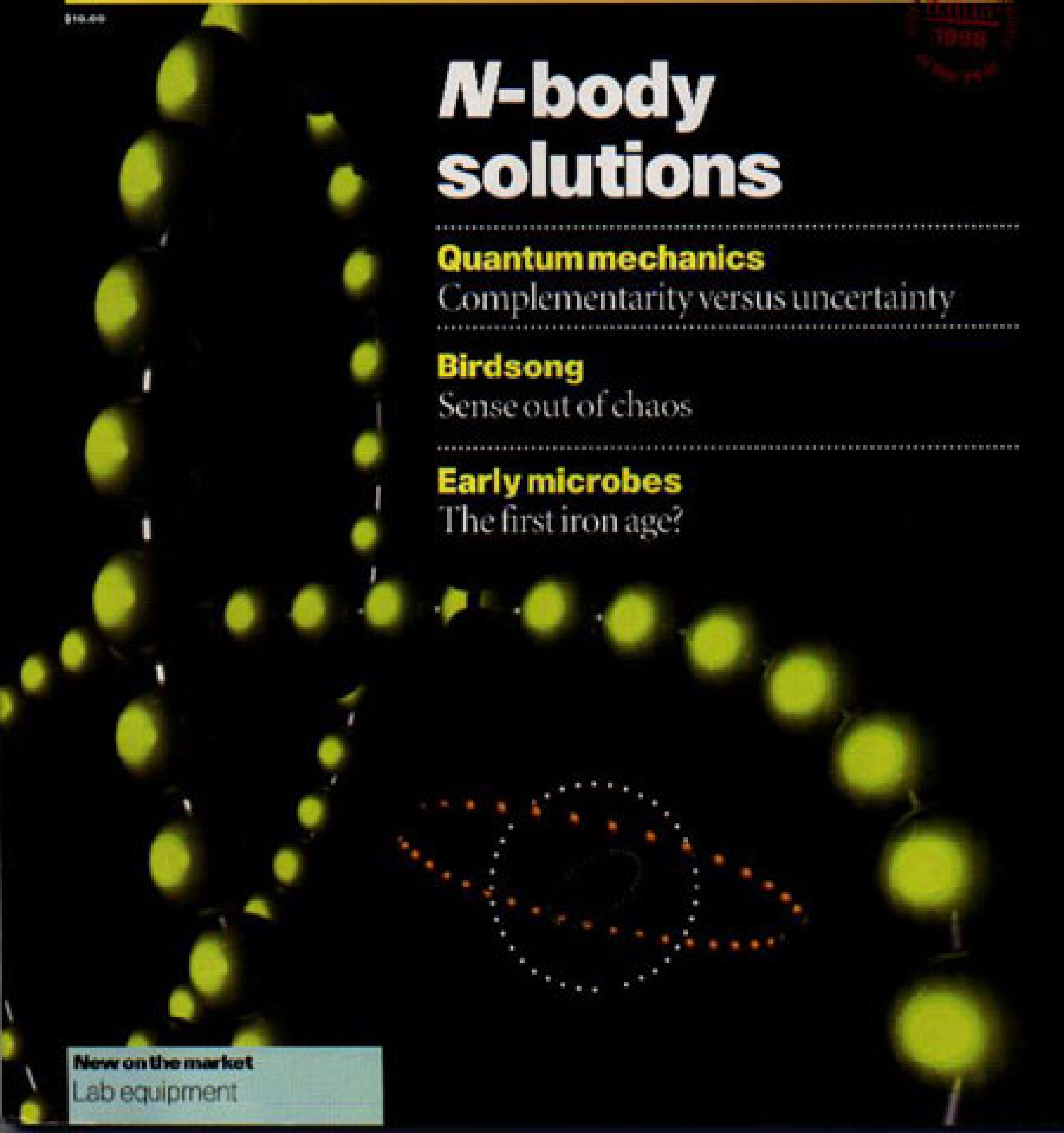
3 September 1998

International weekly journal of science

nature



N-body solutions

Quantum mechanics
Complementarity versus uncertainty

Birdsong
Sense out of chaos

Early microbes
The first iron age?

