附件一

行政院國家科學委員會補助專題研究計畫 ■ 成 果 報 告 □期中進度報告

非線性科學在奈米科技(3/3)

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成果報告類型(依經費核定清單規定繳交)：□精簡報告　■完整報告

本成果報告包括以下應繳交之附件：
□赴國外出差或研習心得報告一份
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■出席國際學術會議心得報告及發表之論文各一份
(國際學術會議 UPoN 在 June 2-6 2008 舉行)
□國際合作研究計畫國外研究報告書一份

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執行單位：國立交通大學物理研究所

中　華　民　國　97　年　8　月　18　日

(I) 中英文摘要

此研究為一跨領域的三年計劃,內容包含生物物理,電子自旋學,及量子混沌三個領域。在第三年的成果摘要如下:

(1) 生物物理

蛋白質負責許多生命功能,他們的工作原理大部分需要涉及構象變化。對於有局部電荷的蛋白質,構象可由外場變化操控。由於這項關聯,蛋白質可以成為能量的轉換者,從無序變化的外場中汲取能量來做功。這機制可視為是種觸媒輪,其中有名的例子包括鈉鉀離子 pump 及 F1-ATPase。

(2) 電子自旋學

考慮一個有 Rashba 自旋軌道耦合的無雜質層,被夾在兩個鐵磁材料中。積分掉游盪載子之後,載子輔助交換偶合的等效偶合可完整地被計算出。理論結果告訴我們該系統的磁性行為很敏感地決定於費米面的拓撲結構。假如費米面從蛋糕型變到甜甜圈型,交互作用將從 RKKY 上下振盪型變到螺旋線型。

(3) 量子混沌。

Bohr 的對應原理告訴我們量子態在古典極限下會收斂到古典態。一個例子是波函數的 Wigner 函數弱收斂到相空間裏的不變機率測度,亦即所謂的量子極限。長久以來兩個問題一直困擾著人們:一為如何對這些機率測度做分類,二為那個機率測度可成為量子極限。在這工作裏,我們找到了一個特殊動態系統,它具有兩個可完全被決定的量子極限。此例可能是所有量子遍歷動態系統中具非單一遍歷的首例。

關鍵詞:

生物馬達,能量轉換,觸媒輪,棘輪,Rashba 自旋軌道耦合,自旋遲豫,Bohr 對應原理,單一量子遍歷。

(1) Biological motor:

Proteins are responsible for many functions in living systems. Its working principle is mostly based on conformational changes. For proteins having partial charges, these changes can be driven by external electric fields. Through this coupling, proteins can function as an energy transducer and do work. This mechanism can be regarded as a catalytic wheel, which is capable of extracting energy from disordered external energy sources and converting this stochastic energy to a usable energy format. Examples of this catalytic wheel include the biological motors Na, K-ATPase and F1-ATPase.

(2) Spintronics:

Consider an intermediate thin layer with Rashba interaction sandwiched between two ferromagnets. After integrating out the itinerant carriers, the effective coupling of the carrier-mediated exchange coupling can be calculated. The magnetic trends obtained this way depend sensitively upon the topology of the Fermi surface. Depending on whether the exchange is "wedding cake" or "donut", the mediated exchange goes from the oscillatory RKKY to the non-collinear spiral interactions. The Fermi surface topology determines which type of magnetic interaction becomes dominant.

(3) Quantum chaos:

Bohr's correspondence principle in quantum mechanics states that in the semiclassical limit $h \rightarrow 0$ classical mechanics emerges and governs quantum mechanical quantities. One example is that the Wignerfunctions of eigenfunctions converge weakly to invariant probability measures on the phase space, the so-called quantum limits (QLs). Two big open problems in this field are how to classify the set of QLs and which invariant measures can occur as QLs. We introduce a class of model systems for which the set of QLs can be precisely determined. This work might provide the first example that a quantum ergodic map is not quantum unique ergodicity.

Keywords:
biological motors, energy transduction, catalytic wheel, ratchet, Rashba spin-orbit interaction, spin relaxation, Bohr's correspondence principle, quantum unique ergodicity.

