U.S. CIVILIAN RESEARCH & DEVELOPMENT FOUNDATION (CRDF)

COOPERATIVE GRANTS PROGRAM

FINAL PROJECT REPORT

GENERAL INSTRUCTIONS

- The completed Final Project Report is due **within 30 days** of the termination date of the award.
- Please indicate your **AWARD NUMBER (format XY#-####)** on all submitted documents.
- The Final Project Report forms are available for download from the CRDF web site at **www.crdf.org.**
- The Final Project Report must be submitted as follows:
    - The US and FSU Principal Investigators must jointly complete the Final Project Report and submit it as ONE electronic document attached to an e-mail message to CRDF (finalreports@crdf.org).
    - One Principal Investigator should send this email message and copy ("cc") the other Principal Investigator to indicate that the Report has been jointly completed and approved by both Principal Investigators.
    - Microsoft Word (.doc) format is preferred. However, Adobe Acrobat (.pdf) or Rich-Text (.rtf) formats are also acceptable. If you feel that you will be unable to submit the report electronically, please contact CRDF.
    - For questions regarding the Final Project Report, please contact:
      Laura Meany, Program Assistant
      Fax: 703-526-9721
      E-mail: finalreports@crdf.org
- Information provided by the Principal Investigators in Section I (Public Summary) of the Project Report will be treated as public information and may be used by CRDF in publicly-distributed materials. Individual responses provided in the other sections will not be made public without the permission of the Principal Investigators. Information identified as business-confidential will be held in strict confidence. *Please do not include business-confidential data in Section I of the Project Report.*
- All grantees must also complete the required **Final Financial Reports**, and submit those separately from this Final Project Report. Please see CRDF's web site (www.crdf.org) for the required forms.
- Please note that under the CRDF Award General Conditions governing this award, the final payments for Individual Financial Support and Institutional Support will not be released until the completed Final Project Report and Final Financial Reports have been received and accepted by CRDF.

FINAL PROJECT REPORT CONTENTS

CRDF COOPERATIVE GRANTS PROGRAM: FINAL PROJECT REPORT

SECTION I: Public Summary

Award Number: UP2-2436-LV-02

INSTRUCTIONS

- **Contents:**

  1) Brief Statement of Major Accomplishment: In one or two sentences, please state succinctly what you feel to be the major accomplishment that your research achieved.

  2) Public Summary (English): The public summary should begin with a sentence that describes the project's original major goal(s) without restating the project title. The summary should then follow with findings and implications stated as concisely and informatively as possible, commenting as appropriate on the techniques or approaches used. Please indicate how your research results represent an advance in scientific knowledge and any potential social or commercial applications. The summary should be written from the point of view of a completed project, and should be self-contained and intelligible to a layperson. Please do not re-submit the proposal abstract. The public summary should be **200-300 words** in length.

  3) Public Summary (FSU Language): Same as #2 above, translated into Russian, Ukrainian, or another language of the former Soviet Union (FSU).

- **Use:** Please note that CRDF may use the public summary in publicly-distributed documents and other materials. **Please do not include proprietary or business-sensitive information.**

1) Brief statement of project's major accomplishment (Please summarize in one or two sentences what you consider to be the major accomplishment achieved during your research):

We derived an exact theoretical description of electronic Raman scattering near a metal-insulator transition. Our solution includes all relevant physical processes (nonresonant, resonant, and mixed) and represents one of the most complex applications of dynamical mean field theory to model systems.

2) Public Summary (English)

The problem of inelastic light scattering off of electrons in strongly correlated materials is one of the most complex problems in solid state physics. It involves the process where photons shine onto a material, interact with the electrons, and are reflected back, but the reflected photon has a different color from the incident photon. The inelastic light scattering function counts how many photons are reflected with a given shift in the color over a period of time. Many experiments have been performed on a wide range of materials, ranging from Kondo insulators to materials close to a metal-insulator transition, to the high-temperature superconductors. The inelastic light scattering function shares a number of similarities in these diverse systems: (i) the ratio of the temperature where a gap forms in the response function to the size of the gap is much smaller than 0.5 and (ii) there is an isosbestic point where the response function is independent of temperature at one specific color shift. Combining the expertise of the Ukrainian and the US teams, we managed to solve the full problem including all relevant types of scattering (the so-called nonresonant, resonant, and mixed terms). This required us to develop a new formalism to perform the analytic continuation of the relevant light scattering functions; this formalism is quite general and can be applied to many different many-body problems. We also initiated a study of finite-dimensional effects, by examining nonresonant light scattering with the dynamical cluster approximation in two dimensions. The computer programs for this work are nearly finished, but the production runs are likely to take a significant amount of time before they will be complete. This is the first attempt to calculate transport with the dynamical cluster approximation in any model system.

3) Public Summary (FSU Language)

Проблема непружнього розсіяння світла на електронах у сильноскорельованих матеріалах є однією з найскладніших проблем у фізиці твердого тіла. Воно включає процеси, при яких фотони опромінюють матеріал, взаємодіють з електронами і відбиваються назад, але відбиті фотони мають інший колір (енергію) ніж налітаючі. Переріз (функція) непружнього розсіяння світла показує скільки відбивається фотонів із заданим зсувом кольору за певний проміжок часу. На даний час виконано багато експериментів для широкого ряду матеріалів включаючи діелектрики Кондо, матеріали поблизу переходу метал-діелектрик і високотемпературні надпровідники. Для всіх цих відмінних систем переріз непружнього розсіяння світла володіє рядом спільних властивостей: (i) відношення температури утворення щілини до розміру самої щілини набагато менше за 0.5 (ii) наявність ізосбестичної точки коли функція відгуку для певного значення зсуву кольору не залежить від температури. Поєднуючи досвід української і американської команд нам вдалося знайти розв’язок загальної проблеми враховуючи усі суттєві типи розсіяння (т.з. нерезонансні, резонансні та змішані доданки). Це вимагало від нас розробки нового формалізму виконання аналітичного продовження для відповідних функцій, що описують непружнє розсіяння; розроблений формалізм є загальний і може бути застосований до багатьох різноманітних проблем багатьох тіл. Ми також започаткували дослідження скінчено-розмірних ефектів шляхом вивчення нерезонансного розсіяння світла у двовимірних системах в рамках наближення динамічного кластера. Відповідні комп’ютерні програми вже написані, але сам рахунок вимагає значного об’єму часу для завершення. Це буде перша спроба розрахувати транспортні явища для довільної модельної системи використовуючи наближення динамічного кластера.

