The effect of elastic vibrations on collisions of fine powder with walls

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Physics of Granular Flows

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Introduction

Collisions of Granular Particles

<u>Restitution Coefficient</u>

$$e \equiv -\frac{v_{\mathrm{f}}}{v_{\mathrm{i}}}$$

$$e = const.$$

$$\updownarrow$$

$$e = e(v)$$

Nonlinear function

Vibration : store and release

Collisions of Granular Particles

Restitution Coefficient

$$e \equiv -\frac{v_f}{v_i}$$

$$e = const.$$

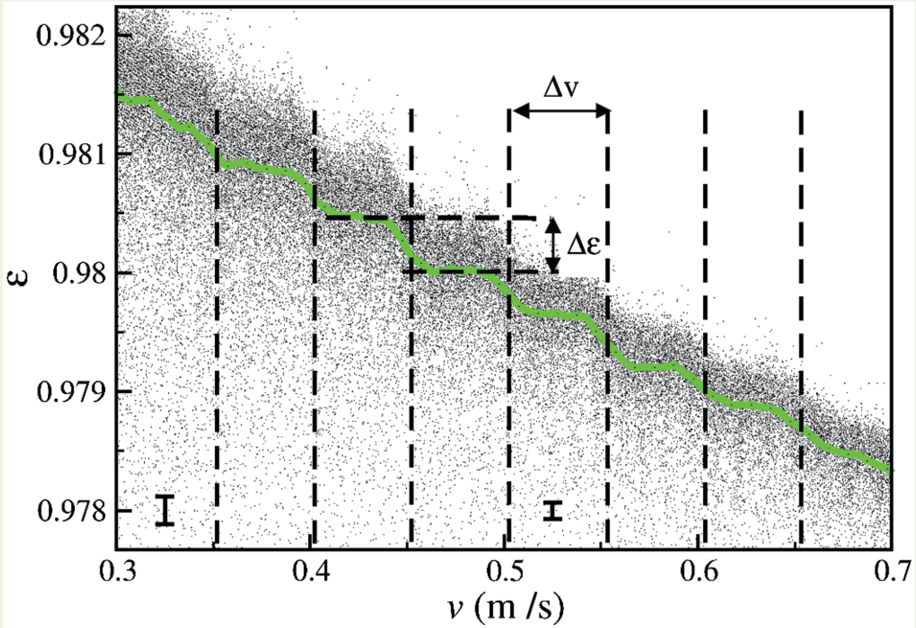
$\updownarrow$

$$e = e(v)$$

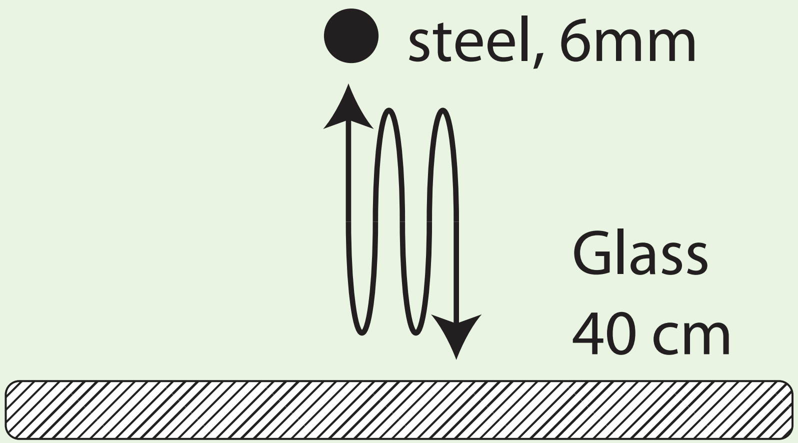
Nonlinear function

Vibration : store and release

Experiment

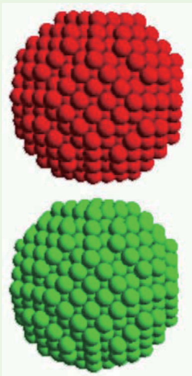


F. Müller, M. Heckel, A. Sack and T. Pöschel, Phys. Rev. Lett. 110, 254301 (2013).



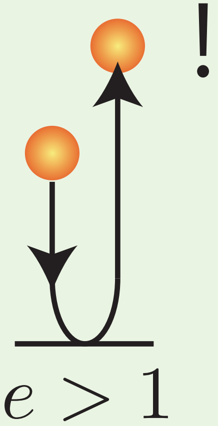
Super Rebounds

Molecular Dynamics



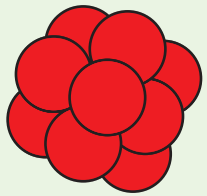
H. Kuninaka and H. Hayakawa,
Phys. Rev. E 79, 031309 (2009).

Super Rebounds



Breaking the second law?

Two Approaches

		
	Molecular Dynamics	Continuum Model
System	Many-Particle	Continuum
Focus on	Microscopic structures	Macroscopic motions
Computational Cost	Depending on the size	Independent of the size
		→ larger than 100 nm

H. Kuninaka and H. Hayakawa, PRE 86, 051302 (2012)

Previous Studies

	Previous Studies	Our Study
	F. Gerl and A. Zippelius, Phys. Rev. E 59, 2361 (1999). H. Hayakawa and H. Kuninaka, Chem. Eng. Sci. 57, 239 (2002).	
Dimension	2D	3D
Impact Velocity	Fast ~ Sound velocity / 10	Ultra-slow ~ Thermal velocity
Attraction	×	○
Viscosity	×	○
Collision with	Wall	Wall, ball

Model

Elastic Wave Equation

Elastic Wave Equation

$$\ddot{\mathbf{u}} = \left(c^{(\mathrm{l})}\right)^2 \nabla\nabla\cdot\mathbf{u} - \left(c^{(\mathrm{t})}\right)^2 \nabla\times(\nabla\times\mathbf{u})$$

Divergence term Rotation term

$c^{(\mathrm{l})}$: Vertical sound velocity

$c^{(\mathrm{t})}$: Horizontal sound velocity

Elastic Wave Equation

Elastic Wave Equation

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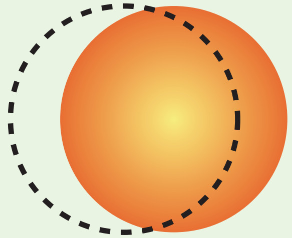
Dipole



$l = 1$

Stress Free Solutions

Spheroidal modes

$$\begin{aligned}\tilde{\mathbf{u}}^{(\mathrm{S})}_{nlm}(\mathbf{x}) &= \left[A_{nlm}\frac{\mathrm{d}j_l(k^{(\mathrm{l})}_{nl}r)}{\mathrm{d}r} + C_{nlm}l(l+1)\frac{j_l(k^{(\mathrm{t})}_{nl}r)}{r}\right]Y_{lm}(\Omega)\mathbf{e}_r \\ &+ \left[A_{nlm}j_l(k^{(\mathrm{l})}_{nl}r) + C_{nlm}\frac{\mathrm{d}\left\{rj_l(k^{(\mathrm{t})}_{nl}r)\right\}}{\mathrm{d}r}\right]\nabla Y_{lm}(\Omega)\end{aligned}$$

$$k^{(\mathrm{t})}_{nl}c^{(\mathrm{t})} = \omega_{nl}$$

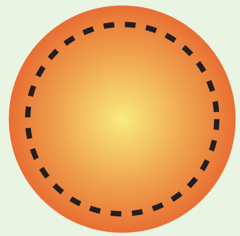
$$k^{(\mathrm{l})}_{nl}c^{(\mathrm{l})} = \omega_{nl}$$

n : Principal quantum number

l : Azimuthal quantum number

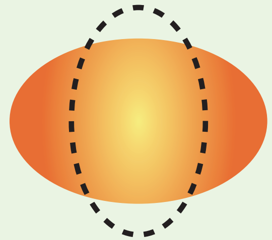
m : Magnetic quantum number

Breathing



$l = 0$

Quadrupole



$l = 2$

Elastic Wave Equation

Elastic Wave Equation

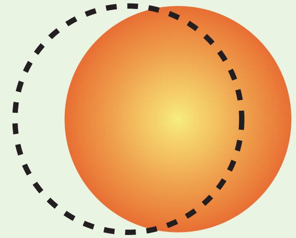
$$\ddot{\mathbf{u}} = \left(c^{(\mathrm{l})}\right)^2 \nabla\nabla\cdot\mathbf{u} - \left(c^{(\mathrm{t})}\right)^2 \nabla\times(\nabla\times\mathbf{u})$$

