# Gravitational Chemistry



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#### Spoken Introduction

Chemistry was revolutionized when Linus Pauling applied the new ideas of quantum mechanics to understand molecular bonding. He was able to derive bond strengths etc, and the energetics of molecule formation and destruction can be understood in terms of this. In particular, he developed the concept of resonance to understand the stability of molecular structures, an idea first introduced by Heisenberg. This uses a perturbation technique not unlike that which will be presented today.

Unlike Pauling, we have had the advantage of computers to study the secrets of complex structures. The deep analytical insights of Douglas Heggie and Michel Henon, the numerical scattering experiments (and accompanying deep insights) of Piet Hut, together with fundamental contributions by others such as Jack Hills and Joe Monaghan, have taught us much about the dynamics of binaries and triples.





Use analytical methods to understand

- how small-N systems are formed and destroyed
- how this depends on the environment

 $\checkmark$  how their stability depends on the state of the system (internal energy and angular momentum  $\rightarrow$  ratio of semis, eccentricities, orientations)



## Gravitational chemistry



Given analytical expressions for E and J transferred during interactions :

- Can do statistics of reactions (cross sections etc)
- Can estimate ``half-life'' of various products
- ♥ Can determine (bounds on) orbital parameters of decay products
- Can understand why some reactions are energetically favoured over others (eg: 2+2 compared to 3+1)







- Complements (CPU-intensive) numerical studies but allows one to cover large parameter space
- Generalizes Heggie's perturbation analysis for distant hyperbolic encounters to include strong encounters and bound systems



#### Small-N processes important in

- ♥ Energetics of star cluster cores (Sverre, Simon)
- ♥ Star formation interactions (Matthew)
- ♥ Planet formation
- Planetary and small body dynamics (Derek)
- ♥ Interacting galaxies





#### new formalism

#### Introduces concept of ``normal modes of a binary"





## stable triples

**example:** 
$$e_{in} = 0, e_{out} = 0.2, a_{out} / a_{in} = 4$$



#### Unstable triple...



download movie separately



### unstable triples

$$e_{in} = 0, \quad e_{out} = 0.5$$

#### example:

(a): 
$$a_{out} / a_{in} = 7$$
  
(b):  $a_{out} / a_{in} = 8$ 





Why is the behaviour so different?

- -- large scale energy transfer in unstable triples
- -- very little energy transferred in stable triples

To move energy around in bulk in a physical system there must be internal <u>**RESONANCE**</u> between different parts of the system.

Thus one needs to identify the *dominant frequencies* in

each part of the system.



09:44

The outer body induces *tidal oscillations* in the inner binary

-- in fact the *orbital elements* oscillate

-- it is natural to try and define the <u>normal modes of oscillation of a binary</u>

unforcedforcedtime dependent  
mode amplitude
$$r \approx a (1 - e \cos M);$$
 $r \approx a_g \left(1 + \sum_{n=-\infty}^{\infty} b_n(t) e^{inM}\right)$ normal mode $f \approx M + 2 e \sin M;$  $f \approx M + \sum_{n=-\infty}^{\infty} a_n(t) e^{inM}$ normal mode



09:44

$$r \approx a_g \left( 1 + \sum_{n = -\infty}^{\infty} b_n(t) e^{inM} \right)$$
$$f \approx M + \sum_{n = -\infty}^{\infty} a_n(t) e^{inM}$$

free modes of oscillation: isolated eccentric binary

Similar to amplitudes of modes of oscillation of **rotating star** in binary



#### forced modes

$$\ddot{\mathbf{r}} + \frac{Gm_{12}}{r^2}\hat{\mathbf{r}} = Gm_3\frac{\partial}{\partial \mathbf{r}}\left(\frac{\alpha_1}{|\mathbf{R} + \alpha_2\mathbf{r}|} + \frac{\alpha_2}{|\mathbf{R} - \alpha_1\mathbf{r}|}\right) \qquad \alpha_i = \frac{m_i}{m_1 + m_2}, \ i = 1, 2$$
$$= Gm_3\sum_{l=2}^{\infty}\sum_{m=-l}^{l}\frac{\partial}{\partial \mathbf{r}}\left(\frac{4\pi}{2l+1}\mathcal{M}_l\frac{r^l}{R^{l+1}}Y_{lm}(\pi/2,\varphi)Y_{lm}^*(\Theta,\psi)\right)$$



 $(r, \theta, \varphi) = (R, \Theta, \psi)$ 

spherical polar coords of m2, m3



#### amplitudes of forced modes

Only a handful of modes are non-zero. Only 1 or 2 of these matter. *quadrupole terms*: (I=2, m=2) dominate in coplanar stellar triples

$$b_{2}(t) = \frac{\Omega_{i}}{2i} \left\{ e^{-i\Omega_{i}t} \int_{t_{0}}^{t} e^{i\Omega_{i}t} F_{22} dt - e^{-3i\Omega_{i}t} \int_{t_{0}}^{t} e^{3i\Omega_{i}t} F_{22} dt \right\}$$
  
