

Quantum Mechanical Ground State of Hydrogen Obtained from Classical Electrodynamics

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Abstract

The behavior of a classical charged point particle under the influence of only a Coulombic binding potential and classical electromagnetic zero-point radiation, is shown to yield agreement with the probability density distribution of Schrödinger's wave equation for the ground state of hydrogen. These results, obtained without any fitting parameters, again raise the possibility that the main tenets of stochastic electrodynamics (SED) are correct, thereby potentially providing a more fundamental basis of quantum mechanics. The present methods should help propel yet deeper investigations into SED.

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The following fact probably comes as a surprise to most physicists. A group of researchers in the past have both proposed and deeply investigated the idea that classical electrodynamics, namely, Maxwell's equations and the relativistic version of Newton's equation of motion, may describe much, if not all, of atomic physical processes, provided one takes into account the appropriate classical electromagnetic random radiation fields acting on classical charged particles. Stochastic electrodynamics (SED) is the usual name given for this physical theory; it was most significantly advanced in the 1960s by Boyer [1],[2] and Marshall [3], [4], [5], although its full history is somewhat more complicated and is reviewed and described in Ref. [6]. Other useful reviews exist such as Refs. [7], [8], and [9].

SED is really a subset of classical electrodynamics. However, it differs from conventional treatments in classical electrodynamics in that it assumes that if thermodynamic equilibrium of classical charged particles is at all possible, then a thermodynamic radiation spectrum must also exist and must be an essential part of the thermodynamic system of charged particles and radiation. As can be shown via statistical and thermodynamic analyses [1], [10], if thermodynamic equilibrium is possible for such a system, then there must exist random radiation that is present even at temperature $T = 0$. This radiation has been termed classical electromagnetic zero-point (ZP) radiation, where the "ZP" terminology stands for $T = 0$, as opposed to "ground state" or "lowest energy state". Either of the following requirements has been shown to enable the derivation of the required functional form of the ZP radiation spectrum: (1) the ZP radiation must possess a Lorentz invariant character [1], and (2) no heat must flow during reversible thermodynamic operations [10],[11],[12]. Deriving the ZP spectral form from (1) follows only from the radiation properties, while (2) involves the interaction of both particles and fields.

Results have been obtained from SED that agree nicely with quantum mechanical (QM) predictions for linear systems [13], such as for systems of electric dipole simple harmonic oscillators [8],[9], and for linear electromagnetic fields in Casimir/van der Waals type situations [6],[12],[14]. Moreover, most physicists, who know of SED, are likely to agree that SED provides a better description of physical processes than does conventional classical electrodynamics without the consideration of ZP and Planckian electromagnetic radiation. Nevertheless, since the late 1970s and early 1980s, the vast majority of physicists have clearly concluded that SED cannot come close to predicting the full range of QM phenomena for nonlinear dynamics found in real atomic systems [15], [16], [17],[18], [19], [20], [9], [6]. In

particular, these past analyses of SED predicted clear disagreements with physical observation, such as that a single hydrogen atom will ionize at $T = 0$ and that the spectra predicted by SED does not agree with QM predictions.

However, as discussed in Refs. [21] and [22], reasons exist to raise some doubts on these conclusions. In particular, for atomic systems, all of the key physical effects should arise from electromagnetic interactions. Examining other nonlinear binding potentials, other than ones arising from Coulombic binding potentials, have no relation to real physical atomic systems. Even though one can place any potential function in Schrödinger's equation, and attempt to solve it, SED does not need to match these solutions as they have little relationship, in detail, to the real physical world of atomic systems. Instead, realistic binding potentials must be examined. Moreover, for perturbation analyses, if one assumes that the small effect of the electric charge is a key part of the perturbation analysis, then this effect must be consistently carried out for the radiation reaction as well as for the binding potential and the effect of the ZP field acting on the orbiting charge [22]. Still, properly accounting for these objections into an improved analytic, or even semi-analytic, reanalysis of SED, has seemed quite difficult.

For that reason, in this article we have turned to attacking one of the more significant problems in SED via simulation methods, namely, the hydrogen atom. The present results certainly seem to bear out the hope that the earlier impasse in SED may have been due to the difficulties of analyzing nonlinear stochastic differential equations, rather than a fundamental physical flaw in the basic ideas of SED.

