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Phase-amplitude solution of the Schrödinger equation with application to free-free absorption

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The phase-amplitude method for solving the Schrödinger equation is implemented for free-free absorption in a hot, dense plasma. The method is benchmarked against two independent direct Schrödinger calculations.

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I. INTRODUCTION

The phase-amplitude method of solving the Schrödinger equation has been of interest for a long time without giving up many practical applications. The time-dependent three-dimensional form was investigated by Bohm [1] as a quantum form of the equations of fluid hydrodynamics. The so-called ''Bohmian dynamics'' has been recently reexamined [2,3] from the point of view of the Lagrangian or moving frame computational scheme, with applications to simple quantum mechanical problems. Although the analog with fluid hydrodynamics may make the method seem attractive from a philosophical point of view, the severe practical problems associated with the three-dimensional (3D) or even 2D solution of the equations of motion in the Lagrangian frame which have beset computational physicists in classical hydrodynamics for many years might give one pause as to why the problem would be any less daunting in quantum physics.

In classical hydrodynamics these difficulties show up as distortions of 2D and 3D meshes, requiring techniques such as arbitrary Lagrangian-Eulerian (ALE) frame mixing, of which Bohmian hydrodynamicists have already had to avail themselves to obtain sensible results [3]. The outcome, at least in classical hydrodynamics, is a theoretical wilderness in which the possibility of meaningful results depends strongly on adjustments to the theoretical methods once reliable laboratory data are in hand.

In this paper our phase-amplitude ambitions are more modest but hopefully more practical: we study the phase-amplitude method for solving the radial Schrödinger equation. Recent papers [4–6] have appeared on this subject which reveal that, notwithstanding the greater computational tractability of the 1D problem, difficulties remain in the production of accurate results, as discussed by Wilson and coworkers [6]. These authors implement a hybrid version of the phase-amplitude method, first used by Burgess and Sheorey [7], in which the radial Schrödinger equation is integrated directly from the origin to a point beyond the classical turning point where it is matched onto a phase-amplitude solution generated from the matching point to infinity or, as the authors discuss, in the ''far field.'' In this paper we integrate the nonlinear equation for the amplitude over all space and find that the solution is numerically stable and accurate. The phase is found from numerical quadrature knowing the amplitude.

II. THEORY AND RESULTS

In phase-amplitude theory the reduced radial wave function is written

$$\psi(r)=y(r)\sin[\varphi(r)]. \tag{1}$$

Substitution into the reduced radial Schrödinger equation yields the equations for the amplitude and phase, respectively,

$$-\frac{1}{2}y''+\left[\frac{L(L+1)}{2r^2}+V(r)-\frac{k^2}{2}\right]y+\frac{k^2}{2y^3}=0, \tag{2a}$$

$$\varphi=\int_0^r dr'\frac{k}{y^2}. \tag{2b}$$

The WKB approximation for the phase, for large L, follows immediately by setting the second derivative in Eq. (2a) equal to zero and solving for the integrand of Eq. (2b),

$$\frac{k}{y^2}=\left[k^2-2V-\frac{L(L+1)}{r^2}\right]^{1/2}. \tag{3}$$

In our application the potential V represents the screened interaction of a free electron with an ion embedded in a plasma and has the analytic form,

$$rU=2rV=\sum a_i e^{-\alpha_i r}, \tag{4}$$

where the parameters are given in Table I. There has been

TABLE I. Cs plasma potential parameters for a temperature of 100 eV and a density of 0.187 g/cm^3 [17].

i	a_i	α_i
1	4.31601	33.89329
2	2.42685	23.46050
3	59.01007	6.30434
4	44.28462	0.20468

much interest recently in dynamic screening, in which the potential depends on the velocity of the projectile, for example in fast photoexcitation in semiconductor physics [8] and in ion-beam plasma interactions [9–11]. It appears that the methods presented here could also be useful in dynamic screening applications.

