Nonlinear Optical Response of SDW Insulators

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(Received September 22, 2018)

We calculate the third order nonlinear optical response in the Hubbard model within the spin density wave (SDW) mean field ansatz in which the gap is due to onsite Coulomb repulsion. We obtain closed-form analytical results in one dimension (1D) and two dimension (2D), which show that nonlinear optical response in SDW insulators in 2D is stronger than both 3D and 1D. We also calculate the two photon absorption (TPA) arising from the stress tensor term. We show that in the SDW, the contribution from stress tensor term to the low-energy peak corresponding to two photon absorption becomes identically zero if we consider the gauge invariant current properly.

KEYWORDS: Third harmonic generation, Two photon absorption, Gauge invariance, SDW insulator

1. Introduction

The realization of ultra fast networking through all-optical switching in modern optical technology requires advanced optical materials with large third-order nonlinear optical susceptibility $\chi^{(3)}$ (Ref. 1). Quasi one dimensional (1D) $\pi$-conjugated polymers offer $\chi^{(3)}$ values of $10^{-12}$ to $10^{-7}$ e.s.u. (electronic system of units). The quasi 1D Mott insulators such as Sr$_2$CuO$_3$, offer $\chi^{(3)}$ values in the range $10^{-8}$ to $10^{-5}$ e.s.u.$^{2,3}$

The canonical model for strongly correlated materials is the standard Hubbard model. In the spin density wave (SDW) mean field approximation, this Hamiltonian reduces to a simple quadratic form that can be diagonalized exactly. Such an SDW Hamiltonian is indeed relevant to several groups of organic materials.$^{4,5}$ The SDW approximation assumes long range order. On the other hand, since such a model is essentially non-interacting, there are no vertex corrections in the current loops and the calculation of $\chi^{(3)}$ is greatly simplified. This simplification allows us to calculate various nonlinear optical processes, including those due to the stress tensor.

Although in one dimensional organic materials, where SDW states have been observed, people have already studied the optical conductivity (linear response), nonlinear optical response in this approximation which admits closed form expressions in 1D and 2D has not
been addressed yet. In this contribution we examine the nonlinear optical response of SDW insulators in one, two and three dimensions. Contrary to commonly accepted intuition that lower dimensions is equivalent to larger optical responses, we find that among SDW insulators, optical response in 2D larger that both one and three dimensions.

Among 1D, 2D and 3D systems with large on-site Coulomb interaction, the 1D system has the largest optical nonlinearity because of the decoupling of spin and charge degrees of freedom.\textsuperscript{9,10} In contrast to this, among SDW-ordered systems, the largest third order optical response appears in 2D.

Another purpose of this contribution is to clarify the importance of gauge-invariant treatment in a simple model. From symmetry point of view, some of optically allowed peaks (such as the case of two photon absorption) may become zero, provided there is charge conjugation symmetry.\textsuperscript{6} But, in SDW case, the mean field factorization of the Hubbard model that leads to SDW Hamiltonian, breaks this symmetry. However, when dealing with the contribution arising from stress tensor terms, we find that the gauge symmetry gives identically zero contribution to mid-gap peak in TPA. This result implies that the mid-gap peak in TPA is solely due to the four-current correlations. This observation is a symmetry property, and as we will explicitly show, is independent of dimension.

This paper is organized as follows: In section 2 we review the SDW mean field treatment of the Hubbard model. In section 3 we discuss the choice of gauge and method of calculation. In section 4 we discuss the four-current contribution to the third harmonic generation (THG) spectrum in 1D, 2D and 3D. In section 5 we consider the effects of stress tensor terms that come through quadratic couplings of gauge field to the electron system and also through the dependence of gauge invariant current to the stress tensor. Finally in section 6, we summarize the results.

2. Model Hamiltonian

The SDW Hamiltonian is obtained from the Hubbard Hamiltonian in the mean field approximation, where the gap is driven by Coulomb repulsion. The Hubbard Hamiltonian is written as:

\[
H = \sum_{k} \epsilon_{k} c_{k}^{\dagger} c_{k} + U \sum_{j} (n_{j\uparrow} - n/2)(n_{j\downarrow} - n/2),
\]

where \( c_{k}^{\dagger} \) creates an electron with momentum \( k \) and spin \( s = \uparrow, \downarrow \). The dimension of the lattice can be arbitrary, but in this derivation let us focus on 1D case. We are interested in half-filled case (\( n = 1 \)). Hereafter we will fix the scale of energy by setting \( 2t_{0} = 1 \), where \( t_{0} \) is the hoping amplitude. In this paper we also use the system of units in which \( \hbar = c = e = a = 1 \), where \( a \) is the lattice constant. The hopping part of this Hamiltonian is characterized by the
dispersion $\epsilon_k = -\cos k$. The SDW mean field approximation amounts to requiring