CRDF COOPERATIVE GRANTS PROGRAM: FINAL PROJECT REPORT

SECTION II: Technical Report

Award Number: UP2-2436-LV-02

INSTRUCTIONS

- **Length:** The technical report should be **no more than 5 pages** in length.
- **Content:** The technical report should outline the goals of the original research project and provide a technical description of how these goals were or were not met, highlighting specific achievements. Please do not re-submit the project narrative from the original proposal.
- **Use:** From time to time, CRDF conducts a review of completed grant projects for possible inclusion in publicity materials, for presentations at symposia, etc. In connection with this, CRDF occasionally asks expert reviewers from the original grant selection panels to review the final technical reports to assist staff in selecting projects for possible feature in such activities. CRDF does not use specific information (except as otherwise indicated in these Final Project Report instructions) about individual projects in publicity activities without the permission of both Principal Investigators.
- **Language:** The technical report must be submitted in English.

Technical Report

Our CGP CRDF grant focused on two major projects: (i) the calculation of resonant Raman scattering using dynamical mean-field theory (DMFT) and (ii) the calculation of finite-dimensional effects on nonresonant Raman scattering using the dynamical cluster approximation (DCA) in two dimensions. The first project has been completed. We have one publication in Physical Review Letters, one long paper in press with Physical Review B, and two conference proceedings. The second project is still underway. We have completed the formalism development and the computer coding and debugging (we need only to parallelize the final version of the codes). We are in the process of making production runs, which are taking somewhat longer than we had anticipated in our original proposal. In addition, we wrote one paper on the equivalence of two different forms for the free energy of the Falicov-Kimball model. This is a project not in our original proposal, but it arose out of discussions we had during the first trip of Jim Freericks to the Ukraine.

Electronic Raman scattering is an important probe of electronic excitations in materials. It has been used to examine different kinds of charge and spin excitations in a variety of different materials, ranging from Kondo insulators [1,2], to high temperature superconductors [3,4], to collossal magneto-resistance materials [5]. Inelastic light scattering involves contributions from scattering processes that depend on the incident photon frequency (so-called mixed and resonant contributions) and processes that are independent of the incident photon frequency (so-called nonresonant contributions). There has been much theoretical work on this problem. In the strong-coupling regime, a perturbative approach has been used, and has illustrated a number of important features of resonant scattering processes [6,7]. The nonresonant case has also been examined, and an exact solution for correlated systems (in large spatial dimensions) is available for both the Falicov-Kimball [8] and Hubbard [9] models. In our CRDF project, we concentrated on an exact solution of the full problem for the Falicov-Kimball model including all resonant and mixed effects.

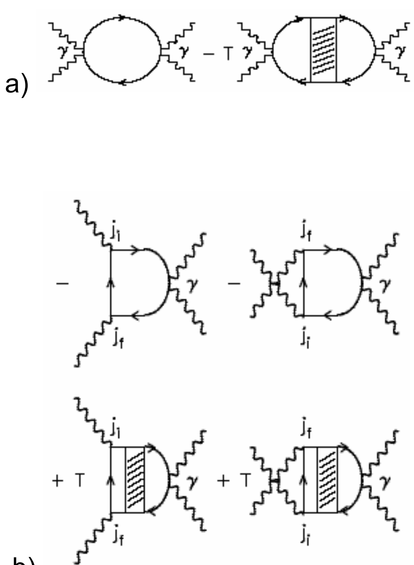
The resonant Raman scattering work represents a tour-de-force of dynamical mean field theory. Normally the Raman response function, $\chi(\Omega)$, which is related to the cross section $R(\Omega)$ by

$$R(\Omega)=\frac{2\pi g^2(\mathbf{k}_i)g^2(\mathbf{k}_f)}{1-\exp(-\beta\Omega)}\chi(\Omega),$$

cannot be easily determined for a many-body system. Here and below, $\mathbf{k}_{i,f}$, $\omega_{i,f}$, $\mathbf{e}^{i,f}$ are the momentum, frequency and polarization of the initial and final states of the photons, respectively, $\mathbf{q}=\mathbf{k}_i-\mathbf{k}_f$, $\Omega=\omega_i-\omega_f$ are the transferred momentum and frequency, and $g(\mathbf{k})$ is the "scattering strength". We analyze three different symmetries for the incident and outgoing light. The A_{1g} symmetry has the full symmetry of the lattice and is measured by taking the initial and final polarizations to be $\mathbf{e}^i=\mathbf{e}^f=(1,1,1,\ldots)$ (we assume nearest-neighbor hopping only). The B_{1g} symmetry is a d-wave-like symmetry that involves crossed polarizers: $\mathbf{e}^i$

= (1,1,1,…) and $\mathbf{e}^f$ = (-1,1,-1,1,…). Finally, the B_{2g} symmetry is another d-wave symmetry rotated by 45 degrees; with $\mathbf{e}^i$ = (1,0,1,0,…) and $\mathbf{e}^f$ = (0,1,0,1,…).

The light-scattering cross section expressions were evaluated by first considering the relevant multi-time correlation functions on the imaginary-time axis, then Fourier transforming to a Matsubara frequency representation, and finally making an analytic continuation from the imaginary to the real frequency axis [V-3] (here and below [V-x] indicate reference x in SECTION V: Bibliography of Project-Related Publications). In the case of nonresonant scattering, the expressions to be analytically continued are constructed from the correlation function of two stress operators $\chi^{(2)}(\tau,\tau')=\langle T\gamma(\tau)\gamma(\tau')\rangle$ and depend on only one frequency; for mixed scattering they are constructed from the correlation function between one stress and two current operators $\chi^{(3)}(\tau,\tau',\tau'')=\langle T\gamma(\tau)j^i(\tau')j^f(\tau'')\rangle$ which depends on two frequencies, and for resonant scattering they are constructed from the correlation function of four current operators $\chi^{(4)}(\tau,\tau_1,\tau_2,\tau_3)=\langle Tj^i(\tau)j^f(\tau_1)j^i(\tau_2)j^f(\tau_3)\rangle$ which depends on three frequencies. The analytic continuation procedure for the mixed and resonant Raman scattering is complicated, because it requires a multi-step procedure, where first the transferred frequency is continued to the real axis, then the individual initial and final frequencies are continued to the real axis. In addition to the analytic continuation, we also must evaluate the dressed multi-time correlation functions. There are renormalizations associated with two-particle ‘‘ladderlike’’ summations for a number of the relevant diagrams (see Fig. 1), but the symmetry of the velocity operator, and of the relevant multi-particle vertex functions (which are local in the large-dimensional limit) imply that there are no parquet-like summations, nor are there any three-particle or four-particle vertex renormalizations [V-3]. Since the two-particle vertex function for the Falicov-Kimball model is already known [10], the full Raman scattering problem can be solved via a straightforward but tedious procedure. The final formulas are cumbersome and appear in Ref. [V-3]. To our knowledge, this calculation is the most complex DMFT calculation completed on any model system.



