SELF-CONSISTENT DESCRIPTION OF NUCLEAR PHOTOABSORPTION CROSS-SECTIONS*

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(Received January 11, 2011)

Several approaches to photonuclear reactions, based on the time-dependent density-functional theory, have been developed recently. The standard linearization leads to the random-phase approximation (RPA) or the quasiparticle-random-phase approximation (QRPA). We have developed a parallelized QRPA computer program for axially deformed nuclei. We also present a feasible approach to the (Q)RPA calculation, that is the finite amplitude method (FAM). We show results of photoabsorption cross-sections for deformed nuclei using the QRPA and FAM calculations. Finally, the canonical-basis approach to the time-dependent Hartree–Fock–Bogoliubov method is presented, to demonstrate its feasibility and usefulness.

DOI:10.5506/APhysPolB.42.609
PACS numbers: 21.10.Re, 21.60.Jz, 24.30.Cz

1. Introduction

Photonuclear reaction cross-sections are the fundamental properties in nuclear systems. In the energy region of giant resonances ($E = 10 \sim 30$ MeV), the absorption process is dominated by the electric dipole excitations. The giant dipole resonance (GDR) has been of significant interest in studies of nuclear structure and reaction. It exhausts almost 100 % of the energy-weighted sum-rule value, corresponding to a collective oscillation of neutrons against the protons. A typical measurement of the GDR in stable nuclei is the photoneutron cross-section measurement using monoenergetic photons [1]. The energy of the GDR peak was found to have a mass dependence

* Presented at the Zakopane Conference on Nuclear Physics "Extremes of the Nuclear Landscape", August 30–September 5, 2010, Zakopane, Poland.

midway between $A^{-1/3}$ and $A^{-1/6}$ which correspond to the Steinwedel–Jensen and Goldhaber–Teller models, respectively [2]. The energy-weighted sum-rule value is larger than the classical Thomas–Reiche–Kuhn (TRK) value by 20% [1] in average. The general trend of the width of the GDR is well correlated with the neutron magic numbers, which may suggest that the main origin of the spreading width is the shape fluctuations in the ground state [3,4]. The double-peak structure in GDR appears for axially deformed nuclei, known as the deformation splitting, because of the different frequencies for vibrations along and perpendicular to the symmetry axis [1].

In a microscopic point of view, one can construct the giant resonance from a superposition of particle-hole excitations. Since dynamics of the giant resonances are basically in a small-amplitude regime, the random-phase approximation (RPA) [2] has been extensively utilized for studies of their properties. Although the spreading width $\Gamma^{\downarrow}$ is not taken into account in the RPA level, main features of the giant resonance are well reproduced. In this paper, we present three theoretical approaches to studies of the nuclear response; the standard quasiparticle RPA (QRPA) [2], the finite amplitude method (FAM) [5], and the canonical-basis time-dependent Hartree–Fock–Bogoliubov (Cb-TDHFB) method [6]. The numerical results will be shown, mainly focused on the photoabsorption cross-section.

2. Quasiparticle random-phase approximation for axially deformed nuclei

The quasiparticle RPA (QRPA) is a standard method to calculate linear response in heavy open-shell nuclei [2]. However, since its application to realistic energy functionals requires a large computational task and a complicated programing, the QRPA calculation for heavy deformed nuclei is still a challenging subject at present.

We have recently developed a parallelized computer code of the QRPA based on the Hartree–Fock–Bogoliubov (HFB) state with the Skyrme functionals, which is an extended version of that developed in Ref. [7], to include the residual spin–orbit interaction. A missing part is only the residual Coulomb interaction that does not significantly affect nuclear response functions (see Sec. 4.2).