$$\langle n_{js} \rangle = \frac{n}{2} + s\epsilon_{k+Q},$$

(2)

where $n$ is the average particle density, and $s = \pm$ for $\uparrow$ and $\downarrow$, respectively, and $Q = \pi$. Ignoring fluctuations, and dropping additive constant of energy, we obtain the quadratic SDW Hamiltonian\(^{11}\)

$$H_{SDW} = H_0 - U m \sum_j e^{iQj} (n_{j\uparrow} - n_{j\downarrow}),$$

(3)

where $H_0$ is the tight-binding band part. This can be written in a more compact form as

$$H_{SDW} = \sum_k \sum_s \chi_{ks}^\dagger H_{ks} \chi_{ks},$$

(4)

where $\chi_{ks}^\dagger = (c_{ks}^\dagger, c_{k+Qs}^\dagger) = (c_{ks}^c, c_{ks}^v)$ and

$$H_{ks} = \left( \frac{\epsilon_k + \epsilon_{k+Q}}{2} + \frac{\epsilon_k - \epsilon_{k+Q}}{2} \right) \sigma^z - U m \sigma^x.$$

Here $k$ runs over the half BZ and $\sigma$’s are Pauli spin matrices. If the perfect nesting property $\epsilon_{k+Q} = -\epsilon_k$ holds, we have a much simpler Hamiltonian

$$H_{SDW}^{SDW} = \epsilon_k \sigma^z - s\Delta \sigma^x,$$

(5)

where the $k$–independent gap parameter $\Delta = U m$ is determined by $U$.

The unitary transformation $\psi_{ks} = U^\dagger \chi_{ks}$, such that $U H_k U^\dagger$ is diagonal, is given by

$$U^\dagger = \begin{pmatrix} u_k & v_k \\ -v_k^* & u_k^* \end{pmatrix}, \quad |u_k|^2 + |v_k|^2 = 1,$$

(6)

with

$$u_k = \frac{i s}{\sqrt{2}} \sqrt{1 + \frac{\epsilon_k}{\epsilon_k}},$$

$$v_k = \frac{-i}{\sqrt{2}} \sqrt{1 - \frac{\epsilon_k}{\epsilon_k}},$$

$$\epsilon_k = \sqrt{\Delta^2 + \epsilon_k^2}.$$

(7)

We also need to note the relations:

$$v_k^2 - u_k^2 = |u_k|^2 - |v_k|^2 = \frac{\epsilon_k}{\epsilon_k},$$

$$-v_k^* u_k - u_k^* v_k = 2 u_k v_k = \frac{s\Delta}{\epsilon_k},$$

(8)

giving

$$U^\dagger \sigma^x U = \frac{s\Delta}{\epsilon_k} \sigma^z - \frac{\epsilon_k}{\epsilon_k} \sigma^x,$$

$$U^\dagger \sigma^z U = \frac{\epsilon_k}{\epsilon_k} \sigma^z - \frac{s\Delta}{\epsilon_k} \sigma^x.$$
that imply:

\[ H_{\text{SDW}}^{\text{SDW}} = \sum_{k_s} \psi_{k_s}^\dagger \varepsilon_k \sigma^z \psi_{k_s}. \]  

(10)

In 1D the density of states for this model is given by (Appendix B)

\[ \rho(\omega) = \sqrt{\frac{1}{\omega^2 - \Delta^2}} \frac{1}{\sqrt{w_1^2 - \omega^2}}, \]  

(11)

where \( w_1 = \sqrt{1 + \Delta^2} \).

One can also consider other quadratic models with gap and coherence factors, such as the \( U = 0 \) limit of the ionic Hubbard model:

\[ H^b = -t_0 \sum_{\ell} \left( a_{\ell}^\dagger b_{\ell+1} + b_{\ell+1}^\dagger a_{\ell} \right) + \sum_{\ell} \epsilon_A a_{\ell}^\dagger a_{\ell} + \sum_{\ell} \epsilon_B b_{\ell}^\dagger b_{\ell}. \]  

(12)

where 'b' stands for band insulator. This Hamiltonian describes simple tight-binding insulator in which the gap is due to difference \( \epsilon_A = -\epsilon_B \equiv \Delta \) in site energy, not the Coulomb correlation (in SDW \( \Delta = Um \)). This model will differ from SDW insulator in the \( \epsilon_k \leftrightarrow \Delta \) replacements in their coherence factors. Such a difference will affect the first order responses dramatically, but it is easy to see that third order optical response of this model is identical to SDW model.