New on the market
Lab equipment

Most smooth closed space curves contain approximate solutions of the *n*-body problem

Gregory Buck

Department of Mathematics, Saint Anselm College, Manchester, New Hampshire 03102, USA

The determination of the exact trajectories of mutually interacting masses (the *n*-body problem[1,2]) is apparently intractable for $n \geqslant 3$, when the generic solutions become chaotic. A few special solutions are known, which require the masses to be in certain initial positions; these are known as 'central configurations' (refs 1–6) (an example is the equilateral triangle formed by the Sun, Jupiter and Trojan asteroids). The configurations are usually found by symmetry arguments. Here I report a generalization of the central-configuration approach which leads to large continuous families of approximate solutions. I consider the uniform motion of equidistributed masses on closed space curves, in the limit when the number of particles tends to infinity. In this situation, the gravitational force on each particle is proportional to the local curvature, and may be calculated using an integral closely related to the Biot–Savart integral. Approximate solutions are possible for certain (constant) values of the particle speed, determined by equating this integral to the mass times the centrifugal acceleration. Most smooth, closed space curves contain such approximate solutions, because only the local curvature is involved. Moreover, the theory also holds for sets of closed curves, allowing approximate solutions for knotted and linked configurations.

Central configurations[1–6] are usually thought of in one of two ways. With appropriate initial velocities, a planar central configuration gives homographic solutions—in which the shape of the initial configuration is preserved, but not necessarily the size (a special case is rigid rotation, where the centrifugal forces exactly balance the attraction due to gravity and size is preserved as well). In our Solar System, the Sun, Jupiter and the Trojan asteroids form an equilateral triangle homographic solution. Alternatively, if a central configuration is allowed to run from rest, then the solution is that the configuration collapses to the centre of mass, while keeping its shape.

Here I generalize the idea of a central configuration, searching for conditions such that a set of masses would move along a given space curve. Let $\mathbf{x}_i$ denote the position vector for the ith mass, and let $\ddot{\mathbf{x}}_i$ denote the acceleration vector of the ith mass. Consider the regular n-gon of equal masses, which is known to be a central configuration for all n. If the velocities are of the correct magnitude and tangent to the circle containing the n-gon, then a relative equilibrium solution is given; the masses move along the circle with uniform speed. Let κ denote the curvature vector—the vector in the direction of the normal with length equal to the curvature. Then in this system we have $\kappa = (1/v^2)\ddot{\mathbf{x}}_i$ for all masses in all positions $\mathbf{x}_i(t)$ along the circle containing the masses, because if a mass travels along a given curve with uniform speed v, $\ddot{\mathbf{x}}_i = \kappa v^2$.

In general, if there were n masses distributed along a closed space curve, moving along the curve with uniform speed v, and the condition $\kappa = (1/v^2)\ddot{\mathbf{x}}_i$ held for all masses in all positions $\mathbf{x}_i(t)$ (all translations of the masses along the curve), then the space curve would contain all the trajectories of the system, and we would have a solution to the n-body problem. In this sense, the equations $\ddot{\mathbf{x}}_i = k\kappa$ can be thought of as a generalization of the central configuration equations $\ddot{\mathbf{x}}_i = k\mathbf{x}_i$.

I now consider the likelihood of finding such curves. The perhaps surprising result is that, in the limit as n (the number of masses) tends to ∞, most smooth closed space curves are such curves. By 'most' we mean curves with bounded curvature, a finite number of inflexion points and without self-intersections. These are generic conditions for smooth space curves.

