_0\cdot\mathbf{r}}+\int G(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}', \quad (17)$$

Y_1 in (12) is transformed to

$$'Y_1'=e^{i\mathbf{k}_0\cdot\mathbf{r}}+\int G(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'+\int\Psi(\mathbf{r}',\mathbf{r})U(\mathbf{r}')e^{i\mathbf{k}_0\cdot\mathbf{r}'}d\mathbf{r}'-\int\Psi(\mathbf{r}',\mathbf{r})U(\mathbf{r}')\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'+\int\int\Psi(\mathbf{r}',\mathbf{r})U(\mathbf{r}')G(\mathbf{r}',\mathbf{r}'')U(\mathbf{r}'')\times\psi(\mathbf{k}_0|\mathbf{r}'')d\mathbf{r}'d\mathbf{r}''. \quad (18)$$

The term $e^{i\mathbf{k}_0\cdot\mathbf{r}}$ may be dropped so that what remains is a variational principle for the scattered part of $\psi(\mathbf{k}_0|\mathbf{r})$.[1] This is the near-field analog to Schwinger's variational principle[2] for the transition amplitude while (12) is analogous to Kohn's principle.[3] Both transition amplitude principles follow immediately by allowing the observation point $\mathbf{r}$ to become infinitely large. For example, in the stationary form (12), the incident plane wave may be first subtracted off and what remains is a variational principle for the scattered wave. Then, in the asymptotic region, it follows after employing (4), that

$$\frac{e^{ikr}}{r}F(\mathbf{k}_0\to\mathbf{k})\equiv\lim_{\hat{k}r\to\infty}(Y_1-e^{i\mathbf{k}_0\cdot\mathbf{r}})$$
$$=\frac{e^{ikr}}{r}f(\mathbf{k}_0\to\mathbf{k})-\int\frac{e^{ikr}}{-4\pi r}\psi(-\mathbf{k}|\mathbf{r}')\times[\nabla'^2+k^2-U(\mathbf{r}')]\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}',$$

or

$$4\pi F(\mathbf{k}_0\to\mathbf{k})=4\pi f(\mathbf{k}_0\to\mathbf{k})+\int\psi(-\mathbf{k}|\mathbf{r}')\times[\nabla'^2+k^2-U(\mathbf{r}')]\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'.$$

This is the Kohn[3] bifunctional variational principle for the amplitude F for scattering into the direction given by the unit vector $\hat{k}$.

It is desirable to find amplitude-independent stationary forms. In the case of (12), the Kohn-type variational principle, we follow the method employed by Moe[4] in finding an amplitude-independent form for the Kohn variational principle on the scattering amplitude. The two wave functions $\psi(\mathbf{k}_0|\mathbf{r})$ and $\Psi(\mathbf{r}',\mathbf{r})$ are divided into perturbed and unperturbed parts,

$$\psi(\mathbf{k}_0|\mathbf{r})=e^{i\mathbf{k}_0\cdot\mathbf{r}}+A\Phi(\mathbf{r}),$$

and

$$\Psi(\mathbf{r}',\mathbf{r})=G(\mathbf{r}',\mathbf{r})+BW(\mathbf{r}',\mathbf{r}),$$

where A and B are constants. These are then substituted into (12) and the requirement

$$\frac{\partial[\Phi(\mathbf{r})]}{\partial A}=\frac{\partial[\Phi(\mathbf{r})]}{\partial B}=0,$$

where

$$[\Phi(\mathbf{r})]\equiv Y_1-e^{i\mathbf{k}_0\cdot\mathbf{r}},$$

leads easily to the following stationary form for $[\Phi(\mathbf{r})]$:

$$[\Phi(\mathbf{r})]=\int G(\mathbf{r}',\mathbf{r})U(\mathbf{r}')e^{i\mathbf{k}_0\cdot\mathbf{r}'}d\mathbf{r}'+\frac{\int G(\mathbf{r}',\mathbf{r})U(\mathbf{r}')\Phi(\mathbf{r}')d\mathbf{r}'\int W(\mathbf{r}',\mathbf{r})U(\mathbf{r}')e^{i\mathbf{k}_0\cdot\mathbf{r}'}d\mathbf{r}'}{\int W(\mathbf{r}',\mathbf{r})[\nabla'^2+k^2-U(\mathbf{r}')]\Phi(\mathbf{r}')d\mathbf{r}'}. \tag{19}$$

