The deconstructed hydrodynamic model for plasmonics

Paul Kinsler

Physics Department, Lancaster University, Lancaster LA1 4YB, United Kingdom, and Cockcroft Institute, Sci-Tech Daresbury, Daresbury WA4 4AD, United Kingdom.

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I give an exact but deconstructed version of the second-order wave-like equation that encapsulates the hydrodynamic model for plasmonics. Comprising two first order equations, the deconstruction has potential uses in understanding or interpreting the hydrodynamic model, since its meaning is not obscured by approximation. However, as the physical interpretation of the deconstructed model is difficult, due to the choice of the polarization as the significant quantity, I also consider an alternate model based on the polarization current. This alternate model has a clear and direct physical interpretation.

I. INTRODUCTION

The hydrodynamic model for plasmonics (HMP) \cite{1} has recently found widespread popularity in the field of plasmonics. One of its key features is that unlike simpler plasmonics approaches based on the Drude model, it incorporates spatial derivatives terms which represent the dynamics of the charge distribution. Although these are often called “non-local” effects, they are more usefully called propagation effects, since they are not non-local in any sense that violates relativistic constraints on the physics. However, although much of its usage in plasmonics is recent, the basic model itself dates back to the 1970’s \cite{2} and has been used in a number of other contexts \cite{3, 4}.

Since it is most efficient to direct the reader interested in the physical basis and assumptions of the HMP to the motivation, derivation, and exposition of Ciraci et. al \cite{1}; here we will simply repeat their relevant equation \eqref{eq:1}, which describes the how the wave-like response of the charge distribution in the material appears as a standard electromagnetic polarization. It is

\[ \partial_t^2 \mathbf{P} + \gamma \partial_t \mathbf{P} - \nabla \beta^2 \nabla \cdot \mathbf{P} = \varepsilon_0 \alpha \beta^2 \mathbf{E}, \tag{1} \]

where we should remember that the polarization field \( \mathbf{P} \equiv \mathbf{P}(t, \mathbf{r}) \) and the driving electric field \( \mathbf{E} \equiv \mathbf{E}(t, \mathbf{r}) \). In the following I prefix all equation numbers from this reference with CPS, so that the above is then (CPS14). In this equation we note that the parameter \( \beta \) is defined by

\[ \beta^2 = \frac{2E_F}{3m_e} \tag{2} \]

where \( E_F \) is the Fermi energy and \( m_e \) is the electron mass. Also, \( \gamma \) is the polarization decay rate, \( \varepsilon_0 \) is the permittivity of vacuum, \( \omega_p = \sqrt{n_e e^2 / \varepsilon_0 m_e} \) is the plasma frequency, \( n_e \) is the background electron number density, and \( e \) the electron charge. Key features of the derivation are (a) the substitution of the polarization \( \mathbf{P} \) for the (polarization) current \( \mathbf{J} \), (b) the dropping of all but the dominant term in the Lorentz force equation, and (c) assuming that the fluctuations in the polarization and/or charge densities are small. Here step (a) in particular results in the above equation for \( \mathbf{P} \), a useful feature when we plan to link the plasmonic behaviour to that of the electric field, since it allows us to define an effective permittivity. However, the replacement of \( \mathbf{J} \) is not strictly necessary, and the derivation can proceed without it.

For the purposes of my discussion here, it is important to note that this model is not exactly equivalent to the starting assumptions used in its derivation. While this is of course completely natural, given the approximations made in the derivation, and is indeed in itself an unremarkable statement, given the ubiquity of the role of approximations in physical model-making, we might still ask the question: What is this approximate HMP model exactly equivalent to?

In Section \textbf{II} I present a physical model which is exactly equivalent to the HMP, and discuss some of the implications, while in Section \textbf{III} I show how an alternative form based on the polarization current \( \mathbf{J} \) has a simpler physical interpretation. Lastly, in Section \textbf{IV} I summarize the results.

II. DECONSTRUCTION OF THE HMP

We can deconstruct the HMP into two first order pieces, one defining how (scaled) charge density gradients drive changes in the dielectric polarization, along with losses; and the other defining how the divergence of the polarization drives changes in a quantity related to the charge density, along with the effect of the electric field potential.