In quick summary, the present simulation work was carried out by tracking individual trajectories of electrons for long lengths of time, assuming classical electrodynamics governed the trajectories. Probability distributions were then obtained in coordinate space based on the length of time the electrons spent in regions of space about the nucleus. References [23],[24], [25], and [26] contain many of the technical details that led to the present work, although these previous works concentrated on the nonlinear dynamical effects of a classical electron, with charge $-e$ and rest mass m , in orbit about an infinitely massive nucleus of charge $+e$, where besides the binding potential acting, only a limited set of plane waves acted on the electron. In that work, as here, we have numerically solved the nonrelativistic

approximation to the classical Lorentz-Dirac equation [27],[28]:

$$m\ddot{\mathbf{z}} = -\frac{e^2\mathbf{z}}{|\mathbf{z}|^3} + \mathbf{R}_{\text{reac}} + (-e) \left\{ \mathbf{E}[\mathbf{z}(t), t] + \frac{\dot{\mathbf{z}}}{c} \times \mathbf{B}[\mathbf{z}(t), t] \right\} ,$$

where the radiation reaction term of \mathbf{R}_{reac} has been approximated by $\mathbf{R}_{\text{reac}} \approx \frac{2}{3} \frac{e^2}{c^3} \frac{d^3\mathbf{z}}{dt^3} \approx \frac{2}{3} \frac{e^2}{c^3} \frac{d}{dt} \left(-\frac{e^2\mathbf{z}}{m|\mathbf{z}|^3} \right)$, and where \mathbf{E} and \mathbf{B} represent the electric and magnetic fields of the radiation acting on the electron. We note that to date we have carried out a fair bit of numerical analysis involving full relativistic computation, but, for the results reported here, the key effects of our present system are adequately represented by the above equations.

The electromagnetic ZP field formally consists of an infinite set of frequencies, which clearly would be impossible to implement fully in any sort of numerical scheme. Consequently, we limited the number of frequencies in the simulation to ranges that had the most significant effect on the electron's orbital motion. We did so in two ways. Often the ZP radiation fields are represented in SED by a sum of plane waves [6]:

$$\mathbf{E}_{\text{ZP}}(\mathbf{x}, t) = \frac{1}{(L_x L_y L_z)^{1/2}} \sum_{n_x, n_y, n_z = -\infty}^{\infty} \sum_{\lambda=1,2} \hat{\epsilon}_{\mathbf{k}_n, \lambda} [A_{\mathbf{k}_n, \lambda} \cos(\mathbf{k}_n \cdot \mathbf{x} - \omega_n t) + B_{\mathbf{k}_n, \lambda} \sin(\mathbf{k}_n \cdot \mathbf{x} - \omega_n t)] ,$$

with n_x , n_y , and n_z integers, $\mathbf{k}_n = 2\pi \left(\frac{n_x}{L_x} \hat{\mathbf{x}} + \frac{n_y}{L_y} \hat{\mathbf{y}} + \frac{n_z}{L_z} \hat{\mathbf{z}} \right)$, $\omega_n = c|\mathbf{k}_n|$, $\mathbf{k}_n \cdot \hat{\epsilon}_{\mathbf{k}_n, \lambda} = 0$, $\hat{\epsilon}_{\mathbf{k}_n, \lambda} \cdot \hat{\epsilon}_{\mathbf{k}_n, \lambda'} = 0$ for $\lambda \neq \lambda'$, and $A_{\mathbf{k}_n, \lambda}$ and $B_{\mathbf{k}_n, \lambda}$ are both real quantities. $\mathbf{B}_{\text{ZP}}(\mathbf{x}, t)$ is expressed by replacing $\hat{\epsilon}_{\mathbf{k}_n, \lambda}$ by $(\hat{\mathbf{k}}_n \times \hat{\epsilon}_{\mathbf{k}_n, \lambda})$ in the above expression for $\mathbf{E}_{\text{ZP}}(\mathbf{x}, t)$. In the above, L_x , L_y , and L_z are dimensions of a rectilinear region in space. Usually at the end of SED calculations, these dimensions are taken to a limit of infinity. For our simulation, we wanted them to be large, but not so large that they created too many plane waves to prohibit numerical simulation. The coefficients $A_{\mathbf{k}_n, \lambda}$ and $B_{\mathbf{k}_n, \lambda}$ were taken to be independent random variables generated once at the start of each simulation, via a random number generator routine, and then held fixed in value for the remainder of the simulation. The random number generator algorithm was designed to produce a Gaussian distribution for these coefficients, with an expectation value of zero, and a second moment of, $\langle A_{\mathbf{k}_n, \lambda}^2 \rangle = \langle B_{\mathbf{k}_n, \lambda}^2 \rangle = 2\pi\hbar\omega_n$. The latter specification corresponds to the energy spectrum of classical electromagnetic ZP radiation of $\rho_{\text{ZP}}(\omega) = \hbar\omega^3 / (2\pi c^3)$ [6].