The amplitude independent form constructed from the various integrals appearing in (18) may be written down at once by analogy with Schwinger's well-known amplitude independent variational principle for the transition or scattering amplitude. That is, the following expression for the scattered wave is also stationary:

$$\text{‘}\Phi(\mathbf{r})\text{’}=\frac{\int G(\mathbf{r},\mathbf{r}')U(\mathbf{r}')\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'\int\Psi(\mathbf{r}',\mathbf{r})U(\mathbf{r}')e^{i\mathbf{k}_0\cdot\mathbf{r}'}d\mathbf{r}'}{\int\Psi(\mathbf{r}',\mathbf{r})U(\mathbf{r}')\psi(\mathbf{k}_0|\mathbf{r}')d\mathbf{r}'-\int\int\Psi(\mathbf{r}',\mathbf{r})U(\mathbf{r}')G(\mathbf{r}',\mathbf{r}'')U(\mathbf{r}'')\psi(\mathbf{k}_0|\mathbf{r}'')d\mathbf{r}'d\mathbf{r}''}. \tag{20}$$

III. ILLUSTRATIONS OF VARIATIONAL PRINCIPLES FOR THE WAVE FUNCTION

The first example applying a variational principle for the wave function will concern the rather trivial one-dimensional scattering for a delta-function interaction. It is amusing to see how the exact solution follows practically by inspection if the stationary form (20) is chosen. Thus, if $U(x)=2g\delta(x)$, then since $G(x,x')=(2ik)^{-1}\exp(ik|x-x'|)$, the scattered wave from (20) is

$$\Phi(x)=\frac{(g/ik)e^{ik|x|}(2g)}{2g-(2g)^2/2ik}=\frac{ge^{ik|x|}}{ik(1-g/ik)}. \tag{21}$$

Therefore,

$$\psi(x)=e^{ikx}+\Phi(x)=e^{ikx}+\frac{ge^{ik|x|}}{ik(1-g/ik)}, \tag{22}$$

the exact solution.

A more realistic example is the general three-dimensional propagation problem which will now be considered in connection with Y_2 in (16). After choosing the undisturbed solutions $\exp(i\mathbf{k}_0\cdot\mathbf{r})$ and $G(\mathbf{r},\mathbf{r}')$ for

[1] A near-field variational principle equivalent to (18) has been derived for the surface scattering problem by Harold Levine. It appears in "Lectures by H. Levine, Variational Methods for Solving Electromagnetic Boundary Value Problems," September 1, 1954 (unpublished), prepared by L. Mower, Sylvania Electric Products, Inc., Mountain View, California.

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[3] W. Kohn, Phys. Rev. **74**, 1763 (1948).

[4] M. M. Moe, thesis, 1956, University of California at Los Angeles (unpublished).

$\psi(\mathbf{k}_0|\mathbf{r})$ and $\Psi(\mathbf{r}',\mathbf{r})$, respectively, it follows that the improved wave function is given by

$$Y_2(\mathbf{r})=\exp(i\mathbf{k}_0\cdot\mathbf{r})\times\exp\left(\frac{-1}{4\pi}\int\frac{\exp(ik\rho-i\mathbf{k}_0\cdot\boldsymbol{\varrho})}{\rho}U(\mathbf{r}-\boldsymbol{\varrho})d\boldsymbol{\varrho}\right), \quad (23)$$

where $\boldsymbol{\varrho}=\mathbf{r}-\mathbf{r}'$. The integral in (23) may be evaluated[5] in terms of an expansion in reciprocal powers of k by a stationary phase method which is based upon the observation that most of the contribution to its value arises for small angles between $\mathbf{k}_0$ and $\boldsymbol{\varrho}$. For exceptionally large k, one obtains[6]