Divergence term   Rotation term

$c^{(\mathrm{l})}$: Vertical sound velocity

$c^{(\mathrm{t})}$: Horizontal sound velocity

Dipole



$l = 1$

Stress Free Solutions

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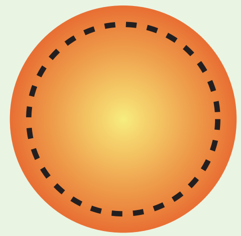
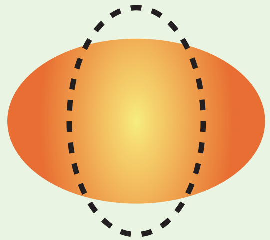
Breathing   Quadrupole



$l = 0$

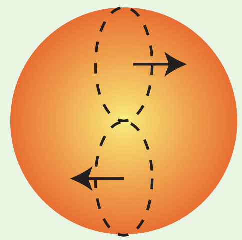


$l = 2$

Torsional modes

$$\tilde{\mathbf{u}}^{(\mathrm{T})}_{nlm}(\mathbf{x}) = B_{nlm}j_l(k^{(\mathrm{t})}_{nl}r)\mathbf{x}\times\nabla Y_{lm}(\Omega) \quad \perp\mathbf{e}_r$$

$l = 2$



No contribution in head-on collisions $\longrightarrow$ Neglected

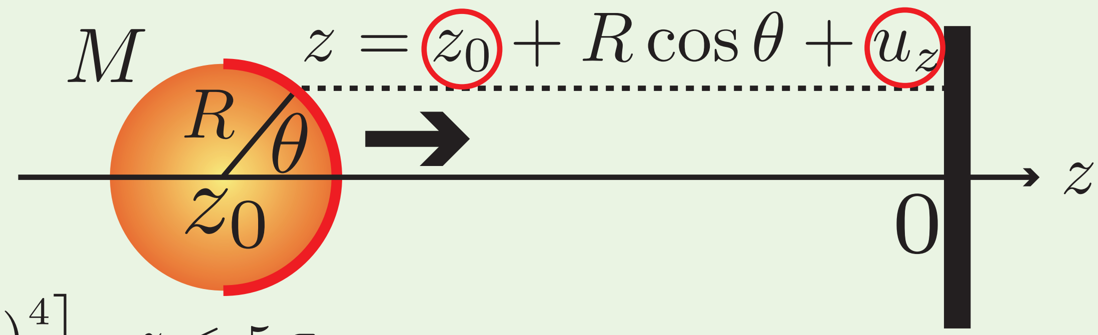
Wall Potential

Equation of motion

ρ : Mass density
M : Mass

$$\ddot{\mathbf{u}} = \left(c^{(\mathrm{l})}\right)^2 \nabla\nabla\cdot\mathbf{u} - \left(c^{(\mathrm{t})}\right)^2 \nabla\times(\nabla\times\mathbf{u}) - \frac{1}{\rho}\frac{\delta V}{\delta \mathbf{u}}$$

Wall Potential



$$V(z_0, Q) = \int_0^{\frac{\pi}{2}} \mathrm{d}\theta \int_0^{2\pi} \mathrm{d}\varphi\, \phi(z)$$

$$\phi(z) = \begin{cases} 4\pi\sigma^2 n\varepsilon \left[\frac{1}{5}\left(\frac{\sigma}{z}\right)^{10} - g\,\frac{1}{2}\left(\frac{\sigma}{z}\right)^4\right] & z < 5\,\sigma \\ 0 & z \geq 5\,\sigma \end{cases}$$

Modified Lennard-Jones

A. Awasthi et al., Phys. Rev. B 76, 115437 (2007).

n : Number density g : Cohesive parameter

ρ n σ ε : borrow from copper

P. M. Agrawal et al., Surf. Sci. 515, 21 (2002).

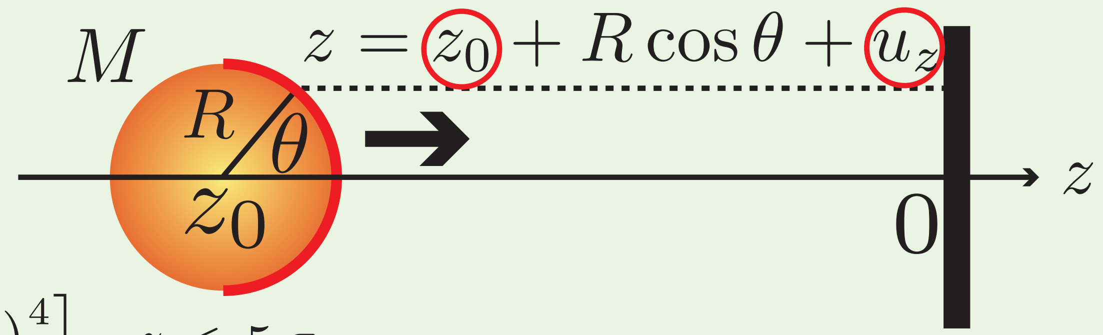
Wall Potential

Equation of motion

$$\ddot{\mathbf{u}} = \left(c^{(\mathrm{l})}\right)^2 \nabla\nabla\cdot\mathbf{u} - \left(c^{(\mathrm{t})}\right)^2 \nabla\times(\nabla\times\mathbf{u}) - \frac{1}{\rho}\frac{\delta V}{\delta \mathbf{u}}$$

ρ : Mass density
M : Mass

Wall Potential



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n : Number density $\quad$ g : Cohesive parameter

$\rho \quad n \quad \sigma \quad \varepsilon$: borrow from copper $\quad$ P. M. Agrawal et al., Surf. Sci. 515, 21 (2002).

$$\mathbf{u}(t,\mathbf{x}) = \sum_{n=0}^{\infty}\sum_{l=0}^{\infty}\sum_{m=-l}^{l} Q_{nlm}(t)\tilde{\mathbf{u}}_{nlm}^{(\mathrm{S})}(\mathbf{x}) \qquad \omega_{nl} < 25c^{(\mathrm{t})}/R$$

$$\longrightarrow \quad M\ddot{Q}_{nlm} = -M\omega_{nl}^2 Q_{nlm} - \frac{\partial V(z_0, Q)}{\partial Q_{nlm}}$$

Center of mass

$$M\ddot{z}_0 = -\frac{\partial V(z_0, Q)}{\partial z_0}$$

Initial Conditions

Center of Mass

$z_0(0)$ Fix : at the position V = 0

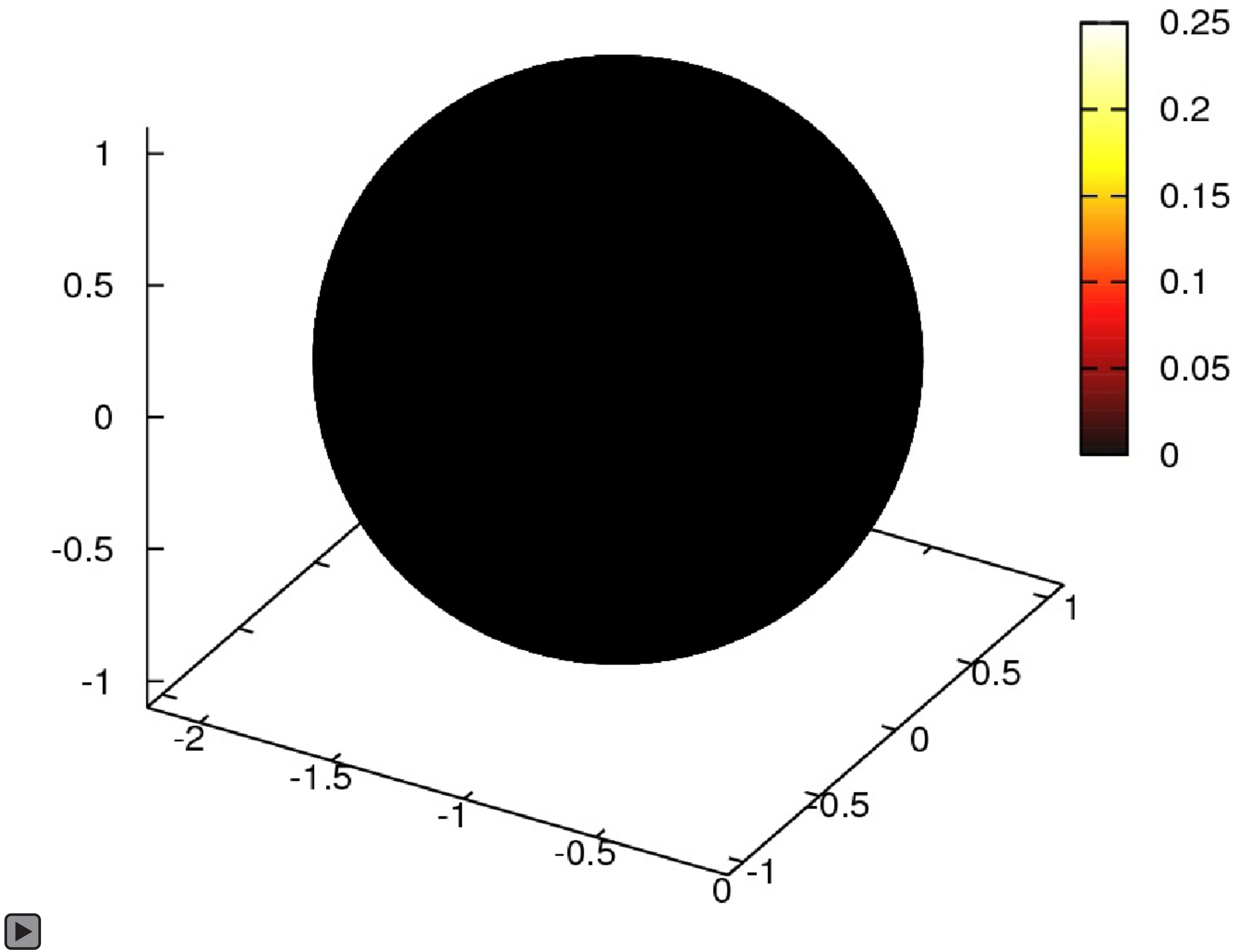
$\dot{z}_0(0) \equiv v_0$ Control : 0.0001 ~ 0.1 sound velocity

