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项目摘要

中文摘要(500字以内):

在本基金的资助下，我们在半导体及石墨稀的自旋动力学方面做了系统的工作。共发表了论文57篇，书中论文1篇。其中PRB 27篇，JAP 9篇，EPL 3篇，其他文章分别发表在PR、PRL、NJP、APL、JPD、JPCM、SSC、SST、PE、JSNM。这些论文被他引304次。在美、日、德、俄、波兰、西班牙、芬兰及土耳其等国的国际会议上受邀作邀请报告12次。特别需要指出的是，在本基金的资助下，受邀在Physics Reports上发表了一篇近200页的Review文章，系统总结了本人近十年在自旋动力学中建立的自旋动力学Bloch方程方法的工作，并总结了该领域的进展。

关键词(不超过5个，用分号分开): 自旋；动力学；半导体；石墨稀

Abstract(limited to 500 words):

Supported by this grant, we have performed systematic investigation on spin dynamics in semiconductors and graphene. We have published 57 papers and contributed one book chapter. In these publications, 27 are published in PRB, 9 in JAP, 3 in EPL and the remaining are published in PR, PRL, NJP, APL, JPD, JPCM, SSC, SST, PE and JSNM. These papers have been cited (excluding self-citation) 304 times. The principal investigator has been invited to present 12 invited talks in international conferences held in US, Japan, Germany, Russia, Poland, Spain, Finland and Turkey. We published an invited review article in Physics Reports. In this around 200-page review, studies based on the kinetic spin Bloch equation approach developed by the principal investigator during the past 10 years have been fully reviewed, together with the development of the whole field.

Keywords(limited to 5 keywords, seperated by;):spin; dynamics; semiconductor; graphene

报告正文

在本基金的资助下，我们在半导体及石墨稀的自旋动力学方面做了系统的工作，共发表了论文57篇（其中7篇为本人指导的论文，但由于对本人来说内容不够新颖，本人贡献只在感谢中标明），书中论文1篇。其中PRB 28篇，JAP 9篇，EPL 3篇，其他文章分别发表在PR、PRL、NJP、APL、JPD、JPCM、SSC、SST、PE、JSNM。这些论文被他引290+14次（14次为本人不署名的论文被他引数）。在美、日、德、俄、波兰、西班牙及土耳其等国的国际会议上受邀作邀请报告12次。担任Elsevier期刊[Physica E: Low-dimensional Systems and Nanostructures](#)的编辑、Springer期刊[J. Supercond. Nov. Magnet.](#)的编委。2010年担任韩国第30届国际半导体大会International Program Committee成员。

特别需要指出的是，在本基金的资助下，受邀在Physics Reports上发表了一篇近200页的Review文章[1]，系统总结了本人近十年在自旋动力学中建立的自旋动力学Bloch方程方法的工作，并总结了该领域的进展。该文在2010年下半年发表后，已被他引63次。

我们将动力学自旋Bloch方程推广到三维体材料系统、包含所有散射的情况，并全面系统地研究了III-V族半导体体材料中的电子自旋弛豫。在一篇长达21页的文章[2]中，我们给出了大量的预言，指出了一些之前被广泛接受的观点的错误，并发现了很多重要的结果。例如，我们预言了在n型和本征型体材料中自旋弛豫时间随电子浓度变化在金属区会有一个峰出现，在本征型体材料中由于库仑散射的非单调性自旋弛豫时间随温度变化会有一个峰出现，在p型体材料中由于屏蔽的变化自旋弛豫时间随空穴浓度会有一个峰出现。此外我们发现，之前人们认为在n型窄带半导体如InSb和InAs中Elliott-Yafet机制占主导的观点是错误的，我们的全微观计算表明Elliott-Yafet机制在所有常见的III-V材料中都不重要。另外Bir-Aronov-Pikus机制在本征型III-V体材料中不重要。我们的研究极大地丰富了人们对体材料中的自旋弛豫的理解。其中我们预言的在n型体材料中自旋弛豫时间随电子浓度变化的峰很快就被美国Colorado大学的Cundiff实验组证实[Krauß, Bratschitsch, Chen, Cundiff, and Schneider, PRB **81**, 035213 (2010); Shen, CPL **26**, 067201 (2009)]。我们关于Elliott-Yafet机制在III-V族半导体中是不重要的预言，已被其后Murdin的实验证实[Litvinenko, Leontiadou, Li, Clowes, Emeny, Ashley, Pidgeon, Cohen, and Murdin, APL **96**, 111107 (2010)]。我们关于在本征III-V半导体中的温度峰的预言，也被Ma等人的实验所证实[Ma, Jin, and Ma, APL **96**, 136102 (2010); Ma, Jin, Wang, and Ma, JAP **109**, 023105 (2011)]。该文章从09年发表以来，已被他引31次。

我们用我们的动力学自旋Bloch方程理论，重新研究了BAP机制对本征及空穴型量子阱

自旋迟豫的贡献,发现以往文献中普遍认为的BAP机制在低温下是决定自旋迟豫的机制是错误的[3]。并指出了以往单体理论错误的原因。该预言已被港大X. D. Cui [Chunlei Yang, Xiaodong Cui, Shun-Qing Shen, Zhongying Xu, and Weikun Ge, Phys. Rev. B **80**, 035313 (2009)] 及德国 Hannover大学的M. Oestreich [S. Oertel, S. Kunz, D. Schuh, W. Wegscheider, J. Hü bner, and M. Oestreich, arXiv:1103.2474]的实验所验证。 该文已被他引17次。