$$\exp(-i\mathbf{k}_0\cdot\boldsymbol{\varrho})=\frac{2\pi i}{k}\left\{\frac{e^{-ik\rho}}{\rho}\delta(\hat{k}_0-\hat{\rho})-\delta(\hat{k}_0+\hat{\rho})\frac{e^{ik\rho}}{\rho}\right\}, \quad (24)$$

where $\hat{k}_0$ and $\hat{\rho}$ are unit vectors. Thus, the leading term for the integral may be written down at once. It is

$$\frac{-i}{2k}\int_0^\infty U(\mathbf{r}-\hat{k}_0 s)ds.$$

Consequently, contributions from the other regions in the space of $\boldsymbol{\varrho}$ give rise to nonclassical or diffraction effects which is, of course, correlated with higher order terms in powers of k^{-1} since the leading term is simply the well-known solution of the Hamilton Jacobi or eikonal equation along a straight line trajectory. Schiff[5] has evaluated the $O(k^{-2})$ term and has indicated a procedure for further integration. The approximate wave function in (23) is not new. It has already been used, although derived in a different way, by Obukhov.[7] His method is essentially equivalent to that of Rytov[8] who substitutes a semiclassical-type wave function

$$\psi(\mathbf{k}_0|\mathbf{r})=\exp(i\mathbf{k}_0\cdot\mathbf{r})\exp\left(\frac{-iw(\mathbf{r})}{\exp(i\mathbf{k}_0\cdot\mathbf{r})}\right) \quad (25)$$

into the wave equation to deduce the following exact nonlinear equation for $w(\mathbf{r})$:

$$(\nabla^2+k^2)w(\mathbf{r})=iU(\mathbf{r})\exp(i\mathbf{k}_0\cdot\mathbf{r})+i\exp(i\mathbf{k}_0\cdot\mathbf{r})\{\nabla[w\exp(-i\mathbf{k}_0\cdot\mathbf{r})]\}^2. \quad (26)$$

Upon dropping the nonlinear term, the solution for $w(\mathbf{r})$ leads to (23).

It is now interesting to develop an approximate solution to the point source problem which parallels (23). Therefore, the free-space Green's function is chosen as trial solution in (8), with the result that

$$S_2(\mathbf{r},\mathbf{p})=G(\mathbf{r},\mathbf{p})\exp\left(\int\frac{G(\mathbf{r}',\mathbf{p})U(\mathbf{r}')G(\mathbf{r}',\mathbf{r})}{G(\mathbf{r},\mathbf{p})}d\mathbf{r}'\right). \quad (27)$$

The leading term in k^{-1} of this integral is evaluated in Appendix II. Thus the approximate solution of the point-source problem for high energies and slowly varying potential functions is the WKB solution[9]:

$$S_2(\mathbf{r},\mathbf{p})=\frac{\exp(ik|\mathbf{r}-\mathbf{p}|)}{-4\pi|\mathbf{r}-\mathbf{p}|}\times\exp\left(\frac{-i}{2k}\int_0^{|\mathbf{r}-\mathbf{p}|}U(\mathbf{p}+\hat{\gamma}s)ds\right), \quad (28)$$

where $\hat{\gamma}$ is a unit vector in the direction $\mathbf{r}-\mathbf{p}$. As one would expect, the free-wave Green's function is merely corrected eikonal-wise for phase change along straight-line trajectories connecting the points $\mathbf{p}$ and $\mathbf{r}$, just as in the case previously discussed in relation to (23).

As further examples, the WKB solutions for $\Psi(\mathbf{r},\mathbf{r}')$ and $\psi(\mathbf{k}_0|\mathbf{r})$ can be used as trial solutions in (12), (16), (18), or (20), and lead to a variety of variationally improved wave functions. Of course, the stationary forms (18) and (20) have the advantage that the trial solutions need only be meaningful in regions of space where the potential is important since the potential limits the domain of integration in each term. Thus, the WKB trial solution

$$\psi(\mathbf{p}_0|\mathbf{r})=\exp\left[i\mathbf{k}_0\cdot\mathbf{r}-\frac{i}{2k}\int_0^\infty U(\mathbf{r}-\hat{k}_0 s)ds\right], \quad (29)$$

which is a sensible approximation at finite distances from the scattering center is best employed in connection with (18) and (20).