Distribution of vibrational modes

$$
\begin{aligned}
p_{\mathrm{can}}\left(Q_{nlm}(0)\right) &= \sqrt{\frac{M\omega_{nl}^2}{2\pi k_{\mathrm{B}}T}} \exp\left[-\frac{1}{k_{\mathrm{B}}T}\frac{1}{2}M\omega_{nl}^2 Q_{nlm}^2(0)\right] \\
p_{\mathrm{can}}\left(\dot{Q}_{nlm}(0)\right) &= \sqrt{\frac{M}{2\pi k_{\mathrm{B}}T}} \exp\left[-\frac{1}{k_{\mathrm{B}}T}\frac{1}{2}M\dot{Q}_{nlm}^2(0)\right]
\end{aligned}
$$

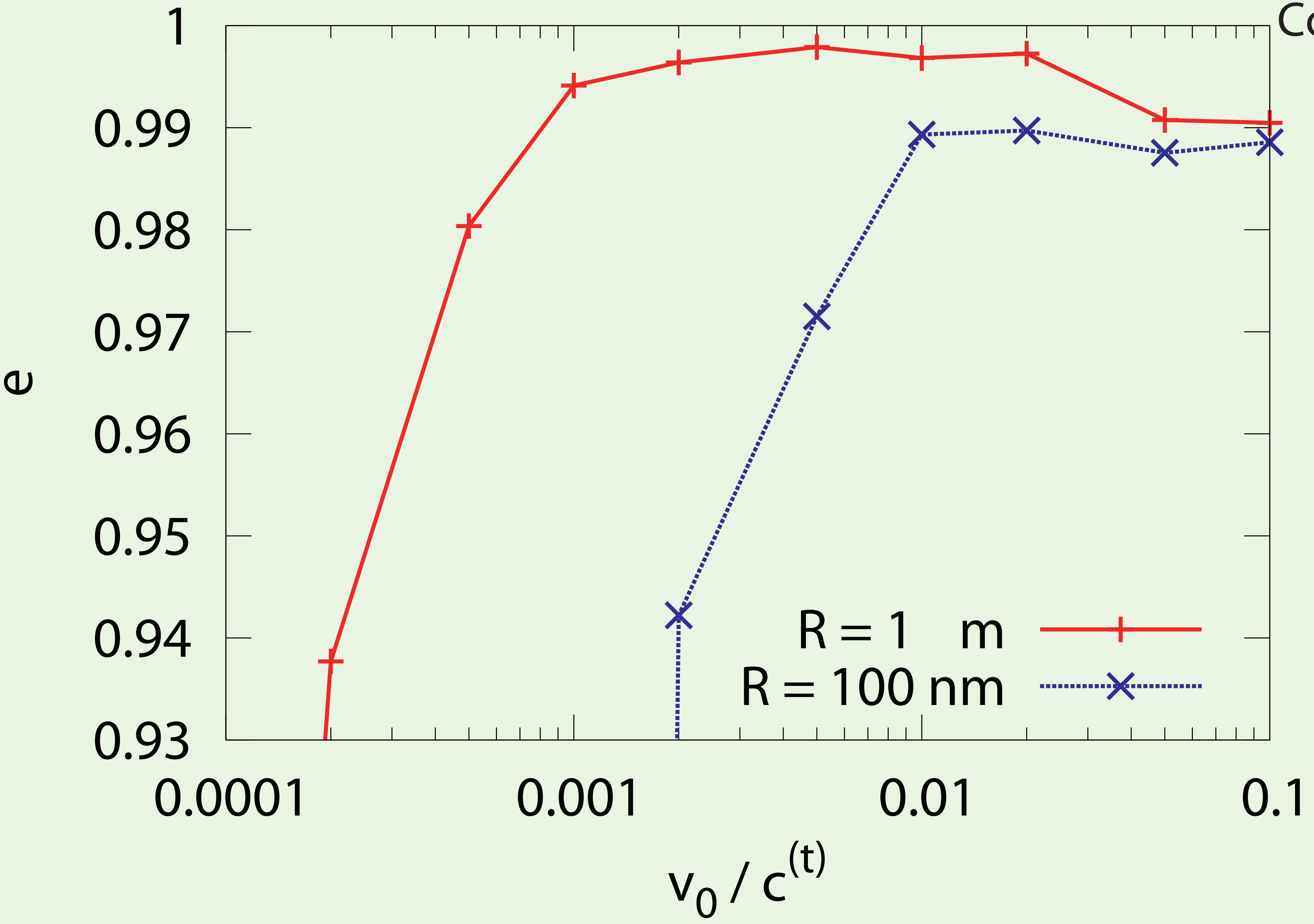
Using normal random number

Results



0.25
0.2
0.15
0.1
0.05