For reasons to be explained shortly, the orbit of the electron was forced to lie in the $x - y$ plane. We retained plane waves in our simulation from the summation expression above for the ZP fields, up to an angular frequency that corresponded to that of an electron in a

circular orbit of radius 0.1 \AA , or, $\omega_{\max} \approx 5.03 \times 10^{17} \text{ s}^{-1}$. For our simulations, we chose $L_x = L_y = 37.4 \text{ \AA}$ and $L_z = 40,850,000 \text{ \AA} \approx 0.41 \text{ cm}$, bearing in mind that this scenario has some similarity to an atom situated in a rectilinear cavity with highly conducting walls of these dimensions; thus, this “cavity”, or region of space, was made very narrow ($\approx 37 \text{ \AA}$), but still fairly large in width compared to the Bohr radius ($\approx 0.53 \text{ \AA}$), and comparatively very long ($\approx 0.41 \text{ cm}$). This procedure was done to keep the number of plane waves needed as small as possible, while still attempting to retain the most important physical effects. By making L_x and L_y so very much smaller than L_z , then if n_x or n_y was anything other than zero, the frequency of the associated plane wave would be greater than $c2\pi/L_x \approx 5.04 \times 10^{17} \text{ s}^{-1}$, thereby enabling us to drop such waves in this approximation scheme. Consequently, only waves traveling in the $+\hat{\mathbf{z}}$ and $-\hat{\mathbf{z}}$ were retained; the value of L_z we chose then resulted in $\approx 2.2 \times 10^6$ plane being used in the simulation. The minimum, nonzero, angular frequency in the simulation was $\omega_{\min} = c2\pi/L_z \approx 4.61 \times 10^{11} \text{ s}^{-1}$, which corresponds to the angular frequency of an electron in a circular orbit of radius $\approx 1.06 \times 10^{-5} \text{ cm}$, or, about 2000 times the size of the Bohr radius, $a_B \approx 0.53 \text{ \AA}$. In this way, we expected to simulate the approximate behavior of the classical electron in the SED scheme, for radii lying between about 0.1 \AA to hundreds of Angstroms.

This approximate method for representing the desired physical situation greatly reduced the number of plane waves required if L_x , L_y , and L_z were all made equal to $\approx 0.41 \text{ cm}$. Although physically this last approach would be more desirable, it would have resulted in an absurd number of plane waves to handle numerically, namely, $(2.2 \times 10^6)^3 \approx 10^{19}$ waves. Nevertheless, even our much reduced number of 2.2×10^6 waves created expensive runs in CPU time. Consequently, we experimented with and found a second approximation method that reduced our CPU times yet further, while still retaining key physical effects. We will refer to this second method as our “window” approximation.

Specifically, as discussed in Refs. [23] and [26], we found that each plane wave effected near-circular orbits most significantly for orbital angular frequencies lying within a fairly narrow range of the angular frequency of the plane wave itself. Figure 9 in Ref. [26] best illustrates this point. Our numerical experiments found that for the average range of plane wave amplitudes in the present simulation scheme, that a window of $\pm 3\%$ about each average radius more than adequately accounted for the most significant effects. We were prepared to examine a much more complicated window algorithm due to elliptical orbit

considerations, based on the work of Ref. [24], but numerical experiments showed that the eccentricity of the orbits remained small throughout the simulation runs, thereby reducing the need for such considerations. Since the angular frequency of the classical electron in a circular orbit is $e/(mr^3)^{1/2}$, the specific algorithm we implemented kept track of the radius r and retained in the simulation the plane waves with angular frequencies that fell within a range of $e/(mr_H^3)^{1/2}$ to $e/(mr_L^3)^{1/2}$, where $r_L = r(1-f)$ and $r_H = r(1+f)$, where f was selected in these simulations to be 0.03, based on resonance width analysis. As r changed, this scheme automatically changed the range of plane wave frequencies included in the summation to act on the electron, but always considered only those specific plane waves already initialized via the random number generation carried out at the beginning of the simulation. Future speedups in the simulation might well profit by lowering the value of f yet further, and/or by treating it as a function of r to better fit resonance width as r varies.