It is, however, important to point out that (29) does not produce any difficulty as a trial solution for the stationary expressions containing the operator $\nabla^2+k^2-U(\mathbf{r})$, although at first sight it would appear erroneous on the basis of the radiation condition (15) which is sufficient for the requirement that the surface term in (14) vanish. It is demonstrated in Appendix III that this surface term does in fact vanish when the trial solution (29) is employed. Consequently, this trial solution is also valid for the stationary forms (12) and (16). The plane wave $e^{i\mathbf{k}_0\cdot\mathbf{r}}$ as trial solution produces no difficulty since δf in (15) is in this case the exact f and the surface term automatically vanishes.

ACKNOWLEDGMENTS

The author wishes to thank Dr. M. M. Moe for several profitable discussions and for making her un-

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[8] S. M. Rytov, Izvestica, AN: U.S.S.R. Physica Series No. 2 (1937).

[9] This WKB solution also appears in I. I. Gol'dman and A. B. Migdal, J. Exptl. Theoret. Phys. U.S.S.R. **28**, 394 (1954) [translation: Soviet Phys. JETP **1**, 304 (1955)].

published thesis available. Her derivation of an exponential-type variational principle for the scattering amplitude furnished the motivation for the extension to the exponential-type stationary forms in the present report. The writer is also grateful to Dr. D. S. Saxon and Dr. P. Molmud for valuable discussion, and is especially indebted to Dr. C. L. Dolph for his keen interest and helpful collaboration during a preliminary stage of this investigation.

APPENDIX I

We wish to evaluate the surface integral

$$\lim_{r'\to\infty}\int_{S'}\left\{\psi(\mathbf{k}_0|\mathbf{r}')\frac{\partial}{\partial r'}\Psi(\mathbf{r}',\mathbf{r})-\Psi(\mathbf{r}',\mathbf{r})\frac{\partial}{\partial r'}\psi(\mathbf{k}_0|\mathbf{r}')\right\}dS',$$

where the asymptotic forms for large r' are given by

$$\psi(\mathbf{k}_0|\mathbf{r}')\sim e^{i\mathbf{k}_0\cdot\mathbf{r}'}+f(\mathbf{k}_0,k\hat{r}')\frac{e^{ikr'}}{r'}$$

and

$$\Psi(\mathbf{r}',\mathbf{r})\sim\frac{e^{ikr'}}{-4\pi r'}\psi(-k\hat{r}'|\mathbf{r}).$$

Here, $\hat{r}'$ is a unit vector taken in the direction of observation in the asymptotic region.

The outgoing part of $\psi(\mathbf{k}_0|\mathbf{r}')$ may be omitted at once since the integrand vanishes exactly for this term. Then, upon employment of (24) for $e^{i\mathbf{k}_0\cdot\mathbf{r}'}$ as $r'\to\infty$, there remains

$$\frac{-2\pi i}{k}\int_{S'}\left\{\left[\frac{e^{ikr'}}{r'}\delta(\hat{k}_0-\hat{r}')-\frac{e^{-ikr'}}{r'}\delta(\hat{k}_0+\hat{r}')\right]\times\frac{ike^{ikr'}}{-4\pi r'}\psi(-k\hat{r}'|\mathbf{r})-\frac{e^{ikr'}}{-4\pi r'}\psi(-k\hat{r}'|\mathbf{r})\times\left[\frac{ike^{ikr'}}{r'}\delta(\hat{k}_0-\hat{r}')+\frac{ike^{-ikr'}}{r'}\delta(\hat{k}_0+\hat{r}')\right]\right\}r'^2d\hat{r}'$$