0
1
0.5
0
-0.5
-1
-2
-1.5
-1
-0.5
0
-1
-0.5
0
0.5
1

Restitution Coefficient vs Impact Velocity



Cohesive Parameter

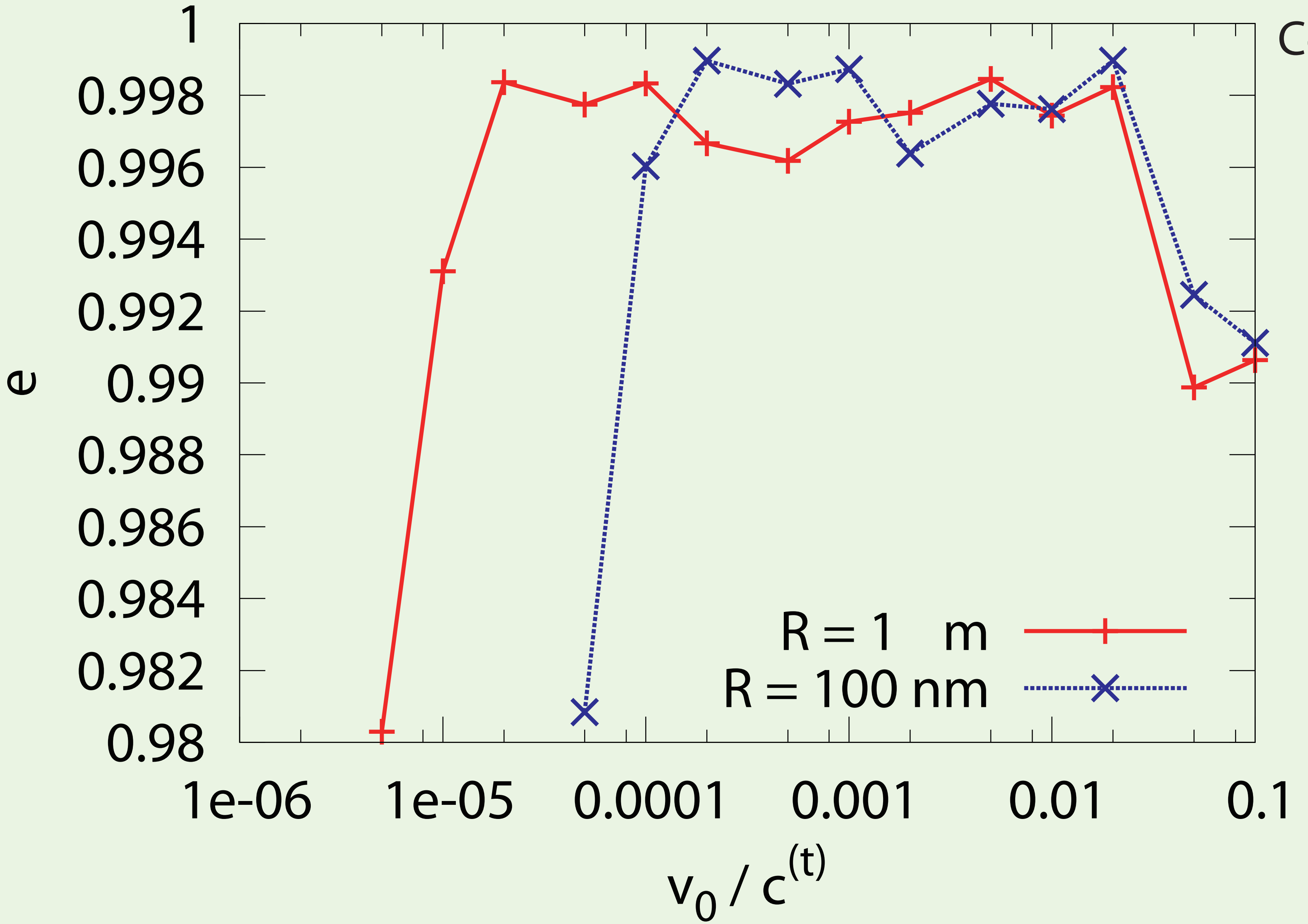
$g = 1$

: No reduce

Temperature

$T = 0$

Restitution Coefficient vs Impact Velocity



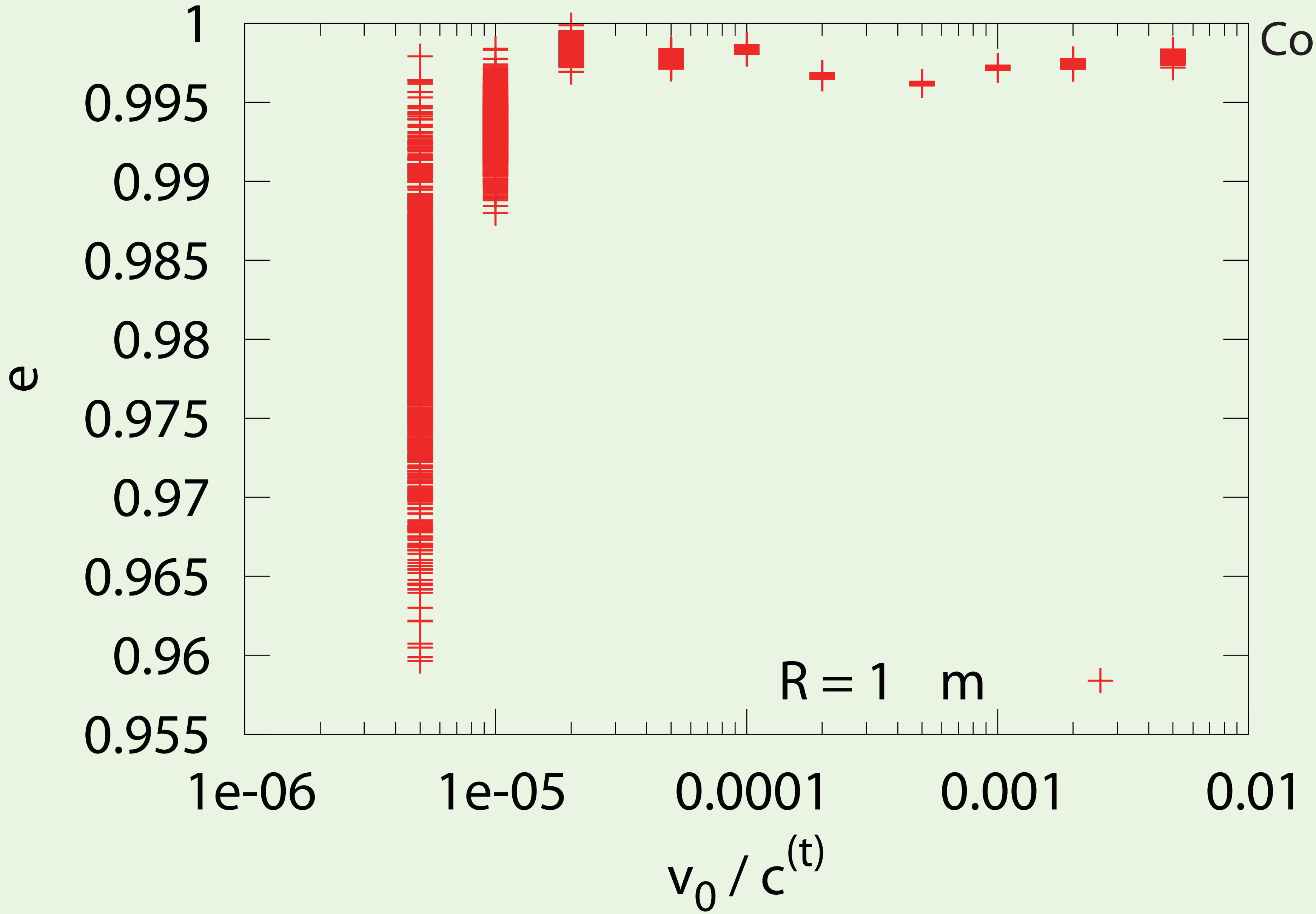
Cohesive Parameter

$$g = 0.2$$

Temperature

$$T = 0$$

Restitution Coefficient vs Impact Velocity



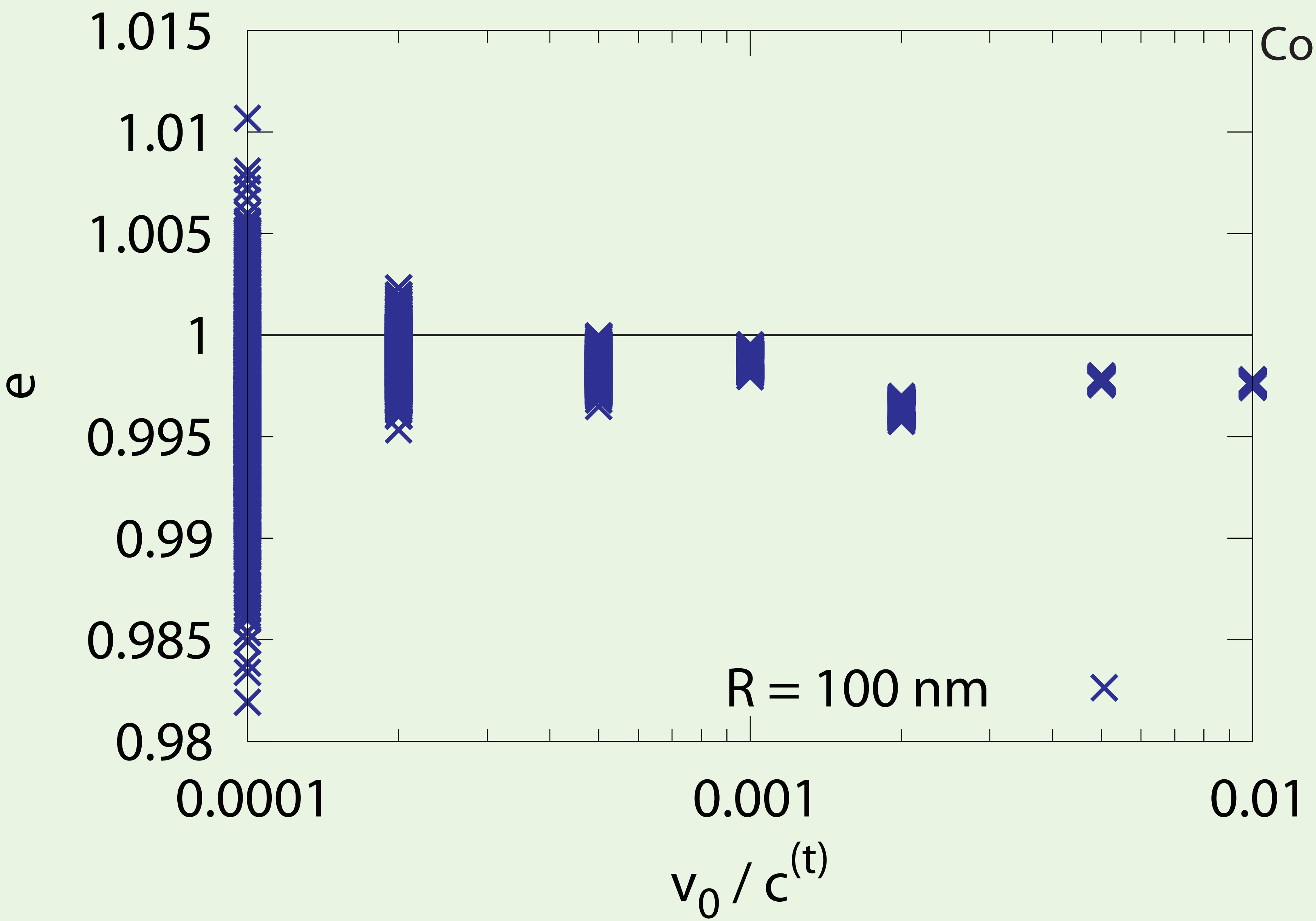
Cohesive Parameter

$g = 0.2$

Temperature

$T = 300\text{K}$

