MD Simulation of Hydrogen bonded Ferroelectrics: Effect of Anion Polarisability and Temperature on Proton Dynamics

4.1 Introduction

4.2 Details of calculations

4.3 Results: Effect of g-parameter and temperature variation on proton motion.

4.4 Results: Effect of variation of double well parameters on transport of proton.

4.5 Phase space plots of atoms in selected lattice sites.

4.6 Discussion
4.1 Introduction

In this chapter the molecular dynamics simulation has been carried out for the proposed model using the computer programmes developed in the previous chapter. The effects of variation of the temperature T, and the core-shell coupling constant g and the double well parameters $\varepsilon_o$ and $u_o$ on the displacement patterns of the proton lattice ($\eta$) and the anion lattice ($\Phi$) are discussed. For convenience of reference the dimensionless equations of motion which have been studied are given below.

$$\frac{m}{\ddot{\Phi}_n} = \gamma_3 (\eta_{n+1} + \eta_{n-1} + 2\eta_n) - 2(\gamma_1 + \gamma_2) \Phi_n + \gamma_1 (\Phi_{n+1} + \Phi_{n-1}) \quad \ldots(4.1a)$$

$$\frac{d^2 \eta_n}{dt^2} = [\gamma_2 + \gamma_4] (\eta_{n+1} \eta_{n-1}) + \gamma_3 \Phi_n - \eta_3^n + \eta_n [1 - 2\gamma - 2\gamma_2 + 2\gamma_4] \quad \ldots(4.1b)$$

where

$\gamma_1$, $\gamma_2$, and $\gamma_3$ are functions of the double well parameters $\varepsilon_o$ and $u_o$.

$\gamma_4$ and $\gamma_5$ are functions of $g$, $\varepsilon_o$ and $u_0$.

4.2 Details of calculation

Simulation has been carried out for different values of $T$ (0.1, 0.5 and 0.8) and $g$ (0 to $10^{15}$ dynes/cm) using the following parameters. The values of the parameters are taken from experimental data available in the literature [28].

$$m_1 = 2.8822 \times 10^{-23} \text{ gm}$$

$$m_2 = 1.66 \times 10^{-24} \text{ gm}$$

$$\varepsilon_o = 3.53 \times 10^{-13} \text{ ergs}$$

$$u_o = 3.9 \times 10^{-9} \text{ cm}$$
\[ f = 5.5 \times 10^5 \text{ dynes/cm} \]
\[ f_1 = 1.0 \times 10^4 \text{ dynes/cm} \]
\[ f_2 = 1.0 \times 10^4 \text{ dynes/cm} \]

By keeping the limitations of computer used in mind the length of the chain is restricted to 1000 unit cells or 2000 particles. The model system is allowed to evolve for sufficiently large number of time steps, i.e. \( 2^{14} \) or 16384 steps.

The value of time step is taken to be \( h = 0.5 \) keeping in mind the numerical stability. In order to eliminate initial bias, the actual beginning is made after 10000 initial time steps. This corresponds to the variable verlet skip \( \rightarrow 10000 \) in the computer programme. Considering the fact that seed for RN generator given in the previous chapter should be large negative, odd digit numbers \([39]\), the value of seed is taken to be \(-93179\). Initial values of \( \eta \) and \( \Phi \) are taken from the analytical solution discussed in the second chapter. In addition, fluctuation is added randomly to the ground state configuration.

\[ \eta \text{ has displacement range from } -0.999 \text{ to } -1.001 \]
\[ \Phi \text{ has displacement range from } -1.999 \text{ to } -2.001 \]

All protons are in the left side of the double well potential. After fixing these values, simulations have been carried out for different value of \( g \) and \( T \).
4.3 Results: Effect of g-parameter and temperature variation on proton motion.