$$=\frac{-2\pi i}{k}\int_{S'}\left(+\frac{2ik}{4\pi}\right)\delta(\hat{k}_0+\hat{r}')\psi(-k\hat{r}'|\mathbf{r})d\hat{r}'$$

$$=+\psi(\mathbf{k}_0|\mathbf{r}).$$

APPENDIX II

In order to evaluate[10] the leading term (order k^{-1}) of the integral

$$I=-\frac{1}{4\pi}\int\frac{e^{ik|\mathbf{r}-\mathbf{r}''|}U(\mathbf{r}'')e^{ik|\mathbf{r}''-\mathbf{r}'|-ik|\mathbf{r}-\mathbf{r}'|}|\mathbf{r}-\mathbf{r}'|d\mathbf{r}''}{|\mathbf{r}-\mathbf{r}''||\mathbf{r}''-\mathbf{r}'|},\tag{A1}$$

we first eliminate $\mathbf{r}$ by the transformation $\boldsymbol{\varrho}=\mathbf{r}-\mathbf{r}'$. Next, the variable of integration is eliminated by transforming to $\boldsymbol{\mu}=\mathbf{r}''-\mathbf{r}'$. Thus,

$$I=-\frac{\rho}{4\pi}\int\frac{\exp[ik|\boldsymbol{\varrho}-\boldsymbol{\mu}|-ik(\rho-\mu)]U(\mathbf{r}'+\boldsymbol{\mu})d\boldsymbol{\mu}}{|\boldsymbol{\varrho}-\boldsymbol{\mu}|\mu}.\tag{A2}$$

For large k and slowly varying U in a length (k^{-1}), the principal contribution to the integral arising from the integration over the angles of $\boldsymbol{\mu}$ occurs when the phase is stationary. Therefore, for the main contribution $\boldsymbol{\varrho}\cdot\boldsymbol{\mu}\sim 1$ and for such small angles θ, one has

$$|\boldsymbol{\varrho}-\boldsymbol{\mu}|-(\rho-\mu)=[\rho^2+\mu^2-2\mu\rho(1-\tfrac{1}{2}\theta^2)]^{\frac{1}{2}}-(\rho-\mu)$$

$$=\pm(\rho-\mu)\left(1+\frac{\mu\rho}{(\rho-\mu)^2}\frac{\theta^2}{2}\right)-(\rho-\mu).$$

Here, the positive sign holds when $\mu<\rho$ and the negative sign is required for $\mu>\rho$.

We first consider the case $\mu<\rho$ for which the phase term is then $[2(\rho-\mu)]^{-1}\mu\rho\theta^2$. Hence, for small θ

$$I=-\frac{\rho}{4\pi}\int\frac{\exp[\frac{1}{2}ik\mu\rho\theta^2/(\rho-\mu)]U(\mathbf{r}'+\boldsymbol{\mu})d\boldsymbol{\mu}}{\mu(\rho-\mu)}.\tag{A3}$$

But $d\boldsymbol{\mu}=\mu^2\sin\theta d\theta d\phi d\mu\cong\mu^2 d\mu d(\theta^2/2)d\phi$, and partial integration over θ can be done at once yielding

$$\int d(\theta^2/2)\exp\left(\frac{ik\mu\rho\theta^2}{2(\rho-\mu)}\right)\times U(x'+\mu\sin\theta\cos\phi,\,y'+\mu\sin\theta\sin\phi,\,z'+\mu\cos\theta)$$

$$=\left|\frac{(\rho-\mu)\exp[\frac{1}{2}ik\mu\rho\theta^2/(\rho-\mu)]U}{ik\mu\rho}\right|_0^\theta-\frac{1}{ik\mu\rho}\int\exp\left(\frac{ik\mu\rho\theta^2}{2(\rho-\mu)}\right)U'd(\theta^2/2).$$