(II) 報告內容:

(II.1) 前言:

此計劃的第三年，研究問題包含生物物理，電子自旋學，及量子混沌幾個領域，成果綜括如下:

(II.2) 研究目的、結果與討論:

(i) Biological motors:

Most proteins have electric dipoles and net charges in the structure and their conformations are susceptible to the electric and magnetic perturbation. The shape of a cell may also amplify an electric field across its plasma membrane. Therefore, a membrane integral protein such as an ion channel, an ion pump, or a molecular motor, is especially amenable to electric perturbation. When an alternating electric field or a fluctuating electric field is employed to actuate a two-state protein oscillator, the dynamics of the conformational change of the protein can be synchronized with the applied field. Through this two-state protein oscillator, we construct a four-state catalytic wheel by coupling an energy transducer mechanism to the two-state protein oscillator [1]. Analysis shows that the catalytic wheel can extract energy from a disordered external energy source, be it electrical, mechanical, or chemical, and convert this stochastic energy source to a usable energy format. The catalytic wheel is tested with the experimental data on the electric field-stimulated cation pumping of Na, K-ATPase. A dipole ratchet model based on the electroconformational coupling concept will also be discussed and compared with the ATP-dependent rotation of a rotary motor F1-ATPase. Since the working principle of this model is simpler than that of F1-ATPase, it provides an easier way to realize a nanoscale rotary motor than artificially reconstructing a F1-ATPase.

(ii) Spintronics:

In Ref. [2], we investigate the carrier-mediated exchange coupling between two ferromagnets, sandwiching an intermediate thin layer with Rashba interaction. The effective exchange coupling is obtained by integrating out the itinerant carriers. It turns out that the magnetic trends depend sensitively upon the topology of the Fermi surface. As the topology changes from "wedding cake" to "donut", the mediated exchange goes from the oscillatory Ruderman-Kittel-Kasuya-Yosida to the non-collinear spiral interactions accordingly. It is rather surprising that the Fermi surface topology determines which type of magnetic interaction becomes dominant. Finally, we also discuss potential applications for carrier-mediated exchange coupling across the junction.

In Ref. [4], the semiclassical path integral method provides a powerful tool to understand the spin dynamics in narrow channels with Rashba SOI. At large w regime (w ≈ 20 μm), the relaxation time $\tau_s \approx 9.7$ ps determined by previous analytical formula agrees with the τ_s calculated from our SPI method up to second decimal; the $\tau_s \approx 11.4$ ps from recent experiments in Ref. [Awschalom, 2006] only slightly deviates from this value. At small w regime (w ≈ 1.4 μm), the peculiar saturation phenomenon of τ_s observed in Ref. [Awschalom, 2006] is confirmed by the SPI method and its unknown reason is clarified. For helix modes, the analytically derived linearity and its slope of $1/\tau_s$ against w^2 in Ref. [Malshukov, 2000] coincide precisely with those calculated by the SPI method. Apart from these consistencies, this work can easily predict τ_s for general systems beyond the few known experimental samples and beyond the strict constraints assumed on the analytical formulae. Finally, a relaxation is conventionally understood as a monotonic exponential decay and it will usually be fitted by an exponential function. This work proves that in low dimensional systems a relaxation can be a process behaving like a Bessel function. To fit this function by an exponential function is not so meaningful, especially when we expect the fitted τ_s to characterize its original relaxation behavior. More rigorously speaking, this fitted τ_s is not representative, because infinitely many different functions can have the same τ_s. This paper brings out the question how to unify a proper definition of relaxation time τ_s for general relaxation processes.