3. Choice of gauge

The coupling of electromagnetic field to matter can be described in two gauges. One is a gauge in which vector potential is zero, but the scalar potential is non-zero and given by \( A_0 = -\mathbf{E} \cdot \mathbf{r} \). In this gauge, the electric field of radiation couples to the dipole moment of electrons, and hence one needs the matrix elements of the position operator \( \mathbf{r} \) to calculate the response of the matter to electromagnetic perturbation. Working in this gauge is suitable for molecules and small clusters. Because of the \( \mathbf{r} \) operator, the calculations in this gauge are sensitive to boundary conditions. Moreover, for periodic boundary conditions, one has problem in choosing the origin of the \( \mathbf{r} \) coordinate. Therefore this gauge is ill-defined in thermodynamic limit, and sensitive to boundary conditions.

On the other hand, we have an alternative choice of working in a gauge in which scalar potential is zero, while the vector potential \( \mathbf{A} \) is non zero. In this gauge the coupling between the external field and electrons at the first order is via the current operator: \( j \cdot \mathbf{A} \). In second order the gauge field couples to electrons via the stress tensor operator as \( \mathbf{A} \cdot \mathbf{\tau} \cdot \mathbf{A} \), etc. Working in this gauge is actually equivalent to Peierls substitution, and hence we call it the Peierls gauge.

Without taking into account the effect of nonlinear couplings, and nonlinear dependence of the gauge-invariant current on the vector potential, the response function at \( n \)’th order is given by:

\[ \chi^{(n)}(\Omega; \omega_1, \ldots, \omega_n) = \frac{n e^2 \delta_{n1}}{\epsilon_0 m \omega_1^2} f + \frac{\chi^{(n)}_{jj}(\Omega; \omega_1, \ldots, \omega_n)}{\epsilon_0 i \omega_1 \ldots \omega_n}, \]  

(13)
where $n$-current correlation function is given by

$$
\chi_{jj}^{(n)}(\Omega; \omega_1, \ldots, \omega_n) = \frac{1}{n!} \left( \frac{i}{\hbar} \right)^n \frac{1}{V} \int dr_1 \ldots dr_n \int dt_1 \ldots dt_n \int dr dt e^{i\Omega t - i k \cdot r} \langle T_c j(r, t) j(r_1, t_1) \ldots j(r_n, t_n) \rangle.
$$

Here $T_c$ is the time-ordering operator along the Keldysh path and $j(r, t)$ is particle current operator.

In general a $m$-point Keldysh Green’s function has a tensor structure due to two time branches. A unitary transformation to the "physical” representation will give $G_{\alpha\beta\gamma\ldots}$ where

$$\alpha, \beta, \gamma \in \{a, r\}$$

Here $a$ stands for "advanced”, while $r$ means ”retarded”. The optical experiments measure the fully retarded components which are given by nested commutators. On the other hand, the sum of nested commutators is generated by $G_{arr\ldots}$, where only one of the indices is equal to $a$ and the rest are equal to $r$ index. As will be shown in appendix A, due to the commutators and appropriate $\theta$ functions, this component of Keldysh Green’s function is very special, in the sense that we do not really need to get into Keldysh machinery in order to calculate the nonlinear optical response. As is shown in appendix A, the fully retarded $G_{arr\ldots r}$ component can always be calculated within the framework of equilibrium quantum field theory. We first calculate the time ordered expectation values and then analytically continue the result to ensure the correct behavior of the poles. If we need other components of Keldysh Green’s functions (the fluctuation functions) that involve anti-commutators, and are related to noise spectroscopy, Keldysh formulation becomes inevitable.

Therefore, in the case of optical response, we can forget the two time branches, and denote the response function at say, third order by $\langle j j j \rangle$, keeping in mind that this is an ordinary time ordered expectation value and should be analytically continued according to prescription of appendix A.

Another important point is that the four-current scheme for calculation of the optical response is reliable far from zero frequency. Therefore, we do not have to worry about the so called zero frequency divergence (ZFD) in our calculations. To remove the unphysical ZFD one has to calculate a few more correlation functions, but as far as the behavior near resonance region is concerned, the $\langle j j j \rangle$ is sufficient. To appreciate this point, let us look at the first order response in two gauges ($\mu$ is the dipole operator and is proportional to $r$; $j$ is current operator, and proportional to $\dot{r}$):

$$
\chi_{\mu\mu}(\omega; \omega_1) = \int_0^\beta d\tau e^{i\omega \tau} \int_0^\beta d\tau_1 e^{i\omega_1 \tau_1} \langle \mu(\tau) \mu(\tau_1) \rangle
$$

