PHYSICAL REVIEW E VOLUME 47, NUMBER 4 APRIL 1993

Short-time electric-field dynamics at a neutral point in strongly coupled plasmas

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(Received 28 October 1992)

Recent theoretical analyses of the two-time joint-probability density for electric-field dynamics in a strongly coupled plasma have included formal short-time expansions. Here we compare the short-time-expansion results for the associated generating function with molecular-dynamics-simulation results for the special case of fields at a neutral point in a one-component plasma with plasma parameter $\Gamma=10$. The agreement is quite good for times $\omega_p t \leq 2$, although more general application of the short-time expansion requires some important qualifications.

PACS number(s): 52.25.$-$b, 05.40.$+$j, 05.20.Gg, 05.90.$+$m

I. INTRODUCTION

The radiative and transport properties of an impurity (ion or atom) in a plasma are determined largely by the local electric field $\mathbf{E}(t)$. The characterization of this field as a function of time provides the primary description of the plasma environment on the impurity. The probability density for finding a field value $\boldsymbol{\varepsilon}$ at a given time $Q(\varepsilon)$ has been studied for some time and there are quite accurate approximations for practical calculation even under conditions of strong coupling [1]. In contrast, the joint distribution for a field value $\boldsymbol{\varepsilon}'$ at time 0 and a value $\boldsymbol{\varepsilon}$ at time t, $Q(\boldsymbol{\varepsilon},t;\boldsymbol{\varepsilon}',0)$, has received little attention until recently [2–5]. Even the results for an ideal-gas environment (Holtsmark limit) are not known for this latter case [6].

References [3] and [4] studied a number of formally exact limits for $Q(\boldsymbol{\varepsilon},t;\boldsymbol{\varepsilon}',0)$. One of these is the short-time limit of the generating function associated with $Q(\boldsymbol{\varepsilon},t;\boldsymbol{\varepsilon}',0)$. It was noted there that the expansion is not uniform and therefore its domain of validity is unknown *a priori* without comparisons to more controlled calculations. Independently, others [5] now have performed computer-simulation studies of this generating function for the special case of fields at a neutral point in a one-component plasma. Strong-coupling conditions were studied, with plasma parameters $\Gamma=1$, 5, and 10 [$\Gamma\equiv(Ze)^2/r_0k_BT$, where Ze is the charge, k_B is Boltzmann's constant, T is the temperature, r_0 is the ion sphere radius ($4\pi n r_0^3/3=1$), and n is the density]. Here we specialize the short-time expansion to this case, describe a suitable approximation to evaluate the coefficients, and report the comparison to simulation results at the strongest coupling conditions considered, $\Gamma=10$. The agreement is quite good for $\omega_p t\leq 2$, where $\omega_p=(4\pi n Z^2e^2/m)^{1/2}$ is the plasma frequency. In the last section we speculate on the utility of short-time expansions for practical calculations at strong coupling.

II. DEFINITIONS AND SHORT-TIME EXPANSION

In this section we review briefly the definitions of the joint-probability density and its generating function, and the short-time expansion of Ref. [4]. The system considered is a one-component plasma (OCP) of N ions with mass m and charge Ze, in a uniform neutralizing background. The electric field at a neutral point (chosen to be the origin) due to the OCP is given by

$$\mathbf{E}\equiv\sum_{i=1}^{N}\mathbf{e}(\mathbf{q}_i),\quad \mathbf{e}(\mathbf{r})\equiv(Ze)(\hat{\mathbf{r}}/r^2)+\mathbf{e}_b\ , \tag{2.1}$$

where N is the number of ions and $\mathbf{e}(\mathbf{q}_i)$ is the electric field due to the ith particle plus a contribution from the uniform background ($\mathbf{E}_b\equiv N\mathbf{e}_b$). The equilibrium probability density for field values $\boldsymbol{\varepsilon}$ is

$$Q(\varepsilon)\equiv\langle\delta(\boldsymbol{\varepsilon}-\mathbf{E})\rangle=(2\pi)^{-3}\int d\boldsymbol{\lambda}\, e^{-i\boldsymbol{\lambda}\cdot\boldsymbol{\varepsilon}}e^{G(\lambda)}\ . \tag{2.2}$$

The second equality defines the associated generating function $G(\lambda)$,

$$G(\lambda)=\ln(\langle e^{i\boldsymbol{\lambda}\cdot\mathbf{E}}\rangle)\ . \tag{2.3}$$

