

BUILDING AND VALIDATING A MODEL FOR INVESTIGATING THE DYNAMICS OF ISOLATED WATER MOLECULES

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THE INTRODUCTION

- Dressel *et. al* have found a system in which single water molecules are isolated with only dipole-dipole interactions and expect to find evidence of ferroelectricity¹
- Computational models are desired for proof-of-concept calculations and verifying deduced understanding of this system
- Efficacy of three popular algorithms investigated

THE MOTIVATION

- Models will increase understanding of fundamental interactions in many sciences
- Greatest potential impact is in biology
- Interpreting results of isolation is difficult, because biological systems are too complex and have too much unknown uncertainty

THE METHODS

Consider a dipole at the origin with only rotational degree of freedom in presence of a constant electric field (setup given in Fig. 1a)

for each algorithm

for each electric field

for each initial angle

Model dynamics for total runtime

Determine frequency of oscillation

end

Determine average frequency

end

Examine average frequency vs. e-field

Fit to power function (Fig. 2a)

Determine predictive stability coefficient ρ (Fig. 2b)

end

THE ALGORITHMS

Euler Method (EM)

- First-point approximation
- Unstable for oscillatory phenomena

$$v_n = v_{n-1} + a(x_{n-1}, t_{n-1})\tau$$

$$x_n = x_{n-1} + v_{n-1}\tau$$

Euler-Aspel Method (EAM)

- Last-point approximation
- Stable for oscillatory phenomena

$$v_n = v_{n-1} + a(x_{n-1}, t_{n-1})\tau$$

$$x_n = x_{n-1} + v_n\tau$$

Beeman Method (BM)

- Uses weighted average of information from previous two timesteps
- Not self-starting

$$x_n = x_{n-1} + v_{n-1}\tau + \frac{\tau^2}{6}(4a(x_{n-1}, t_{n-1}) - a(x_{n-2}, t_{n-2}))$$

$$v_n = v_{n-1} + \frac{\tau}{6}(2a(x_n, t_n) + 5a(x_{n-1}, t_{n-1}) - a(x_{n-2}, t_{n-2}))$$

THE ANALYSIS

FIG. 4 The results from fitting the data (to Fig. 2a) and determining the predictive stability coefficient (Fig. 2b) are summarized. The units for a are $(\sqrt{N/C})$. Data and best-fits given in Fig. 3a.

| Model | a | | n | | ρ | |
|-------|------------------|--------------------|------------------|-----------------|--------|---------|
| | full | limited | full | limited | full | limited |
| EM | 0.16 ± 0.65 | $4,500 \pm 6,200$ | -0.01 ± 0.17 | 0.40 ± 0.07 | 1.02 | 0.20 |
| EAM | $54,000 \pm 390$ | $45,000 \pm 7,700$ | 0.51 ± 0.01 | 0.50 ± 0.01 | 0.02 | 0.01 |
| BM | $44,000 \pm 320$ | $38,000 \pm 7,500$ | 0.51 ± 0.01 | 0.50 ± 0.01 | 0.02 | 0.01 |

- EAM and BM are superior in both ranges
- Limited range in which EM is effective
- EAM determined most effective, because it also better predicts coefficient ($a = 56,000$)

THE FUTURE WORK

- Determine ρ for more sophisticated algorithms
- Investigate nearest-neighbor interactions (setup given in Fig. 1b)
- Further analyze Prelim. Results for two dipoles (Fig. 3b)
- Look for evidence of ferroelectricity

THE GRATITUDE

- Drs. Michael Crosser, Jennifer Heath, Joelle Murray of Linfield College
- Prof. Dr. Martin Dressel of Stuttgart Universität
- Linfield Physics and Mathematics Departments