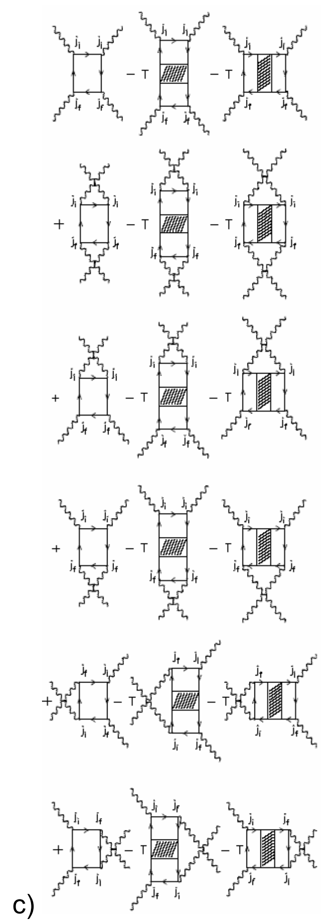


Fig. 1. Feynman diagrams for a) nonresonant, b) mixed, and c) resonant Raman scattering. The wavy lines denote photon propagators and the solid lines denote electron propagators. The cross-hatched rectangle is the reducible charge vertex.

With the use of DMFT, we solved for the full Raman response for all frequencies of incident light in the Falicov-Kimball model. Since the Falicov-Kimball model can be tuned across a metal-insulator transition, we were able to study the evolution of electronic Raman scattering from the metallic to the insulating states, and we have investigated the light scattering on both sides of the quantum critical point that occurs at $U=\sqrt{2}$. Resonant, non-resonant, and mixed contributions have all been treated on an equal footing and we allowed for an analysis of the dependence of Raman scattering with temperature, interactions, and different light polarizations.

Our results confirm a number of previously held beliefs about resonant effects in strongly correlated systems. First, we found a strong resonant enhancement of the charge-transfer peak in Raman scattering when the incident photon energy lies near the charge-transfer energy. This behavior is robust to temperature and polarization changes due to the local nature of the charge-transfer excitation in our model. Second, we found a polarization-independent "double-resonance" enhancement when the transferred frequency of the light approaches the incident light frequency. This feature survives in the insulating phase because of the pseudogap nature of the insulator on the hypercubic lattice and the long lifetime of the pseudogap states near the chemical potential.

Our main results are summarized in Fig. 2. In the left panel, we plot the Raman scattering response function in a correlated insulator for three different scattering geometries (A_{1g}, B_{1g} and B_{2g}). The results are plotted for different values of the incident photon frequency as a function of the transferred photon frequency at moderate temperature. Surprisingly, the resonant effects do not just enhance the nonresonant curve, but can change the shape of the response function, especially when the incident photon frequency is close to the interaction energy $U=2$. The response separates into a low-energy feature around $\Omega\approx0.5$ and a charge-transfer feature around $\Omega\approx U=2$ (the charge-transfer peak is absent in the B_{2g} symmetry, and is suppressed in the A_{1g} sector due to a cancellation of the nonresonant and mixed diagrams until $\omega_i>>U$). In addition, there is a sharp peak when $\omega_i\to\Omega$ due to purely resonant effects. In the right panel, we focus on the low-energy peak (at $\Omega=0.5$) and plot the resonant profile as a function of the incident photon energy. We find an interesting joint resonance of this low energy peak with the charge transfer peak when the photon energy is close to U (not shown here). This kind of joint resonance is seen in many strongly correlated materials [3] and was first explained theoretically by our work [V-2, V-5].

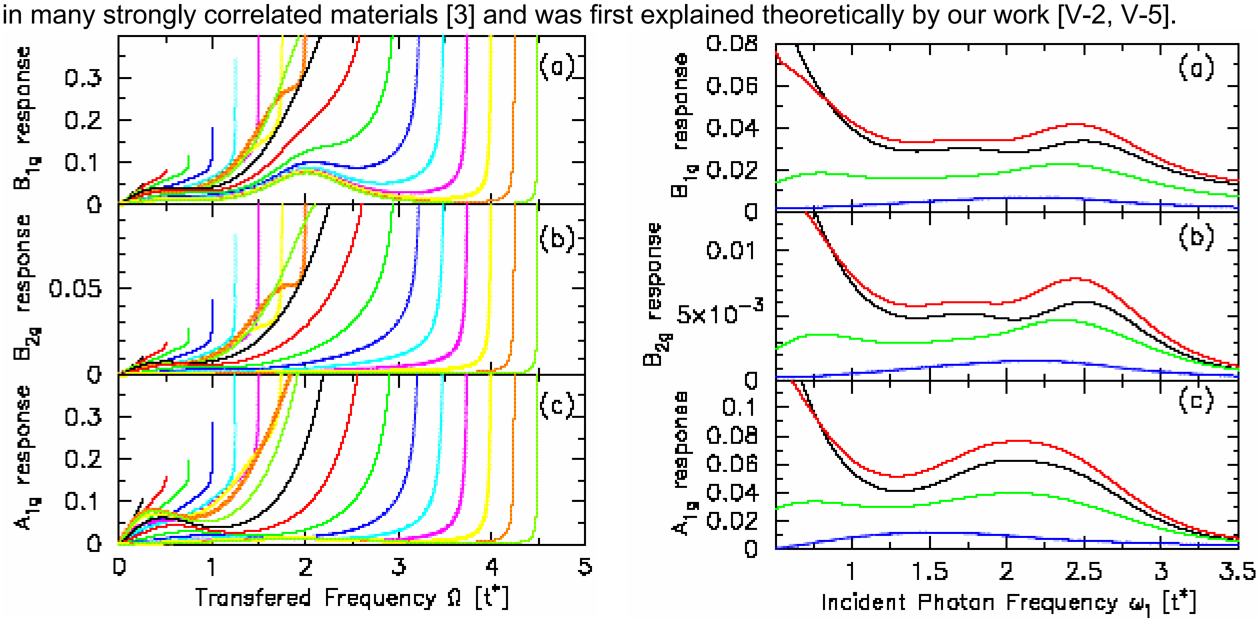


Fig. 2. Resonant Raman scattering for $U=2$ which is just on the insulating side of the Mott transition. The left panel is the Raman scattering for different incident photon frequencies ω_i as a function of the transferred frequency Ω at $T=0.5$, while the right panel fixes the transferred frequency at $\Omega=0.5$ and varies ω_i, with the different curves corresponding to different temperatures $T=1$ (black), $T=0.5$ (red), $T=0.2$ (green), and $T=0.05$ (blue).