The deconstructed HMP (D-HMP) equations are

\[ \partial_t \mathbf{P} = \nabla \Psi - \gamma \mathbf{P} \tag{3} \]
\[ \partial_t \Psi = \nabla \cdot \mathbf{P} + \alpha \phi \tag{4} \]

where \( \Psi(t, \mathbf{r}) = \sigma \mathbf{J}(t, \mathbf{r}) \) and there is a scalar electric potential \( E(t, \mathbf{r}) = \nabla \phi(t, \mathbf{r}) \). Although we could have put the driving electric field in \eqref{eq:4}, it would have to have been in the form of the time-integral of the field, and so disrupting the causal interpretation of the equation \cite{5}.

Note that these two equations are very similar to a modified and reinterpreted version of “p-acoustics” \cite{6, 7, 8}, albeit with extra driving terms.
A. Equivalence

To demonstrate that these two coupled first-order D-HMP equations are in fact equivalent to the second-order HMP equation, we can combine them. We first take the time derivative of (3), then substitute in (4), so that

\[
\frac{\partial^2}{\partial t^2} P = \nabla \frac{\partial}{\partial t} \Psi - \gamma \partial_i P \\
= \nabla \frac{\partial}{\partial t} \sigma^{-1} \Psi - \gamma \partial_i P \\
= \nabla \sigma^{-1} \frac{\partial}{\partial t} \Psi - \gamma \partial_i P \\
= \nabla \sigma^{-1} \nabla \cdot P + \nabla \sigma^{-1} \alpha \phi - \gamma \partial_i P \\
= \nabla \sigma^{-1} \nabla \cdot P + \sigma^{-1} \alpha \nabla \phi - \gamma \partial_i P \\
= \nabla \sigma^{-1} \nabla \cdot P + \sigma^{-1} \alpha \mathbf{E} - \gamma \partial_i P. \tag{10}
\]

In doing this we have necessarily made some assumptions, namely that \( \sigma \) is a fixed parameter with no time or space dependence, and that \( \alpha \) has no space dependence. These assumptions are unremarkable, since both the original HMP model and this one are predicated on being in a homogeneous background. However, with this new D-HMP, we could allow them to vary and so derive a more general version of (10).

Although (10) is structurally similar to (1), to show they are identical we need to fix the parameters \( \sigma \) and \( \alpha \). By comparing terms, we straightforwardly find that

\[
\sigma = \beta^{-2} = \frac{3n_e}{2E_F}, \tag{11}
\]

and

\[
\sigma^{-1} \alpha = \varepsilon_0 \omega_0^2 = \frac{3n_e e^2}{2E_F}. \tag{12}
\]

Hence our D-HMP equations have combine to form exactly the HMP model equation from (1), i.e.

\[
\frac{\partial^2}{\partial t^2} P + \gamma \partial_i P - \nabla \beta^2 \nabla \cdot P = \varepsilon_0 \omega_0^2 \mathbf{E}. \tag{13}
\]

Now, let us briefly reiterate the distinction between the two models, a difference which exists despite the fact that (1) and (13) are identical:

- Eqn. (1) is an approximation to the HMP’s starting point, which considers the dynamics of an electron fluid dynamics on an otherwise homogeneous background, i.e. (CPS3) and following equations.
- Eqn. (13) is an exact counterpart to the D-HMP’s starting point of coupled polarization and charge density equations on an otherwise homogeneous background, i.e. (5), (6).

B. Interpretation

The two equations (5), (6) are not seen in the usual derivation (1). The distinction is primarily due to the fact that the HMP starting point in (1) focuses on charge density, charge fluid velocity, and current; whereas the result looks at polarization \( \mathbf{P} \), which is the time integral of the current. This time-integral property of the polarization can make interpretations somewhat tricky\(^1\), as here, although the drawbacks are usually minor compared to the advantage it provides in allowing us to use it as an input to macroscopic electrodynamics, i.e. in writing \( \mathbf{D} = \varepsilon_0 \mathbf{E} + \mathbf{P} \).

Since the D-HMP is a deconstruction of the HMP result, this means that the other D-HMP quantities are, like polarization, also time integrated quantities – hence the appearance of the scalar electric potential \( \phi \) in place of the electric field \( \mathbf{E} \).

The \( \Psi, \psi \) quantities are likewise related to the time integral of the number and/or charge densities, which might therefore be thought of as (called) “accumulations” rather than densities.