A typical simulation produced roughly circular orbits that would grow and shrink in radius over time, as seen in Fig. 1. We carried out 11 simulations, each with the starting condition of $r = 0.53 \text{ \AA}$, but with different seeds in the random number generation scheme to create a different set of plane waves. Consequently, the trajectory of each of these simulations was completely different, although the general character of each was similar. We used a Runge-Kutta 5th order algorithm, with an adaptive stepsize. The simulation code was written in C; the runs were carried out on 11 separate Pentium 4 PCs, each with 1.8 GHz processing speed and 512 MB of RAM. The CPU times for each run was about 5 CPU days, with some more and some less, as we attempted to have all electrons tracked for reasonably close to the same length in time. However, for those electrons spending more time near the nucleus, the calculations took longer because of the faster fluctuations involved. The net time for all runs was about 55 CPU days.

Each of the four snapshots in Fig. 2 show the radial probability density curve, $P_{QM}(r)$ vs. r , from Schrödinger's wave equation for the ground state of hydrogen, versus the probability distribution calculated at the indicated snapshot in time. In Fig. 2(a), the simulated trajectories still strongly show the character of the initial condition of $r = 0.53 \text{ \AA}$. However, each succeeding snapshot shows a striking convergence toward $P_{QM}(r)$. Moreover, the probability distribution for the end of each of the individual eleven runs has a reasonable resemblance to $P_{QM}(r)$, although combining all of the results together provides a better match, presumably due to the net longer simulation run and the greater sampling over field

conditions. We anticipate that future tests of interest will involve other initial starting points, deeper testing for ergodicity, etc.

These simulation results follow the qualitative idea that Boyer originally suggested in 1975 [29] that for larger radial orbits, the dominant part of the ZP spectrum that will effect the orbit will be the low frequency regime, which has a low energetic contribution, thereby leading on average to a decaying behavior of the orbit. However, for orbits of smaller radius, then the electron will interact most strongly with the higher frequency components of the ZP field, which have a larger energetic contribution. Hence, for smaller radii, the probability greatly increases that the ZP field will act to increase the orbit size. In this way, a stochastic-like pattern should emerge for the electron [Fig. 1].

Without question, the simulations presented here do not “prove” that SED works for atomic systems. There are far more tests and phenomena to still be examined, such as atomic spectra, many electron situations, spin, an understanding of how “photon” behavior arises, relativistic corrections and very high frequency effects. We are presently investigating some of these areas. Nevertheless, there is also the very real possibility, far stronger now that we see predictions for the hydrogen atom in fairly close agreement with physical observation, that the core ideas of SED provide a fundamental perspective on nature and a potential basis for QM phenomena.

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Figure Captions

Figure 1: Typical plot of r vs. t for one trajectory realization via the methods described here. The inset shows the probability density $P(r)$ vs r computed for this particular trajectory.

Figure 2: Plots of the radial probability density vs. radius. The solid line was calculated from the ground state of hydrogen via Schrödinger's equation: $P(r) = 4\pi r^2 |\Psi(\mathbf{x})|^2 = \frac{4r^2}{a_B^3} \exp\left(-\frac{2r}{a_B}\right)$, where $a_B = \hbar^2/mc^2$. The dotted curves are the simulation results, calculated as a time average for all eleven simulation runs from time $t = 0$ to the average time indicated: (a) 1.559×10^{-11} sec; (b) 4.950×10^{-11} sec; (c) 6.275×10^{-11} sec; (d) 7.977×10^{-11} sec.