Consider a sub-arc of such a curve, and let n, the number of equal masses distributed along the curve, be large enough that the change in curvature is small between successive masses (Fig. 1). Choose a mass m_i. The components of $\ddot{\mathbf{x}}_i$ come in pairs, taking the effect from m_{i+1} together with the force from m_{i-1}, m_{i+2} with m_{i-2}, and so on. As the masses are equidistributed along the curve, and the curve is nearly 'flat' between successive masses, this pairing cancels the tangential component of the force from the nearest neighbours. To first approximation we are left with the component of the force in the direction of κ.

Next I consider the limit of a distribution along the curve, keeping the total mass constant (say 1), and letting there be n masses of mass $1/n$, and letting $n \to \infty$. Suppressing for the moment G, the gravitational constant, and ρ, the line density (mass per unit length), which both enter as scalars, the computation of $\ddot{\mathbf{x}}$ becomes an integral, $\int_c (\mathbf{x} - \mathbf{y})/|\mathbf{x} - \mathbf{y}|^3$, where $\mathbf{x}$ is a particular point on the curve c, and $\mathbf{y}$ varies along the curve. The cancellation of tangent forces mentioned above means that the integral, near the point $\mathbf{x}$, can be approximated by $(\kappa/|\kappa|)\int(\cos\alpha)/|\mathbf{x} - \mathbf{y}|^2$, where α is the angle between the vector $\mathbf{x} - \mathbf{y}$ and κ, the curvature vector at $\mathbf{x}$. This integral is divergent as $\mathbf{y}$ approaches $\mathbf{x}$. The $\cos\alpha$ cancels one power of $\mathbf{x} - \mathbf{y}$ at the singularity, but the curvature gives a coefficient to this cancellation. The remaining inverse power gives us a logarithmic singularity at $\mathbf{x} = \mathbf{y}$ (Fig. 1). Let R be the local radius of curvature, and δ the small particle size $(1/n)$. Then in the limit as $n \to \infty$ we have $\ddot{\mathbf{x}}_i \to G\rho\log(R/\delta)\kappa$. Here I used the case of equal masses for ease of exposition. The analysis requires only the equidistribution of mass along the curve.

Let the particles move along the curve with uniform speed v given by $v^2 = G\rho\log(R/\delta)$. ($R$ weakly varies over c, but as $n \to \infty$ it tends to

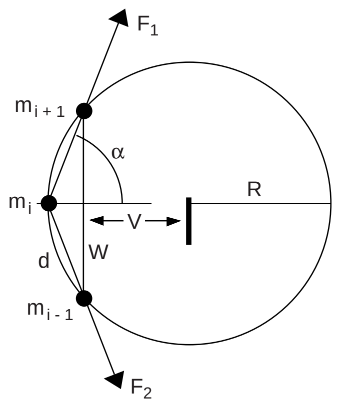


Figure 1 The gravitational force vectors $\mathbf{F}_1$ and $\mathbf{F}_2$ result from the effect of m_{i+1} and m_{i-1} on m_i. As m_{i+1} and m_{i-1} approach m_i symmetrically along the circle, the components of $\mathbf{F}_1$ and $\mathbf{F}_2$ tangential to the curve (here the circle) cancel, leaving only the contribution in the direction of the curvature vector. Passing to the continuous case, it is necessary to analyse $\int(\cos\alpha)/d^2$. But using $d^2 = w^2 + (R - v)^2$, we have $\cos\alpha/d^2 = (1/d)[(R - v)/d^2] = (1/d)[(R - v)/(2R^2 - 2Rv)] = (1/d)(1/2R)$, so the integral becomes $(1/2)\kappa\int(1/d)$, which is the logarithmic singularity times the curvature vector. The analysis for the general case is given by considering the osculating circle at the given point on the curve. This analysis is similar to the calculation carried out in fluid dynamics in the analysis of the dynamics of vortex filaments. In that case, the force is in the direction of the binormal of the underlying curve (the vortex filament), as opposed to the normal, and the logarithmic singularity is regularized, giving the local induction approximation: the vortex filament's self induction is given by speed that is the norm of the curvature, in the direction of the binormal vector[7,8].