我们研究了ZnO及GaN的自旋轨道耦合[4]。该文发表后, 不断被各国同行引用并用于解释实验。该文已被他引21次。

我们研究了硅中的自旋迟豫机制, 指出了Elliot-Yafet机制中的相干相消作用[5]。 该文已被他引18次。

我们用动力学自旋Bloch方程方法系统地研究了GaAs体材料中的空穴自旋弛豫。在我们的研究中很好的处理了重(轻)空穴带的带内关联, 从而可以对 D'yakonov-Perel' 机制和 Elliott-Yafet机制在空穴自旋弛豫过程中的相对重要性作出定量的比较。在室温下本征GaAs 中, 我们的计算结果和实验符合的很好[D. J. Hilton and C. L. Tang, PRL **89**, 146601 (2002)]。 我们发现带内关联在空穴自旋动力学中是十分重要的,因此以往文献中忽略带内关联研究空穴自旋动力学是不对的[M. Krauß, M. Aeschlimann, and H. C. Schneider, PRL **100**, 256601 (2008)]。 我们首次指出空穴-光学声子的非极化相互作用在空穴自旋动力学过程中也有很大的贡献。在这个工作中,我们还研究了空穴自旋弛豫时间的温度、浓度依赖关系,预言了弛豫时间的很多有意思的非单调行为。另外, 我们发现Elliott-Yafet机制通常要比D'yakonov-Perel' 重 要, 但是在低温高掺杂与中等温度(100 K左右)低掺杂情况下, 两者的贡献可以相比[6]。

我们用动力学自旋Bloch方法研究了石墨烯中的自旋弛豫。我们的结果表明高温下库仑散射对石墨烯的自旋弛豫有很大贡献, 而这一贡献均被之前石墨烯自旋弛豫的研究所忽略。 我们还预言由库仑Hartree-Fock项导致的纵向有效磁场会极大地延长大极化下的自旋弛豫时间, 而这一效应即使在室温下仍然十分显著。另外, 我们还发现由于石墨烯中的库仑散射不够强, 热电子的稳态分布并不符合之前广泛使用的分布公式, 我们基于计算结果提出了一个新的近似分布公式[7]。 我们用动力学的自旋Bloch方程方法研究了SiO₂衬底上石墨单层里电子的自旋扩散和输运。由于衬底和表面附着原子的影响, 石墨单层里电子感受到的 Rashba场得到加强, 幅度达到0.1 meV的量级。在这个Rashba场下, 我们计算得到的自旋扩散/输运长度在1-10微米量级, 和实验测量值可比拟。 我们的研究发现, 在强散射条件下, 自旋扩散/输运不受散射的影响。此外, 自旋扩散/输运还表现出对注入的自旋极化方向的各向异性依赖。当注入的自旋极化方向处在由与石墨表面垂直的方向和自旋注入方向定义的平面内时, 自旋扩散/输运的长度是相同的, 但是要大于当注入的自旋极化方向与该平面垂

直时的自旋扩散/输运长度。电子浓度、电场对自旋输运的影响在这个工作中也得到了研究[8]。我们利用Floquet理论讨论了强太拉赫兹场下石墨烯中的光学响应。我们的结果表明对于足够大的动量，准能谱中的带隙会消失。正是由于这些大动量态的贡献，态密度中的带隙并不会出现。这一发现纠正了之前文献中的误解 [T. Oka and H. Aoki, PRB **79**, 081406(R) (2009)]。另外，我们发现石墨烯中动力学 Franz-Keldysh效应与半导体中的有很大差别，并作出很多预言。比如光电导的频率依赖会呈现出多台阶状的行为；对低费米面的情况，谷出现在探测光频率等于赫兹场频率的整数倍处；当费米面取某些特定值，会出现一系列的峰。这些发现有待实验的验证[9]。

我们基于s-d模型，从动力学自旋Bloch方程出发，系统地研究了铁磁半导体磁矩动力学的Landau-Lifshitz-Gilbert方程。我们推导了铁磁半导体中的Gilbert damping系数，指出在铁磁半导体中自旋轨道相互作用的存在使自旋守恒散射会影响巡游电子的自旋寿命，从而对damping系数有贡献。我们还预言了，当体系存在自旋流的情况下，自旋流与自旋轨道耦合的共同作用会对Gilbert damping有额外的贡献[10]。我们进一步推导了存在磁矩空间梯度的情况下铁磁半导体中巡游载流子的自旋动力学方程并计算了相应的磁扭矩。我们得到的磁矩的一阶梯度对磁扭矩的贡献与极化电流成线性关系，这个结果和之前的研究一致。我们提出从磁矩的二阶梯度给出来的扭矩除了通常的自旋刚度(spin stiffness)以外，还存在一项与磁性材料的非绝热参数 β 成正比的垂直自旋刚度。通过计算我们发现这项额外的磁扭矩对铁磁半导体磁畴壁的结构有重要修正，因此在研究铁磁半导体的磁矩动力学过程中需要在Landau-Lifshitz-Gilbert(LLG)加入该项的贡献[11]。最后，我们用微观模型计算了GaMnAs的LLG系数[12]。

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已培养博士2人、博士后2人。

在本基金资助下，2008-2011年四年中，共邀请了国内外学者86人次访问科大讲学。具体目录可见在<http://wu.ustc.edu.cn/wu/> 的COLLOQUIA & SEMINARS链接中找到。

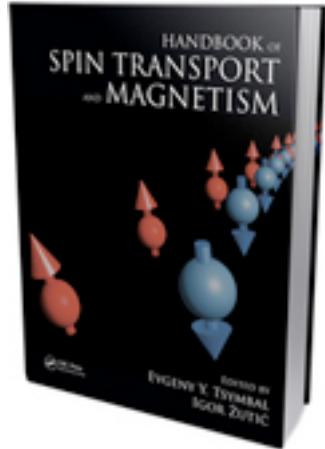
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