The integral on the right is to be dropped since it is of order $(k\mu\rho)^{-1}$ relative to the first term since another partial integration will introduce an additional power of $(k\mu\rho)$ in the denominator. Furthermore, the upper limit in the first term contains the rapidly oscillating factor $k\mu\rho$ and is small compared with the lower limit. Hence the leading term in (k^{-1}) is given by

$$I=\frac{1}{2ik}\int_0^\rho U(x',y',z'+\mu)d\mu=\frac{-i}{2k}\int_0^\rho U(\mathbf{r}'+\hat{\rho}\mu)d\mu,\tag{A4}$$

where $\hat{\rho}$ is a unit vector in the direction $\boldsymbol{\varrho}$. When $\mu>\rho$,

$$|\boldsymbol{\varrho}-\boldsymbol{\mu}|-(\rho-\mu)=-2(\rho-\mu)-\left(\frac{\mu\rho}{\rho-\mu}\right)\frac{\theta^2}{2},$$

and it now follows that the final integral over μ which

[10] The basic idea employed in the analysis of this integral follows Schiff[5] in his reduction of the integral in Eq. (23) of the present report.

remains after the angular integration is

$$\frac{1}{2ik}\int_{\rho}^{\infty} e^{2ik(\mu-\rho)}U(x',y',z'+\mu)d\mu,$$

and yields, therefore, terms of order (k^{-2}) and higher. Consequently, the leading term arises from the domain $\mu<\rho$ and is given by (A4). It is to be mentioned that no difficulty relative to the angular integration can occur for $\mu=\rho$. In this case, for small angles,

$$|\boldsymbol{\varrho}-\boldsymbol{\mu}|-(\rho-\mu)\cong\mu\theta,$$

with the result that the leading term of the integral over angles is now

$$\frac{-\mu}{4\pi}\int\frac{e^{ik\mu\theta}}{\mu^2\theta}U(\mathbf{r}'+\boldsymbol{\mu})\mu^2\theta d\theta d\phi=\frac{-2\pi\mu}{4\pi}\left|\frac{e^{ik\mu\theta}U(\mathbf{r}'+\boldsymbol{\mu})}{ik\mu}\right|_0^{\theta}$$

$$=\frac{1}{2ik}U(x',y',z'+\mu),$$

as before.

APPENDIX III

We wish to demonstrate here that the wave function

$$\psi(\mathbf{k}_0|\mathbf{r})=e^{i\mathbf{k}_0\cdot\mathbf{r}+\alpha(\mathbf{r})},$$

where

$$\alpha(\mathbf{r})=\frac{-i}{2k}\int_0^{\infty}U(\mathbf{r}-\hat{k}_0s)ds,$$

can be used as a trial solution in connection with the variational principles for $\psi(\mathbf{k}_0|\mathbf{r})$ which contain the Schrödinger operator $\nabla^2+k^2-U(\mathbf{r})$. Of course, the associated trial solution for the point source problem is everywhere outgoing. Therefore, it is required to prove that the surface integral

$$\int_{S'}\left\{\Psi(\mathbf{r},\mathbf{r}')\frac{\partial}{\partial r'}\delta\psi(\mathbf{k}_0|\mathbf{r}')-\delta\psi(\mathbf{k}_0|\mathbf{r}')\frac{\partial}{\partial r'}\Psi(\mathbf{r},\mathbf{r}')\right\}dS' \quad \text{(A5)}$$

vanishes in the limit $r'\to\infty$ when

$$\lim_{r'\to\infty}\delta\psi(\mathbf{k}_0|\mathbf{r}')=\lim_{r'\to\infty}[\text{trial }\psi(\mathbf{k}_0|\mathbf{r}')-\text{exact}\psi(\mathbf{k}_0|\mathbf{r}')]$$

$$=e^{i\mathbf{k}_0\cdot\mathbf{r}'+\alpha(\mathbf{r}')}-\left(e^{i\mathbf{k}_0\cdot\mathbf{r}'}+f(\mathbf{k}_0\to k\hat{r}')\frac{e^{ikr'}}{r'}\right)$$

$$=e^{i\mathbf{k}_0\cdot\mathbf{r}'}(e^{\alpha(\mathbf{r}')}-1)-f(\mathbf{k}_0\to k\hat{r}')\frac{e^{ikr'}}{r'},$$

and when

$$\lim_{r'\to\infty}\Psi(\mathbf{r},\mathbf{r}')\sim\frac{e^{ikr'}}{r'}A(\hat{r}',\mathbf{r}).$$

As indicated in (4), $A(\hat{r}',\mathbf{r})=\psi(-k\hat{r}'|\mathbf{r})$ when $\Psi(\mathbf{r},\mathbf{r}')$ is exact.