In addition, we find a number of new features of light scattering in correlated insulators. We find that low-energy spectral features, related to thermal populations of elementary excitations, show a resonance behavior when the incident light is tuned to the much higher frequency of the charge-transfer energy. This is a specific case where the correlations are crucial, since in uncorrelated materials, this would correspond to off-resonant conditions. Yet due to the many-body nature of the correlated band, spectral features well separated from the charge-transfer peak have a non-trivial resonance profile. We believe that these may be potentially useful to understand the complex nature of charge excitations in correlated materials as it would impact both electronic and phononic Raman scattering at low frequencies. Finally, we find that the presence of an isosbestic point in the Raman response for correlated insulators results from a symmetry-dependent combination of all resonant, mixed, and non-resonant terms, and appears to be generic.

We end our discussion of this sub-project with a summary of the technical achievements and of the potential applications of this work. To begin, this project is a significant advance in formalism for the many-body problem, as it shows how to explicitly calculate retarded three and four particle response functions, which are not normally discussed, and have never been treated in DMFT before (our analytical continuation formalism can be applied to other problems that require three or four particle response functions). This work is also more complex than most transport problems in DMFT because there are a number of vertex corrections that enter for many of the diagrams that we calculate. In most applications to date with DMFT, such vertex corrections vanished due to symmetry reasons. Finally, our work provides the first theoretical calculations that can frame the experimental results that have been generated over the past ten years on strongly correlated materials. We find that virtually all of the anomalies seen in experiment are also seen in our theory, and we have found some additional features that would be interesting to look for in experimental systems.

In addition to this major Raman scattering project, we also completed a short project on the free energy of the Falicov-Kimball model. Falicov and Kimball proposed a mean-field theory form for the free energy that was made exact by Plishke [11]. This work predated the development of DMFT. Brandt and Mielsch developed an apparently different formalism to calculate the free energy within DMFT [12]. It was well known that numerical calculations of these two different forms for the free energy always agreed, but there was no derivation that showed how to go from one form to the other. This is what we accomplished in a short project early in the grant period [V-1]. While this work does not have significant applications, it provides an important missing piece to the understanding of the solutions of the Falicov-Kimball model. We also spent time examining the feasibility of solving the static Su-Schrieffer-Heeger model [13] (this model couples the phonons to the electron hopping rather than to the electron charge as in the Holstein model). The Su-Schrieffer-Heeger model is an interacting electron-phonon problem that has not been exactly solved in the thermodynamic limit on any lattice. We have generalized the DMFT approach for systems with correlated hopping and obtained the equations for the DMFT solution. We believed that we might be able to solve these equations and provide the first exact solution of this model, but due to the infinite dimensionality of the order parameters it appears impossible to perform a complete analysis of the possible orderings and to calculate the phase diagram.

We completed much work on our other major project for the grant proposal---namely the calculation of finite dimensional effects on the nonresonant Raman response function. This calculation can be performed with the so-called dynamical cluster approximation [14], which adds, in a systematic fashion, the momentum dependence to the self energy and the irreducible vertex functions, that allows us to calculate both the Raman response function and the optical conductivity; neither have ever been done before. This means that we can see how the DMFT results evolve into the finite-dimensional results and we can come up with quantitative predictions for the effects of momentum dependence on the response functions and transport.

We have already completed some preliminary results for this problem on a two-dimensional lattice in Fig. 3. Here we plot the Raman response function for the A_{1g} symmetry and different temperatures on a 4×4 lattice (left panel) and at a fixed temperature ($T = 0.5$) for different cluster sizes in the right panel. The response function includes short-range charge fluctuations in addition to the local fluctuations, due to an irreducible vertex function that has explicit momentum dependence.

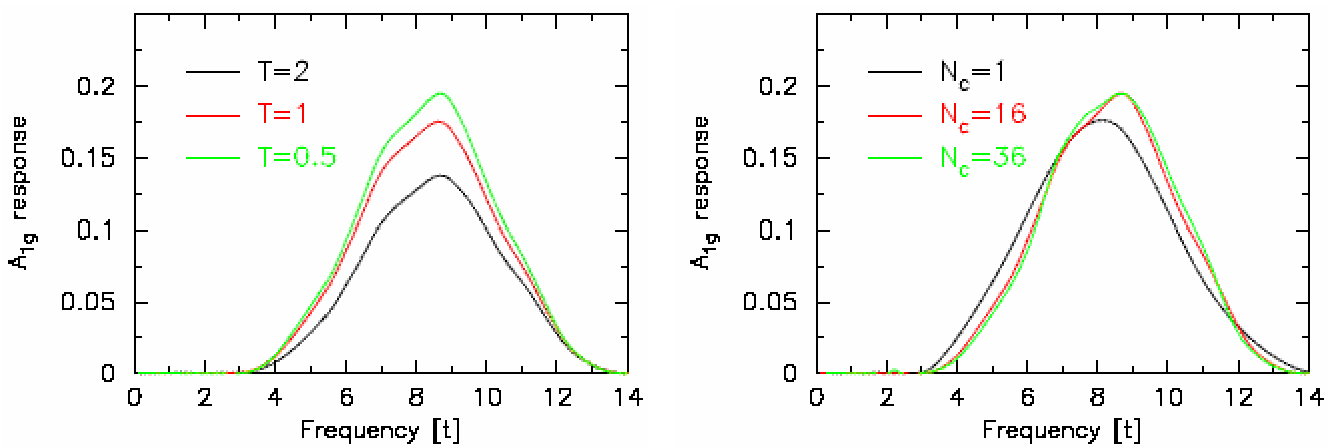


Fig. 3. Nonresonant Raman response for U=8 which is just on the insulating side of the Mott transition (which occurs at $U\approx 6$). The left panel is for different temperatures on a 4×4 lattice, while the right panel is at T=0.5 for different cluster sizes ($N_c = 1$, $N_c = 16$, and $N_c = 36$).

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CRDF COOPERATIVE GRANTS PROGRAM: FINAL PROJECT REPORT

SECTION III: FSU Team Data
(to be completed by the FSU Principal Investigator only)

Award Number: UP2-2436-LV-02

A. Research Information

1. Scientific Results

a. Were the scientific and technical objectives of your original proposal accomplished?
Yes ☒ No ☐

The specific research objectives changed. ☐

b. If specific research objectives were *not* accomplished, please briefly describe the factors that impeded their successful completion (e.g., unanticipated research results, difficulty in communications, administrative or financial complications, etc.).

c. If specific research objectives *changed*, please describe:

d. Please indicate the type of accomplishments achieved under your project (please check all that apply):

☒ New theoretical results
☐ Elaboration of known topic
☐ New experimental results
☒ New techniques developed or techniques improved
☐ Development of "know-how"
☐ Prototype development
☐ Patent Application
  ☐ Pending
  ☐ Received
☒ Publication of results in journal
☒ Other (please describe) (Presentations at conferences)

Invited oral presentations at international conferences

2. Collaborative Benefits

a. Describe the benefits of having conducted your research in collaboration with U.S. counterparts rather than independently.