Results for free-free absorption are presented in terms of the Gaunt factor,

$$g = \frac{\sqrt{3}}{2\pi k_i k_f} \sum L[M^2_{k_i k_f, LL-1} + M^2_{k_i k_f, L-1L}], \qquad (5)$$

where the radial matrix elements are defined in the acceleration gauge,

$$M_{k_i k_f LL'} = \int_0^\infty dr\, \psi_{k_f, L'} \frac{dU}{dr} \psi_{k_i L}\,. \qquad (6)$$

The acceleration gauge is the obvious choice owing to the long range of the integrands belonging to dipole matrix element in the length or velocity gauges. It would be of interest in future work to make comparison calculations in all three gauges, for which results appear not to be widely available for free-free absorption [12]. The agreement of the results for the different gauges is a sensitive test of the accuracy of the wave functions, a result which has been widely exploited in bound-free and bound-bound absorption. In these transitions one or both of the wave functions respectively is bound with exponential decay at large distances from the nucleus, thereby facilitating studies in all three gauges [13] since the radial matrix elements are rapidly convergent in all three gauges. Free-free absorption on the other hand has rapidly convergent matrix elements only in the acceleration gauge, such that the length and velocity gauge calculations are usually carried out [12,14,15] with the use of an exponentially decaying cutoff factor in the matrix element, and the results of a series of calculations are extrapolated to a result corresponding to unit cutoff factor. The length and velocity gauge matrix elements are convergent only through the phase mismatch of the initial and final radial waves, such that one really requires an analytic representation of the wave functions in order to use these gauges with complete reliability. For this reason we do not pursue a gauge study further at this time.

Equation (2a) is integrated backwards from large r into the origin, with $y=1$ as initial value at large r. At small r, y is dominated by the solution irregular at the origin, $y \approx r^{-L}$. The phase goes as $\varphi \approx r^{2L+1}$ and ψ [Eq. (1)] as $\psi \approx r^{L+1}$, or the Schrödinger solution regular at the origin. It is necessary only to stop the backward solution far enough from the origin to avoid overflows in y and at the same time satisfy that ψ is negligibly small. This procedure is illustrated in Figs. 1 and 2, where the amplitude and the wave function from the phase amplitude solution [Eq. (1)] and from the direct integration of the Schrödinger equation are plotted versus r. Note the agreement perfect within graphical accuracy of the wave functions from the two different methods. We have used the automatic error control ordinary differential equation (ODE) method due to Bulirsch and Stoer [16].

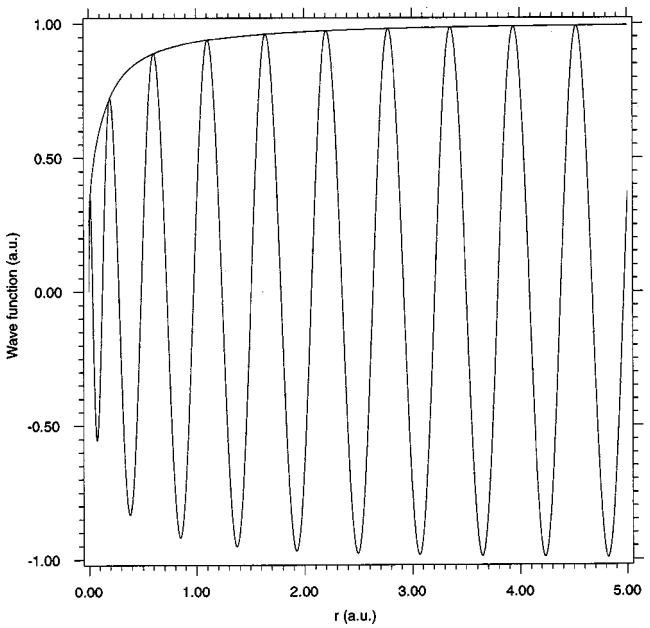

FIG. 1. Wave function for $L=0$ and $k=10.5$ a.u. Upper curve: $y(r)$. Lower curves: $\psi(r)=y(r)\sin[\varphi(r)]$ and ψ from the direct solution of the reduced radial Schrödinger equation.

A selection of phase-amplitude and direct Schrödinger results is given in Table II. The two Schrödinger calculations serve as a benchmark for the accuracy of the phase-amplitude results. The GSFC Schrödinger calculation was performed in quadruple precision, using ODE procedures based on the Nordsieck method.