First, we solve the following self-consistent HFB equation for the quasiparticle states

$$\begin{pmatrix} h-\lambda & \Delta \\ -\Delta^* & -(h-\lambda)^* \end{pmatrix} \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix} = E_\mu \begin{pmatrix} U_\mu \\ V_\mu \end{pmatrix}, \tag{1}$$

where the single-particle Hamiltonian $h[\rho,\kappa]$ and the pair potential $\Delta[\rho,\kappa]$ are functionals of the density ρ and the pairing tensor κ. The self-consistent solution of Eq. (1) determines the ground-state densities (ρ_0,κ_0) and the

ground-state Hamiltonians (h_0, Δ_0). To describe the nuclear deformation and the pairing correlations, simultaneously, in good account of the continuum, we solve the HFB equations in the cylindrical coordinate space. We assume axial and reflection symmetries in the ground state. To reduce the QRPA-matrix dimension, we introduce a cut-off energy $E_c^{2qp} = 60$ MeV for the two-quasiparticle states. For instance, the number of two-quasiparticle states becomes about 38,000 for the $K^\pi = 0^-$ excitation in ^{154}Sm. Then, we calculate the QRPA matrix elements and diagonalize the matrix, to obtain the QRPA normal modes.

$$\sum_{\gamma\delta} \begin{pmatrix} A_{\alpha\beta,\gamma\delta} & B_{\alpha\beta,\gamma\delta} \\ -B_{\alpha\beta,\gamma\delta} & -A_{\alpha\beta,\gamma\delta} \end{pmatrix} \begin{pmatrix} X_{\gamma\delta} \\ Y_{\gamma\delta} \end{pmatrix} = \hbar\omega \begin{pmatrix} X_{\alpha\beta} \\ Y_{\alpha\beta} \end{pmatrix} . \tag{2}$$

Since the spreading effect is missing in this calculation, the dipole strength of each discrete eigenmode is folded by the Lorentzian curve with a smoothing parameter Γ. A more detailed description can be found in Ref. [8].

We show in Fig. 1 the photoabsorption cross-section for ^{154}Sm. The HFB calculation with the SkM* parameters produces the ground state in a prolate deformation of $\beta = 0.31$. It clearly shows a deformation splitting due to a prolate deformation of the ground state. The experimental data [3] are well reproduced in the calculation. We have carried out a systematic analysis on Nd and Sm isotopes and have found that the spreading effect with $\Gamma = 2$ MeV can well reproduce experimental data from spherical, transitional, to deformed nuclei [8]. Especially, the agreement on the evolution of the GDR width as a function of the neutron number is excellent.

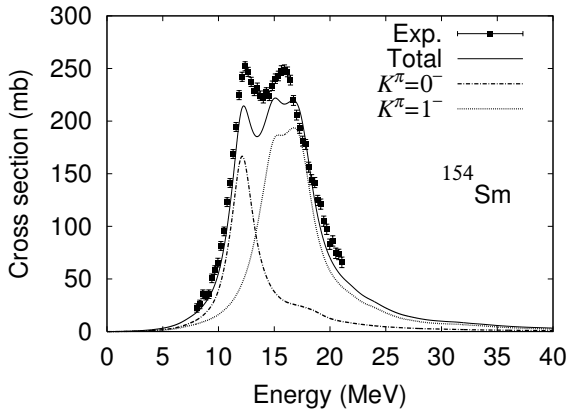


Fig. 1. Calculated (lines) and experimental (symbols) photoabsorption cross-section in ^{154}Sm. The SkM* parameter set and the smoothing parameter of $\Gamma = 2$ MeV is used. See text for details. Experimental values are taken from Ref. [3].

3. Finite amplitude method

In this section, we recapitulate the methodology of the finite amplitude method (FAM) we have developed for small-amplitude oscillations based on the time-dependent density-functional theory [5,9].

3.1. FAM without pairing correlations

First, we discuss the case that the energy density functional is represented by normal density ρ only. In this case, the density can be expressed by the Kohn–Sham orbitals, $\rho = \sum_i |\phi_i\rangle\langle\phi_i|$, where the subscript i indicates the occupied orbitals ($i = 1, 2, \ldots, A$). The linear-response equation to a weak external field with a fixed frequency, $V_{\rm ext}(\omega)$, can be expressed in terms of the forward and backward amplitudes, $|X_i(\omega)\rangle$ and $\langle Y_i(\omega)|$

$$\omega\,|X_i(\omega)\rangle = (h_0 - \epsilon_i)\,|X_i(\omega)\rangle + \hat{P}\,\{V_{\rm ext}(\omega) + \delta h(\omega)\}\,|\phi_i\rangle\,, \tag{3}$$

$$-\omega\,\langle Y_i(\omega)| = \langle Y_i(\omega)|\,(h_0 - \epsilon_i) + \langle\phi_i|\,\{V_{\rm ext}(\omega) + \delta h(\omega)\}\,\hat{P}\,, \tag{4}$$