Case (i) \( T = 0.1 \) (  \( \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg, } u_0 = 3.9 \times 10^{-9} \text{ cm.} \)  

When \( g \) is small (\( g = 0, 10^{-15}, 10^{-5}, 10^{-2} \)) all protons oscillate in the left well (i.e. around \(-1\)) independently. This corresponds to small amplitude protons oscillations. \( \Phi \) shows unrealistically large values (Fig. 4.1)

When \( g = 1 \), there is no major change in \( \eta \) dynamics. \( \Phi \) value starts to come down. This value of \( g \) may be considered as transition region as far as \( \Phi \) is concerned. (Fig. 4.2)

If \( g \) is larger (\( 10^2 \)) proton dynamics (\( \eta \)) shows phonons dressed solitons. This collective behaviour is due to co-operative excitation of protons. \( \Phi \) results show that it is still in the transition region (Fig. 4.3)

As the value of \( g \) is further increased (\( 10^5, 10^{15} \)) both proton (\( \eta \)) and anion (\( \Phi \)) show the same behaviour. i.e. both solutions are kink like solutions (Fig.4.4). The reason for the similar behaviour will be discussed at the end of the section.

Case (ii) \( T = 0.5 \)

For low \( g \) values (0, \( 10^{-15}, 10^{-5} \)), unlike low amplitude phonon solution in the case of low temperature (0.1) proton motion also shows soliton solution. Again, similar to low temperature regime, \( \Phi \) shows unrealistic values (Fig.4.5).
At large \( g \) values \((10^{-2}, 1, 10^2)\) \( \eta \) shows soliton solution while \( \Phi \) starts to have reasonable value (Fig. 4.6).

At still higher values of \( g \) \((10^5, 10^{15})\), number of solitons increase which implies that large amplitude phonons (non-linear phonon or periodon) and kink solutions coexist (Fig. 4.7).

Case (iii) \( T = 0.8 \)

If \( g \) is low \((0, 10^{-15}, 10^5)\), \( \eta \) shows cooperative kink solution whereas \( \Phi \) shows unrealistic values (Fig. 4.8).

If \( g \) is large \((10^{-2}, 1, 10^2)\) there is no major change in the behaviour of \( \eta \) but \( \Phi \) starts to show reasonable values.

For very large \( g \) values \((10^5, 10^{15})\) there are no solitons but only large amplitude phonons (periodon) seem to exist. Both \( \eta \) and \( \Phi \) behave in a similar fashion (Fig. 4.9).

### 4.4 Results: Effect of variation of double well parameters on transport of proton.

In this section the effect of variation of double well parameters such as barrier height \( (\varepsilon_0) \) and distance between the two minima \( (u_0) \) on the chain dynamics is investigated.
(1) Standard value \((u_0 = 3.9 \times 10^{-9} \text{ cm}; \ T = 0.1)\)

a) \(\varepsilon_0 = 5.29 \times 10^{-13} \text{ erg} \) (1.5 times that of standard value of \(\varepsilon_0\)).

There is no marked change in the proton displacement pattern (Fig. 4.10) when compared with the results reported in the previous section for standard \(\varepsilon_0\) value (Fig. 4.3).

b) \(\varepsilon_0 = 1.765 \times 10^{-15} \text{ erg} \) (0.5 times that of standard value of \(\varepsilon_0\)).

For \(g = 0, 10^{-15}, 10^{-5} \text{ and } 10^{-2}\), \(\eta\) solutions oscillate around -1, i.e. implying phonon oscillation of protons at the left well (Fig. 4.11).

At \(g = 1\), solitons appear unlike in the case of \(\varepsilon_0 = 3.53 \times 10^{-13}\) where solitons start appearing only at \(g = 10^2\) (Fig. 4.12).

Further increase of \(g\) values \((10^2)\) soliton disappears and all protons now are in the right well oscillating around +1 (Fig. 4.13).

In all cases we started with the initial value of \(\eta\) around -1 (left well) and the previous results showed the presence of small amplitude phonons, solitons and large amplitude phonons or peridons. However, in the present case the solution is of the type _temporal Autowaves_ i.e. we start with one equilibrium and end in another equilibrium with time evolution. It is still a small amplitude phonon solution or oscillatory solution, i.e. all protons in the model are oscillating at the right side of the double well.
When $g = 10^5$, almost all protons are in the left well and oscillate around -1.

At large $g$ value ($10^{15}$), solitons start reappearing (Fig.4.14).

(2) $u_o = 3 \times 10^{-9}$ cm, $T = 0.1$

a) $\varepsilon_o = 3.53 \times 10^{-13}$ erg

At low $g$ values ($0, 10^{-15}$), MD simulation reveals $\eta$ solution is kink type and $\Phi$ shows unrealistic values (Fig.4.15).

