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Approximate Green function for a semi-infinite solid with varying properties

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Abstract. An expression is derived for the spatially dependent Green function or response function in a solid occupying a half-space and having generally varying properties. The expression is valid in the same range as the WKB approximation, namely for slowly varying properties. Some generalisation is indicated and the time-dependent Green function or the resolvent is obtained as a Fourier transform.

1. Introduction

An electric field penetrating into a semi-infinite solid interacts with the particles in the medium. An example of this situation is the excitonic polariton studied by Hopfield and Thomas (1963), Maradudin and Mills (1973), Balslev (1981) and Lagois (1981). The mathematical formulation of the problem leads to a set of differential equations inhomogeneous in the electric field, which are customarily solved by means of Green functions, resolvents, response functions, etc. The methods of solution are of interest in a broader range of problems as well.

A Schrödinger equation for a semi-infinite medium with space-varying properties has been solved using the WKB (Wentzel–Kramers–Brillouin) approximation by Goodman (1971) who discussed the validity of his solution. Green functions in a homogeneous half space were obtained by Oliveros and Tilley (1982, 1983). In this paper we consider a half-space with spatially varying properties and propose an approximation for the Green function. Because of the connection of the method to the WKB solution of differential equations (Fröman and Fröman 1965, Jacobsson 1966), we start by studing this problem first.

2. A differential equation

The differential equation for the half space $x \geqslant 0$,

$$[(\mathrm{d}^2/\mathrm{d}x^2) + q^2(x)]f(x) = 0 \tag{1}$$

with $\operatorname{Im} q(x) > 0$, has the well known approximate WKB solution

$$f(x) = \frac{a}{\sqrt{q(x)}} \exp\left(\mathrm{i} \int^x q(\xi)\, \mathrm{d}\xi\right) + \mathrm{O}\left(\frac{q'''}{q^4}, \frac{(q')^2}{q^4}\right) \tag{2}$$

a being a constant. The error terms indicate that the solution is accurate when the variation of $q(x)$ is slow, i.e. in the so-called long wavelength limit. If (1) is the Schrödinger equation, then

$$q^2 = 2M[E - V(x)]/\hbar^2 \tag{3}$$

M being the mass, E the energy and $V(x)$ the potential. In this context equation (2) represents a semi-classical approximation, which arises from a series expansion of the exact, exponential solution of (1), namely

$$f(x) = a \exp \mathrm{i} \int^x Q_+(\xi)\, \mathrm{d}\xi \tag{4}$$

where Q_+ satisfies the nonlinear differential equation for $Q(x)$:

$$Q^2(x) - q^2(x) - \mathrm{i}\, \mathrm{d}Q(x)/\mathrm{d}x = 0 \tag{5}$$

where $\mathrm{Im}\, Q_+(x) > 0$. WKB type solutions are obtained by regarding the third term in (5) as small. Twice iterated solutions of (5) are

$$Q_\pm = \pm q + (\mathrm{i}/2)\, \mathrm{d} \ln q/\mathrm{d}x + \ldots \tag{6}$$

where $\mathrm{Im}\, Q_-(x) < 0$. To the written accuracy Q_+ leads to (2).

3. Spatial Green function

Surprisingly, no analogous expression seems to exist in the scientific literature for the Green function $G(x, x')$, defined for $x, x' \geqslant 0$ by the equation:

$$[(\partial^2/\partial x^2) + q^2(x)]G(x, x') = -4\pi\delta(x - x') \tag{7}$$

and subject to some boundary conditions, e.g. the Dirichlet boundary condition: $G(0^+, x') = 0$, or the Neumann boundary condition: $\partial G(x, x')/\partial x = 0$ as $x \to 0^+$; $G \to 0$ as x or $x' \to \infty$ (Morse and Feshbach 1953, Blinder 1975).

Equation (7) describes the behaviour of the system in the positive half-space x in which a unit force or source acts at a point x'. The effect of a distribution of sources can be obtained by superposition of solutions. We wish to show that the WKB-type Green function, subject to the same errors as in (2), is

$$G(x, x') = \frac{2\pi \mathrm{i}}{\sqrt{q(x) q(x')}} \left[\exp\left(\mathrm{i} \int_{\min(x,x')}^{\max(x,x')} q(\xi)\, \mathrm{d}\xi \right) - U \exp\left(\mathrm{i} \left[\int_0^x + \int_0^{x'} \right] \right) q(\xi)\, \mathrm{d}\xi \right] + \mathrm{O}\left(\frac{q'^2}{q^4}, \frac{q'''}{q^4} \right) \tag{8}$$

where max and min represent the greater and the lesser of the two arguments; $U = 1$ for Dirichlet boundary conditions, $U = -1$ for Neumann boundary conditions and U takes some intermediate value for other boundary conditions.