where the operator $\hat{P}$ denotes the projector onto the particles space, $\hat{P} = 1 - \sum_i |\phi_i\rangle\langle\phi_i|$. Usually, the residual field $\delta h(\omega)$ is expanded to the first order with respect to $|X_i(\omega)\rangle$ and $|Y_i(\omega)\rangle$. This leads to the well-known matrix form of the linear-response equation, known as the RPA. For deformed nuclei, the calculation of these matrix elements is time-consuming in practice and their storage requires a large memory capacity. In the FAM, we do not explicitly linearize the equations. Instead, we utilize the fact that the linearization can be numerically achieved for $\delta h(\omega) = h[\rho_0 + \delta\rho(\omega)] - h_0$, if the transition density $\delta\rho(\omega)$ is small enough to validate the linear approximation. The FAM is nothing but a trick to perform this numerical differentiation in the single-particle (Kohn–Sham) Hamiltonian $h[\rho]$.

The residual field $\delta h(\omega)$ depends only on the forward "ket" amplitudes $|X_i(\omega)\rangle$ and backward "bra" ones $\langle Y_i(\omega)|$. In other words, it is independent of bras $\langle X_i(\omega)|$ and kets $|Y_i(\omega)\rangle$. This is related to the fact that the transition density $\delta\rho(\omega)$ depends only on $|X_i(\omega)\rangle$ and $\langle Y_i(\omega)|$

$$\delta\rho(\omega) = \sum_i \{|X_i(\omega)\rangle\langle\phi_i| + |\phi_i\rangle\langle Y_i(\omega)|\}\,. \tag{5}$$

We calculate the residual field by introducing a small real parameter η to realize the linear approximation [5]

$$\delta h(\omega) = \frac{1}{\eta}\,(h\,[\rho_\eta] - h_0)\,, \tag{6}$$

where h_0 is the Hamiltonian for the ground state and ρ_η are defined by

$$\rho_\eta \equiv \sum_i \{(|\phi_i\rangle + \eta|X_i(\omega)\rangle)(\langle\phi_i| + \eta\langle Y_i(\omega)|)\}\,. \tag{7}$$

Once $|X_i(\omega)\rangle$ and $\langle Y_i(\omega)|$ are given, the calculation of $h[\rho_\eta]$ is an easy task. This does not require complicated programming, but only needs a small modification in the calculation of $h[\rho]$. Of course, eventually, we need to solve Eqs. (3) and (4) to determine the forward and backward amplitudes. We use an iterative algorithm to solve this problem. Namely, we start from initial amplitudes $|X_i^{(0)}\rangle$ and $\langle Y_i^{(0)}|$, then update them in every iteration, $(|X_i^{(n)}\rangle, \langle Y_i^{(n)}|) \to (|X_i^{(n+1)}\rangle, \langle Y_i^{(n+1)}|)$, until the convergence. In each step, we calculate $\delta h(\omega)$ using the FAM as Eq. (6). For more details, readers are referred to the reference [5].

We have developed a parallelized computer program of the FAM for a Skyrme functional in the three-dimensional (3D) coordinate-space representation [9]. Currently, we are performing a systematic calculation of the electric dipole response in even–even nuclei. So far, we have calculated the photoabsorption cross-section in nuclei with $A \lesssim 100$. In Fig. 2, we demonstrate a part of our achievement for nuclei up to Ca isotopes.