For moderate values of $g$ ($10^{-2}, 1, 10^2$) kink solutions continue and their width increases with increase of $g$ values (Fig.4.16).

At large values of $g$ ($10^5, 10^{15}$) number of kinks or solitons increases with $g$ values (Fig.4.17).

b) $\varepsilon_o = 5.295 \times 10^{-13}$ erg

If $g$ is small ($0, 10^{-15}, 10^{-5}, 10^{-2}, 1$) there are no kink solutions and the solution oscillates around -1 (Fig.4.18).

At $g = 10^2$, kinks appear (Fig.4.19). For higher value of $g$, number of kinks increases with increase of $g$ value (Fig.4.20).
c) \( \varepsilon_0 = 1.765 \times 10^{-13} \text{ erg} \)

For small \( g \) values \( (0, 10^{-15}, 10^{-5}) \) there is no kink solution (Fig. 4.21).

If \( g = 10^{-2} \), one kink appears (Fig. 4.22) Further increase of \( g \) i.e. \( 10^2 \), the kink solution gets destroyed and all protons oscillate around +1 (Fig. 4.23).

At very large values of \( g \) \( (10^5, 10^{15}) \) kinks again appear and their numbers increase with \( g \) value (Fig. 4.24).

(3) \( \nu_o = 4.9 \times 10^{-9} \text{ cm}, \ T = 0.1 \)

a) \( \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \)

If \( g = 10^{-15} \), \( \eta \) dynamics shows kink behaviour (Fig. 4.25).

If \( g = 10^{-5}, 10^{-2} \), soliton solution gets destroyed and all protons oscillate around -1, i.e. only small amplitude phonons are present. (Fig. 4.26).

At \( g = 1 \), soliton again reappears (Fig. 4.27).

For \( g = 10^2 \), number of solitons decreases and almost all protons oscillate around +1 suggesting temporal auto wave behaviour (Fig. 4.28).

When \( g = 10^5, 10^{15} \) number of solitons increases with \( g \) value (Fig. 4.29).
b) $\varepsilon_o = 5.295 \times 10^{-13} \text{ erg}$

For $g = 0, 10^{-15}, 10^{-5}$, there are no kink solutions. All protons oscillate around $\pm 1$ (Fig. 4.30) indicating small amplitude phonons.

For $g = 10^{-2}$, solitons start appearing indicating co-operative behaviour is evident in the solution (Fig. 4.31).

When $g = 10^2$, number of solitons decreases (Fig. 4.32) drastically.

At high $g$ values (of the order of $10^5, 10^{15}$) number of kinks decreases with increase of $g$ values (Fig. 4.33).

c) $\varepsilon_o = 1.765 \times 10^{-13} \text{ erg}$

For $g = 10^{-15}, 10^{-5}, 10^{-2}$, width of kink+antikink decreases with increase of $g$ value (Figs. 4.34, 4.35). This width becomes minimum at $g = 1$ (Fig. 4.36). Once again it increases at higher $g$ values - i.e. at $10^5, 10^{15}$ (Fig. 4.37).

4.5 Phase space plots of atoms in selected lattice sites.

During MD simulation, velocity and displacement of 250th, 500th and 750th particles are stored at each time step and phase space graph is plotted between the dynamical variables $\eta$ and $\eta'$ for standard double well parameter values (Fig. 4.38). Figs. 4.38 to 4.46 depict the phase space plots for $\eta$ and $\eta'$ for different $g$ and temperature ($T$) values.
The following results have been arrived at from the phase portraits.

(i) Variation of $T$ and $g$ give the same effect.

(ii) At low values of $g$ or $T$, two equilibrium positions can be seen and as the value, of the variables increase the two equilibrium positions become blurred. At high $g$ values, both equilibria cannot be distinguished. This is indicative of non-linear oscillations or large amplitude phonons or periodons.

(iii) In some cases ($g = 10^2$, 500th particle, $T = 0.1$) the motion of proton from left to right equilibrium and then from right to left is clearly seen.

(iv) Again phase portraits show, some interesting behaviour around $g = 10^2$, where $\Phi$ starts to have to reasonable values.

(v) At large $g$ values phonons, solitons and periodons are found to coexist.