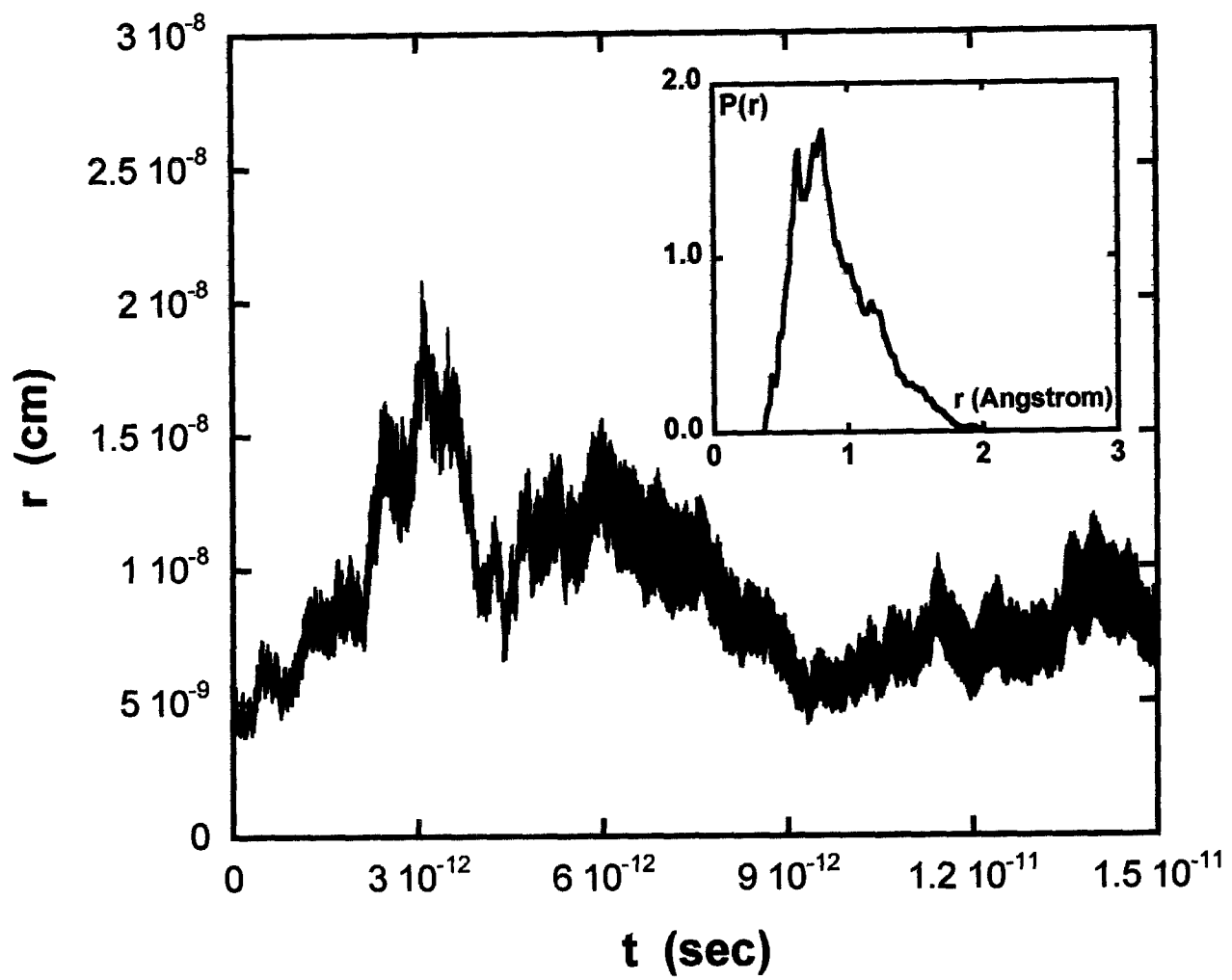


Fig. 1