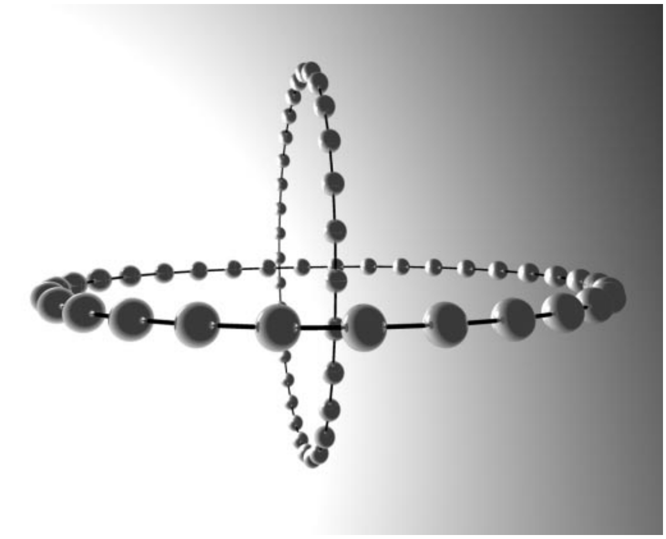


Figure 2 Schematic representation of a simple link approximate solution.

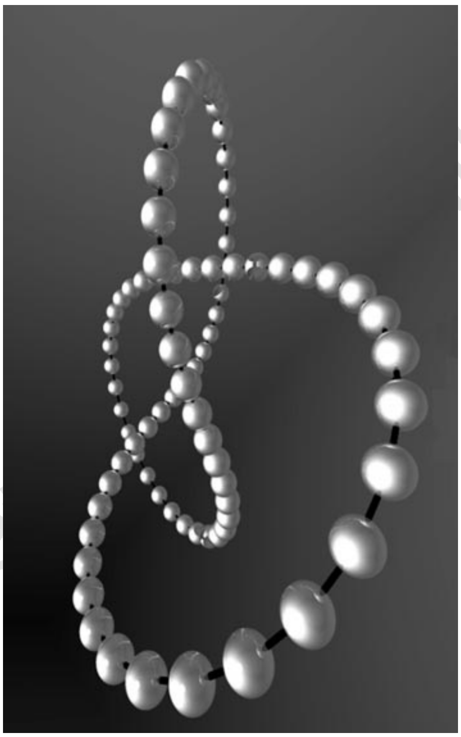


Figure 3 Schematic representation of a knotted approximate solution. One way to measure the rate of convergence (in n) to the infinite speed solution for a particular curve is by subtracting off the logarithmic singularity at each point. Consider the double integral $E(c) = \int\int |[(x-y)/|x-y|^3] - [(x-S)/|x-S|^3]|$, where the interior integral is computed by holding x fixed and letting y vary over the curve c, and letting S vary over the osculating circle to c at x. For the exterior integral, let x vary over c. The integral is finite for the curves which satisfy our conditions. $E(\text{circle}) = 0$, as the osculating circle for the circle is the circle itself. A higher E value indicates that more masses may be required for a better approximate solution. For example, if the curve self-intersects, $E(c) = \infty$, and near self-intersections have high $E(c)$. $E(c)$ is closely related to 'energy' functions for knots and links that have recently been studied[9–12]. Such functions have been found to be remarkably effective at simplifying complex tangles (R. Scharein, Knot-Plot, program available at http://www.cs.ubc.ca/nest/imager/contributions/scharein/KnotPlot.html; K. Brakke, Evolver, program available at http://www.geom.umn.edu), and have found applications in biochemistry[13,14].

a uniform value, so for uniform motion a representative constant should be chosen). Then Newton's equations of motion are nearly satisfied for all times.