Restitution Coefficient vs Impact Velocity



Cohesive Parameter

$g = 0.2$

Temperature

$T = 300\mathrm{K}$

Excitation Energy

ΔH_{nlm} : Excitation energy of each mode

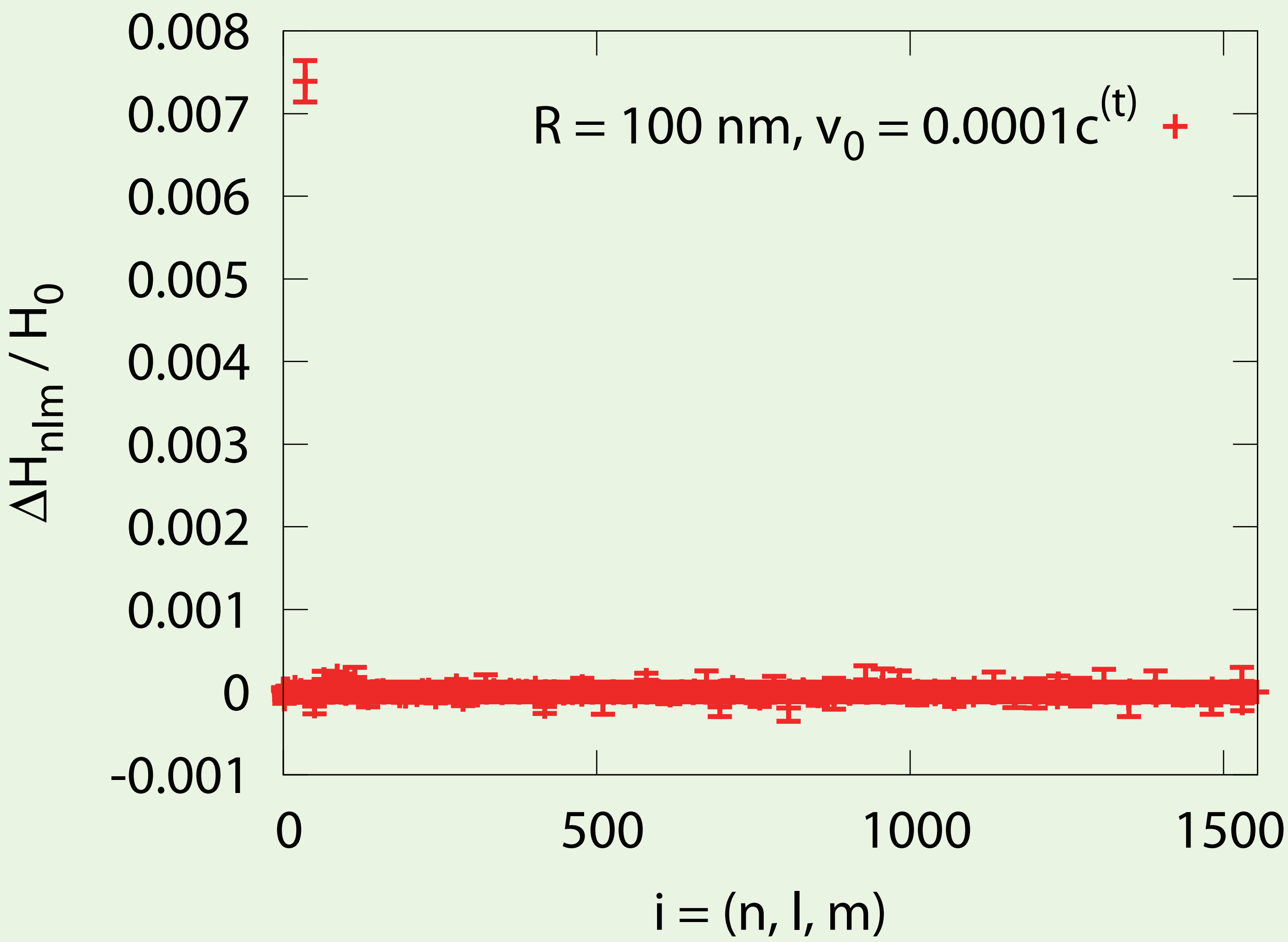
$H_0 = \frac{1}{2} M v_0^2$: Initial kinetic energy

Cohesive Parameter

$$g = 0.2$$

Temperature

$$T = 300\mathrm{K}$$



Excitation Energy

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Cohesive Parameter

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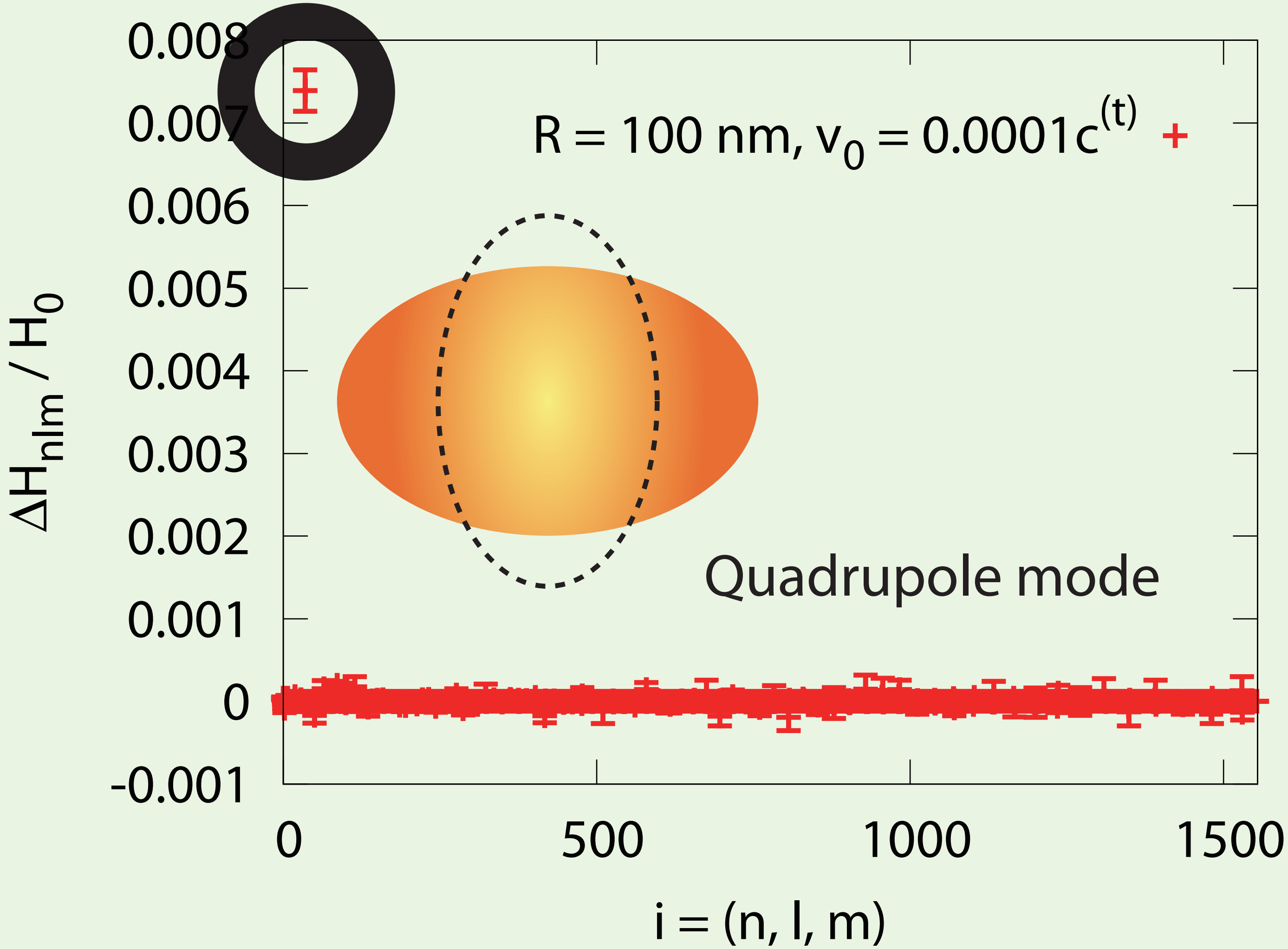