☒ Exchange of ideas
☒ Access to new facilities
☒ Joint publications
☒ Access to new research methods
☐ Other (please describe)
☒ Complementary expertise in particular research area
☒ Access to new or previously unavailable information
☒ Access to new geographical research area
☒ Educational effect on young researchers/students

b. Describe any difficulties related to the collaborative nature of the effort.

- ☐ Language barriers
- ☐ Procuring equipment or supplies
- ☒ Other time commitments
- ☒ Travel/Visas
- ☐ Other (please describe)
- ☐ E-mail/Internet difficulties
- ☐ Paperwork
- ☐ Intellectual Property Rights issues
- ☐ Financial Issues

c. Will the collaboration with the U.S. team continue? Yes ☒ No ☐

d. If "Yes", by which of the following means? (check all that apply)

- ☒ Future joint publications
- ☐ Joint patents
- ☒ E-Mail contact
- ☒ New grant proposals
- ☒ Exchange visits
- ☐ Other (please describe)

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3. Additional Support

a. Have you submitted applications to any funding agencies for support of your collaborative research? Yes ☒ No ☐

b. If "Yes", please indicate which funding agencies you applied to for possible funding (check all that apply).

- ☒ CRDF (Program: CGP ____________)
- ☐ ISTC/STCU
- ☐ INTAS
- ☐ FSU Government Agency/Ministry
- ☐ NATO
- ☐ European Community Sixth Framework Programme
- ☒ U.S. Department of Energy (DOE)
- ☐ U.S. Department of Defense
- ☐ National Institutes of Health (NIH) (Please specify NIH institute: ________________________)
- ☐ For-Profit Company (Please identify: ______________)
- ☐ Other: __________________________

c. If you received any funding to continue your collaborative research, please identify the source(s) from which you have received this funding (check all that apply).

- ☐ CRDF (Program:_____________)
- ☐ ISTC/STCU
- ☐ INTAS
- ☐ FSU Government Agency/Ministry
- ☐ NATO
- ☐ European Community Sixth Framework Programme
- ☐ U.S. Department of Energy (DOE)
- ☐ U.S. Department of Defense
- ☐ National Institutes of Health (NIH) (Please specify NIH institute: ________________________)
- ☐ For-Profit Company (Please identify: ______________)
- ☐ Other: __________________________

d. In the future, do you plan to apply for support for continuation of your collaborative research? Yes ☒ No ☐

e. If "Yes," please specify which funding source(s) you plan to apply to for support (check all that apply).

- ☒ CRDF (Program: CGP __________)
- ☐ ISTC/STCU
- ☐ INTAS
- ☒ FSU Government Agency/Ministry
- ☐ NATO
- ☐ European Community Sixth Framework Programme
- ☒ U.S. Department of Energy (DOE)
- ☐ U.S. Department of Defense
- ☐ National Institutes of Health (NIH) (Please specify NIH institute: ________________________)
- ☐ For-Profit Company (Please identify: ______________)
- ☐ Other: __________________________

4. **Technology Commercialization**

a. Are you pursuing commercial application of your research results? Yes ☐ No ☒

b. If "Yes", please check all that apply:

- ☐ Planning joint patent application
- ☐ Approved joint patent application
- ☐ Contract with for-profit company
- ☐ Marketing
- ☐ Licensing
- ☐ Other: (please describe)
- ☐ Planning country-specific patent application
- ☐ Approved country-specific patent application
- ☐ Prototype development
- ☐ Seeking venture capital investment
- ☐ Manufacturing

c. If "Yes," please provide a paragraph with details about the above-checked plans:

5. **Transition to Civilian Science**

a. Did your project include researchers who were formerly actively engaged in weapons-related research? Yes ☒ No ☐ (*if you check No, please skip to Question 6*)

b. Did the CRDF research project provide a positive means for engaging and retaining former weapons scientist(s) in civilian science? Yes ☒ No ☐

c. If Yes, please describe: **individual support and support for travelling**

d. Did any of the former weapons researchers on your team change institutional affiliation or country of residency during this project? Yes ☐ No ☒

e. If Yes, please describe:

f. What percentage of research time did the former weapons researchers spend on civilian research?
100 %

6. **Research Infrastructure**

a. How did you use technological information resources (such as the Internet, e-mail) to support your CGP project? (check all that apply)

- ☒ To obtain data or information
- ☒ To consult with co-investigator by e-mail
- ☒ To consult with other researchers working on the same or related topics by e-mail
- ☒ To identify future research collaborators
- ☒ To identify funding sources
- ☒ To promote/market the results of the research project
- ☒ To help educate student researchers
- ☒ To aid in the submission of additional collaborative research proposals and publications
- ☐ Other (please describe)

b. Over the course of the award, did you or your laboratory/institute develop new linkages (international or in-country) with any of the following in order to carry out the research project? (check all that apply)

- ☒ Academy of Sciences Research institutions
- ☐ Government Research Institutions
- ☒ FSU Universities
- ☒ Other Universities
- ☐ For-Profit Companies
- ☐ Other (please describe)

c. Please briefly identify and describe the institutional linkages developed (e.g., “developed arrangement to share access to research equipment with XXX Institute”):

Computer clusters at the Ukrainian site have been accessed from Georgetown and used to run computer codes.

d. Over the course of the award, did you have the opportunity to utilize equipment (for project-related purposes) at your U.S. collaborator’s institution or other foreign or FSU institutions?

Yes ☒ No ☐

If ”Yes”, please describe:

Use of computers and compilers, use of the library, and electronic journals.

B. Administrative Information

1. **Project Personnel**

a. List <u>all</u> members of your CGP research team (<u>including those who worked on the project but did not receive individual financial support from CRDF</u>) including name, date of birth, gender, and affiliation (if different from Principal Investigator’s institution). Please include and identify students. Please identify as “Former Weapons Researchers” those project participants who were formerly or are currently actively engaged in research at a current or former weapons laboratory or institution. *<u>For those researchers only</u>*, please indicate the type of defense-related research by using the code list provided in the Appendix.