+ free terms(e<sub>i</sub>, phase) overlap integral

$$F_{lm} = l \,\mathcal{M}_l \mathcal{C}_{lm} \left(\frac{m_3}{m_{12}}\right) \left(\frac{a_i}{R}\right)^{l+1} e^{-im\psi}$$

procedure picks out active modes



#### dynamical evolution of a stable triple



#### amplitudes of forced modes

<u>octopole terms</u>: these are important in close planetary systems. Also responsible for secular evolution when  $m_1 \neq m_2$ 

$$l = 3, \ m = 3$$
  

$$b_{3}(t) = \frac{\Omega_{i}}{2i} \left\{ e^{-2i\Omega_{i}t} \int_{t_{0}}^{t} e^{2i\Omega_{i}t} F_{33} dt - e^{-4i\Omega_{i}t} \int_{t_{0}}^{t} e^{4i\Omega_{i}t} F_{33} dt \right\}$$
  
+ free terms(e<sub>j</sub>, phase)  

$$l = 3, \ m = 1$$
  

$$b_{1}(t) = \frac{\Omega_{i}}{2i} \left\{ \int_{t_{0}}^{t} F_{31} dt - e^{-2i\Omega_{i}t} \int_{t_{0}}^{t} e^{2i\Omega_{i}t} F_{31} dt \right\} + \text{free terms}(e_{j}, \text{phase})$$

integrands contain terms like  $sin(n \Omega_i t - m \psi)$ 

 $\rightarrow$ opportunity for resonance

stable planetary systems are able to be more closely packed than stellar systems. Thus resonances such as 3:2 can be important. 09:44

17

#### non-coplanar systems

Use of spherical harmonics makes it easy to study arbitrary orientations

-- Wigner  $\mathcal{D}$ -functions from quantum mechanics

other modes may dominate

coplanar systems: I=2 modes: m=0, m=2 I=3 modes: m=1, m=3

<u>non-coplanar</u> systems: I=2 modes: m=0, <u>m=1</u>, m=2 I=3 modes: <u>m=0</u>, m=1, <u>m=2</u>, m=3

*Example*: i=180 deg .... I=2, m=0 mode dominates

The standard averaging procedure gives the

secular evolution of the orbital elements of a system.

The formalism is an *normal mode* procedure which

isolates the dominant modes governing dynamical evolution

### energy exchange

$$\dot{E}_{\rm i} = \frac{\mu_i}{2\pi} \int_0^{2\pi} \dot{\mathbf{r}} \cdot \mathbf{F} \, dM_i$$

$$\Delta E_i(t) = \int_0^t \dot{E}_i \, dt'$$



$$\Omega_i$$
 = inner orbital frequency

$$\phi_i$$
 = initial phase of inner binary

$$e_i$$
 = inner eccentricity

For one entire outer orbit: can approximate overlap integrals with asymptotic expressions

$$\begin{array}{l} \displaystyle \frac{\Delta E_i}{E_i}\simeq \sum_{lm} \left(X_{lm}^2-2\,e_i\,X_{lm}\sin\Phi_{lm}\right) & \text{no secular}\\ \displaystyle \sum_{lm} \left(\sum_{i=1}^{n}e_i\right) & \text{terms} \end{array}$$

$$X_{22} = \left(\frac{m_3}{m_{12}}\right) f(e_o) \,\sigma^{5/2} \,e^{-\sigma g(e_o)}$$

asymptotic expression (Heggie) -adiabatic invariance of  $E_i/\Omega_i$ 

$$\Phi_{22} = \phi_i - \sigma \phi_o + 2(\varpi_i - \varpi_o) \qquad \text{(coplanar)}$$

 $\sigma$  = period ratio (outer/inner)

 $e_o$  = outer eccentricity

 $\lim_{e_o \to 1} \sigma g(e_o) \text{ finite} \qquad 21$ 

09:44

#### angular momentum exchange

$$\dot{\mathbf{J}}_{i} = \frac{\mu_{i}}{2\pi} \int_{0}^{2\pi} \mathbf{r} \times \mathbf{F} \, dM_{i} \qquad \qquad \Delta \mathbf{J}_{i}(t) = \int_{0}^{t} \dot{\mathbf{J}}_{i} \, dt'$$

-- changes in all orbital elements may be calculated as well as the back effect on the outer orbit

-- may contain secular terms...

some applications of new formalism

- Properties of ``decay products'' of unstable triples
- Decay timescales (half lives) of unstable triples
- Cheap scattering experiments
- ♥ Stability



Characteristics of decay products

What are the orbital parameters of the binary left behind when a triple decays?





