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Theoretical Concept and Model of Metal Surface Response

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Abstract: ***To calculate the response of a metal surface from microscopic quantum mechanical models in a formidable task of heavy computation. It is the therefore desirable to drive the answer to question of metal optics from macroscopic relation between fields, current and charge densities. Such a phenomenological approach is simpler to handle often more transparent and easier adaptable to real experiments The HD with ABC is the most successful approximation for this purpose.***

Keywords: Additional Boundary condition, Theoretical Physics, Metal Optics

1. Introduction

The dielectric function ε is related by linear response theory to a microscopic description of the system. The response functions are generally tensors and nonlocal in space and time. A system is called spatially dispersive and its response function depends on wave vector K which is mathematically related to the non-locality. Much effort have been spent in calculating $\varepsilon(\bar{k},\omega)$ for bulk metals. But the knowledge of the bulk response is not sufficient to solve the problem of metal optics since the surface breaks the translational invariance of the system. Then $\varepsilon(\bar{k},\omega)$ depend on $\bar{r}$ and $\bar{r}'$ separately and not only on the difference $(\bar{r}-\bar{r}')$. There have been many attempts to driven the response near the surface from the known response function of the bulk. The hydrodynamic approximation is the simplest approach and the one used most successfully.

2. Additional Boundary Condition or Susceptibility

The hydrodynamic model in conjunction with additional boundary conditions as presented is one way to treat optical problems at metal surfaces. Due to its simplicity transparency, and flexibility this method has been widely used for the interpretation of experiments. In this chapter we have discussed other attempts to calculate electromagnetic fields at metal surfaces. A response theory on an intermediate level, which describes measurable response properties such as reflectivity, absorbance etc in terms of certain surface response functions, but which does not try to calculate surface electromagnetic fields.

Attempts to calculate surface electromagnetic fields have been made by many authors with many different model assumptions, mostly on a phenomenological, but also on a microscopic level. This microscopic theory introduced the surface on the quantum mechanical level of wave functions. Linear response theory then yields the electromagnetic response of the system with surface in terms of a certain susceptibility, e.g. in the form.

$$j(r,\omega) = \int d^3r^1 \overleftrightarrow{\sigma}(r,r^1,\omega)E(r^1,\omega) \qquad ..(1)$$

With an explicit expression for the nonlocal conductivity $\overleftrightarrow{\sigma}$. Together with Maxwell's equations, the material equation (1) yields a set of couple Integra-differential equation, which determines uniquely the response to incoming electromagnetic radiation. Microscopic calculations require a substantial amount of computational work.

The phenomenological approaches attempts to use the knowledge of bulk response. This leads to the long standing problem of additional boundary condition (ABC) in phenomenological optics, which has been a matter of debate since PEKAR[1] proposal in the context of excitation polarization in semiconductors. According to the manner in which the bulk response properties are introduced, the read for ABC become apparent or not. Some auther[2-4] claimed that it is not necessary to worry about ABC, because mathematics automatically solves the problem. They argued that, if the homogeneous bulk medium responds according to

$$j(r,\omega) = \int d^3r^1 \overleftrightarrow{\sigma}(r-r^1,\omega)E(r',\omega) \qquad ..(2)$$

The response of the system containing the medium only in the half space z>0 is given by the same expression (2) provide both r and r^1 are restricted to the half space. For this surface model which was termed the "dielectric approximation", the susceptibility is obtained from the corresponding bulk susceptibility simply by truncation.

$$\overleftrightarrow{\sigma}^{DA}(r,r^1,\omega) = \theta(z)\theta(z^1)\overleftrightarrow{\sigma}^{h}(r-r^1,\omega) \qquad \ldots (3)$$

With θ(z) = 1 for z>0, θ(z) = 0 for z<0 BISHOP and MARADUDIN[5] pointed out that, in the case of a spatially dispersive semiconductor, model (3) leads to a discontinuity of the energy current at the surface, which then acts as a source or sink of energy. They tried to repair this defect by introducing additional surface forces.

In fact, (3) is not a necessary mathematical consequence of (2).