4.6 Discussion

Even though the proposed model is suitable to study both soft mode and proton transport in one dimensional lattice, we studied only proton dynamics as anharmonic polarisation gets linearised by SPA approximation. This avoids mathematical complication arising out of handling two non-linear terms in the equations of motion.

As thermal averaged SPA is applied, $g$ has a similar effect like that of the temperature. In addition to the temperature like effect of $g$, one can visualise additional physical mechanisms through the proposed model when $g$ is varied.
(a) when $g$ is small ($\sim 0$ i.e. core-shell force constant is very weak), the core and shell move independently. As only shell is connected with proton, core will be unaffected by the proton dynamics. This is evident as $\Phi$ shows unrealistically large values.

(b) At high $g$ values ($\sim 10^{15}$ i.e. rigid shell-core coupling), core and proton couple indirectly. For this reason $\eta$ and $\Phi$ behave similarly. But large values of temperature and low $g$ values do not produce this effect. In this case $g$ effect is not the same as that of the temperature effect.

Let us summarise the different types of solutions and their associated possible mechanisms in the proposed model.

(i) At low temperature (0.1) thermal energy is not sufficient to lift the proton from one minimum to another. Proton simply oscillates in one minimum (say left well) independently and it is called small amplitude oscillation. Pictorially it can be represented as in Fig.4.47

![Fig.4.47 Proton motion in double well potential](image)

(ii) At high temperature (0.5), thermal energy fluctuation is enough to lift the particles from one minimum to another minimum. Results show cluster like pattern. In one cluster which spreads over several unit cells, all protons are in the left well and in the next cluster all
protons are in the right well. And this pattern repeats. This type of co-operative behaviour of the system is clearly observed in the kink solution (Fig.4.47).

(iii) At still higher temperature (0.8), proton executes large amplitude oscillation across the well and no barrier effect is felt (Fig.4.47). This large amplitude oscillation is called non-linear phonon or periodon[16]. For this reason at high temperature, soliton solution gets destroyed.

(iv) In some cases (Fig.4.39), results indicate that all types of solutions i.e. phonon (arising due to small amplitude oscillation), kink(co-operative behaviour) and non-linear phonon or periodon (large amplitude phonon) co-exist together.

(v) In some other cases (Fig.4.40), all protons jump over to the right well from the left well and execute small amplitude oscillations independently. This solution is called temporal autowaves.

Another interesting result is that, for low potential barriers the protons go from one minimum to another minimum easily without the appearance of solitons for low and intermediate g values even at low temperatures. Phonon, periodon and temporal autowave behaviour is very evident. For high potential barriers and low g values protons remain in the left well. However, as g increases solitons appear suggesting a longer range co-operative behaviour, i.e. protons in the left minima are shifted to the right minima over several unit cells. No temporal autowave effect is apparent.
In Chapter II the phonons, periodons and solitons were obtained as analytical solutions under specific condition. Temperature was not explicitly introduced. In the M.D. simulation where temperature is explicitly introduced one observes all these solutions. Solitons are essentially low energy solutions (low temperature) whereas periodons are essentially high temperature solutions.

The phase space diagram of specific protons in the chain clearly demonstrates the mechanism of their movement from one minimum to another depending on g and T values.

In hydrogen bonded systems there are two ways to look at phase transition mechanism. The first one involves the dynamics of protons alone. Above the phase transition temperature the protons are statistically distributed over both the minima. As one comes close to the $T_c$ the protons have large oscillations (or quantum mechanical tunneling). Below $T_c$ the protons choose one of the minima (left or right) and execute harmonic motion about those minima. The dynamics involves non-linear phonons and relaxations.

The second model attributes the phase transition to the anion lattice soft mode and associated polarisation. Bilz et.al. model essentially works on this principle [1,2]. Very low g values lead to the soft mode behaviour.