THE FIGURES

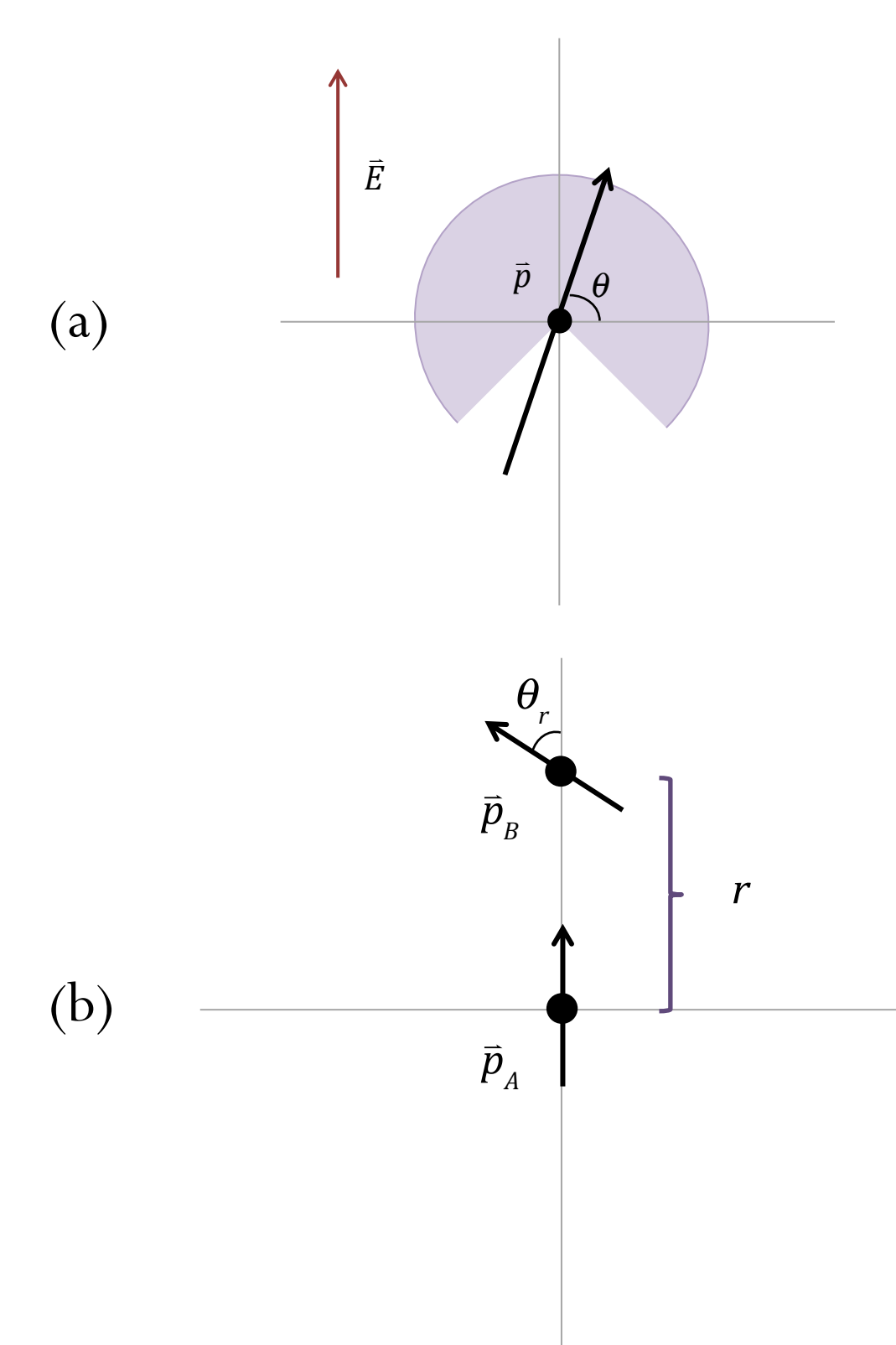


FIG. 1 (a) The setup for The Methods is given. The purple region represents possible initial angles. (b) The setup for The Future Works is given. Two dipoles are separated by a distance r and start with initial relative angle θ_r .

$$y = ax^n$$

$$\rho = \left| 1 - \frac{n}{n_0} \right|$$

FIG. 2 (a) The equation to which the data is fitted. (b) The definition for the predictive stability coefficient. (Note: Here, $n_0 = 1/2$)