Temperature

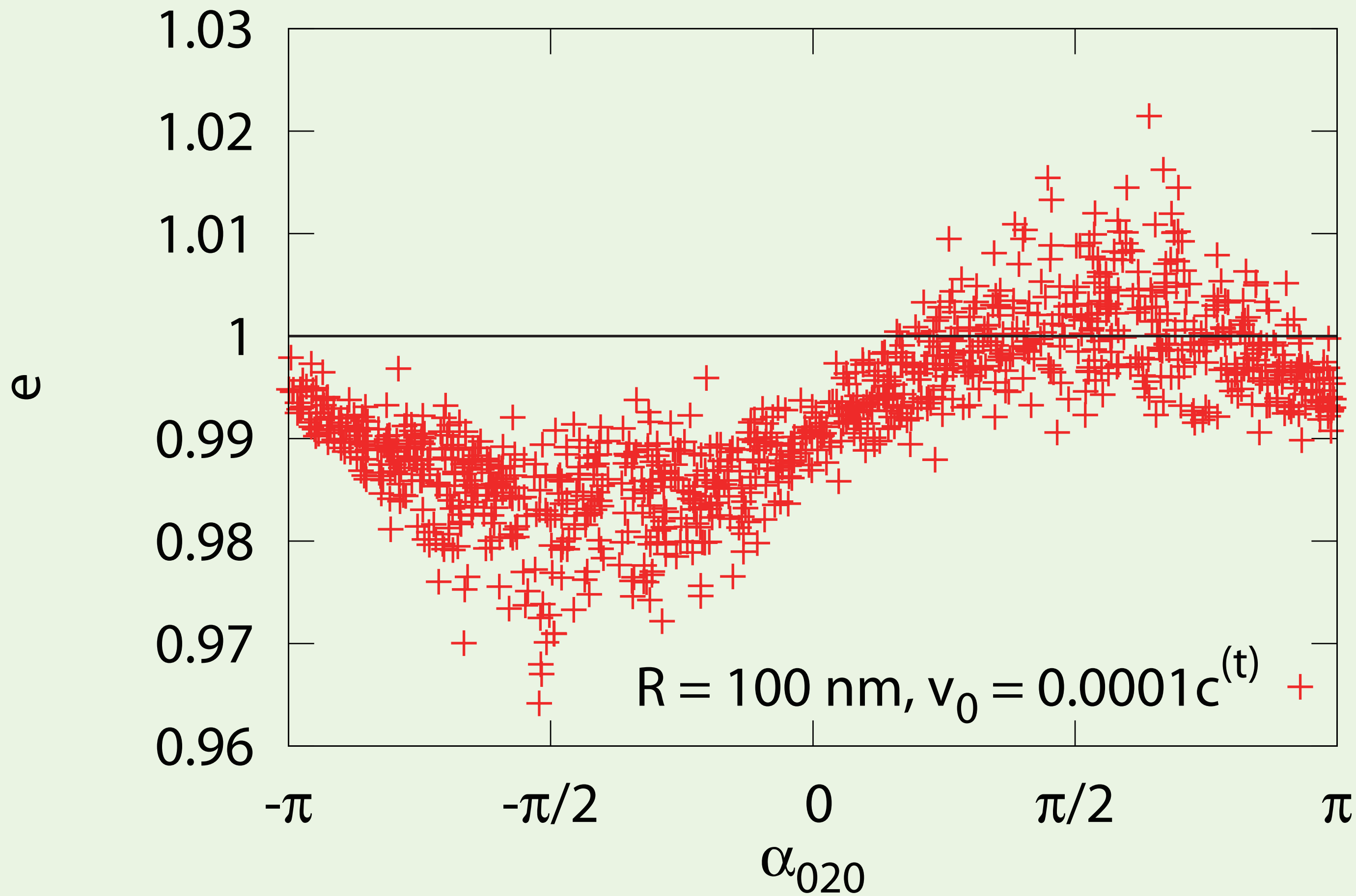
$T = 300\text{K}$

Restitution Coefficient vs Initial Phase

$$Q_{nlm}(0) = a_{nlm}(0)\sin\alpha_{nlm}(0)$$
$$\dot{Q}_{nlm}(0) = \omega_{nl} a_{nlm}(0)\cos\alpha_{nlm}(0)$$

a_{nlm} : Amplitude

α_{nlm} : Phase



Cohesive Parameter

$$g = 0.2$$

Temperature

$$T = 300\mathrm{K}$$

Discussion

Perturbation Theory

Unit

M : Mass
R : Radius
v_0 : Initial velocity

$$\begin{aligned}\tilde{z}_0 &\equiv z_0/R\\ \tilde{Q}_{nlm} &\equiv Q_{nlm}/R\\ \tilde{t} &\equiv tv_0/R\\ \tilde{V} &\equiv V/Mv_0^2\end{aligned}$$

$$\begin{aligned}\frac{\mathrm{d}^2\tilde{Q}_{nlm}}{\mathrm{d}\tau^2} + \tilde{\omega}_{nl}^2\tilde{Q}_{nlm} &= -\varepsilon^2\frac{\partial\tilde{V}\left(\tilde{z}_0,\tilde{Q}\right)}{\partial\tilde{Q}_{nlm}}\\ \frac{\mathrm{d}^2\tilde{z}_0}{\mathrm{d}\tilde{t}^2} &= -\frac{\partial\tilde{V}\left(\tilde{z}_0,\tilde{Q}\right)}{\partial\tilde{z}_0}\end{aligned}$$

$\varepsilon \equiv v_0/c^{(\mathrm{t})}$ $\quad\tau \equiv \tilde{t}/\varepsilon$

Expansion

$$\begin{aligned}\tilde{Q}_{nlm} &= \tilde{Q}_{nlm}^{(0)} + \varepsilon\tilde{Q}_{nlm}^{(1)} + \varepsilon^2\tilde{Q}_{nlm}^{(2)} + \ldots\\ \tilde{z}_0 &= \tilde{z}_0^{(0)} + \varepsilon\tilde{z}_0^{(1)} + \varepsilon^2\tilde{z}_0^{(2)} + \ldots\end{aligned}$$

0th order

$$\begin{aligned}\frac{\mathrm{d}^2\tilde{Q}_{nlm}^{(0)}}{\mathrm{d}\tau^2} + \tilde{\omega}_{nl}^2\tilde{Q}_{nlm}^{(0)} &= 0\\ \frac{\mathrm{d}^2\tilde{z}_0^{(0)}}{\mathrm{d}\tilde{t}^2} + \frac{\partial\tilde{V}\left(\tilde{z}_0^{(0)},0\right)}{\partial\tilde{z}_0} &= 0\end{aligned}$$