The second term in $\delta\psi$, the standard radiation condition, may be omitted at once. Thus, the problem reduces to evaluating

$$\lim_{r'\to\infty}\int_{S'}A(\hat{r}',\mathbf{r})\frac{e^{ikr'}}{r'}\left[\frac{\partial}{\partial r'}\{e^{i\mathbf{k}_0\cdot\mathbf{r}'}(e^{\alpha(\mathbf{r}')}-1)\}-e^{i\mathbf{k}_0\cdot\mathbf{r}'}(e^{\alpha(\mathbf{r}')}-1)ik\right]r'^2d\hat{r}', \quad \text{(A6)}$$

$$=\lim_{r'\to\infty}\int_{S'}A(\hat{r}',\mathbf{r})\frac{e^{ikr'}}{r'}\left[(e^{\alpha(\mathbf{r}')}-1)\frac{\partial}{\partial r'}e^{i\mathbf{k}_0\cdot\mathbf{r}'}-(e^{\alpha(\mathbf{r}')}-1)e^{i\mathbf{k}_0\cdot\mathbf{r}'}ik\right]r'^2d\hat{r}'$$

$$+\int_{S'}A(\hat{r}',\mathbf{r})\frac{e^{ikr'}}{r'}e^{i\mathbf{k}_0\cdot\mathbf{r}'}\frac{\partial}{\partial r'}e^{\alpha(\mathbf{r}')}r'^2d\hat{r}'. \quad \text{(A7)}$$

Let us first consider the integral on the left. The term in brackets, after incorporating the asymptotic form for $e^{i\mathbf{k}_0\cdot\mathbf{r}'}$ is

$$\frac{-2\pi i}{k}\left[(e^{\alpha(\mathbf{r}')}-1)ik\left\{\frac{e^{ikr'}}{r'}\delta(\hat{k}_0-\hat{r}')+\delta(\hat{k}_0+\hat{r}')\times\frac{e^{-ikr'}}{r'}-\frac{e^{ikr'}}{r'}\delta(\hat{k}_0-\hat{r}')+\delta(\hat{k}_0+\hat{r}')\frac{e^{-ikr'}}{r'}\right\}\right]$$

$$=+4\pi\delta(\hat{k}_0+\hat{r}')\frac{e^{-ikr'}}{r'}(e^{\alpha(\mathbf{r}')}-1),$$

and upon performing the integration over angles, the result for this part of the surface integral is

$$4\pi A(-\hat{k}_0,\mathbf{r})\{\exp[\alpha(-\hat{k}_0r')]-1\}. \quad \text{(A8)}$$

But,

$$\alpha(-\hat{k}_0r')=\frac{-i}{2k}\int_0^{\infty}U(-\hat{k}_0r'-\hat{k}_0s)ds$$

$$=\frac{-i}{2k}\int_{-\infty}^{-r'}U(0,0,t)dt=0 \text{ in the limit } r'\to\infty.$$

Hence, (A8) vanishes.

The integral on the right in (A7), when handled in a similar manner, reduces easily to

$$\lim_{r'\to\infty}\frac{2\pi i}{k}\left[A(\hat{k}_0,\mathbf{r})e^{2ikr'}\exp[\alpha(\hat{k}_0r')]\frac{\partial}{\partial r'}\alpha(\hat{k}_0r')-A(-\hat{k}_0,\mathbf{r})\exp[\alpha(-\hat{k}_0r')]\frac{\partial}{\partial r'}\alpha(-\hat{k}_0r')\right].$$