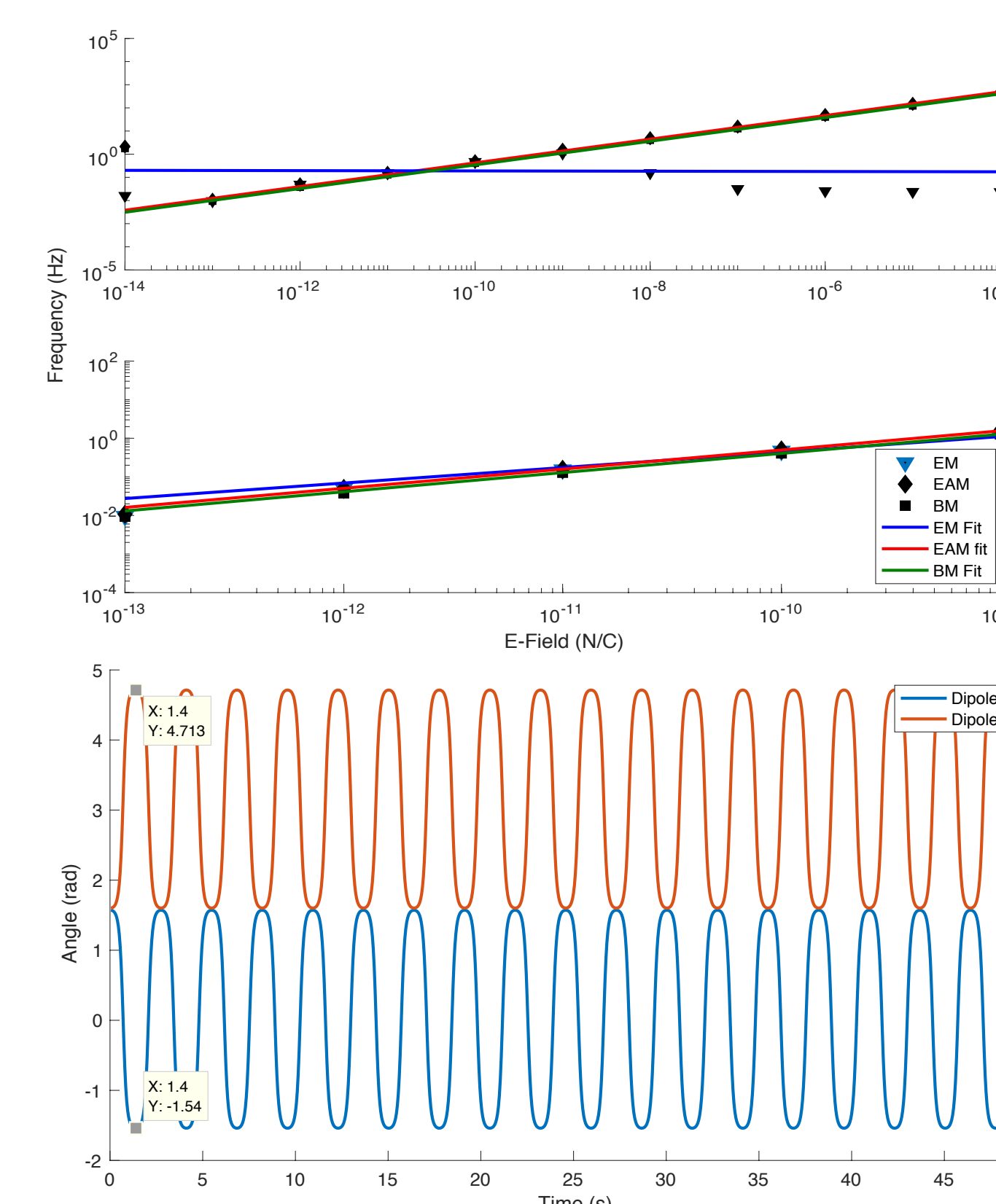


FIG. 3 (a) The results from probing the full range of e-fields (top; $E = 10^{-14}$ to 10^{-4} N/C) and the limited range (bottom; $E = 10^{-13}$ to 10^{-9} N/C) and (b) the preliminary results from The Future Work are shown.

¹M. Dressel, B. Gorshunov Broad-band optical spectroscopy of low-energy excitations of water molecules confined in nano-cages of beryl crystal lattice (2016).