The proposed model in this work account for the motion of protons from one minimum to another minimum in terms of co-operative soliton behaviour over several unit cells. However, this is critically dependent on the values of the coupling constant g and temperature T. Lower g
values and intermediate temperature values are conducive to transport of protons from one minimum to the next. Higher $g$ values and temperatures lead to large amplitude phonons involving oscillations between the two minima rather than proton transport. In Bilz model high $g$ values correspond to low electric polarisation. It is only natural that high $g$ and high $T$ values correspond to a paraelectric phase.
Fig. 4.1a

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^{15} \]

Fig. 4.2a

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 1 \]

Fig. 4.3a

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^2 \]
Fig. 4.1b

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \epsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^{-15} \]

Fig. 4.2b

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \epsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 1 \]

Fig. 4.3b

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \epsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^2 \]
Fig. 4.4a

\[ T = 0.1 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^5 \]

Fig. 4.5a

\[ T = 0.5 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^{-13} \]

Fig. 4.6a

\[ T = 0.5 \]
\[ u_0 = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 1 \]
Fig. 4.4b

$T=0.1$
$u_0=3.9 \times 10^{-9} \text{ cm}$
$\varepsilon_0=3.53 \times 10^{-13} \text{ erg}$
$g=10^3$

Fig. 4.5b

$T=0.5$
$u_0=3.9 \times 10^{-9} \text{ cm}$
$\varepsilon_0=3.53 \times 10^{-13} \text{ erg}$
$g=10^{-15}$

Fig. 4.6b

$T=0.5$
$u_0=3.9 \times 10^{-9} \text{ cm}$
$\varepsilon_0=3.53 \times 10^{-13} \text{ erg}$
$g=1$
Fig. 4.7a

\[ T=0.5 \]
\[ u_0=3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0=3.53 \times 10^{-13} \text{ erg} \]
\[ g=10^5 \]

Fig. 4.8a

\[ T=0.8 \]
\[ u_0=3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0=3.53 \times 10^{-13} \text{ erg} \]
\[ g=0 \]

Fig. 4.9a

\[ T=0.8 \]
\[ u_0=3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0=3.53 \times 10^{-13} \text{ erg} \]
\[ g=10^{15} \]
Fig. 4.7b

$T=0.5$

$u_0=3.9 \times 10^{-9} \text{ cm}$

$\varepsilon_0=3.53 \times 10^{-13} \text{ erg}$

$g=10^5$

---

Fig. 4.8b

$T=0.8$

$u_0=3.9 \times 10^{-9} \text{ cm}$

$\varepsilon_0=3.53 \times 10^{-13} \text{ erg}$

$g=0$

---

Fig. 4.9b

$T=0.8$

$u_0=3.9 \times 10^{-9} \text{ cm}$

$\varepsilon_0=3.53 \times 10^{-13} \text{ erg}$

$g=10^{13}$
Fig. 4.10a

$T = 0.1$

$u_0 = 3.9 \times 10^9 \text{ cm}$

$\epsilon_0 = 5.295 \times 10^{-13} \text{ erg}$

$g = 10^2$

Fig. 4.11a

$T = 0.1$

$u_0 = 3.9 \times 10^9 \text{ cm}$

$\epsilon_0 = 1.765 \times 10^{-13} \text{ erg}$

$g = 10^{14}$

Fig. 4.12a

$T = 0.1$

$u_0 = 3.9 \times 10^9 \text{ cm}$

$\epsilon_0 = 1.765 \times 10^{-13} \text{ erg}$

$g = 1$
\( \Phi \) - Dynamics

**Fig. 4.10b**

\[
\begin{align*}
T &= 0.1 \\
\nu_o &= 3.9 \times 10^{-9} \text{ cm} \\
\epsilon_o &= 5.295 \times 10^{-13} \text{ erg} \\
g &= 10^2
\end{align*}
\]

**Fig. 4.11b**

\[
\begin{align*}
T &= 0.1 \\
\nu_o &= 3.9 \times 10^{-9} \text{ cm} \\
\epsilon_o &= 1.765 \times 10^{-13} \text{ erg} \\
g &= 10^{14}
\end{align*}
\]

**Fig. 4.12b**

\[
\begin{align*}
T &= 0.1 \\
\nu_o &= 3.9 \times 10^{-9} \text{ cm} \\
\epsilon_o &= 1.765 \times 10^{-13} \text{ erg} \\
g &= 1
\end{align*}
\]
Fig. 4.13a
\[ T=0.1 \]
\[ u_0=3.9 \times 10^{-9} \text{ cm} \]
\[ \epsilon_0=1.765 \times 10^{-12} \text{ erg} \]
\[ g=10^2 \]