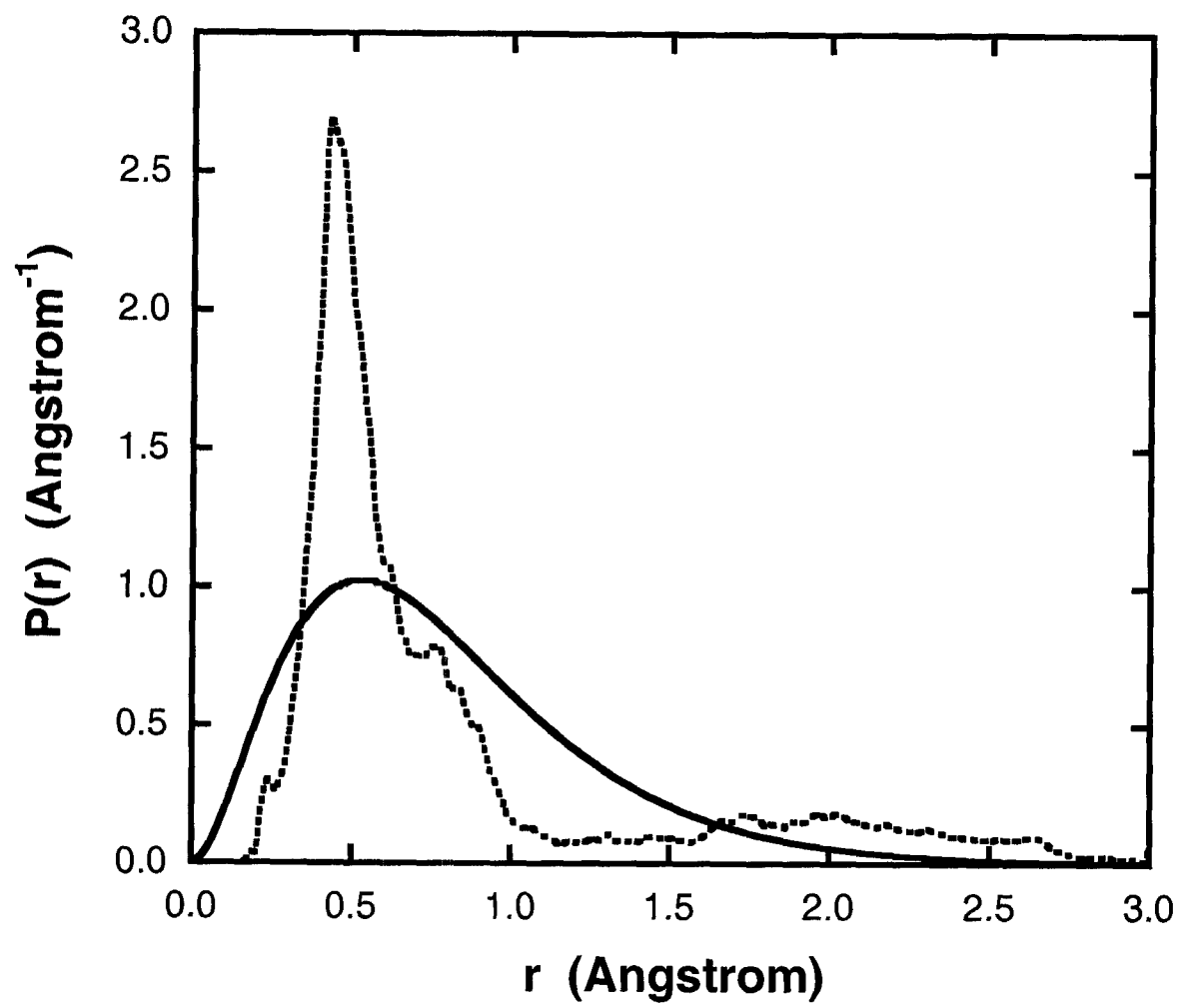


Fig. 2(a)