$$
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$$

$$
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$$
where a factor of $2\pi\delta(\omega + \omega_\sigma)$, with $\omega_\sigma = \omega_1$ does also multiply the right hand side. We integrate by parts with respect to both time variables $\tau$ and $\tau_1$ to obtain:

$$\chi_{\mu\mu}(\omega; \omega_1) = \int_0^{\beta} d\tau e^{i\omega_1\tau} \int_0^{\beta} d\tau_1 \frac{\langle \mu(\tau)\mu(\tau_1) \rangle}{i\omega_1}$$

$$= \frac{1}{i\omega_1} \int_0^{\beta} d\tau e^{i\omega_1\tau} \left[ \langle \mu(\tau)\mu(\beta) \rangle - \langle \mu(\tau)\mu(0) \rangle \right]$$

$$- \frac{1}{i\omega_1} \frac{1}{i\omega} \int_0^{\beta} d\tau_1 e^{i\omega_1\tau_1} \left[ \langle \mu(\beta)\mu(\tau_1) \rangle - \langle \mu(0)\mu(\tau_1) \rangle \right]$$

$$+ \frac{1}{i\omega_1} \frac{1}{i\omega} \chi_{\mu\mu}(\omega; \omega_1)$$

where we have used the fact that both $\omega_1$ and $\omega$ are bosonic Matsubara frequency, $e^{i\omega_1\beta} = 1$.

Hence we see that the relation $\chi_{\mu\mu}(\omega; \omega_1) = \frac{1}{i\omega_1} \frac{1}{i\omega} \chi_{\mu\mu}(\omega; \omega_1)$, often used to relate the response in two gauges is not quite correct. Inclusion of the boundary terms (first two lines of the above equation) compensates the frequency denominators appearing in $\langle \gamma \rangle$ scheme. Similar consideration applies to higher order correlations such as $\langle \gamma \gamma \rangle$.

If we keep nonlinear coupling between the gauge field and electrons that comes through the stress tensor operator $\tau$, and also dependence of gauge invariant current to powers of gauge field $A$, a simple perturbation theory gives expressions of the type $\langle \gamma \gamma \rangle$ that again appear in fully retarded combination of nested commutators. The simplicity of SDW and our band model allows us to consider these terms as well.

4. Four-current response

The particle current operator is given by

$$j = it_0 \sum_\ell \left( c_{\ell+1}^\dagger c_\ell + c_\ell^\dagger c_{\ell+1} \right)$$

(18)

The momentum space representation of this operator for the band and SWD insulators is given by:

$$j = \sum_{ks} \chi_{ks}^\dagger \gamma_k \sigma^z \chi_{ks}, \quad \gamma_k = 2t_0 \sin k$$

(19)

which in terms of new fermions is

$$j_{\text{SDW}} = \sum_{ks} \psi_{ks}^\dagger \left( \frac{\gamma_k \epsilon_k^2}{\epsilon_k} \sigma^z - \frac{\gamma_k \Delta}{\epsilon_k} \sigma^x \right) \psi_{ks}$$

(20)

The coefficient of $\sigma^z$ in the above expression describes \textit{intra}-band transitions, while the coefficient of $\sigma^x$ causes \textit{inter}-band transitions. Let us define the corresponding coefficients by

$$g \epsilon_k = \sin k \cos k, \quad h \epsilon_k = s \Delta \sin k,$$

(21)

The THG susceptibility corresponding to photon frequency $\nu$ (or $i\nu$ in imaginary time) is given by
A few comments are in order: The trace operator arises from closing the current loop, and enormously simplifies the calculations. This trace is taken with respect to the indices of Pauli matrix. But since Pauli matrices along with unit matrix have a closed algebra, and that only the unit operator survives the trace, the sums of 16 terms in the case of first order response, and of 256 terms in the case of third order response are considerably simplified.

We need one more physical considerations to further simplify the calculations. At half filled situation of interest to us, the intra-band terms at zero temperature do not contribute to optical absorption. In calculating general expectation value of say $\langle ABCD \rangle$, where $A, B, C, D$ can be any operators contributing to the coupling of light with matter, we are interested in dominant processes in which terms containing $g$ (intra-band matrix element) in the rightmost and leftmost operators $A$ and $D$ do not contribute. Similarly in $B$ and $C$ operators the $h$ term should be dropped.