Fig. 4.14a
\[ T=0.1 \]
\[ u_0=3.9 \times 10^{-9} \text{ cm} \]
\[ \epsilon_0=1.765 \times 10^{-13} \text{ erg} \]
\[ g=10^{15} \]

Fig. 4.15a
\[ T=0.1 \]
\[ u_0=3.0 \times 10^{-9} \text{ cm} \]
\[ \epsilon_0=3.53 \times 10^{-13} \text{ erg} \]
\[ g=0 \]
Fig. 4.13b
\[ T = 0.1 \]
\[ u_o = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_o = 1.765 \times 10^{-13} \text{ erg} \]
\[ g = 10^2 \]

Fig. 4.14b
\[ T = 0.1 \]
\[ u_o = 3.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_o = 1.765 \times 10^{-13} \text{ erg} \]
\[ g = 10^{13} \]

Fig. 4.15b
\[ T = 0.1 \]
\[ u_o = 3.0 \times 10^9 \text{ cm} \]
\[ \varepsilon_o = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 0 \]
Fig. 4.16a
\( T=0.1 \)
\( u_0=3.0 \times 10^{-9} \text{ cm} \)
\( \varepsilon_0=3.53 \times 10^{-13} \text{ erg} \)
\( g=1 \)

Fig. 4.17a
\( T=0.1 \)
\( u_0=3.0 \times 10^{-9} \text{ cm} \)
\( \varepsilon_0=3.53 \times 10^{-13} \text{ erg} \)
\( g=10^{13} \)

Fig. 4.18a
\( T=0.1 \)
\( u_0=3.0 \times 10^{-9} \text{ cm} \)
\( \varepsilon_0=5.295 \times 10^{-13} \text{ erg} \)
\( g=0 \)
Fig. 4.16b

$T=0.1$

$u_0 = 3.0 \times 10^{-9}\text{ cm}$

$\varepsilon_0 = 3.53 \times 10^{-13}\text{ erg}$

$g=1$

Fig. 4.17b

$T=0.1$

$u_0 = 3.0 \times 10^{-9}\text{ cm}$

$\varepsilon_0 = 3.53 \times 10^{-13}\text{ erg}$

$g=10^{13}$

Fig. 4.18b

$T=0.1$

$u_0 = 3.0 \times 10^{-9}\text{ cm}$

$\varepsilon_0 = 5.295 \times 10^{-13}\text{ erg}$

$g=0$
Fig. 4.19a

$T=0.1$
$u_0=3.0 \times 10^{-9} \text{ cm}$
$\varepsilon_0=5.295 \times 10^{-13} \text{ erg}$
$g=10^2$

Fig. 4.20a

$T=0.1$
$u_0=3.0 \times 10^{-9} \text{ cm}$
$\varepsilon_0=5.295 \times 10^{-13} \text{ erg}$
$g=10^{13}$

Fig. 4.21a

$T=0.1$
$u_0=3.0 \times 10^{-9} \text{ cm}$
$\varepsilon_0=1.765 \times 10^{-17} \text{ erg}$
$g=10^{-13}$
Fig. 4.19b

$T=0.1$

$u_o = 3.0 \times 10^{-9}$ cm

$\epsilon_o = 5.295 \times 10^{-13}$ erg

$g=10^2$

---

Fig. 4.20b

$T=0.1$

$u_o = 3.0 \times 10^{-9}$ cm

$\epsilon_o = 5.295 \times 10^{-13}$ erg

$g=10^{13}$

---

Fig. 4.21b

$T=0.1$

$u_o = 3.0 \times 10^{-9}$ cm

$\epsilon_o = 1.765 \times 10^{-13}$ erg

$g=10^{13}$
\( \eta - \text{Dynamics} \)

**Fig. 4.22a**

\[
\begin{align*}
T &= 0.1 \\
u &= 3.0 \times 10^9 \text{ cm} \\
\epsilon_o &= 1.765 \times 10^{13} \text{ erg} \\
g &= 10^2
\end{align*}
\]

**Fig. 4.23a**

\[
\begin{align*}
T &= 0.1 \\
v &= 3.0 \times 10^9 \text{ cm} \\
\epsilon_o &= 1.765 \times 10^{13} \text{ erg} \\
g &= 10^2
\end{align*}
\]