Proof. An exact solution of (7) is of the form

$$G(x, x') \equiv G_1 + G_2 = g_s(x') \exp\left(\mathrm{i} \int^x Q_s(\xi)\, \mathrm{d}\xi \right) + G_2(x, x') \tag{9}$$

where G_2 is a solution of the homogeneous equation for G, ensuring that the boundary conditions are satisfied by G,

$$s = \text{sign}(x - x') \tag{10}$$

and Q_s is one of the solutions of (5). In order that the first term in (9) shall match the inhomogeneous part of (7), $\partial G(x, x')/\partial x$ must exhibit a jump of -4π as x crosses x' from below. Evaluating the derivative at $x = x' \pm 0$ we obtain

$$\begin{aligned}(\partial/\partial x)G_1(x, x') &= \mathrm{i}g_s(x')Q_s(x')\exp\left(\mathrm{i}\int^x Q_s(\xi)\,\mathrm{d}\xi\right) \qquad \text{as } x \to x' \\ &= s2\pi(-1).\end{aligned} \tag{11}$$

We have equated (11) with -2π for $x = x' + 0$ and with 2π for $x = x' - 0$, thus obtaining the desired -4π jump. We can solve for g_s and arrive at

$$G(x, x') = \frac{2\pi\mathrm{i}}{sQ_s(x')}\exp\left(\mathrm{i}\int_{x'}^{x} Q_s(\xi)\,\mathrm{d}\xi\right) + G_2(x, x'). \tag{12}$$

At $x = 0$, $s = -$, whence

$$G_2(x, x') = U\frac{2\pi\mathrm{i}}{Q_-(x')}\exp\left[-\mathrm{i}\left(\int_0^{x'} Q_-(\xi) - \int_0^{x} Q_+(\xi)\right)\mathrm{d}\xi\right]$$

is appropriate to satisfy the boundary conditions there. In the WKB limit (equation (6)) one obtains the solution given in (8). Higher-order corrections are provided by Jacobsson (1966).

4. Time dependence

To obtain the time-dependent Green function (Morse and Feshbach 1953, Blinder 1975) satisfying

$$[(\partial^2/\partial x^2) + q^2(x, \partial/\partial t)]G(x, t; x', t') = -4\pi\delta(x - x')\delta(t - t') \tag{13}$$

we make one Fourier transformation (denoted by a horizontal bar)

$$\bar{G}(x, \omega; x', t') = \int_{-\infty}^{\infty} \mathrm{e}^{\mathrm{i}\omega t}\, G(x, t; x', t')\,\mathrm{d}t$$

which is the solution of

$$[(\partial^2/\partial x^2) + q^2(x, -\mathrm{i}\omega)]\bar{G}(x, \omega; x', t') = -4\pi\delta(x - x')\,\mathrm{e}^{\mathrm{i}\omega t'}.$$

Now clearly

$$\bar{G}(x, \omega; x', t')\,\mathrm{e}^{-\mathrm{i}\omega t'} \equiv G(x, x'; \omega)$$

is independent of t' and is in fact the solution of the purely spatial equation, (7), with the addition that in q^2 there now appears ω as a parameter. Using for $G(x, x'; \omega)$ either the formal solution, given in (12), or the WKB approximation, appearing in (8), we transform back to obtain the formal solution

$$G(x, t; x', t') = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}\omega\, \exp[\mathrm{i}\omega(t' - t)]G(x, x'; \omega). \tag{14}$$

Physical applications of our results to the reflectivity of a medium with spatial dispersion will be the subject of a later publication.

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References

Balslev I 1981 *Solid State Commun.* **39** 359–62

Blinder S M 1975 *Configuration Space Green's Functions* in *International Review of Science, Physical Chemistry, Series Two* vol 1, ed A D Buckingham and C A Coulson (London: Butterworths) pp 1–41

Fröman N and Fröman P O 1965 *JWKB Approximation* (Amsterdam: North-Holland)

Goodman F O 1971 *J. Chem. Phys.* **55** 5742–53

Hopfield J J and Thomas D G 1963 *Phys. Rev.* **132** 563–72

Jacobsson R 1966 *Light Reflection From Films of Continuously Varying Refractive Index* in *Progress of Optics* vol 5, ed E Wolf (Amsterdam: North-Holland) pp 247–86

Lagois J 1981 *Phys. Rev.* B **23** 6611–20

Maradudin A A and Mills D L 1973 *Phys. Rev.* B **7** 2787–810

Morse P M and Feshbach H 1953 *Methods of Theoretical Physics Part I* ch 7 (New York: McGraw-Hill)

Oliveros M C and Tilley D R 1982 *J. Phys. C: Solid State Phys.* **15** 4289–304

—— 1983 *J. Phys. C: Solid State Phys.* **16** 487–502