A physical interpretation is to think of the bodies as restricted to the space curve, like beads on a wire, and ask how much force is used to keep the beads on the wire as they traverse it (at speed v). In a solution, such as a relative equilibrium, no force at all is required. In an approximate solution this force should be small. In this spirit I offer a definition of periodic approximate solution—other definitions are certainly possible. In a solution to the n-body problem, Newton's equations of motion

$$m_i \ddot{\mathbf{x}}_i = \sum_{j=1, i\neq j}^{n} \frac{G m_i m_j (\mathbf{x}_j - \mathbf{x}_i)}{|\mathbf{x}_i - \mathbf{x}_j|^3}$$

hold for all masses. In an approximate solution, which is a set of trajectories $\mathbf{X}(t) = \mathbf{x}_1(t), \mathbf{x}_2(t), \ldots \mathbf{x}_n(t)$, the equations nearly hold. It is necessary to define 'nearly'. Let

$$E_i = \left| m_i \ddot{\mathbf{x}}_i - \sum_{j=1, i\neq j}^{n} \frac{G m_i m_j (\mathbf{x}_j - \mathbf{x}_i)}{|\mathbf{x}_i - \mathbf{x}_j|^3} \right|$$

For periodic trajectories, let Er denote the maximum over the n masses of $E'_i\omega$, where ω is the period and E'_i is the maximum of E_i over $0 \leqslant t \leqslant \omega$. If Er is small, there is a sort of uniform bound on the 'error' along each trajectory and I will call $\mathbf{X}(t)$ an approximate solution. For the trajectories along closed curves described above $Er \rightarrow 0$ as $n \rightarrow \infty$. Simpler sets of curves, such as the Hopf link (Fig. 2), require fewer masses to make Er small. Measures of complexity of curves may give us estimates of the number of masses required (Fig. 3).

Questions remain regarding the exact relationship of these approximate solutions to n-body initial value problems. In particular, consider the initial value problem of many masses equidistributed along a closed curve, with initial velocities which are tangent to the curve and have constant magnitude $v = (G\rho \log(R/\delta))^{1/2}$. The existence of the approximate solutions would seem to give an idea of the behaviour of the initial value problem for some time interval—the masses nearly follow the underlying curve: the question is how long a time interval.

A long-standing open question in celestial mechanics is whether there exist continuous families of central configuraitons for a given set of masses. We can construct approximate collapse solutions consisting of masses distributed along circles about the centre of mass, where the density of the distribution on a given circle of radius R is R^2 (so we have $\ddot{\mathbf{x}}_i = k\mathbf{x}_i$ for masses on each circle). As the local contribution along the curve dominates, the orientation of the

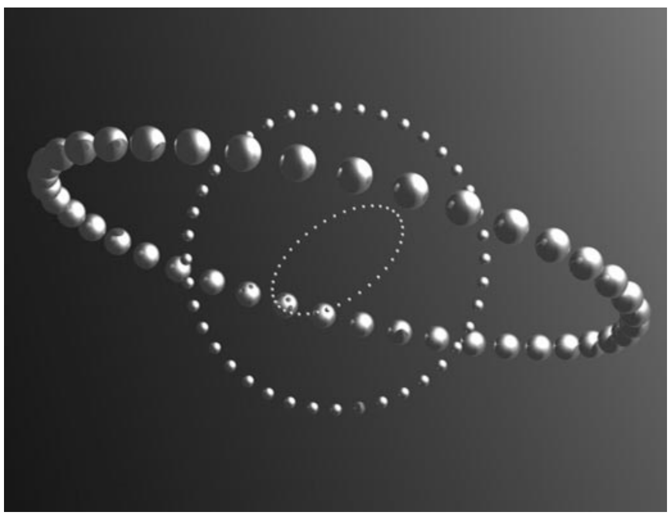


Figure 4 Schematic of approximate collapse solutions.

circles to one another makes no difference, and in the limit we have continuous families of collapse solutions (Fig. 4).