To calculate the time ordered product within the framework of equilibrium quantum field theory, we use the Matsubara technique. The summation over fermion loop frequency $i \omega_n$ can be done with standard contour integration techniques. Also, if we ignore the momentum from the incident light, the momentum $k$ running in the current loop must be the same for all fermion propagators. After contracting various fermion spinors to get the appropriate Greens’ functions we obtain

$$\frac{1}{\nu^4} \langle J_\mu J_\mu \rangle = \sum_k \frac{1}{\nu^4 \epsilon_k^x} \times$$

$$\frac{8(4 \epsilon_k^x + \nu^2) \Delta^2 \cos(k)^2 \sin(k)^4}{(2\epsilon_k - 3\nu)(2\epsilon_k + 3\nu)(2\epsilon_k - 2\nu)(2\epsilon_k + 2\nu)(2\epsilon_k - \nu)(2\epsilon_k + \nu)}.$$

The analytic continuation $\nu \rightarrow \nu + i0^+$ is implicitly understood.

It is also important to note that, as far as the behavior of response functions near the resonance is concerned (that is away from $\nu = 0$), four-current response functions, $\langle J_\mu J_\mu \rangle$ give the same qualitative features as that of four-dipole response functions, $\langle \mu \mu \mu \mu \rangle$, where $\mu$ is the dipole moment operator. To appreciate this point, let us go back to the expression of the current operator for the SDW insulator. The inter-band matrix element for the current operator is $j_k = s \Delta \sin \frac{k}{\epsilon_k}$, that via the equation of motion for the dipole moment operator $\mu$, would imply that the dipole matrix elements are:

$$\mu_k = s \Delta \sin \frac{k}{2\epsilon_k^x}.$$

Similar procedure that lead to equation (23) gives:

$$\langle \mu \mu \mu \mu \rangle = \sum_k \frac{1}{2\epsilon_k^x} \times$$

$$\frac{(4 \epsilon_k^x + \nu^2) \Delta^2 \cos(k)^2 \sin(k)^4}{(2\epsilon_k - 3\nu)(2\epsilon_k + 3\nu)(2\epsilon_k - 2\nu)(2\epsilon_k + 2\nu)(2\epsilon_k - \nu)(2\epsilon_k + \nu)}.$$

Now we can see that up to a numerical factor of the order of unity, the "near resonance" behavior of both expression is the same. Because after analytic continuation, the imaginary
Fig. 1. Plot of imaginary part of $\chi_{THG}^D(\nu)$ vs. $\nu$ in the SDW model in $D = 1, 2, 3$ dimensions. The unit of energy is $2t_0 = 1$, and in all calculations we have assumed $\Delta = 0.3$. The gap is given by $E_g = 2\Delta = 0.6$. We see that the response in $D=2$ is stronger than $D=1,3$. Values of $D=1,3$ are magnified by factors of 10 and 100, respectively, for eye assistance.

The imaginary part of THG susceptibility can now be written as

$$\Im \chi_{THG}^D(\nu) = \frac{27}{2} f_D \left( \frac{3\nu}{2} \right) - 8 f_D(\nu) + \frac{1}{2} f_D \left( \frac{\nu}{2} \right),$$

$$f_D(\nu) = \sum_k \frac{\pi \Delta^2 \cos^2 k \sin^4 k}{24 \varepsilon_k^6} \delta(\varepsilon_k - \nu), \quad (25)$$

where $D$ is the dimension of space. In 1D this integral can be evaluated as follows:

$$f_1(\nu) = \int d\varepsilon \rho(\varepsilon) \frac{\pi \Delta^2 (\varepsilon^2 - \Delta^2)(w_1^2 - \varepsilon^2)^2}{12 \varepsilon^6} \delta(\varepsilon - \nu)$$

$$= \frac{\pi \Delta^2}{24 |\nu|^5} (w_1^2 - \nu^2)^{3/2} (\nu^2 - \Delta^2)^{1/2}. \quad (26)$$

Using the Kramers-Kronig relation

$$\Re \chi(\omega) = \frac{1}{\pi} \rho \int d\nu \frac{\Im \chi(\nu)}{\nu - \omega}, \quad (27)$$

one can obtain a closed form expression for the real part of the above retarded susceptibility in terms of Elliptic functions of various kind.

In 2D still we can obtain closed form results by transforming to tight binding coordinates.
\[ f_2(\nu/2) = \frac{\Delta^2}{6\pi\nu\lambda} \int_{\Delta}^{\nu_2} d\varepsilon \int_{0}^{\pi/4} d\xi \frac{\delta(\nu/2 - \varepsilon)}{\sqrt{1 - \beta \cos^2(2\xi)}} \]

\[ = \frac{\Delta^2}{90\pi\nu\lambda} E \left( \sqrt{\beta} \right) \left[ 548\beta^2 - 1258\beta - 708 \right] \]

\[ + \frac{\Delta^2}{90\pi\nu\lambda} K \left( \sqrt{\beta} \right) \left[ (60\beta^2 - 226\beta + 177) \right]. \] (28)