#	**Name/Institutional Affiliation**	**Date of Birth (MM/DD/YYYY)**	**Gender [M/F]**	**Student?**	**Former Weapons Researcher?**	**Weapons Research Code (see Appendix for code)**
1	**Shvayka A.M./ICMP**	**11/8/1960**	**M**	☐	☒	**A1**
2	**Danyliv O.D./ICMP**	**8/7/1970**	**M**	☐	☐	
3	**Vorobyov O.A./ICMP**	**5/11/1977**	**M**	☒	☐	
4				☐	☐	
5				☐	☐	
6				☐	☐	
7				☐	☐	
8				☐	☐	
9				☐	☐	
10				☐	☐	

b. Did any of the participating students complete a thesis in whole or in part based on research directly related to the CRDF-sponsored project? Yes ☐ No ☒

c. If "Yes", check all that apply: ☐ Doctoral/Candidat ☐ Undergraduate

2. **Project-Related Travel**

a. How many FSU team members traveled to the United States for project-related purposes during the term of the grant?	2
b. Of these, how many were students?	1
c. How many FSU team members traveled to countries other than the U.S. for project-related purposes such as presenting CGP research results at an international conference?	3
d. Of these, how many were students?	1
e. How many FSU team members left the FSU for six months or more during the grant period to take a position in a foreign laboratory or organization?	1
f. Of these, how many were students?	0

For all participants in Question "e" above, please provide the following information:

	Student?	**Period of Time Abroad**				**Destination**		
		< 1 year	**1-2 years**	**> 2 years**	**Returned home**	**USA**	**Other FSU Country**	**Other (please specify)**
Team member 1	☐	☐	☐	☐	☐	☐.	☐	☐
Team member 2	☐	☐	☒	☐	☐	☐	☐	☒ U.K.
Team member 3	☐	☐	☐	☐	☐	☐	☐	☐

3. **Award Administration**

a. Did you encounter any administrative difficulties during the course of the project? Yes ☒ No ☐

b. If "Yes", please identify the type of problem encountered by checking the appropriate box below (check all that apply).

☐ Individual financial support payments
☒ Purchase of materials & services
☒ Institutional support payments
☐ Other (please describe)
☒ Travel /Visa Issues
☐ Cost-share payments
☐ Communication with CRDF staff

c. Please comment on how these difficulties were addressed and/or resolved.

4. **CRDF Performance**

On a scale of 1 to 5, rate the performance of CRDF staff in administering your award.

Poor 1 ☐ 2 ☐ *Good* 3 ☐ 4 ☐ *Excellent* 5 ☒

Please provide any additional comments regarding CRDF's performance.

CRDF COOPERATIVE GRANTS PROGRAM: FINAL PROJECT REPORT

SECTION IV: US Team Data
(to be completed by the US Principal Investigator only)

Award Number: UP2-2436-LV-02

A. Research Information

1. **Scientific Results**

a. Were the scientific and technical objectives of your original CGP proposal accomplished?
Yes ☒ No ☐

Research objectives changed ☐

b. If specific research objectives were not accomplished, please describe the factors that impeded their successful completion (e.g., unanticipated research results, difficulty in communications, administrative or financial complications, etc.).

c. If specific research objectives were *changed*, please describe:

d. Please indicate the type of accomplishments achieved under your project (please check all that apply):

☒ New theoretical results
☐ Elaboration of known topic
☐ New experimental results
☒ New techniques developed or techniques improved
☐ Prototype development
☐ Development of "know-how"
☐ Patent Application
  ☐ Pending
  ☐ Received
☒ Publication of results in journal
☒ Other (please describe) Presentations at conferences

Invited oral presentations at international conferences

2. **Collaborative Benefits**

a. Describe the benefits of having conducted your research in collaboration with FSU counterparts rather than independently.

☒ Exchange of ideas
☐ Access to new facilities
☒ Joint publications
☐ Access to new research methods
☐ Other (please describe)
☒ Complementary expertise in particular research area
☐ Access to new or previously unavailable information
☐ Access to new geographical research area
☒ Educational effect on young researchers/students

b. Describe any difficulties related to the collaborative nature of the effort.

☐ Language barriers
☒ Procuring equipment or supplies
☐ Other time commitments
☒ Travel/Visas
☐ Other (please describe)
☒ E-mail/internet difficulties
☐ Paperwork
☐ Intellectual Property Rights issues
☐ Financial Issues

c. Will your collaboration with the FSU team continue? Yes ☒ No ☐

d. If "Yes," by which of the following means? (please check all that apply)

- ☒ Future joint publications
- ☐ Joint patents
- ☒ E-Mail contact
- ☒ New grant proposals
- ☒ Exchange visits
- ☐ Other (please describe)

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3. Additional Support

a. Do you feel your work on this project helped to enable you or your institution to obtain support for continuation of your collaborative research from sources other than CRDF? Yes ☐ No ☒

b. If "Yes," please check the sources below:

- ☐ National Institutes of Health (Please indicate institute: ________________________)
- ☐ National Science Foundation (Please indicate Program Area/Division: ___________)
- ☐ DOE
- ☐ NASA
- ☐ U.S. Department of Defense:
- ☐ Other:

c. In the future, do you plan to apply for support for continuation of your collaborative research from sources other than CRDF? Yes ☒ No ☐

d. If "Yes," list potential sources. Please be as specific as possible about citing the appropriate funding division of a large agency (for example, for NIH, please cite specific NIH institute; for NSF, please cite specific program area or division):

- ☐ National Institutes of Health (Please indicate institute: ________________________)
- ☐ National Science Foundation (Please indicate Program Area/Division: ___________)
- ☒ DOE
- ☐ NASA
- ☐ U.S. Department of Defense:
- ☐ Other:

---

4. Technology Commercialization

a. Are you pursuing commercial application of your research results? Yes ☐ No ☒

b. If "Yes," please check all that apply:

- ☐ Planning joint patent application
- ☐ Approved joint patent application
- ☐ Contract with for-profit company
- ☐ Marketing
- ☐ Licensing
- ☐ Other (please describe)
- ☐ Planning country-specific patent application
- ☐ Approved country-specific patent application
- ☐ Prototype development
- ☐ Seeking venture capital investment
- ☐ Manufacturing

c. If "yes," please provide a paragraph with details about the above-checked plans:

B. Administrative Information

1. Project Personnel

List all U.S. members of your CGP research team including name, age, gender, and affiliation (if different from Principal Investigator's institution). Include and identify students, even if not paid.

#	Name/Institutional Affiliation	Date of Birth (MM/DD/YYYY)	Gender [M/F]	Student?
1	**Jim Freericks/Georgetown**	**11/21/1963**	**M**	☐
2	**Mark Jarrell/Cincinnati**	**9/19/1960**	**M**	☐
3	**Tom Devereaux/Waterloo**	**5/5/1964**	**M**	☐
4	**Juana Moreno/South Dakota**	**12/24/1964**	**F**	☐
5				☐
6				☐
7				☐
8				☐
9				☐
10				☐

Please indicate if any of the student researchers defended theses in conjunction with this project:

2. Project-Related Travel

a. How many U.S. team members traveled to the FSU for project-related purposes during the term of the grant?	1
b. Of these, how many were students?	0
c. How many U.S. researchers traveled to non-FSU countries for project-related purposes such as presenting CGP research results at an international conference?	2
d. Of these, how many were students?	0

3. Award Administration

a. Describe any administrative difficulties encountered during the course of the CGP grant.

- ☐ Graduate student stipend payments
- ☐ Purchase of materials and services
- ☐ Cost-share payments
- ☒ Travel/Visa Issues
- ☐ Communication with CRDF staff
- ☐ Other (please describe)

b. Please comment on how these difficulties were addressed and/or resolved.