The analysis involved an integral of the same form as the Biot–Savart integral, a much studied integral which arises in several contexts in magneto-hydrodynamics. This connection invites further investigation. The results may be of use in particle systems where filamentary distributions tend to arise, such as cosmic strings. Also, because the acceleration of a filamentary equidistribution is approximated by the curvature, connections to curvature driven flows are possible. □

Received 20 January; accepted 6 July 1998.

1. Diacu, F. & Holmes, P. *Celestial Encounters* (Princeton Univ. Press, 1996).
2. Meyer, K. & Hall, G. R. *Introduction to Hamiltonian Dynamical Systems and the N-Body Problem* (Springer, New York, 1992).
3. Saari, D. On the role and properties of n-body central configurations. *Celest. Mech.* **21,** 9–20 (1980).
4. Moeckel, R. On central configurations. *Math. Z.* **205,** 499–517 (1990).
5. Buck, G. On clustering in central configurations. *Proc. Am. Math. Soc.* **108,** 801–810 (1990).
6. Llibre, J. On the number of central configurations in the n-body problem. *Celest. Mech.* **50,** 89–96 (1991).
7. Ricca, R. L. Rediscovery of Da Rios equations. *Nature* **352,** 561–562 (1990).
8. Saffman, P. G. *Vortex Dynamics* (Cambridge Univ. Press, 1992).
9. Buck, G. Four-thirds power law for knots and links. *Nature* **392,** 238–239 (1998).
10. Buck, G. & Simon, J. Thickness and crossing number of knots. In *Topol. Appl.* (in the press).
11. Moffatt, H. K. The energy spectrum of knots and links. *Nature* **347,** 367–369 (1990).
12. O'Hara, J. Energy of a knot. *Topology* **30,** 241–247 (1991).
13. Simon, J. in *Proc. 1994 IMA Summer Program on Molecular Biology* (eds Mesirov, J. P., Schulten, K. & Sumners, D. W.) 39–58 (IMA Vol. 82, Springer, New York, 1996).
14. Stasiak, A. *et al.* Electrophoretic mobility of DNA knots. *Nature* **384,** 122 (1996).

Acknowledgements. This work was supported in part by the National Science Foundation.

Correspondence and requests for materials should be addressed to the author (e-mail: gbuck@anselm.edu).

Strong exciton–photon coupling in an organic semiconductor microcavity

D. G. Lidzey*†, D. D. C. Bradley*†, M. S. Skolnick*, T. Virgili*†, S. Walker‡ & D. M. Whittaker§

** Department of Physics, † Centre for Molecular Materials, University of Sheffield, Hicks Building, Hounsfield Road, Sheffield S3 7RH, UK*
‡ Department of Electronic and Electrical Engineering, University of Sheffield, Sir Frederick Mappin Building, Mappin Street, Sheffield S1 3JD, UK
§ Toshiba Cambridge Research Centre Ltd, 260 Cambridge Science Park, Milton Road, Cambridge CB4 4WE, UK

The modification and control of exciton–photon interactions in semiconductors is of both fundamental[1–4] and practical interest, being of direct relevance to the design of improved light-emitting diodes, photodetectors and lasers[5–7]. In a semiconductor microcavity, the confined electromagnetic field modifies the optical transitions of the material. Two distinct types of interaction are possible: weak and strong coupling[1–4]. In the former perturbative regime, the spectral and spatial distribution of the emission is modified but exciton dynamics are little altered. In the latter case, however, mixing of exciton and photon states occurs leading to strongly modified dynamics. Both types of effect have been observed in planar microcavity structures in inorganic semiconductor quantum wells and bulk layers[1–8]. But organic semiconductor microcavities have been studied only in the weak-coupling regime[9–18]. Here we report an organic semiconductor microcavity that operates in the strong-coupling regime. We see characteristic mixing of the exciton and photon modes (anti-crossing), and a room-temperature vacuum Rabi splitting (an indicator of interaction strength) that is an order of magnitude larger than the previously reported highest values for inorganic semiconductors. Our results may lead to new structures and device concepts incorporating hybrid states of organic and inorganic excitons[19], and suggest that polariton lasing[20–22] may be possible.