In this expression \( \lambda^2 = \nu^2/4 - \Delta^2 \). Here \( E \) and \( K \) are elliptic functions of second and first kinds, respectively.\(^{17}\) The second term near the band edge behaves like \( \sqrt{\nu/2 - \Delta} \log(\nu/2 - \Delta) \) which remains finite, while the first term give a divergent contribution of the form \( f_2(\nu/2) \sim 1/\sqrt{\nu/2 - \Delta} \). The main THG peak is due to \( f_2(3\nu/2) \sim 1/\sqrt{3\nu/2 - \Delta} \) which occurs at \( \nu = 2\Delta/3 \), with \( 2\Delta \) being the excitation gap.

In three dimensions \( f_3(\nu) \) and hence \( \Im \chi_{THG}(\nu) \) can be calculated numerically. Figure 1 shows \( \Im \chi_{THG}(\nu) \) for \( D = 1, 2, 3 \) and the gap parameter \( \Delta = 0.3 \). The 3D result is magnified 100 times (dotted line), and the 1D result (dashed line) is magnified 10 times. In the SDW system, inverse square root divergence in 2D has no counterpart in 1D and 3D. To understand this, notice that, one can always replace a \( k \) integration with a energy integration weighted by DOS, and so such an enhancement in 2D compared to 1D and 3D can be traced back to the nature of singularities of DOS (appendix B). This figure demonstrates that if we have a insulator in which gap is due to SDW type of order, the phase space effect (DOS) along with SDW coherence factors \( (u_k, v_k) \) generate larger nonlinear response in 2D compared to 1D and 3D.

5. Stress tensor terms

The simplicity of SDW model, along with possibility of obtaining closed form results in one and two dimensions allows us to investigate the role of stress tensor terms in nonlinear optical processes. The first place that stress tensor appears is via the coupling of external field to matter at second order which is \( \tau.A.\tau \). Then the gauge invariant current (particle current plus a correction from external field) involves the stress tensor itself, and to first order is given by:\(^{15}\)

\[ \mathcal{J}^m = j^m - \tau^{mn}A_n, \] (29)

Therefore the third order response of gauge invariant current involves the response of both \textit{particle-current} operator \( (j^m) \) above and also the response of stress tensor operator \( (\tau^{mn}) \) above. The third order response due to particle-current is

\[ \langle j_\tau j \rangle + \langle \tau jj \rangle. \] (30)

while the third order response due to \( \tau \) operator is

\[ \langle jj\tau \rangle \] (31)
These expressions are of the type given in (A·10). The first two corresponds to $A, Q \to j$, $B \to \tau$, and $A \to \tau$, $B, Q \to j$, respectively, while the third one corresponds to $A, B \to j$, $Q \to \tau$.

To obtain the appropriate matrix elements, let us begin by writing the stress tensor in 1D as

$$
\tau = -t_0 \sum_{ns} \left( c_{ns}^\dagger c_{n+1s} + c_{n+1s}^\dagger c_{ns} \right),
$$

or equivalently

$$
\tau = \sum_{ks} \chi_{ks}^\dagger \epsilon_k \sigma^z \chi_{ks},
$$

that eventually becomes

$$
\tau_{\text{SDW}} = \sum_{ks} \psi_{ks}^\dagger \left( \frac{\epsilon_k^2}{\epsilon_k} \sigma^z - \frac{s \Delta \epsilon_k}{\epsilon_k} \sigma^x \right) \psi_{ks}.
$$

The matrix elements we need are given in table I, where $s$ is $\pm 1$ for $\uparrow$ and $\downarrow$ spins,

|       | $j_{\text{inter}}$ | $j_{\text{intra}}$ | $\tau_{\text{inter}}$ | $j_{\text{inter}}$ | $j_{\text{intra}}$ | $\tau_{\text{inter}}$ |
|-------|---------------------|---------------------|-------------------------|---------------------|---------------------|-------------------------|
| SDW   | $\Delta^2 \sin^2 k \cos^2 k/\varepsilon_k^3$ | $s \Delta^2 \sin^2 k \cos^2 k/\varepsilon_k^3$ |

Table I. Inter band and intra band matrix elements in the SDW model.

respectively. Since the matrix elements involve both sin and cos, in 1D the transitions at zone center and zone boundary are suppressed, and hence there is no divergence. But in 2D again SDW response will be divergent.