A whole class of susceptibilities for the surface problem.

$$\overleftrightarrow{\sigma}^{(U)}(r,r^1,\omega) = \theta(z)\theta(z^1)\left[\overleftrightarrow{\sigma}^{h}(r-r^1,\omega)+U\overleftrightarrow{\sigma}^{h}(r-r^1,\omega)\vec{\alpha}\right] \quad \ldots. \quad (4)$$

Where U is a model parameter and

$$\vec{\alpha} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad \ldots.. (5)$$

Describe reflection at the surface, is compatible with the bulk formula (2) and has been considered in the Literature[6-11] the special value U = +1 can be physically motivated by specular reflection arguments, and implies simple and reasonable boundary conditions for currents and fields. In general, the choice of model susceptibility uniquely determines the response of the system and consequently, the behaviour of currents and field at the surface, although it may not be possible to express this behaviour in terms of simple boundary condition (e.g. for U = 1). If boundary conditions are imposed by physical requirements, the admissible susceptibilities will be restricted.

The relation between ABC and susceptibility becomes especially transparent, if the information about the response of the homogeneous bulk medium is not directly taken from the real space material equation (2), but from this Fourier transform $j(k,\omega) = \overleftrightarrow{\sigma}^{h}(k,\omega)E(k,\omega)$. The latter is formally equivalent with an equation of the type

$$\vec{W}j(r,\omega) = E(r,\omega) \quad \ldots\ldots (6)$$

In real space, where $\vec{W}$ is a differential operator containing spatial derivatives, an example, the hydrodynamic model[12] can be cast into this form with

$$\overleftrightarrow{W}_{HD}j = \frac{4\pi}{i\omega\omega_p}\left[\omega(\omega+i\gamma)j+\beta\nabla(\nabla.j)\right] \ldots (7)$$

the nonlocal conductivity $\vec{\sigma}(r,r^1,\omega)$ is an inverse of the operator$\vec{W}$, i.e. Green's function of (6). Since in general the corresponding homogeneous equation$[(6) or\ E = 0]$ has non-trivial solutions, boundary conditions are necessary to uniquely determine the Green's function, i.e. the conductivity. In the homogeneous bulk case, these are the conditions of outgoing plane waves, which are automatically taken into account by the Fourier Transform, and lead to (2)

3. Discussion

In the form (6) it is clear how to use the bulk response properties right up the surface: all the material parameters defining $\vec{W}[(e.g.\omega_p,\gamma,\beta\ in\ (7)]$ all have their bulk values up to the surface plane. To complete the surface model, boundary condition (the ABC) must be specified and then the Green's function $(r,r^1,\omega)$for the surface problem is uniquely defined. As an example one consider a generation of the hydrodynamic model which allows a satisfy alternatively two different sets of reasonable ABC leading to different results for$\vec{\sigma}(r,r^1,\omega)$. The result for Pekar's ABC, $j(z=0^+)=0$, is not of the form (4) and cannot be expressed in terms of bulk conductivity $\vec{\sigma}(r-r^1,\omega)$. The mentioned phenomenological approaches both have their merits and limitations. To hydrodynamic and similar approximation are easy to handle, and (6) together with Maxwell's equation can be solved, even without explicit evaluation of the Green's function, by a suitable ersatz of partial waves. The method is also easily adapted to metal-metal interfaces. However, his method works only if the differential operator $\vec{W}$ in (6) is sufficiently simple, if the bulk conductivity has a complicated analytical dependence on the wave vector k, as e.g. the Lind hard function which contains branch cut, the method cannot be applied. The specular reflection model and related models, (4) are on the other hand, free from this limitation and work for any bulk response function. They are however not easily generalized to metal-metal interfaces, although attempts in this direction have recently been made[13]. Moreover, there are sets of physically reasonable ABC, which cannot be satisfied by this method.

4. Conclusion

One focus attention on the free vacuum-metal surface, and in the phenomenological discussion, on sharp, single-stepped surface Hydrodynamic models of the form (6) with position-dependent material parameters inter polluting smoothly between the metal and vacuum side have also been considered[15-17]. These models usually require a lot of computational work, already for the evaluation of the material equation.

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