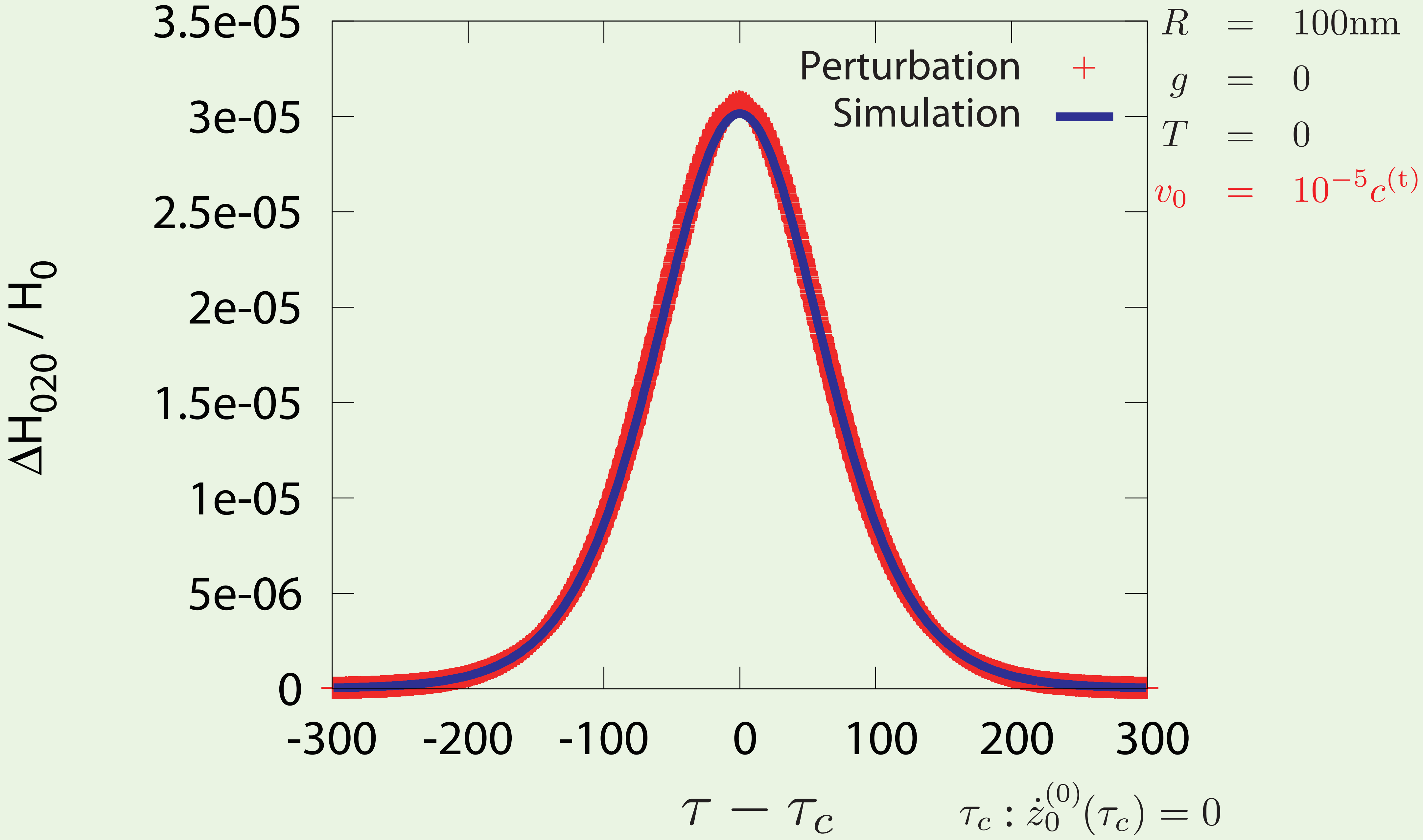
1th order

$$\tilde{Q}_{nlm}^{(1)} = 0$$

2th order

$$\frac{\mathrm{d}^2\tilde{Q}_{nlm}^{(2)}}{\mathrm{d}\tau^2} + \tilde{\omega}_{nl}^2\tilde{Q}_{nlm}^{(2)} = -\frac{\partial\tilde{V}\left(\tilde{z}_0^{(0)},0\right)}{\partial\tilde{Q}_{nlm}}$$

Perturbation vs Simulation



Phase Dependence

ΔH_{nlm}	: Excitation energy
$H_0(0) = \frac{1}{2} M v_0^2$	: Initial kinetic energy

$$1 - e^2 = \sum_{nlm} \frac{\Delta H_{nlm}}{H_0(0)}$$ Energy conservation

$$= 2 \sum_{nlm} \left[\frac{\mathrm{d}\tilde{Q}^{(0)}_{nlm}}{\mathrm{d}\tau} \frac{\mathrm{d}\tilde{Q}^{(2)}_{nlm}}{\mathrm{d}\tau} + \tilde{\omega}^2_{nl} \tilde{Q}^{(0)}_{nlm} \tilde{Q}^{(2)}_{nlm} \right] + 2\varepsilon^2 \sum_{nlm} \left[\frac{1}{2} \left(\frac{\mathrm{d}\tilde{Q}^{(2)}_{nlm}}{\mathrm{d}\tau} \right)^2 + \frac{1}{2} \tilde{\omega}^2_{nl} \left(\tilde{Q}^{(2)}_{nlm} \right)^2 \right] + O(\varepsilon^3)$$

$$= 2 \sum_{nlm} \sqrt{2 \tilde{H}^{(2)}_{nlm}} \tilde{\omega}_{nl} \tilde{a}_{nlm} \cos\left(\alpha_{nlm} + \tilde{\omega}_{nl} \tau_c \right) + 2\varepsilon^2 \tilde{H}^{(2)}_{\mathrm{vib}} + O(\varepsilon^3)$$

Averaging out → except α_{020}

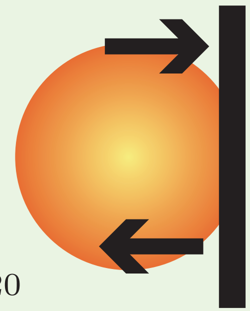
$$2 \sqrt{2 \tilde{H}^{(2)}_{020}} \underline{\tilde{\omega}_{02} \tilde{a}_{020} \cos\left(\alpha_{020} + \tilde{\omega}_{02} \tau_c \right)} + 2\varepsilon^2 \tilde{H}^{(2)}_{\mathrm{vib}} + O(\varepsilon^3)$$

$$= \frac{\mathrm{d}\tilde{Q}^{(0)}_{020}(\tau_c)}{\mathrm{d}\tau} \qquad \tau_c : \dot{z}_0(\tau_c) = 0$$

$$\tilde{H}_{nlm} = \frac{1}{2} \left(\frac{\mathrm{d}\tilde{Q}_{nlm}}{\mathrm{d}\tau} \right)^2 + \frac{1}{2} \tilde{\omega}^2_{nl} \tilde{Q}^2_{nlm}$$
$$Q_{nlm} = a_{nlm} \sin \alpha_{nlm}$$
$$\dot{Q}_{nlm} = \omega_{nl} a_{nlm} \cos \alpha_{nlm}$$

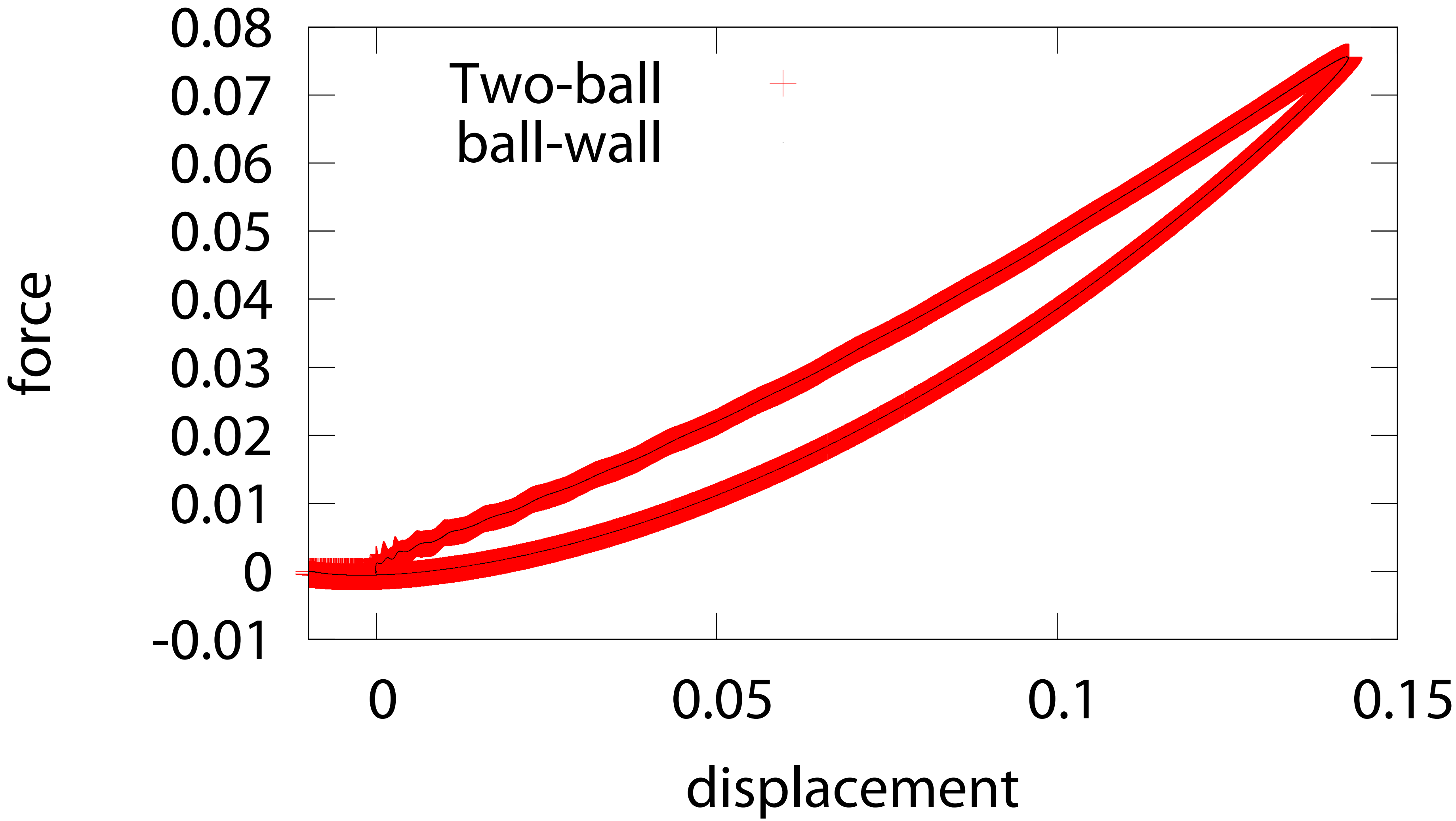
$$Q_{020}(\tau_c) = 0$$
$$\dot{Q}_{020}(\tau_c) = \omega_{02} a_{020}$$

$$Q_{020}(\tau_c) = 0$$
$$\dot{Q}_{020}(\tau_c) = -\omega_{02} a_{020}$$



Two Ball Collisions

$$M\ddot{Q}_{nlm} = -M\omega_{nl}^2\left(Q_{nlm} + \gamma\dot{Q}_{nlm}\right) - \frac{\partial V}{\partial Q_{nlm}}$$



Conclusion

Simulation

Super rebounds are found when the radius, the temperature and the velocity are 100 nm, 300 K and 10^{-4} sound velocity, respectively.