Let us look at the two photon absorption (TPA) contribution arising from $\tau$ operator carefully. In ordinary case of $\langle jjjj \rangle$, the TPA corresponds to $\omega_1 = \omega_2 = -\omega_3 = \nu$. In the case of stress tensor TPA corresponds to $\omega_1 = \omega_2 = \nu$. If we denote the denominators of the first, second and third lines of the expression (A·10) by $\ell_1, \ell_2, \ell_3$, respectively, after decomposing to partial fractions we have

$$
\ell_{1,2} = \frac{1}{2\epsilon_k (\nu + i\eta - \epsilon_k)} - \frac{1}{2\epsilon_k (\nu + i\eta - 2\epsilon_k)},
$$

$$
\ell_3 = \frac{1}{2\epsilon_k (\nu + i\eta - 2\epsilon_k)},
$$

where a $(\nu + i\eta \to -\nu - i\eta)$ term also is present in the time ordered correlation function. Putting in the matrix elements, the TPA susceptibility becomes

$$
(j_{\text{inter}})^2 \tau_{\text{intra}} [\ell_1 + \ell_2 - \ell_3] + j_{\text{inter}} j_{\text{intra}} \tau_{\text{inter}} \left[ (\ell_2 + \ell_3) + (\ell_3 + \ell_1) - (\ell_1 + \ell_2) \right],
$$

where we have not simplified the second line deliberately to emphasize the role of gauge invariant current. Obviously what we measure is the gauge invariant current. The minus sign in third terms of the each line in the above equation comes from the minus sign in equation (29), which is essential for the cancellation that takes place in the second line of the above equation, leaving a contribution proportional to $\propto \ell_3$. 

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Now let us concentrate on the first line of this equation. Here the matrix element have opposite signs for up and down spins (which ultimately comes from the coherence factors of the SDW state). Therefore their contributions identically cancel each other, and we are left only with a term coming from denominator of $\ell_3$ only, which peaks at the gap $2\Delta$. In 1D as we mentioned, the presence of sin and cos suppresses the transitions at band edge and zone center. So let us calculate this term in 2D in the SDW insulator:

$$\langle (J_x J_x \tau_{xx}) \rangle^{SDW} = -\frac{\pi \Delta^2}{4} \sum_{k_x, k_y} \delta(\nu/2 - \varepsilon_k) \frac{\sin^2 k_x \cos^2 k_x}{\varepsilon_k^4}$$

$$= -\frac{\pi \Delta^2}{4} \int \int \frac{dxdy \sin^2 x \cos^2 x}{2\pi^2} \frac{\delta(\nu/2 - \varepsilon)}{\varepsilon^4}$$

$$= -\frac{\Delta^2}{8\pi} \int \int \frac{d\lambda d\xi \sin^2 x \cos^2 x}{J} \frac{\delta(\nu/2 - \varepsilon)}{\varepsilon^4}$$

$$= -4\Delta^2 \frac{\lambda(12\beta - 23)K(\sqrt{\beta})}{3\pi \nu^4} - 16 \frac{(23 - 22\beta)E(\sqrt{\beta})}{3\pi \lambda \nu^4},$$

where in the last line again delta function picks up the value of $\lambda = \sqrt{\nu^2/4 - \Delta^2}$, $\beta = 1 - \lambda^2/4$ as in the appendix B. The logarithmic divergence of the first term gets suppressed by $\lambda \sim \sqrt{\nu - 2\Delta}$ factor, but the second term still shows inverse square root divergence in 2D. Therefore in the case of stress tensor terms too, the 2D SDW systems offer larger response than 1D.

We would also like to emphasize that, the requirement of gauge invariance cancels the singularity at $\Delta = E_g/2$, in $\tau$’s contribution and leaves us with a square root singularity in $2\Delta = E_g$ in 2D SDW systems. In other words, in SDW insulator the peak at $E_g/2$ may solely be due to four-current correlations and the contribution from stress tensor to this peak is identically zero.

6. Summary and conclusions

In conclusion, we have calculated the nonlinear optical responses in the SDW insulator in which the gap is due to on-site Coulomb repulsion. The linear response of SDW model has the characteristic inverse square root divergence in 1D which due to larger amount of nesting is further enhanced by a logarithmic factor in 2D and is entirely suppressed in 3D. The THG spectrum of SDW model has no divergence in 1D, but diverges as inverse square root in 2D and becomes finite again in 3D. Therefore the optical responses (linear and nonlinear) of SDW insulators is maximal in 2D as a function of dimensionality.

The model calculations presented in this work suggests that nesting as a possible mechanism of nonlinearity enhancement which works best in 2D, contrary to common intuition that lower spatial dimensions are better for nonlinear optical materials. This mechanism does not work in 1D. It was found that in 1D such an enhancement can arise from the spin-charge separation.$^9,10$

The simplicity of the quadratic model treated in this investigation allowed us to exactly
calculate the contributions of stress tensor in nonlinear optical response. We showed that (i) in TPA measurements in the SDW systems, the structure at the mid-gap ($E_g/2$) has essentially no contribution from the stress tensor term, and (ii) when these contributions are non-zero, have comparable effect to that of usually considered four-current terms. Stress term has even parity and in nonlinear processes can lead to dipole-forbidden transition. This hints to the importance of gauge invariant treatment of currents in nonlinear optics, which is usually neglected in the literature.