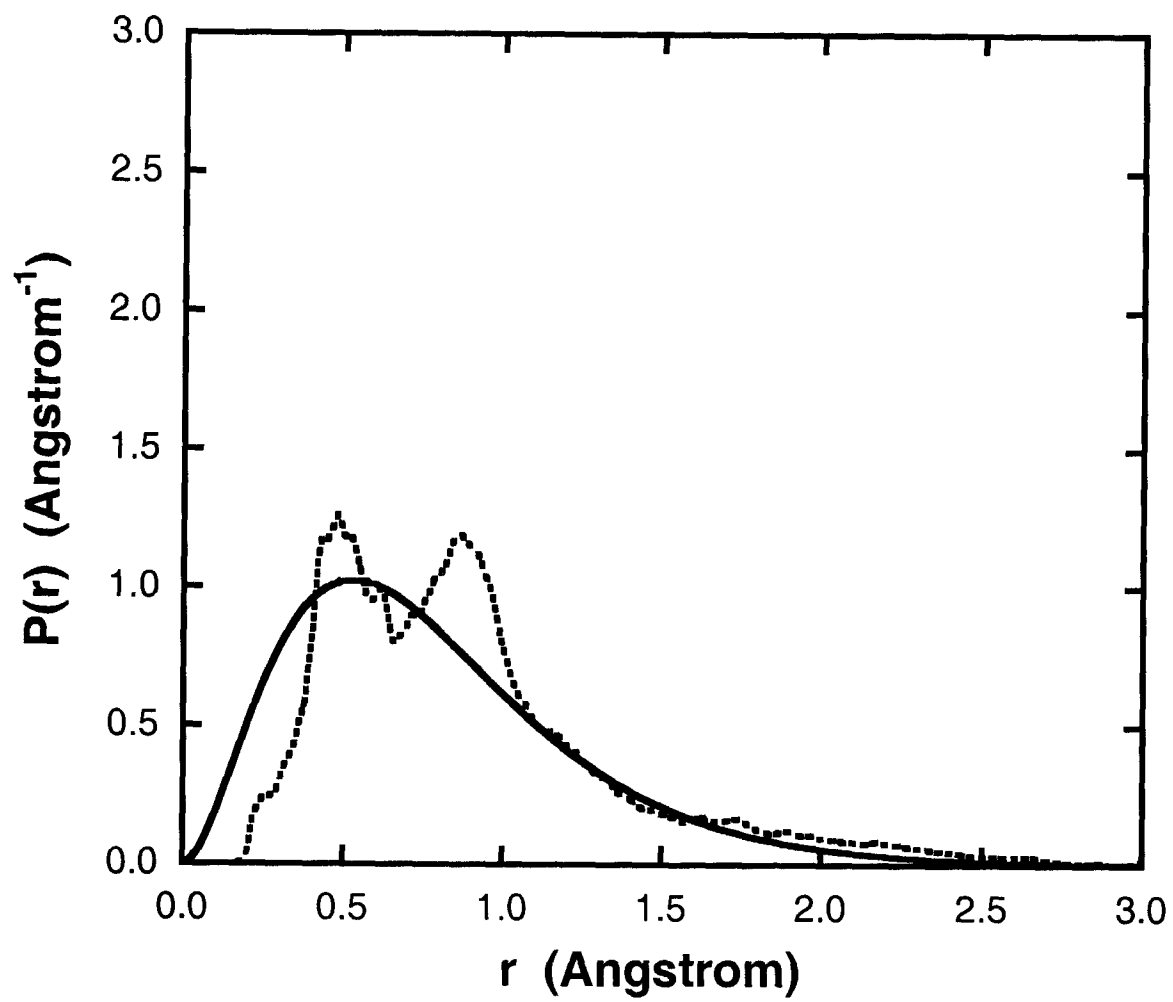


Fig. 2(b)

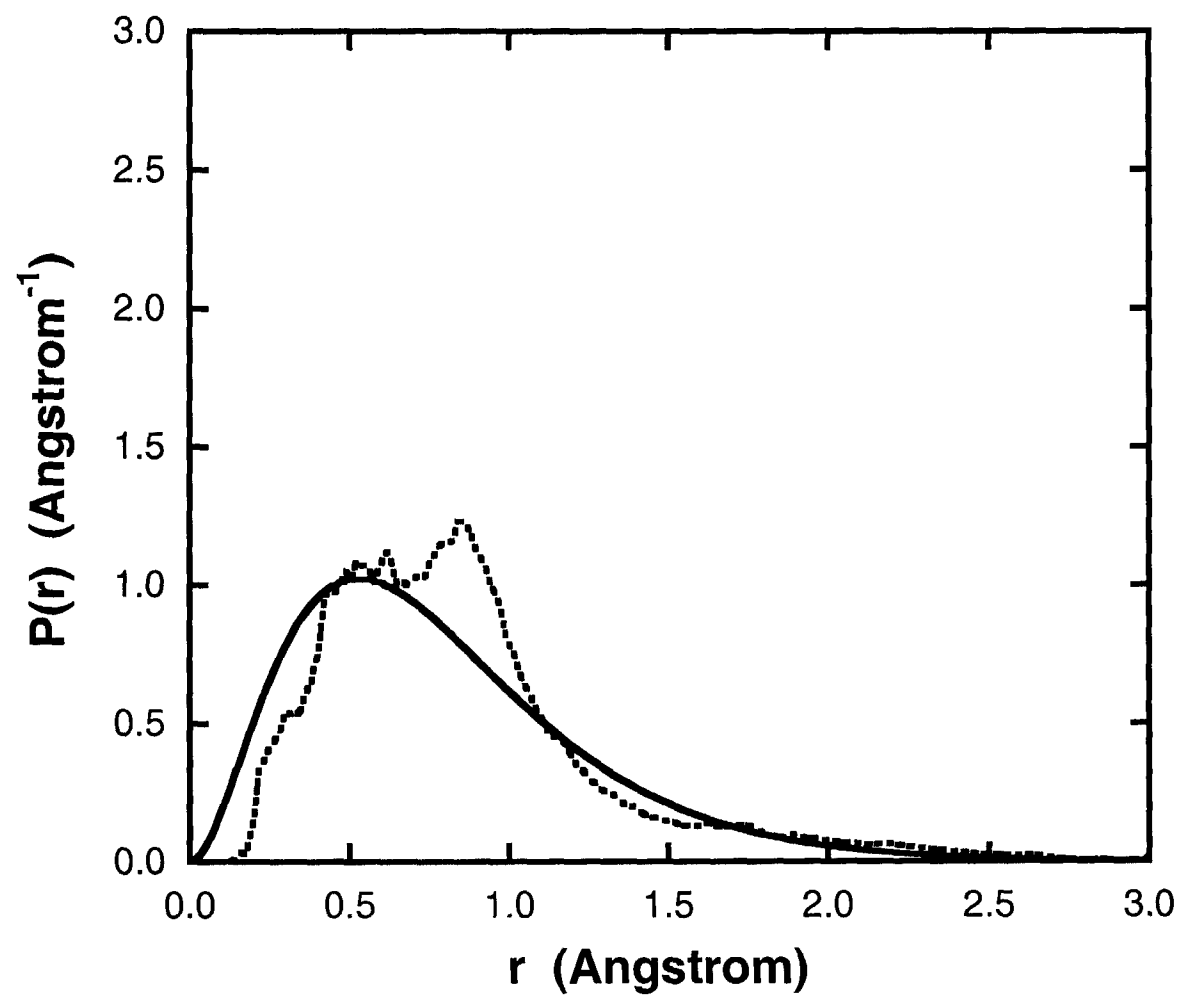


Fig. 2(c)