The joint distribution for a field value $\boldsymbol{\varepsilon}'$ at $t=0$ and a field value $\boldsymbol{\varepsilon}$ at time t is given by

$$\begin{aligned}Q(\boldsymbol{\varepsilon},t;\boldsymbol{\varepsilon}',0)&\equiv\langle\delta(\boldsymbol{\varepsilon}-\mathbf{E}(t))\delta(\boldsymbol{\varepsilon}'-\mathbf{E})\rangle\\&=(2\pi)^{-6}\int d\boldsymbol{\lambda}\,d\boldsymbol{\lambda}'\,e^{-i\boldsymbol{\lambda}\cdot\boldsymbol{\varepsilon}-i\boldsymbol{\lambda}'\cdot\boldsymbol{\varepsilon}'}e^{G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)}\ .\end{aligned} \tag{2.4}$$

The generating function in this case is given by

$$G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)=\ln(\langle e^{i\boldsymbol{\lambda}\cdot\mathbf{E}(t)}e^{i\boldsymbol{\lambda}'\cdot\mathbf{E}}\rangle)\ . \tag{2.5}$$

The initial and final values for $Q(\boldsymbol{\varepsilon},t;\boldsymbol{\varepsilon}',0)$ are $\delta(\boldsymbol{\varepsilon}-\boldsymbol{\varepsilon}')Q(\boldsymbol{\varepsilon}')$ and $Q(\boldsymbol{\varepsilon})Q(\boldsymbol{\varepsilon}')$, respectively. The corresponding values for the generating function are

$$\begin{aligned}&G(\boldsymbol{\lambda},\boldsymbol{\lambda}';0)=G(|\boldsymbol{\lambda}+\boldsymbol{\lambda}'|)\ ,\\&G(\boldsymbol{\lambda},\boldsymbol{\lambda}';\infty)=G(\lambda)+G(\lambda')\ .\end{aligned} \tag{2.6}$$

Now consider the direct expansion of $G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)$ in powers of t, for fixed $\boldsymbol{\lambda},\boldsymbol{\lambda}'$, from Eq. (2.5). The leading two terms are found to be [4]

$$G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)=G(|\boldsymbol{\lambda}+\boldsymbol{\lambda}'|)+(t^2/2)\lambda_i\lambda_j'F_{ij}(|\boldsymbol{\lambda}+\boldsymbol{\lambda}'|)+\cdots\ , \tag{2.7}$$

$$F_{ij}(\lambda)\equiv(nk_BT/m)\int d\mathbf{r}\left[\frac{\partial e_i(r)}{\partial r_l}\right]\left[\frac{\partial e_j(r)}{\partial r_l}\right]\tilde{g}(\mathbf{r};\boldsymbol{\lambda})\ , \tag{2.8}$$

$$n\tilde{g}(\mathbf{r};\boldsymbol{\lambda})\equiv\langle n(\mathbf{r})e^{i\boldsymbol{\lambda}\cdot\mathbf{E}}\rangle/\langle e^{i\boldsymbol{\lambda}\cdot\mathbf{E}}\rangle\ , \tag{2.9}$$

where $n(\mathbf{r})$ is the local number density of ions near the impurity. The quantity $\tilde{g}(\mathbf{r};\boldsymbol{\lambda})$ is closely related to the correlation function for an ion-impurity pair, restricted to states distorted by the local field [7]. It is shown elsewhere that it may be determined from a functional derivative of $G(\lambda)$ [7],

$$n\tilde{g}(\mathbf{r};\boldsymbol{\lambda})=\frac{\delta G(\lambda)}{\delta(i\lambda e(r))}\ , \tag{2.10}$$

where $e(r)$ is the magnitude of the single-particle field in (2.1). Thus all of the terms in (2.7) can be calculated from a suitable approximation for $G(\lambda)$ alone. As noted in the introduction, this is a well-studied problem with good approximations available [1].