The first equation (5) is force-law like:

\[
\partial_t P = \nabla \psi - \gamma P,
\]

with changes in polarization \( P \) following from gradients in the potential–like accumulation field \( \psi \); and from linear losses proportional to \( \gamma \).

The second equation (6) is conservation-law like:

\[
\partial_t \Psi = \nabla \cdot \mathbf{P} + \alpha \phi,
\]

with changes in the the accumulation field \( \Psi \) following from the divergence – local inflows or outflows – of the polarization; whilst also being augmented by driving from the electric scalar potential.

The fact that this conservation equation is for this new (and perhaps somewhat mysterious) accumulation field \( \Psi \), and further, is driven by the electric potential rather than the electric field, is a result of the requirement for a dynamic equation for \( \mathbf{P} \) rather than a well-defined microscopic quantity such as (e.g.) current \( \mathbf{J} \).

III. CURRENT-BASED FORM: THE J-HMP

We have seen above that the interpretation of the standard D-HMP model is physically rather unsatisfactory. However, this situation can be avoided by instead using an equation for the polarization current \( J(t, \mathbf{r}) \), rather than its time integral, the polarization \( \mathbf{P}(t, \mathbf{r}) \) itself. We can generate such an expression by simply taking the time-derivative of (1) and substituting \( \mathbf{J} \) for \( \partial_t \mathbf{P} \); but for the interested reader it is nevertheless worth-while to revisit the derivation of Ciraci et. al (1), and seeing that it still follows without the substitution. The modified current-based version of (CPS14) and (1) is

\[
\frac{\partial^2}{\partial t^2} \mathbf{J} + \gamma \partial_i \mathbf{J} - \nabla \beta^2 \nabla \cdot \mathbf{J} = \varepsilon_0 \omega_0^2 \partial_t \mathbf{E}. \tag{14}
\]

We can deconstruct this “J-HMP” into two first order pieces, one defining how charge density gradients drive changes in the polarization current, along with losses; and the

\footnotetext{1}{See also e.g. Faraday’s Law [9]}
other defining how the divergence of the polarization current drives changes in the charge density.

The deconstructed J-HMP (DJ-HMP) equations are

$$\partial_t J = \nabla \sigma \eta - \gamma J + \alpha' \beta E$$  \hspace{1cm} (15)

$$\partial_t N = \nabla \cdot J$$ \hspace{1cm} (16)

where \(N(t, r) = \sigma \eta(t, r)\). Here \(N\) is a linear polarization charge density (in units \(C/m\)), and \(\eta\) is a closely related “current velocity” quantity (in units \(C/m^2\)).

Note the different handling of the driving field in this version, which can now act straightforwardly on the polarization current without introducing problems.

### A. Equivalence

To demonstrate that these two coupled first-order DJ-HMP equations are in fact equivalent to the second-order J-HMP equation, we can combine them. We first take the time derivative of (3), then substitute in (4), so that

$$\partial_t^2 J = \nabla \partial_t \eta - \gamma \partial_t J + \alpha' \partial_t E$$ \hspace{1cm} (17)

$$= \nabla \partial_t \sigma^{-1} N - \gamma \partial_t J + \alpha' \partial_t E$$ \hspace{1cm} (18)

$$= \nabla \sigma^{-1} \partial_t N - \gamma \partial_t J + \alpha' \partial_t E$$ \hspace{1cm} (19)

$$= \nabla \sigma^{-1} \nabla \cdot J - \gamma \partial_t J + \alpha' \partial_t E.$$ \hspace{1cm} (20)

Here we have, as previously, assumed that \(\sigma\) is a fixed parameter with no time or space dependence, and also that \(\alpha'\) is independent of time. These assumptions are unremarkable, since both the original HMP model, the J-HMP one, and this one are predicated on being in a homogeneous background. However, with this new DJ-HMP, just as with the D-HMP, we could allow them to vary and so derive a more general version of (20).

Although (20) is structurally similar to (14), to show they are identical we need to fix the parameters \(\sigma\) and \(\alpha'\). Fortunately these are the same as for the D-HMP model, but with a driving strength \(\alpha' = \sigma^{-1} \alpha\). Hence our DJ-HMP equations combine to form exactly the J-HMP model equation from (14), i.e.

$$\partial_t^2 J + \gamma \partial_t J - \nabla \beta \partial_t \nabla \cdot J = \epsilon_0 \omega_0^2 E.$$ \hspace{1cm} (21)

The distinctions between the J-HMP model and the DJ-HMP model are exactly analogous to the distinctions between the HMP model and the D-HMP one.