(iii) Quantum chaos:

The correspondence principle in quantum mechanics states that in the semiclassical limit h → 0 classical mechanics emerges and governs quantum mechanical quantities for small de Broglie wavelength. One manifestation of this principle is that the Wignerfunctions of eigenfunctions converge weakly to invariant probability measures on phase space, the so-called quantum limits (QLs). It is one of the big open problems in the field to classify the set of QLs, and it is in general not known which invariant measures can occur as QLs. For ergodic classical systems, the celebrated quantum ergodicity theorem states that almost all eigenfunctions have the ergodic Liouville measure as QL. If all eigenfunctions converge to the Liouville measure, it is called quantum unique ergodicity (QUE). Possible exception for QUE is strong scarring, i.e., QLs concentrated on periodic orbits and mixed classical systems, i.e., the phase space has several invariant components of positive measure. Less is known to what extent the quantum mechanical system respects the splitting of the classical system into invariant components. In Ref. [3], we introduce a class of model systems for which the set of QLs can be determined very precisely. This work provides a very rare example that a quantum ergodic map is not QUE.

While the scattering phase in semiclassical methods can be exactly derived in several one-dimensional potentials, less is known in multi-dimensional quantum systems. Ref. [5]

work demonstrates a simple recipe to extend the phase knowledge from one-dimensional to multi-dimensional systems. The result is illustrated in the example of Bogomolny's transfer operator method applied in two quantum wells bounded by step potentials of different heights. The semiclassical method modified by that recipe accurately determines the energy spectrum of the systems, which indicates the substantial role of the proposed phase correction. Theoretically, the result paves a way for generalizing other semiclassical methods, such as Gutzwiller trace formula, dynamical zeta functions, and Landauer-B\"uttiker formula. In practice, the recipe facilitates the application of semiclassical methods on multi-dimensional quantum systems bounded by general potentials.

(II.4) 參考文獻

(a) Papers (2007/01-2008/08)

編號	著作名稱(含期刊名稱, 卷期, 及發表年)	作者	出版年月
[1]	Energy transduction in molecular machines, Nano 2, No. 5, 273–280 (2007)	C.-H. **Chang** T.-Y. Tsong	2007/10
[2]	Carrier-mediated exchange coupling and Fermi surface topology, International Journal of Modern Physics B, 22, Nos. 1 & 2 88-93 (2008)	W.-M. Huang, H.-H. Lai, C.-H. **Chang**, H.-H. Lin	2008/01
[3]	Quantisations of piecewise parabolic maps on the torus and their quantum limits, Communication in Mathematical Physics 282, 395–418 (2008)	C.-H. **Chang**, T. Krueger, R. Schubert, S. Troubetzkoy	2008/09
[4]	Semiclassical path integral approach on spin relaxations in quasi-1D wires	C.-H. **Chang**, J.-J. Tsai, H.-F. Lo, A.G. Mal'shukov	Submitted
[5]	Scattering phase correction for semiclassical methods in multi-dimensional quantum systems	W.-M. Huang, C.-Y. Mou, C.-H. **Chang**	Preprint

(b) 學生畢業論文:

謝宏慶 (Energy transduction in microscopic systems)

劉唐宇 (Transport properties in biological systems)

(II. 5) 計畫成果自評

(a) 研究內容與原計畫相符程度及達成預期目標情況

在這三年計劃的最後一年，獲得的成果和原計劃的差距較大。有些是原計劃延伸出去的問題，有些是前一個計劃有了重大突破，大方向和原計劃一樣，但成果和原計劃的相似度只有約四成。

(b) 研究成果之學術或應用價值及是否適合在學術期刊發表或申請專利

3 篇論文已於年初陸續發表在以上表列的期刊

1 篇 preprint 已 submit，另 1 篇 preprint 將在近期 submit

(c) 主要發現或其他有關價值等:

[1] 闡述在分子馬達裏，能量轉換的效能問題。

[2] 研究在兩層鐵磁材料中夾一層 Rashba 交互作用層，由載子造成的交換偶合，費米面拓撲對磁交互作用的影響，及可能的應用。

[3] 指出 correspondence principle 中量子狀態在古典極限時會收斂到不同的非零測度的古典極限，此 model 可能是此問題第一個實例。

[4] 用 path integral 方法解釋 Awschalom 實驗結果的迷惑，驗證並推廣 Malshukov 的理論結果。

[5] 提出簡單方法將一維位能的 scattering phase 推展到二及三維，提升半經典方法在實際系統的可用性，也使推廣到其他半經典方法變得可能。