**Fig. 4.24a**

\[
\begin{align*}
T &= 0.1 \\
v &= 3.0 \times 10^9 \text{ cm} \\
\epsilon_o &= 1.765 \times 10^{13} \text{ erg} \\
g &= 10^{13}
\end{align*}
\]
$\Phi$ - Dynamics

**Fig. 4.22b**

$T=0.1$

$u_0=3.0 \times 10^{-9} \text{ cm}$

$\varepsilon_0=1.765 \times 10^{-13} \text{ erg}$

$g=10^2$

**Fig. 4.23b**

$T=0.1$

$u_0=3.0 \times 10^{-9} \text{ cm}$

$\varepsilon_0=1.765 \times 10^{-13} \text{ erg}$

$g=10^2$

**Fig. 4.24b**

$T=0.1$

$u_0=3.0 \times 10^{9} \text{ cm}$

$\varepsilon_0=1.765 \times 10^{13} \text{ erg}$

$g=10^{13}$
\textbf{Fig. 4.25a}

\(T = 0.1\)
\(u_0 = 4.9 \times 10^{-9}\) cm
\(\varepsilon_0 = 3.53 \times 10^{-13}\) erg
\(g = 10^{-13}\)

\textbf{Fig. 4.26a}

\(T = 0.1\)
\(u_0 = 4.9 \times 10^{-9}\) cm
\(\varepsilon_0 = 3.53 \times 10^{-13}\) erg
\(g = 10^{-5}\)

\textbf{Fig. 4.27a}

\(T = 0.1\)
\(u_0 = 4.9 \times 10^{-9}\) cm
\(\varepsilon_0 = 3.53 \times 10^{-13}\) erg
\(g = 1\)
**Fig. 4.25b**

\[ T = 0.1 \]

\[ u_o = 4.9 \times 10^{-9} \text{ cm} \]

\[ \varepsilon_o = 3.53 \times 10^{-13} \text{ erg} \]

\[ g = 10^{-15} \]

**Fig. 4.26b**

\[ T = 0.1 \]

\[ u_o = 4.9 \times 10^{-9} \text{ cm} \]

\[ \varepsilon_o = 3.53 \times 10^{-13} \text{ erg} \]

\[ g = 10^{-5} \]

**Fig. 4.27b**

\[ T = 0.1 \]

\[ u_o = 4.9 \times 10^{-9} \text{ cm} \]

\[ \varepsilon_o = 3.53 \times 10^{-13} \text{ erg} \]

\[ g = 1 \]
**η - Dynamics**

**Fig. 4.28a**

\[ T = 0.1 \]
\[ u_0 = 4.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^2 \]

**Fig. 4.29a**

\[ T = 0.1 \]
\[ u_0 = 4.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 3.53 \times 10^{-13} \text{ erg} \]
\[ g = 10^{13} \]

**Fig. 4.30a**

\[ T = 0.1 \]
\[ u_0 = 4.9 \times 10^{-9} \text{ cm} \]
\[ \varepsilon_0 = 5.295 \times 10^{-13} \text{ erg} \]
\[ g = 0 \]
Fig. 4.28b
$T=0.1$
$u_0=4.9 \times 10^{-9} \text{ cm}$
$e_0=3.53 \times 10^{-13} \text{ erg}$
$g=10^2$

Fig. 4.29b
$T=0.1$
$u_0=4.9 \times 10^{-9} \text{ cm}$
$e_0=3.53 \times 10^{-13} \text{ erg}$
$g=10^{11}$

Fig. 4.30b
$T=0.1$
$u_0=4.9 \times 10^{-9} \text{ cm}$
$e_0=5.295 \times 10^{-13} \text{ erg}$
$g=0$
Fig. 4.31a

- $T=0.1$
- $u_o = 4.9 \times 10^{-9}$ cm
- $\varepsilon_o = 5.295 \times 10^{-13}$ erg
- $g = 10^2$

Fig. 4.32a

- $T=0.1$
- $u_o = 4.9 \times 10^{-9}$ cm
- $\varepsilon_o = 5.295 \times 10^{-13}$ erg
- $g = 10^2$