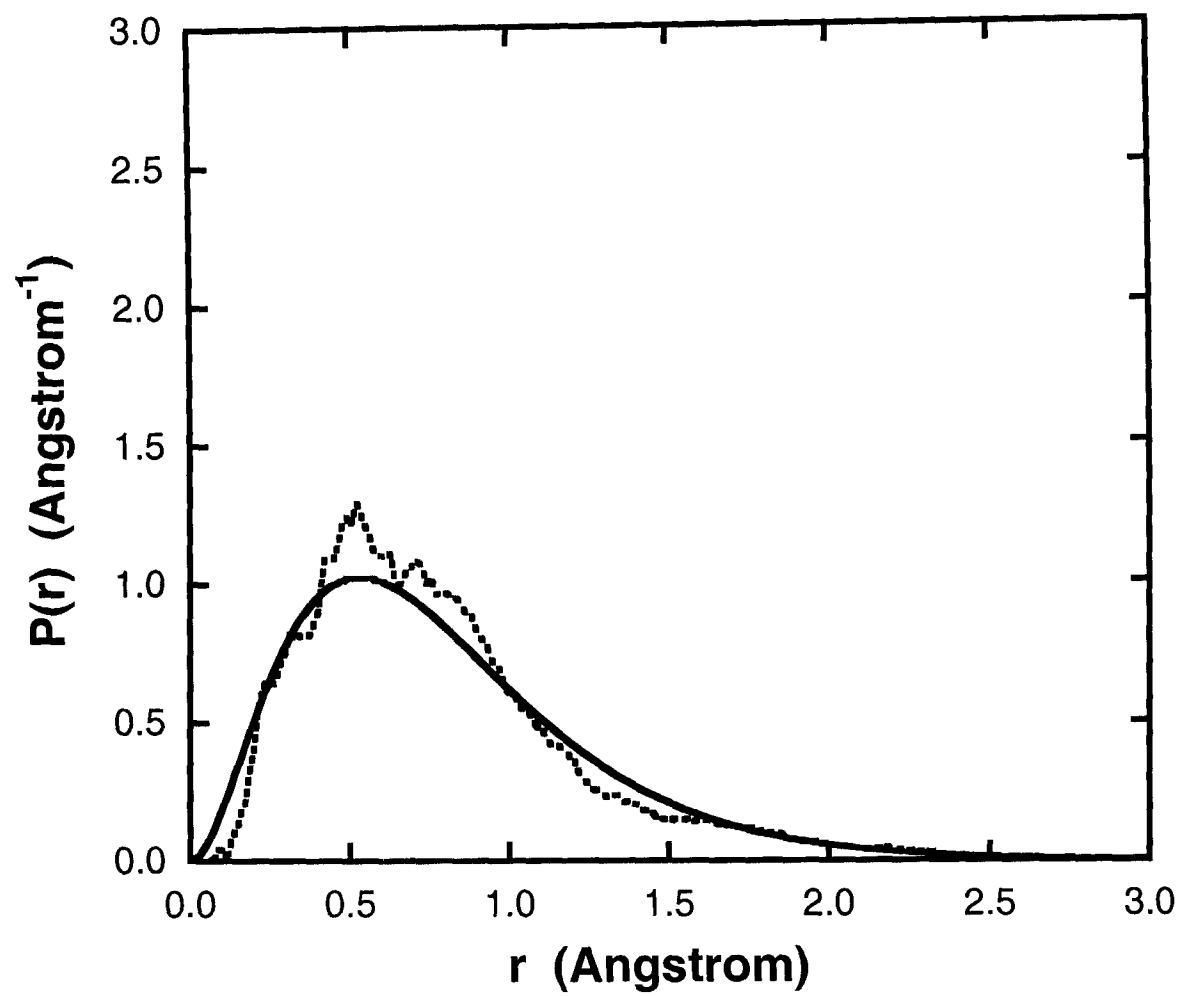


Fig. 2(d)