However,

$$\frac{\partial}{\partial r'}\alpha(\pm\hat{k}_0 r') = \frac{-i}{2k}\frac{\partial}{\partial r'}\int_0^\infty U(\pm\hat{k}_0 r' - \hat{k}_0 s)ds$$

$$= \frac{-i}{2k}\frac{\partial}{\partial r'}\int_{-\infty}^{\pm r'} U(0,0,t)dt,$$

where we have chosen z' in the direction $\hat{k}_0$. Therefore,

$$\frac{\partial}{\partial r'}\alpha(\pm\hat{k}_0 r') = \frac{-i}{2k}U(0,\,0,\,\pm r'),$$

and vanishes in the limit $r'\to\infty$ for bounded potentials. This concludes the proof that (A1) vanishes asymptotically.

PHYSICAL REVIEW VOLUME 109, NUMBER 5 MARCH 1, 1958

Phonon-Polaron Problem*

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(Received October 30, 1957)

The method of moments is employed to determine the ground state of the phonon-polaron system. The trial function employed in this calculation is a bare-electron wave function. It appears that the method is convergent for this problem. Although the energy is in general a complicated function of the parameter and must be determined numerically, it is possible to formally construct a power series expansion for the energy about the unperturbed energy in powers of the coupling constant. The first term in this series has been determined and agrees with the result of conventional perturbation theory. The second term has not yet been evaluated to all orders but it appears that it will have the opposite sign from the corresponding term in perturbation theory. The second and higher terms in some orders of approximation are singular for small values of the cutoff.

I. INTRODUCTION

THE phonon-polaron problem has been extensively studied both because of its intrinsic physical interest and because it is one of the simplest models of a field theory. Physically the system represents the interaction of the longitudinal optical mode of a polar crystal with an electron. The derivation of an appropriate Hamiltonian has been discussed at length[1] and in the present work the primary concern will be the mathematical discussion of this operator.

There are several quantities which it is of interest to calculate in this model. The simplest are the energy level and structure of the ground state. More complicated quantities are the scattering cross sections and the structure of the excited states. The description of the ground state has been carried out at considerable length and quite successfully by several authors.[1,2] The purpose of the present work is to describe an alternate method of approach. The results obtained are not quite as strong as some previously attained; however, it seems likely that the present method can be extended to improve them. There also is an interesting suggestion on the existence of the power series expansion.

The Hamiltonian[1] is

$$H = \frac{p^2}{2m} + \omega\sum_{\mathbf{k}} a_{\mathbf{k}}^* a_{\mathbf{k}} + \sum_{\mathbf{k}}(a_{\mathbf{k}} V_{\mathbf{k}} e^{i\mathbf{k}\mathbf{r}} + a_{\mathbf{k}}^* V_{\mathbf{k}}^* e^{-i\mathbf{k}\mathbf{r}}).$$

The sums are cut off for $k>K$. The first two terms in this expression represent the energy of the noninteracting systems, $p^2/2m$ is the kinetic energy of the electrons and $a_{\mathbf{k}}^* a_{\mathbf{k}}$ is the number of phonons of wave number $\mathbf{k}$. The number of phonons multiplied by the energy ω which is independent of $\mathbf{k}$ gives the total energy in the phonon field. The a's are the usual creation and annihilation operators with the commutation rule $[a_{\mathbf{k}}, a_{\mathbf{k}'}^*] = \delta_{\mathbf{k}\mathbf{k}'}$. The second term is the coupling of the electron to the phonon field. The V's, which are defined by

$$V_k = -\frac{i\omega}{k}\left(\frac{4\pi\alpha}{V}\right)^{\frac{1}{2}}\left(\frac{1}{2m\omega}\right)^{\frac{1}{4}},$$

are the amplitudes for the emission and absorption of phonons, while the exponential factors take into account the electron recoil. The dimensionless number α gives the strength of coupling. In units in which $\hbar$ and c are unity, H/ω is dimensionless and it is the operator H/ω which is considered in the following discussion.

* This work was supported by the Office of Naval Research and the U. S. Atomic Energy Commission.

† A portion of this work was carried out while the author was employed at the Radiation Laboratory, University of California, Berkeley, California.

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