In order to run down the small differences between the two Schrödinger calculations, we calculated a single LLNL result in quadruple precision for photon energy 0.01 eV and

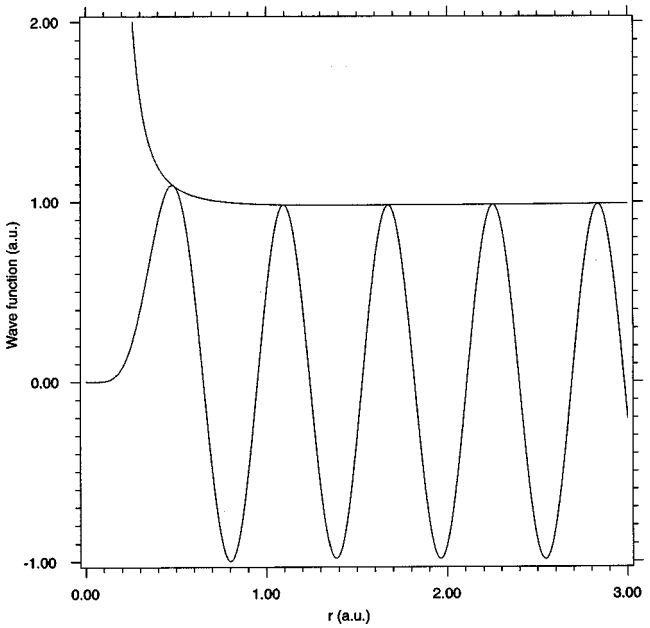

FIG. 2. Wave function for $L=5$ and $k=10.5$ a.u. Upper curve: $y(r)$. Lower curves: $\psi(r)=y(r)\sin[\varphi(r)]$ and ψ from the direct solution of the reduced radial Schrödinger equation.

TABLE II. Comparison of results for Gaunt factor. [Gaunt factors have been obtained by solving the Schrödinger equation at Goddard Space Flight Center (GSFC) and at Lawrence Livermore National Laboratory (LLNL). These have also been calculate by the phase-amplitude method (LLNL). E_{ph} is the photon energy and E_i the incident electron energy. $L_{\max}$ is the number of partial waves required to obtain convergence.]

			Gaunt factor		
			Schrödinger		Phase amplitude
E_{ph} (eV)	E_i (eV)	$L_{\max}$	(GSFC)	(LLNL)	(LLNL)
0.01	100	36	258.944	259.086	258.387
	500	54	641.588	640.446	641.363
	1000	120	936.642	936.604	936.476
	1500	130	1155.49	1155.23	1155.06
80.7	100	22	493.228	492.683	492.649
	500	38	748.379	748.234	748.020
	1000	46	993.365	993.319	993.060
	1500	76	1200.59	1200.08	1199.99
246.0	100	15	659.046	658.648	657.984
	500	33	848.959	848.769	848.746
	1000	50	1053.51	1051.99	1051.72
	1500	70	1227.65	1227.25	1226.81
1312.0	100	9	1355.75	1354.81	1355.29
	500	14	1433.14	1432.39	1432.83
	1000	16	1524.92	1524.01	1524.44
	1500	22	1612.67	1611.19	1611.55

electron energy 1000 eV. It is 936.654, which compares more favorably with the GSCF result of 936.642 than does our double precision result of 936.604 presented in Table II. Remaining difference are likely due to different numerical procedures used by the two authors.

The speedup in computational time due to using the phase-amplitude method has been examined by others [6], and we do not belabor the point here. Obviously the phase and amplitude can be tabulated on a coarse mesh with substantial savings in computational time; however the speedup for the matrix element requires techniques such as those developed in [6] in which the slowly varying part of the integrand is fitted to a linear functional form and the rapidly varying part is evaluated analytically. Our concern here is to show that the nonlinear equation for the amplitude [Eq. (2a)] can be integrated over all r to obtain a numerically stable result. Wilson *et al.* [6] have stated that the amplitude equation is unstable; we find no evidence to support this assertion.

III. CONCLUSIONS

Although the phase-amplitude method has been investigated since the early days of quantum mechanics, most notably in its approximate form, the WKB approximation, it has not been widely implemented in atomic or plasma physics applications. Previous applications have suffered from inaccuracies [5] or from hybrid phase-amplitude-Schrödinger procedures [6,7] which we believe are unnecessary in today's era of fast high-precision computing.

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