It is instructive to consider the limiting case for which there are no interactions among the plasma particles. Then $G(\lambda)$ is given by Holtsmark distribution,

$$G(\lambda)\rightarrow n\int d\mathbf{r}(e^{i\boldsymbol{\lambda}\cdot\mathbf{e}(\mathbf{r})}-1)\ , \tag{2.11}$$

$$\tilde{g}(\mathbf{r};\boldsymbol{\lambda})\rightarrow e^{i\boldsymbol{\lambda}\cdot\mathbf{e}(\mathbf{r})}\ . \tag{2.12}$$

The short-time expansion for this case can be calculated analytically, with the result

$$\begin{aligned}G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)=&-c_1|\boldsymbol{\lambda}+\boldsymbol{\lambda}'|^{3/2}\\&-c_2(\lambda\lambda')^2(1-x^2)|\boldsymbol{\lambda}+\boldsymbol{\lambda}'|^{-7/2}(\omega_pt)^2\\&+O(t^4)\ ,\end{aligned} \tag{2.13}$$

with $x=\hat{\boldsymbol{\lambda}}\cdot\hat{\boldsymbol{\lambda}}'$, $c_1=e_0^{3/2}2(2\pi)^{1/2}/5$, $c_2=e_0^{1/2}9(2\pi)^{1/2}/8$. Here $e_0=Ze/r_0^2$ is the field due to an ion at the ion-sphere radius. This illustrates some limitations of the formal expansion in time. The coefficient of t^2 is singular if $\boldsymbol{\lambda}=-\boldsymbol{\lambda}'$. Furthermore, derivatives with respect to $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}'$ are singular at $\boldsymbol{\lambda}=\boldsymbol{\lambda}'=\mathbf{0}$, so the expansion is not uniform with respect to $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}'$. Its applicability is limited to a time scale that depends on the values of $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}'$ considered. Thus it is of some interest to determine these time scales by direct comparison with computer simulation, as considered here.

III. RENORMALIZATION AT STRONG COUPLING

The generating function $G(\lambda)$ can be considered as a functional of $\phi(\boldsymbol{\lambda},\mathbf{r})=-1+\exp(i\boldsymbol{\lambda}\cdot\mathbf{e}(\mathbf{r}))$, so that $G\equiv G[\phi]$ [8,9]. Truncation of the functional Taylor-series expansion in ϕ (Baranger-Mozer series [10]) leads to a sequence of approximations. At first order in ϕ one obtains the Holtsmark approximation (2.11). Correlations among particles appear at second order in ϕ; beyond second order practical calculation becomes prohibitively difficult. However, the second-order approximation fails for strong coupling ($\Gamma\geq 1$). To describe conditions of strong coupling a renormalization of the Baranger-Mozer series is required. First, we define a "renormalized" functional, $G[\phi]\equiv G_R[\phi^*]$, with ϕ^* defined by

$$\phi^*(\boldsymbol{\lambda},\mathbf{r})\equiv-1+\exp[i\boldsymbol{\lambda}\cdot\mathbf{e}^*(\mathbf{r})]\ . \tag{3.1}$$

The new single-particle electric field $\mathbf{e}^*(\mathbf{r})$ is directed along $\mathbf{r}$ but otherwise has a functional form chosen below to optimize the expansion. The functional transformation from ϕ to ϕ^* is seen to be simply

$$\phi(\boldsymbol{\lambda},\mathbf{r})=-1+[1+\phi^*(\boldsymbol{\lambda},\mathbf{r})]^{R(r)}\ , \tag{3.2}$$

where $R(r)=\hat{\mathbf{r}}\cdot\mathbf{e}(\mathbf{r})/\hat{\mathbf{r}}\cdot\mathbf{e}^*(\mathbf{r})$. A new functional Taylor series in ϕ^* is now truncated to yield a renormalized succession of approximations. The leading two terms are

$$G_R(\lambda)=G_R^{(1)}(\lambda)+G_R^{(2)}(\lambda)+\cdots\ , \tag{3.3}$$

$$G_R^{(1)}(\lambda)\equiv n\int d\mathbf{r}_1R(r_1)\phi^*(\boldsymbol{\lambda},\mathbf{r}_1)\ , \tag{3.4}$$

$$\begin{aligned}G_R^{(2)}(\lambda)\equiv\frac{n}{2}\int d\mathbf{r}_1d\mathbf{r}_2R(r_1)R(r_2)\phi^*(\boldsymbol{\lambda},\mathbf{r}_1)\phi^*(\boldsymbol{\lambda},\mathbf{r}_2)\\\times\{n[g(|\mathbf{r}_1-\mathbf{r}_2|)-1]\\+R(r_1)[R(r_2)-1]\phi^*(\boldsymbol{\lambda},\mathbf{r}_1)\\\times\phi^*(\boldsymbol{\lambda},\mathbf{r}_2)\delta(|\mathbf{r}_1-\mathbf{r}_2|)\}\ .\end{aligned} \tag{3.5}$$