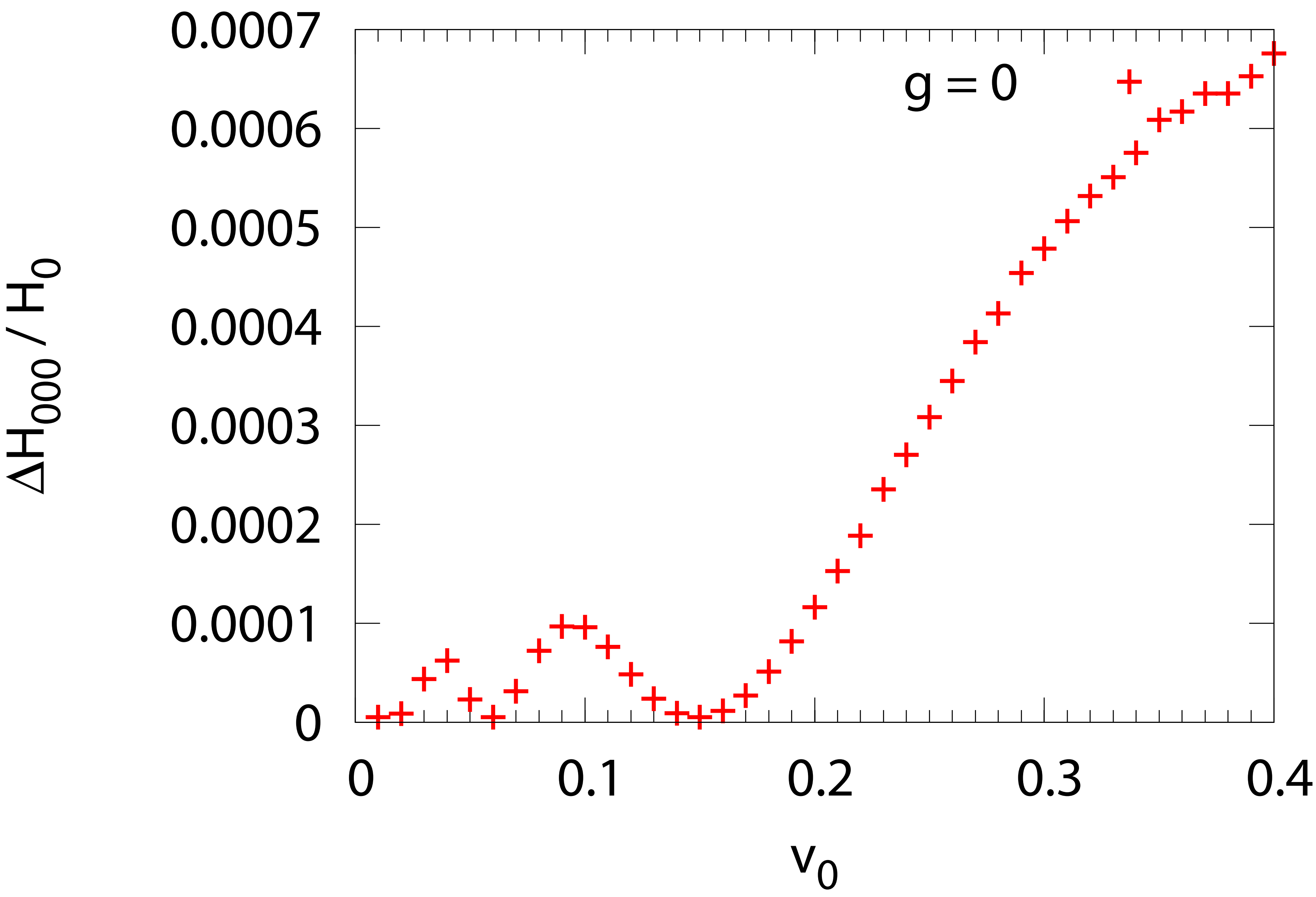
The quadrupole mode is the most excited in this condition.

Sinusoidal structure is found in the restitution coefficient as a function of the initial phase of the quadrupole mode.

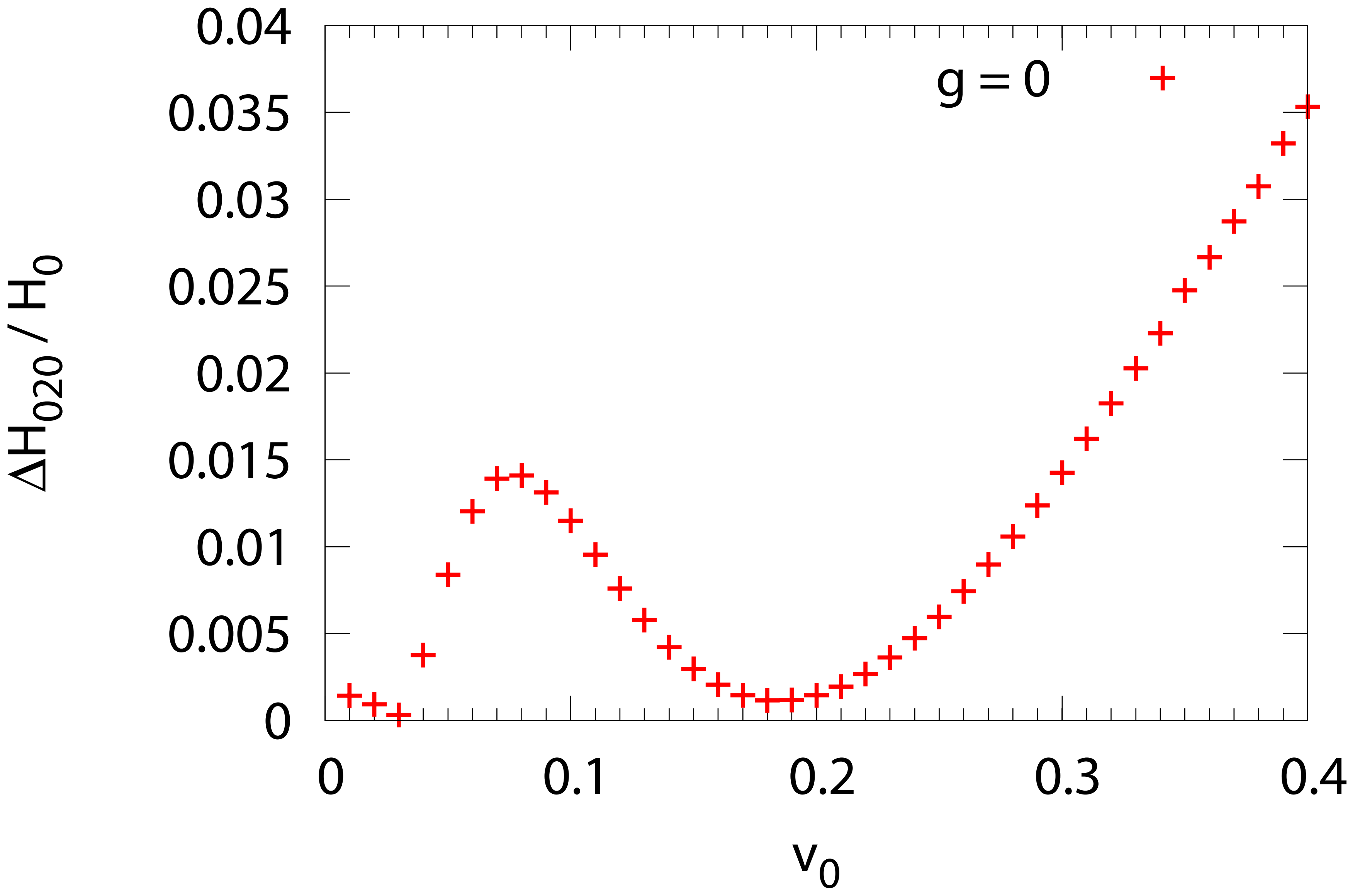
Perturbation theory

The perturbation theory is good agree with our simulation when the initial velocity is lower than 10^{-5} sound velocity.

The sinusoidal structure of the restitution coefficient is derived using this theory.



0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
0
0
0.1
0.2
0.3
0.4
g = 0
$\Delta H_{000} / H_0$
v_0



g = 0
0.04
0.035
0.03
0.025
0.02
0.015
0.01
0.005
0
0.1
0.2
0.3
0.4
$\Delta H_{020} / H_0$
v_0