### B. Interpretation

Examining the DJ-HMP model equations (15) and (16) we see that we now have a very much more straightforward interpretation.

The first equation (15) is force-law like:

$$\partial_t J = \nabla \eta - \gamma J + \alpha' \beta E,$$

with changes in polarization current \(J\) following from gradients in the scaled charge density (i.e. \(\eta = \sigma^{-1} N\)), from linear losses proportional to \(\gamma\), and the driving effect of the electric field \(E\).

The second equation (16) is conservation-law like:

$$\partial_t N = \nabla \cdot J,$$

with changes in the polarization charge density \(N\) following from the divergence – local inflows or outflows – of the polarization current.

The single drawback of this form is that, without a direct expression for \(P\), it is not as simple to construct the effective permittivity resulting from the plasmonic response. However, it is easy enough – we just have to time-integrate the polarization current \(J\); either that, or take a more microscopic view of solving Maxwell’s equations.

### IV. CONCLUSION

The proposal made here is that when trying to understand the behaviour of the HMP, it can be useful to (first) understand it in terms of the D-HMP. This is because the D-HMP equations do not suffer from the conflated effects of the serial approximations used in the HMP derivation. While a discussion of the behavior of the HMP model might easily get bogged down over ambiguities introduced by any of the approximations utilised in the HMP derivation, this possibility is avoided in the D-HMP equations.

However, we also see that the D-HMP equations have a somewhat obscure physical interpretation. This lead us to reformulate the plasmonic response in terms of the polarization current in the DJ-HMP model, an uncomplicated procedure that clarified the physical meaning, but left us without a direct expression for the behaviour of the polarization.
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Appendix: HMP for $\Psi$

As an exercise, I do the substitution in the reverse order to derive a second order wave-like equation for $\Psi$. We have

\begin{align}
\partial_t^2 \Psi &= \nabla \cdot \partial_t \mathbf{P} + \alpha \partial_t \phi \\
&= \nabla \cdot (\nabla \Psi - \gamma \mathbf{P}) + \alpha \partial_t \phi \\
&= \sigma^{-1} \nabla \cdot \nabla \Psi - \gamma \nabla \cdot \mathbf{P} + \alpha \partial_t \phi \\
&= \sigma^{-1} \nabla \cdot \nabla \Psi - \gamma (\partial_t \Psi - \alpha \phi) + \alpha \partial_t \phi \\
&= \nabla \cdot \beta^2 \nabla \Psi - \gamma \partial_t \Psi + n_0 m_e \left( \frac{3e}{2Ef} \right)^2 (\partial_t \phi + \gamma \phi) .
\end{align}

Not unexpectedly, we see the same phase velocity $\beta$. Less conveniently, the driving term is no longer simply dependent on $\mathbf{E}$, depending instead on a combination of its time derivative and a loss-dependent fraction of itself.

However, if the driving electric field is CW at a frequency $\omega_0$ and wavevector $\mathbf{k}$, so that

$$\phi = \phi_0 \exp [i (\omega_0 t - \mathbf{k} \cdot \mathbf{r})].$$

Along the propagation direction, we know that $k$ is the spatial derivative of the potential, so that with $E_0 = k\phi_0$

$$E = E_0 \exp [i (\omega_0 t - \mathbf{k} \cdot \mathbf{r})].$$

Thus simplifying and assuming that propagation is along $x$ with $\bar{\alpha} = \alpha |\omega_0 + \gamma| \mathbf{k}$, and absorbing any phase into $\phi$,

\begin{align}
\partial_t^2 \Psi &= \nabla \cdot \beta^2 \nabla \Psi - \gamma \partial_t \Psi + i \alpha (\omega_0 + \gamma) k^{-1} E_0 e^{(\alpha x - kx + \phi)} \\
&= \nabla \cdot \beta^2 \nabla \Psi - \gamma \partial_t \Psi + \bar{\alpha} E_0 e^{(\alpha x - kx + \phi)} .
\end{align}