So far this rearrangement is only formal. To optimize convergence, the arbitrary field $\mathbf{e}^*(\mathbf{r})$ is chosen such that the first term alone is exact through order λ^2. This gives the constraint

$$\begin{aligned}\int d\mathbf{r}_1e_i(\mathbf{r}_1)(e_j^*(\mathbf{r}_1)-e_j(\mathbf{r}_1))\\=n\int d\mathbf{r}_1d\mathbf{r}_2e_i(\mathbf{r}_1)e_j(\mathbf{r}_2)[g(|\mathbf{r}_1-\mathbf{r}_2|)-1]\ .\end{aligned} \tag{3.6}$$

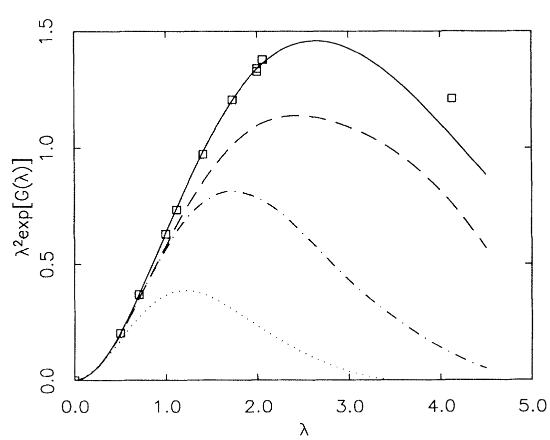

FIG. 1. Generating function density for the time-independent microfield distribution, $\lambda^2\exp[G(\lambda)]$, as a function of λ at $\Gamma=10$; molecular dynamics (□), two terms of renormalized series (——), one term (APEX) of renormalized series (— — —), two terms Baranger-Mozer series (—·—·—·), and Holtsmark (· · · ·).

This does not specify $\mathbf{e}^*(\mathbf{r})$ uniquely. In practice it is useful to choose a Debye-like field with screening parameter chosen to enforce (3.6). The resulting first approximation, $G_R^{(1)}$, is known as the adjustable parameter exponential (APEX) approximation [8]. Figure 1 shows the comparison of results for $\exp[G(\lambda)]$ as a function of λ (in units of e_0) obtained using G_{H} (Holtsmark), G_{BM} (first two terms of the Baranger-Mozer series), APEX equal to $G_R^{(1)}$, and $G_R = G^{(1)} + G^{(2)}$ at $\Gamma = 10$. Also shown are recent molecular-dynamics-simulation results [5]. The main conclusion from this is that the renormalization procedure including *two* terms is required for such strong coupling.

To obtain the short-time coefficient from these approximations, Eq. (2.10) is used,

$$n\tilde{g}(\mathbf{r};\boldsymbol{\lambda}) = \frac{\delta}{\delta(i\lambda e(r))}[G_R^{(1)}(\lambda) + G_R^{(2)}(\lambda) + \cdots] = n\exp[i\boldsymbol{\lambda}\cdot\mathbf{e}^*(\mathbf{r})] + \cdots . \quad (3.7)$$

In the numerical results reported below, the contribution $G_R^{(2)}$ has been included in the calculation of $G(\lambda)$ but not in the calculation of $\tilde{g}(\mathbf{r};\boldsymbol{\lambda})$. To clarify this point, we first note that Fig. 1 shows large differences between the Holtsmark approximation and that obtained using only $G_R^{(1)}$ (APEX). This suggests the need for $G_R^{(2)}$ for an accurate microfield distribution. Conversely, the comparison of these two approximations in the determination of $F_{ij}(\lambda)$ shows only a few percent difference and suggests that contributions from $G_R^{(2)}$ are not important in this case. It appears that short-time dynamics at a neutral point is dominated by ideal gas behavior.

IV. RESULTS

The generating function $G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)$ depends on the four parameters λ, λ', θ, and t, where θ is the angle between $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}'$. The comparison between molecular-dynamics data and the short-time expansion is most compact in terms of the magnitude, $l \equiv [\lambda^2 + \lambda'^2 + 2\lambda\lambda'\cos(\theta)]^{1/2}$. The specific values of λ, λ', and θ for each l are given in Table I (where λ and λ' are measured in units of e_0) Table II shows the comparison of the molecular dynamics (MD) and short time results for the range of l and times considered in Ref. [5]. Except for the largest time, $\omega_p t = 3.46$, the differences are typically of the order of a few percent. This is within the range of accuracy of the MD data and the numerical calculations of the short-time coefficients. Although Fig. 1 shows that the accuracy of $G_R(\lambda)$ is quite good, the small errors propagate in time. The quality of the second term of (2.7) can be determined independently from that of $G_R(\lambda)$ by normalizing the short-time expansion to that of the simulation data at $t = 0$. Typical results are shown in Figs. 2 and 3.