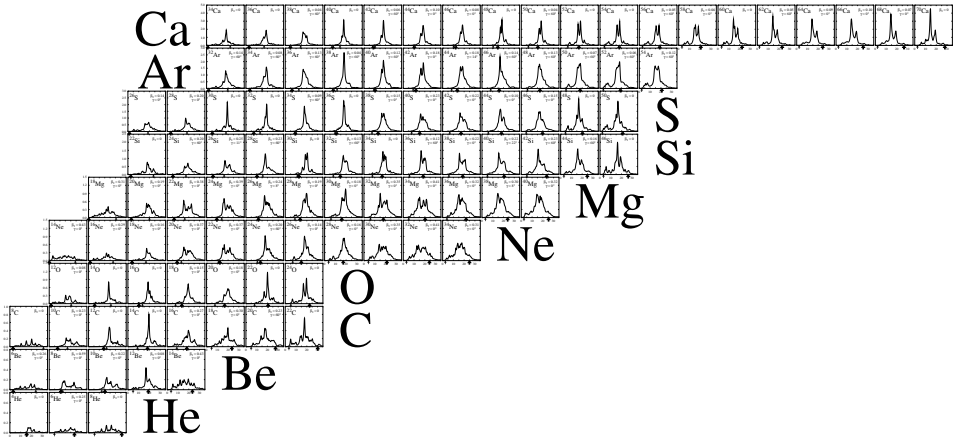


Fig. 2. Electric dipole strength distribution in light nuclei. The horizontal axis corresponds to excitation energy of $0 \sim 35$ MeV. The SkM* parameter set and the smoothing parameter of $\Gamma = 1$ MeV is used.

For nuclei with $A \leq 40$, the observed strength up to 30 MeV exhausts only $60 \sim 100\,\%$ of the TRK sum-rule value [10]. This indicates that the considerable amount of the GDR strength is located above 30 MeV in light nuclei. We also observe that, although the RPA (FAM) calculation reproduces a gross feature of the dipole strength distribution, it systematically underestimates the GDR peak energy by a few MeV for light nuclei [9].

3.2. FAM with pairing correlations

The FAM in the previous section can be extended to superfluid nuclei, namely, to the QRPA with the HFB formalism. A self-consistent solution of Eq. (1) determines the ground-state densities (ρ_0, κ_0) and the ground-state Hamiltonians (h_0, Δ_0). Then, following the same argument as that in Ref. [5], we can derive equations for the residual fields, $\delta h(\omega)$ and $\delta\Delta(\omega)$ as follows

$$\delta h(\omega) = \frac{1}{\eta}\left(h[\rho_\eta, \kappa_\eta] - h_0\right), \tag{8}$$

$$\delta\Delta(\omega) = \frac{1}{\eta}\left(\Delta[\rho_\eta, \kappa_\eta] - \Delta_0\right), \tag{9}$$

where the density and pairing tensor (ρ_η, κ_η) are defined by

$$\rho_\eta = (V^* + \eta U X)(V + \eta U^* Y)^{\mathrm{T}}, \tag{10}$$

$$\kappa_\eta = (V^* + \eta U X)(U + \eta V^* Y)^{\mathrm{T}}. \tag{11}$$

Here, the forward and backward amplitudes $(X_{\mu\nu}, Y_{\mu\nu})$ have subscripts $\mu\nu$ to specify two-quasiparticles. On the other hand, the subscripts of $(U_{k\mu}, V_{k\nu})$ indicate a basis of the single-particle space (k) and the quasiparticle (μ). Again, utilizing an iterative algorithm for solution of the QRPA equation, we can solve the QRPA linear-response equation without explicitly calculating the residual interactions.

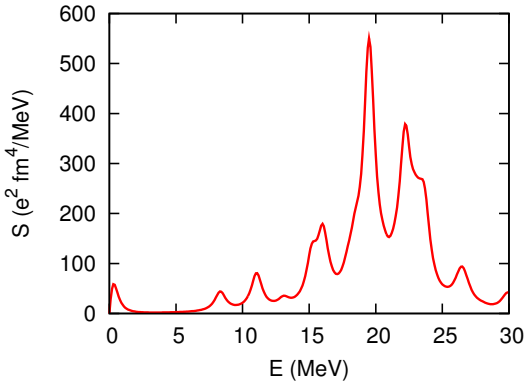


Fig. 3. Calculated isoscalar monopole strength distribution for ^{50}Ca. The SkM* parameter set and the smoothing parameter of $\Gamma = 1$ MeV is used.

We show in Fig. 3 an example of our FAM calculation for isoscalar monopole response in ^{50}Ca. We use the same parameter set and the same pairing energy functional as those in Ref. [11]. The quasiparticle states are

truncated by the maximum quasiparticle energy of $E_{\rm qp} = 200$ MeV. The result agrees with Fig. 1 in Ref. [11]. The peak near zero energy should be associated with a small mixture of the spurious mode (pairing rotation).

4. Canonical-basis time-dependent HFB method

In Secs. 2 and 3, we discuss methods to calculate linear response in nuclei, based on the time-dependent density-functional theory. In this section, we will show a feasible real-time method which is, in principle, applicable to the non-linear regime as well.