Strong coupling manifests itself in anti-crossing of the coupled modes and the appearance, on resonance, of two equal-intensity transitions separated by the vacuum Rabi splitting. These new cavity polariton modes can be considered an admixture of the optical transitions of the material and the cavity photon modes, and have a radiative lifetime determined by the cavity photon lifetime. Strong coupling is evident when the interaction strength (Rabi splitting) exceeds the optical transition and cavity mode damping. Under these conditions, a periodic exchange of energy (Rabi oscillation) can occur between the coupled modes before the excitation decays. In the perturbative weak-coupling regime, the interaction strength is less than the damping. Anti-crossing is then no longer observed and whilst significant changes in the spectral and spatial distribution of transition probability do still occur, no dramatic changes in recombination dynamics are expected.

Up until now, strong coupling in a semiconductor microcavity has only been achieved using inorganic materials. A typical structure consists of a high finesse Fabry–Pérot resonator with distributed Bragg reflector mirrors and a series of quantum wells placed close to the confined field antinode. The largest Rabi splitting reported for a III–V (GaAs) based microcavity structure is[23] 9.4 meV. Larger values, namely 17.5 meV, have been reported for II–VI (ZnCdSe)-based microcavities[8]. The splitting depends on the exciton oscillator strength and the magnitude of the confined field, and is maximized for matched cavity and optical transition linewidths[1–4,24]. The enhanced Rabi splitting for II–VI semiconductors is principally due to their larger oscillator strengths.

Organic semiconductors have recently attracted much interest for applications in electroluminescent displays and as gain media. Microcavity structures[9–18] have been fabricated to allow control of the emission energy, linewidth, intensity and directionality for light-emitting diodes, as prototypical colour displays and as laser resonators. Large oscillator strengths are a characteristic feature of these materials. Strong coupling has not, however, been reported. The large exciton linewidths[25] that result from inhomogeneous broadening and the presence of a vibronic progression make strong coupling difficult to observe. This situation is not, however, universally true and we have identified several candidate materials that have sufficiently narrow exciton linewidths that strong-coupling might be expected to be seen in a typical microcavity structure.

We report experiments that use tetra-(2,6-*t*-butyl)phenol-porphyrin zinc (4TBPPZn) as the organic semiconductor. This molecule has

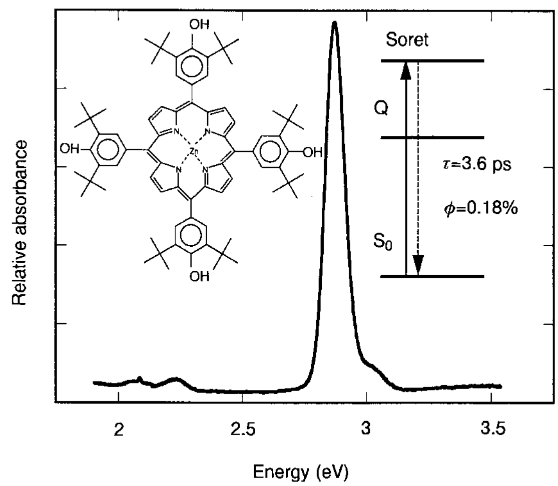


Figure 1 The absorption spectrum of a blend film of 4TBPPZn in polystyrene. The insets show the chemical structure and electronic energy-level scheme[26,27] for 4TBPPZn. The Soret band peaks at 2.88 eV and the Q-band absorbance is seen as a weak double peak structure between 2.0 and 2.26 eV. The Soret-band exciton decay time is expected to be $\tau = 3.6$ ps and the emission yield $\phi = 0.18\%$, due to rapid relaxation to the Q-band exciton[27].