TABLE I. Values of dimensionless λ, λ', θ, and $l = [\lambda^2 + \lambda'^2 + 2\lambda\lambda'\cos(\theta)]^{1/2}$ for molecular dynamics results reported in Ref. [5].

l	λ	λ'	θ
0.707	0.5	0.5	$\pi/2$
1.12	0.5	1.0	$\pi/2$
1.414	1.0	1.0	$\pi/2$
1.732	1.0	1.0	$\pi/3$
1.732	1.0	2.0	$2\pi/3$
2.0	2.0	2.0	$2\pi/3$
2.06	0.5	2.0	$\pi/2$
2.83	2.0	2.0	$\pi/2$
4.13	4.0	1.0	$\pi/2$

The differences at $\omega_p t = 3.46$ are large, indicating a breakdown of the short-time expansion. Thus we estimate that the short-time expansion has validity limited to $\omega_p t \leq 2$ for the conditions considered. This estimate is consistent with a short-time analysis of the field autocorrelation function, $\langle \mathbf{E}(t)\cdot\mathbf{E}\rangle$ in Ref. [5], which shows that the first three terms of an exact short-time expansion are quite accurate up to $\omega_p t = 2$ with significant differences from the simulation results occurring at $\omega_p t = 3.46$. An analysis of the autocorrelation function at other values of Γ also shows that the domain of the short-time expansion decreases at weaker coupling.

V. DISCUSSION

For many applications, e.g., spectral line broadening, the relevant time scales are of the order of a few $\omega_p t$. Thus it would be very useful to conclude from the above that short-time expansions of $G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)$ are sufficient to study complex nonlinear dependencies on electric-field

TABLE II. Values of the generating function $\exp[G(\lambda,\lambda';t)]$ from molecular dynamics (MD) and from the short-time expansion (ST); t in units of ω_p^{-1}.

	$t=0.0$		$t=0.693$		$t=1.39$		$t=1.73$		$t=3.46$	
l	MD	ST	MD	ST	MD	ST	MD	ST	MD	ST
0.707	0.739	0.741	0.729	0.731	0.712	0.708	0.702	0.691	0.680	0.565
1.12	0.585	0.592	0.578	0.586	0.561	0.566	0.551	0.554	0.518	0.457
1.414	0.489	0.495	0.479	0.487	0.456	0.461	0.443	0.444	0.394	0.323
1.732	0.403	0.402	0.401	0.401	0.401	0.401	0.403	0.399	0.404	0.391
1.732	0.403	0.402	0.380	0.388	0.324	0.347	0.296	0.320	0.204	0.160
2.0	0.335	0.335	0.300	0.308	0.231	0.238	0.200	0.197	0.107	0.040
2.06	0.325	0.321	0.324	0.319	0.315	0.316	0.309	0.312	0.278	0.284
2.83	0.191	0.181	0.180	0.175	0.159	0.162	0.153	0.151	0.107	0.380
4.13	0.071	0.062	0.069	0.061	0.063	0.060	0.061	0.057	0.043	0.050

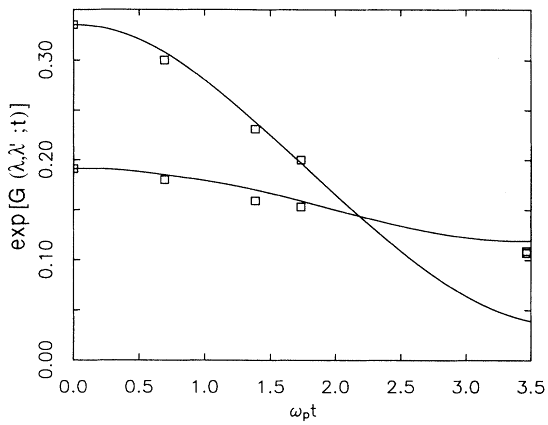

FIG. 2. Comparison of $\exp(G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t))$ as a function of time at $\Gamma=10$, $\lambda=\lambda'=2$; molecular dynamics (□), and short-time expansion (——). Top curve is for $\hat{\boldsymbol{\lambda}}\cdot\hat{\boldsymbol{\lambda}}'=\cos(2\pi/3)$, bottom curve is for $\cos(\pi/2)$. Theoretical results are normalized to those of molecular dynamics at $t=0$.