The time-dependent Hartree–Fock (TDHF) method in the 3D coordinate representation is a well established method to study nuclear dynamics [12]. However, it cannot describe particle–particle (hole–hole) pairing correlations. The pairing correlations are supposed to be very important not only for static properties but also for nuclear dynamics. For instance, it is well known that the life time of spontaneous fission is very different between even and odd nuclei, which is supposed to be due to the pairing correlations. A straightforward extension of the TDHF including the pairing correlations is, of course, the time-dependent Hartree–Fock–Bogoliubov (TDHFB) theory [13]. However, it uses the quasi-particle orbitals instead of the occupied orbitals whose number is, in principle, infinite. Thus, the accurate calculation of TDHFB is presently impractical and a new feasible approach is highly desirable.

In this section, we present the equations of motion of "Canonical-basis TDHFB" (Cb-TDHFB) method which we have developed recently [6]. Then, we apply the method to the linear-response calculations using the full Skyrme functional to show its reliability. For more details, readers should be referred to the reference [6].

4.1. Basic equations

Our starting point is that the TDHFB state can be written in the canonical form as

$$|\Psi(t)\rangle = \prod_{k>0} \left\{ u_k(t) + v_k(t) c_k^\dagger(t) c_{\bar{k}}^\dagger(t) \right\} |0\rangle \,, \tag{12}$$

where the creation operator of particles at the canonical state $|\phi_k(t)\rangle$ is expressed as $\hat{c}_k^\dagger(t) = \sum_\sigma \int d\vec{r} \phi_k(\vec{r}\sigma; t) \hat{\psi}^\dagger(\vec{r}\sigma)$. Here, the state k and $\bar{k}$ are not necessarily related to each other by the time reversal, and the time-dependent (u, v) factors are complex numbers. Using the density matrix and pairing tensor appearing in the HFB equation (1), one can write $\rho_k(t) = |v_k(t)|^2$ and $\kappa_k(t) = u_k^*(t) v_k(t)$ as

$$\rho_k(t) = \sum_{\mu\nu}\langle\phi_k(t)|\mu\rangle\rho_{\mu\nu}(t)\langle\nu|\phi_k(t)\rangle = \sum_{\mu\nu}\langle\phi_{\bar{k}}(t)|\mu\rangle\rho_{\mu\nu}(t)\langle\nu|\phi_{\bar{k}}(t)\rangle\,, \quad (13)$$

$$\kappa_k(t) = \sum_{\mu\nu}\langle\phi_k(t)|\mu\rangle\langle\phi_{\bar{k}}(t)|\nu\rangle\kappa_{\mu\nu}(t)\,. \quad (14)$$

Then, utilizing the TDHFB equation, we obtain the following equations for the time evolution of $\rho_k(t)$ and $\kappa_k(t)$

$$i\frac{d}{dt}\rho_k(t) = \kappa_k(t)\Delta_k^*(t) - \kappa_k^*(t)\Delta_k(t)\,, \quad (15)$$

$$i\frac{d}{dt}\kappa_k(t) = (\eta_k(t)+\eta_{\bar{k}}(t))\,\kappa_k(t) + \Delta_k(t)\,(2\rho_k(t)-1)\,, \quad (16)$$

where

$$\Delta_k(t) \equiv -\sum_{\mu\nu}\Delta_{\mu\nu}(t)\langle\phi_k(t)|\mu\rangle\langle\phi_{\bar{k}}(t)|\nu\rangle\,, \quad (17)$$

$$\eta_k(t) \equiv \langle\phi_k(t)|h(t)|\phi_k(t)\rangle + i\left\langle\frac{\partial\phi_k}{\partial t}|\phi_k(t)\right\rangle\,. \quad (18)$$

So far, there is no approximation in addition to the TDHFB is involved. Now, we need to introduce an approximation for the pair potential. Namely, the pair potential is assumed to be diagonal in the canonical basis

$$\Delta_{\mu\nu}(t) = -\sum_{k>0}\Delta_k(t)\,\{\langle\mu|\phi_k(t)\rangle\langle\nu|\phi_{\bar{k}}(t)\rangle - \langle\nu|\phi_k(t)\rangle\langle\mu|\phi_{\bar{k}}(t)\rangle\}\,. \quad (19)$$