4. **CRDF Performance:** On a scale of 1 to 5, rate the performance of CRDF staff in administering your
5. award.

Poor		*Good*		*Excellent*
1 ☐	2 ☐	3 ☐	4 ☐	5 ☒

Please add any additional comments regarding CRDF's performance.

CRDF COOPERATIVE GRANTS PROGRAM: FINAL PROJECT REPORT

SECTION V: Bibliography of Project-Related Publications

Award Number: UP2-2436-LV-02

INSTRUCTIONS

- **Format:** Please use the following format to list publications:

  Also, please note that it is imperative to list the country of publication in addition to other citation information.

  - *For a journal or magazine article:*
    Author Name(s). "Article Title." Journal Name Volume (Year): Page Numbers. (**Country of publication**)

    Journal/Article Example:
    Feldstein, M.M., I.M. Raigarodskii, A.L. Iordanskii, and J. Hadgraft. "Modeling of percutaneous drug transport in vitro using skin-imitating Carbosil membrane." Journal of Controlled Release 52 (1998): 25-40. (**Country of publication**)

  - *For a book:*
    Author Name. Title. Place: Publisher, Copyright Year.

    Book Example:
    Ebbing, Darrell D. General Chemistry. Boston: Houghton Mifflin Company, 1996.

- Please do not abbreviate the titles of journals or other publications.
- Please do not include abstracts from conferences and conference proceedings. Such abstracts should be cited in Section VI, Conference Presentation List.
- If you include items that have been submitted for publication but have not yet been accepted for publication, please clearly mark these items as "submitted for publication."

If you do not have any project-related publications to cite, please check here and explain: ☐
- Are you planning on publishing in the near future? ☐
  - If so, please provide details about planned publication and expected publication dates.

BIBLIOGRAPHY OF PROJECT-RELATED PUBLICATIONS

1. **Shvaika A.M., Freericks J.K. "Equivalence of the Falicov-Kimball and Brandt-Mielsch forms for the free energy of the infinite-dimensional Falicov-Kimball model." Physical Review B: Condensed Matter and Materials Physics 67 (2003): 153103 (3 pages). (U.S.A.)**
2. **Shvaika A.M., Vorobyov O., Freericks J.K., and Devereaux T.P. "Resonant Enhancement of Inelastic Light Scattering in Strongly Correlated Materials" Physical Review Letters 93 (2004): 137402 (4 pages). (U.S.A.)**
3. **Shvaika A.M., Vorobyov O., Freericks J.K., and Devereaux T.P. "Electronic Raman scattering in correlated materials: A treatment of nonresonant, mixed, and resonant scattering with dynamical mean field theory" Physical Review B: Condensed Matter and Materials Physics 70 (2004): *in print* (18 pages). (U.S.A.) Preprint arXiv:cond-mat/0408400.**
4. **Shvaika A.M., Vorobyov O., Freericks J.K., and Devereaux T.P. "Resonant electronic Raman scattering near a quantum critical point" Physica B: Condensed Matter accepted for publication (2 pages). (The Netherlands) Preprint arXiv:cond-mat/0406305.**
5. **Shvaika A.M., Vorobyov O., Freericks J.K., and Devereaux T.P. "Resonant Enhancement of Electronic Raman Scattering" Journal of Physics and Chemistry of Solids submitted for publication (4 pages). (U.K.) Preprint arXiv:cond-mat/0407120.**

CRDF COOPERATIVE GRANTS PROGRAM: FINAL PROJECT REPORT

SECTION VI: Conference Presentation List

Award Number: UP2-2436-LV-02

INSTRUCTIONS

- **Format:** Please use the following format to list conference presentations:

  Presenter's Name(s). "Presentation Title, (Type of Presentation*), Conference/Workshop Name, Dates of Conference, Location of Conference.

  Example:

  Iordanskii, A. L. "Diffusion Modeling of the Propranol Drug Delivery from a Hydrophilic Transdermal Therapeutic System," (Oral Presentation), Third Spanish-Portuguese Conference on Controlled Drug Delivery, September 6-9, 1998, Lisbon, Portugal.

**** For "Type of Presentation," please indicate either "Oral Presentation" or "Poster Presentation."***

If you have not made any conference presentations, please check here and explain: ☐

- Are you planning on making any conference presentations in the near future? ☐
  If so, please describe planned presentations and list the dates and locations of the respective conferences.

LIST OF PROJECT-RELATED CONFERENCE PRESENTATIONS

1. Freericks, J. K. "Inelastic light scattering and the correlated metal-insulator transition," (Oral Presentation), International Conference on Strongly Correlated Electron Systems, July 10-13, 2002, Krakow, Poland.
2. Freericks, J. K. "Theoretical description of the high-temperature phase of Yb and Eu intermetallics," (Oral Presentation), European Conference "Physics of Magnetism," July 1-5, 2002, Poznan, Poland.
3. Freericks, J. K. "Inelastic light scattering and the correlated metal-insulator transition," (Oral Presentation), NATO Advanced Research Workshop on Concepts in Correlations and 2nd Hvar Workshop on Strongly Correlated Electrons, October 3-8, 2002, Hvar, Croatia.
4. Freericks, J. K. "Inelastic light scattering and the correlated metal-insulator transition," (Oral Presentation), Advanced Photon Source colloquium, Argonne National Laboratory, May 14, 2003 Argonne, Illinois.
5. Devereaux, T.P. "Inelastic light scattering in strongly correlated metals and insulators," (Oral Presentation), International Conference on Low Energy Electrodynamics of Solids (LEES 02), October 13-18, 2002, Montauk (Long Island), New York.
6. Devereaux, T.P. "Inelastic X-ray scattering in correlated metals and insulators," (Oral Presentation), IXS-CAT Workshop, Argonne National Laboratory, January 20-24 2003 Argonne, Illinois.
7. Devereaux, T.P. "Inelastic X-ray scattering in correlated Mott insulators," (Oral Presentation), March meeting of the American Physical Society, March 22-26, 2004, Montreal, Quebec, Canada.
8. Devereaux, T.P. "Shining Light on Quantum Criticality in Correlated Materials," (Oral Presentation), CIAR Quantum Materials Meeting, May 28-30, 2004, Toronto, Canada.