Fig. 4.33a

- $T=0.1$
- $u_o = 4.9 \times 10^{-9}$ cm
- $\varepsilon_o = 5.295 \times 10^{-13}$ erg
- $g = 10^{15}$
Fig. 4.31b

\begin{align*}
T &= 0.1 \\
u_o &= 4.9 \times 10^{-9} \text{ cm} \\
\epsilon_o &= 5.295 \times 10^{-13} \text{ erg} \\
g &= 10^2 
\end{align*}

Fig. 4.32b

\begin{align*}
T &= 0.1 \\
u_o &= 4.9 \times 10^{-9} \text{ cm} \\
\epsilon_o &= 5.295 \times 10^{-13} \text{ erg} \\
g &= 10^2 
\end{align*}

Fig. 4.33b

\begin{align*}
T &= 0.1 \\
u_o &= 4.9 \times 10^{-9} \text{ cm} \\
\epsilon_o &= 5.295 \times 10^{-13} \text{ erg} \\
g &= 10^{13} 
\end{align*}
**Fig. 4.34a**

- $T=0.1$
- $v_0 = 4.9 \times 10^{-9} \text{ cm}$
- $\epsilon_0 = 1.765 \times 10^{-13} \text{ erg}$
- $g = 10^{-3}$

**Fig. 4.35a**

- $T=0.1$
- $v_0 = 4.9 \times 10^{-9} \text{ cm}$
- $\epsilon_0 = 1.765 \times 10^{-13} \text{ erg}$
- $g = 10^{-3}$

**Fig. 4.36a**

- $T=0.1$
- $v_0 = 4.9 \times 10^{-9} \text{ cm}$
- $\epsilon_0 = 1.765 \times 10^{-13} \text{ erg}$
- $g = 1$
**Fig. 4.34b**

$T=0.1$

$u_o=4.9 \times 10^{-9} \text{ cm}$

$\varepsilon_o=1.765 \times 10^{-13} \text{ erg}$

$g=10^{-13}$

---

**Fig. 4.35b**

$T=0.1$

$u_o=4.9 \times 10^{-9} \text{ cm}$

$\varepsilon_o=1.765 \times 10^{-13} \text{ erg}$

$g=10^{-5}$

---

**Fig. 4.36b**

$T=0.1$

$u_o=4.9 \times 10^{-9} \text{ cm}$

$\varepsilon_o=1.765 \times 10^{-13} \text{ erg}$

$g=1$
**Fig. 4.37a**

- \( T = 0.1 \)
- \( u_0 = 4.9 \times 10^9 \text{ cm} \)
- \( \varepsilon_0 = 1.765 \times 10^{13} \text{ erg} \)
- \( g = 10^{15} \)

**Fig. 4.37b**

- \( T = 0.1 \)
- \( u_0 = 4.9 \times 10^2 \text{ cm} \)
- \( \varepsilon_0 = 1.765 \times 10^{13} \text{ erg} \)
- \( g = 10^{15} \)
Phase Space (\eta)

Fig 4.38 (T=0.1, g=10^5)

250^{th} Particle

500^{th} Particle

750^{th} Particle
Phase Space ($\eta$)

Fig 4.39 ($T=0.1$, $g=10^2$)
Phase Space ($\eta$)

Fig 4.40 ($T=0.1$, $g=10^{15}$)

250th Particle

500th Particle

750th Particle
Phase Space (η)

Fig 4.41 (T=0.5, g=10^{-5})

250^{th} Particle

500^{th} Particle

750^{th} Particle
Phase Space \( \eta \)

Fig 4.42 \((T=0.5, \ g=10^2)\)

250\(^{th}\) Particle

500\(^{th}\) Particle

750\(^{th}\) Particle
Phase Space (η)

Fig 4.43 (T=0.5, g=10^{15})

.250th Particle

500th Particle

750th Particle
Phase Space ($\eta$)

Fig 4.44 ($\gamma=0.8$, $g=10^{-5}$)

250th Particle

500th Particle

750th Particle
Phase Space ($\eta$)

Fig 4.45 ($T=0.8$, $g=10^2$)

250th Particle

500th Particle

750th Particle
Phase Space ($\eta$)

Fig 4.46 ($T=0.8, \ g=10^{15}$)

250th Particle

500th Particle

750th Particle