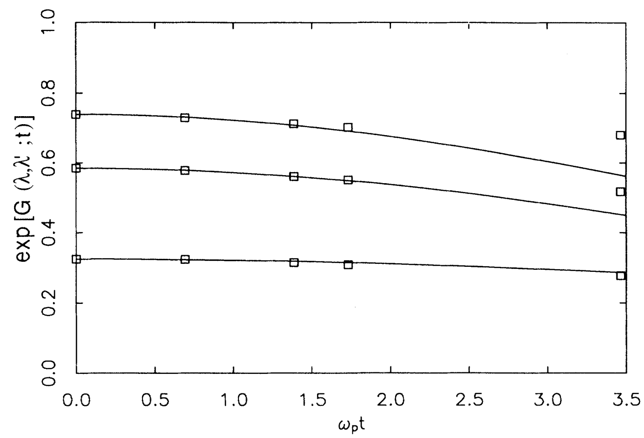

FIG. 3. Same as Fig. 1, except all curves have $\hat{\boldsymbol{\lambda}}\cdot\hat{\boldsymbol{\lambda}}'=\cos(\pi/2)$ and $\lambda=0.5$; top curve ($\lambda'=0.5$), middle curve ($\lambda'=1$), bottom curve ($\lambda'=2$).

dynamics. However, the exact Holtsmark result (2.13) shows that the short-time expansion has some important limitations. To illustrate, consider three exact derived quantities, the electric-field autocorrelation function,

$$\left[\frac{\partial^2}{\partial\lambda_i\partial\lambda_j'}G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)\right]_{\lambda=\lambda'=0}=-\langle E_i(t)E_j\rangle\ , \qquad (5.1)$$

the conditional average of the electric field,

$$\begin{aligned}Q(\boldsymbol{\varepsilon})\langle \mathbf{E}(t);\boldsymbol{\varepsilon}\rangle &\equiv \langle \mathbf{E}(t)\delta(\boldsymbol{\varepsilon}-\mathbf{E})\rangle\\ &=(2\pi)^{-3}\int d\boldsymbol{\lambda}e^{-i\boldsymbol{\lambda}\cdot\boldsymbol{\varepsilon}+G(\lambda)}\\ &\quad\times\left[-i\frac{\partial}{\partial\lambda_i'}G(\boldsymbol{\lambda}',\boldsymbol{\lambda};t)\right]_{\lambda'=0}\ ,\end{aligned} \qquad (5.2)$$

and the time-independent distribution of electric-field derivatives [5],

$$\begin{aligned}P(\eta)&\equiv\langle\delta(\boldsymbol{\eta}-\mathbf{E})\rangle=(2\pi)^{-3}\int d\boldsymbol{\lambda}\,e^{-i\boldsymbol{\lambda}\cdot\boldsymbol{\eta}}e^{J(\lambda)}\ ,\\ J(\boldsymbol{\lambda})&\equiv\lim_{t\to 0}G\left[\frac{\boldsymbol{\lambda}}{t},\frac{-\boldsymbol{\lambda}}{t};t\right]\ .\end{aligned} \qquad (5.3)$$

If the short-time expansion of $G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)$ is used to calculate the conditional field from Eq. (5.2), the correct result to order t^2 is obtained. However, divergent results are obtained for the field autocorrelation function (5.1) and for the distribution of field derivatives (5.3). This is due to the fact that moments of the joint-probability density are nonanalytic functions of t near $t=0$ for fields at a neutral point. Thus the short-time expansion for the generating function cannot be used to describe directly the short-time behavior of all derived properties of interest, and some care is required. It is likely that the domain $\omega_p t\le 2$ can be described by short-time representations for the conditions considered here, but not necessarily by the single expansion (2.7). For example, as noted above, a short-time expansion of the autocorrelation function is accurate over the same range as that of $G(\boldsymbol{\lambda},\boldsymbol{\lambda}';t)$. However, the latter is analytic in t while the former is not, and the two representations are unrelated. The case of electric-field dynamics at a charged point is expected to be simpler in this respect since the corresponding moments are analytic in time and the short-time expansion of the generating function is expected to be uniform in $\boldsymbol{\lambda}$ and $\boldsymbol{\lambda}'$. Unfortunately, there are no corresponding detailed computer-simulation results available for this case at present.

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