#### Characteristics of decay products



The ability to place bounds on orbital characteristics of decay products allows one to do statistics such as *induced collision rates*.

It is also possible to predict the likelyhood of exchange during such an process.

Given system parameters (masses, eccentricities, semis), how long does a triple take to decay to a binary + a single?

A long-lived triple can bring an N-body calculation to it knees!

Also an interesting question in its own right!



#### distribution of energy exchange during **one** outer orbit:



$$Y = \frac{\Delta E_i}{E_i(0)} = X^2 + e_i X \sin \phi$$

 $\phi$  uniformly distributed in  $[0, 2\pi]$ 

$$\int_{X^2 - e_i X}^{X^2 + e_i X} f(Y) \, dY = 1$$



09:44

Change in orbital energy of inner binary after N outer orbits:



For large N,  $Z_N$  distributed normally (central limit theorem)



Distribution of ``first passage time" (first passage N)



On what timescale does an unstable triple decay? --dominated by last few orbits

$$\tau \simeq N_{\rm esc}^{3/2} \left[ \zeta(\frac{3}{2}, 1 - N_{\rm esc}) - \zeta(\frac{3}{2}) \right] T_o(0)$$

 $\zeta(a,b)$  = Riemann zeta function



<u>Scattering studies</u>: scattering of Kuiper belt by stellar flyby



Kenyon & Bromley 2004: 20 CPU days

#### formalism 100,000 times faster!



## Project (with J. Hurley): to study the effect of flybys on planetary systems in star clusters.

Flybys can render planetary systems unstable.



## Gravitational chemistry????



Making new molecules generally involves **exchange** 

requires  $\Delta E_i > -E_i$ 

and for  $m_3$  to form a new binary with  $m_1$  or  $m_2$ 

tricky but possible with new formalism...



Stability and resonance

 $X^2$  term fundamental for strong interactions.

Unstable triples = strong interactions.



## resonance 2 planets 2:1 resonance: Tout = 2 Tin

#### Energy exchange tends to be in same direction at conjunction



# resonance overlap \_\_\_\_ KAM, Chirikov chaos



09:44

Can use formalism to calculate resonance boundaries...

derive an DE for resonance angle...

 $\forall$  ... it will be a pendulum equation:  $\ddot{\Phi} = -\omega^2 \sin \Phi$ 

 $\mathbf{\Psi}$   $\omega$  is a simple function of system parameters

easy to see where they overlap...

Practical application: using simple analytical expressions (functions of orbital parameters, masses), determine if system is inside more than one resonance (simple inequalities).

Resonance overlap vs numerical experiments:

$$m_1 = m_2 = m_3, \quad e_{in} = 0, \quad i = 0$$



39

Resonance overlap vs numerical experiments:

$$m_1 = 1, m_2 = m_3 = 0.001, e_{in} = 0, i = 0$$



ratio of orbital frequencies

Resonance overlap vs numerical experiments:

$$m_1 = 1, m_2 = 0.001, m_3 = 10 e_{in} = 0, i = 0$$



ratio of orbital frequencies

09:45

$$m_1 = 1, \quad m_2 = 1, \quad m_3 = 0.1, \quad e_{in} = 0, \quad i = 0$$



09:45

#### **non-zero inner eccentricity:** $m_1 = m_2 = m_3$ , $e_{in} = 0.4$ , i = 0



43

inclined: 
$$m_1 = 1$$
,  $m_2 = 1$ ,  $m_3 = 0.5$ ,  $e_{in} = 0.5$ ,  $i = 30^\circ$ 



44

09:45

retrograde: 
$$m_1 = m_2 = m_3$$
,  $e_{in} = 0.3$ ,  $i = 180^\circ$ 





### perpendicular orbits: $m_1 = m_2 = m_3 = 1$ , $e_{in} = 0$ , $i = 90^\circ$



high outer mass: 
$$m_1 = 1$$
,  $m_2 = 1$ ,  $m_3 = 30$ ,  $e_{in} = 0$ ,  $i = 0$ 



exchange dominates

Outer periastron (units if inner semi) vs outer eccentricity

high outer mass, perpendicular orbits:

$$m_1 = 1$$
,  $m_2 = 1$ ,  $m_3 = 10$ ,  $e_{in} = 0$ ,  $i = 90^\circ$ 





#### **Stable or not?**



<sup>09:45</sup> Using sensitivity to initial conditions to determine stability

50

## stability: mass dependence

Stability Boundary for ein=0 and eout=0.5



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