9. Shvaika, A.M. “Dynamical mean field theory of correlated hopping,” (Oral Presentation), International Conference on Strongly Correlated Electron Systems, July 10-13, 2002, Krakow, Poland.
10. Shvaika, A.M. “Electronic Raman scattering in correlated materials: exact treatment of nonresonant, mixed, and resonant scattering with dynamical mean field theory,” (Oral Presentation), March meeting of the American Physical Society, March 22-26, 2004, Montreal, Quebec, Canada.
11. Shvaika, A.M. “Correlated hopping in infinite dimensions: rigorous local approach,” (Poster Presentation), European Conference “Physics of Magnetism,” July 1-5, 2002, Poznan, Poland.
12. Shvaika, A.M. “Spin and charge fluctuations in the dynamical mean field theory of strongly correlated electron systems,” (Poster Presentation), European Conference “Physics of Magnetism,” July 1-5, 2002, Poznan, Poland.
13. Shvaika, A.M. “Local approach in the dynamical mean-field theory of correlated hopping,” (Poster Presentation), NATO Advanced Research Workshop on Concepts in Correlations and 2nd Hvar Workshop on Strongly Correlated Electrons, Octoder 3-8, 2002, Hvar, Croatia.
14. Shvaika, A.M. “Resonant Enhancement of Electronic Raman Scattering,” (Poster Presentation), 7th International Conference on Spectroscopies in Novel Superconductors (SNS2004), July 11-16, 2004, Sitges-Barcelona, Spain.
15. Shvaika, A.M. “Exact Treatment of Electronic Raman Scattering with Dynamical Mean-Field Theory,” (Poster Presentation), International Conference on Strongly Correlated Electron Systems (SCES'04), July 26-30, 2004, Karlsruhe, Germany.
16. Danyliv, O.D. “Thermodynamics of pseudospin-electron model in self-consistent GRPA approach,” (Poster Presentation), 19th General Conference of the Condensed Matter Division of the European Physical Society (CMD19), April 7-11, 2002, Brighton, UK.
17. Vorobyov, O. “One-dimensional proton conductor with strong short-range interactions,” (Poster Presentation), March meeting of the American Physical Society, March 22-26, 2004, Montreal, Quebec, Canada.
18. Vorobyov, O. “DMFT treatment of Raman scattering in strongly-correlated materials,” (Poster Presentation), 20th General Conference of the Condensed Matter Division of the European Physical Society (CMD20), July 19-23, 2004, Prague, Czech Republic.

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SECTION VII: SUPPLEMENTAL INFORMATION (optional)

Award Number: UP2-2436-LV-02

CRDF appreciates receiving supplemental information, such as **photographs, publicity articles, publication copies, Power Point presentations, or other materials.** Please send such materials directly to the CRDF contacts listed in the General Instructions on page 2.

If you submit photographs, please be sure to identify all persons pictured and indicate their roles in the CRDF project. Please be aware that unless you indicate otherwise, CRDF reserves the right to use photographs and other materials above in publicly-distributed CRDF documents.

If you do not have any supplemental materials to submit, please check here: ☐

We add photos, copies of our published articles, and some of our talks. We don't have any publicity articles.

All supplemental materials (total size 29.2 Mb) can be downloaded from
http://ph.icmp.lviv.ua/~ashv/crdf/supplement/

Persons in photographs (from left to right):

100_0313.JPG – Andrij Shvaika at Cherry Blossom 2004, Washington, DC

100_0501.JPG – Andrij Shvaika, Jim Freericks with his son Carl, and Oleg Vorobyov

100_1339.JPG – Andrei Mishchenko (CREST, Tsukuba, Japan; Kurchatov Institute, Moscow, Russia), Andrij Shvaika, Arno Kampf (Universität Augsburg, Germany), Tom Devereaux at SNS2004 conference (Sitges-Barcelona, Spain)

100_1652.JPG – Jim Freericks in Lviv (August 2004)

100_1656.JPG – Andrij Shvaika and Jim Freericks in front of the Opera House in Lviv (August 2004)

DSCN0106.JPG – Oleg Vorobyov at APS March Meeting 2004

DSCN0188.JPG – Andrij Shvaika giving an oral presentation at the APS March Meeting 2004

DSCN0250.JPG – Tom Devereaux giving an oral presentation at the APS March Meeting 2004

DSCN0643.JPG – Andrij Shvaika, Oleg Vorobyov, and Jim Freericks visiting CRDF Headquarters

DSCN1776.JPG – Oleg Vorobyov at the CMD20 conference (Prague, Czech Republic) 2004

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APPENDIX
CODES FOR WEAPONS-RELATED RESEARCH

INSTRUCTIONS
This code list is to be used in Section III, FSU Team Data, to identify project participants who are currently or were formerly actively engaged in research at a current or former weapons laboratory or institution. Please fill in the code listed below which corresponds most closely to the *primary* area of the participant's weapons-related experience.

CATEGORY A: MISSILE TECHNOLOGY EXPERTS	
CODE	**DESCRIPTION**
A1	Design, construction and performance of air, space, surface and underwater - launched missiles. Materials and technologies for these missiles. Production of engines, fuels, composites, integrated elements, radio-electronic equipment, different testing devices for missiles.
A2	Techniques for guidance and control of missiles from launching to impact. Includes optical guidance, television guidance, wire guidance, present and terminal guidance, internal guidance, command guidance, and homing guidance.
A3	Missile handling and launching, including transportation, storage, and preparation for launching. Air, space, surface and underwater launching and support equipment and technologies; Checkout equipment and procedures. Guided missile ranges.
A4	Techniques and systems for tracking missiles as defensive measures. Can be from surface installations or air and space-borne platforms.
CATEGORY B: CHEMICAL WEAPONS EXPERTS	
B1	Design and performance of missile warheads and rockets for delivery of chemical weapons.
B2	Materials, facilities and performance processes needed for the production of chemical weapon agents and their key precursors.
B3	Dissemination of chemical weapon agents.
B4	Basic knowledge on CW design and their effect on human system.
CATEGORY C: BIOLOGICAL WEAPONS EXPERTS	
C1	Design and performance of missile warheads and rockets for delivery of biological weapons.
C2	Biopolymer production related to biological warhead capabilities.
C3	Dissemination of biological weapon agents.
C4	Basic knowledge on BW design and their effect on human system.
CATEGORY D: NUCLEAR WEAPONS EXPERTS	
D1	Basic knowledge of Nuclear Weapons design, construction, characteristics and the effect on human system.
D2	Design, construction and performance of missile warheads for delivery of nuclear weapons.
D3	Design, construction and performance of the equipment and Components for Uranium and Plutonium separation.
D4	Design, construction and performance of the equipment connected with Heavy Water Production.
D5	Design, construction and performance of the equipment for Development of Detonators.
D6	Design, construction and performance of Explosive Substances and Related Equipment.
D7	Design, construction and performance of the equipment and Components for Nuclear Testing.
D8	Design, construction, performance and operation of production-type nuclear reactors for fissile and tritium-content materials production (breeding).
D9	Design, construction, performance of nuclear reactors and units for submarine and for military space program.
CATEGORY E: OTHER	
E1	Design, construction, and performance of powerful laser facilities for military applications.
E2	Design, construction and performance of accelerator facilities for military applications in space programs.
E3	Others