In the static limit, this is identical to the BCS approximation. With the approximation of Eq. (19), one can derive the following simple equations for the time-dependent canonical states

$$i\frac{\partial}{\partial t}|\phi_k(t)\rangle = (h(t)-\eta_k(t))|\phi_k(t)\rangle\,, \qquad i\frac{\partial}{\partial t}|\phi_{\bar{k}}(t)\rangle = (h(t)-\eta_{\bar{k}}(t))|\phi_{\bar{k}}(t)\rangle\,. \quad (20)$$

In summary, the Cb-TDHFB equations consists of Eqs. (20), (15), and (16). To derive these equations from the TDHFB equations, we have assumed the diagonal property of the pair potential, Eq. (19).

4.2. Linear response calculation in real time

We have applied the Cb-TDHFB method to study electric dipole resonances in Ne and Mg isotopes [6]. Here, we apply the method to GDR in the deformed ^{154}Sm nucleus. We calculate the time evolution of the electric

dipole moment, starting from the HF+BCS ground state with a perturbative instantaneous external dipole field. Then, we perform the Fourier transform to obtain the response function. The details of the calculation can be found in Ref. [6].

We show in Fig. 4 the calculated photoabsorption cross-section in ^{154}Sm. Although the pair potential is simplified in the Cb-TDHFB calculation, the result is almost identical to the QRPA calculation shown in Fig. 1, except for a small difference seen in the second peak. We have examined the origin of this difference and found that the neglect of the residual Coulomb in the QRPA calculation is responsible for this small discrepancy. Thus, we may conclude that the Cb-TDHFB can reproduce the QRPA result at its small amplitude limit.

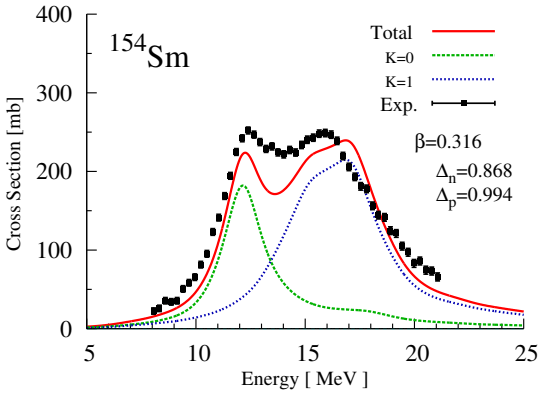


Fig. 4. Calculated (lines) and experimental (symbols) photoabsorption cross-section in ^{154}Sm. The SkM* parameter set and the smoothing parameter of $\Gamma = 2$ MeV is used. See text for details.

It should be emphasized that the computational cost of the Cb-TDHFB is significantly smaller than the QRPA. The present calculation in the full 3D space can be achieved in roughly 50 CPU hours, while the QRPA calculation in Fig. 1, that is restricted to the axially symmetric nuclei, requires roughly 1,000 CPU hours. This is because the Cb-TDHFB treats only the canonical states whose number is the same order as the particle number. In contrast, in the QRPA (or in the TDHFB), we need to treat the quasiparticle states whose number is the same as the dimension of the model space.

5. Conclusion

We have presented our recent developments for studies of nuclear response functions. The parallelized quasiparticle random-phase-approximation (QRPA) code is now ready for investigation for heavy axially deformed

nuclei. The finite-amplitude method (FAM) was applied to systematic investigation of the photoabsorption cross-section in light nuclei. Recently, the QRPA version of the FAM has been developed for superfluid nuclei, including the pairing correlations. We also presented the canonical-basis formulation of the TDHFB. This is applicable to large-amplitude nuclear dynamics beyond the linear approximation.

The work is supported by Grant-in-Aid for Scientific Research (Nos. 21340073 and 20105003). Computational resources were provided by the Joint Research Program at Center for Computational Sciences, University of Tsukuba, and by the Large Scale Simulation Program of High Energy Accelerator Research Organization (KEK). The numerical calculations were also performed on RIKEN Integrated Cluster of Clusters (RICC). We would like to thank the JSPS Core-to-Core Program "International Research Network for Exotic Femto Systems" and the UNEDF SciDAC Collaboration under DOE grant DE-FC02-07ER41457.

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