7. Acknowledgments

This work was supported by Grant-in-Aid for Scientific Research, MEXT of Japan, CREST, and NAREGI. S.A.J. was supported by JSPS fellowship P04310.

Appendix A: Analytic continuation

In nonlinear response theory, we need to calculate fully retarded expectation value of nested commutators. For example in the case of nonlinear dielectric response of an electron gas to a fast moving ion, the nested commutator of density operators at different times appears. In the general theory of nonlinear response, we might have the fully retarded combination of nested commutators of arbitrary operators. These operators are determined by nature of coupling (linear, quadratic, etc.) between the system and the external perturbation, and also the observable being studied. For example the second order coupling of the electromagnetic field to matter via the stress tensor operator $\tau$, leads to a fully retarded current response of the form $\langle [j, [j, \tau]] \rangle$. The general framework to study this type of expectation values is the non-equilibrium quantum field theory. However, within the standard formulation of quantum field theory, with appropriate analytic continuation, one can obtain these kind of expectation values that correspond to $G_{arr...r}$ component in Keldysh Green’s function language. In optical measurements always this kind of expectation values appear. In noise spectroscopies the other components of Keldysh Green’s function appear that can not be treated as straightforward as $G_{arr...r}$ component, and use of Keldish formulation becomes necessary.

For the problem in which external perturbation couples linearly to the system, through operator $A_j$, and quadratically through $B_{kl}$, where we are interested in variations of quantity $Q_i$, one can write the retarded response at third order as:

$$
\phi^{R}_{ijkl}(t; t_1, t_2) = +\theta(t - t_2)\theta(t_2 - t_1)\langle [A_j(t_1), [B_{kl}(t_2), Q_i(t)]] \rangle
$$

$$
+ \theta(t - t_1)\theta(t_1 - t_2)\langle [B_{kl}(t_2), [A_j(t_1), Q_i(t)]] \rangle
$$

$$
+ (j \rightarrow k \rightarrow l \rightarrow j) + (j \rightarrow k \rightarrow l \rightarrow j)^2.
$$

(A-1)
On the other hand, the time-ordered product of these three operators is given by:

\[
\phi^T_{ijkl}(t_1, t_2) = \langle T A_j(t_1) B_{kl}(t_2) Q_i(t) \rangle = \\
+ \theta(t_1 - t_2)\theta(t_2 - t)\langle A_j(t_1) B_{kl}(t_2) Q_i(t) \rangle \\
+ \theta(t - t_2)\theta(t_2 - t_1)\langle Q_i(t) B_{kl}(t_2) A_j(t_1) \rangle \\
+ \theta(t_2 - t_1)\theta(t_1 - t)\langle B_{kl}(t_2) A_j(t_1) Q_i(t) \rangle \\
+ \theta(t - t_1)\theta(t_1 - t)\langle Q_i(t) A_j(t_1) B_{kl}(t_2) \rangle \\
+ \theta(t - t_2)\theta(t - t_1)\langle A_j(t_1) Q_i(t) B_{kl}(t_2) \rangle \\
+ \theta(t_2 - t)\theta(t - t_1)\langle B_{kl}(t_2) Q_i(t) A_j(t_1) \rangle \\
+ \text{permutations.}
\]

The signs are all positive, since operators \(A, B, Q\) are quadratic in fermion operators.

Now let us expand the commutators in definition of retarded expectation value to obtain

\[
\phi^R_{ijkl}(t_1, t_2) = \\
+ \theta(t - t_2)\theta(t_2 - t_1)\langle A_j(t_1) B_{kl}(t_2) Q_i(t) \rangle \\
- \theta(t - t_2)\theta(t_2 - t_1)\langle A_j(t_1) Q_i(t) B_{kl}(t_2) \rangle \\
- \theta(t - t_2)\theta(t_2 - t_1)\langle B_{kl}(t_2) Q_i(t) A_j(t_1) \rangle \\
+ \theta(t - t_2)\theta(t_2 - t_1)\langle Q_i(t) B_{kl}(t_2) A_j(t_1) \rangle \\
+ \theta(t - t_1)\theta(t_1 - t_2)\langle B_{kl}(t_2) A_j(t_1) Q_i(t) \rangle \\
- \theta(t - t_1)\theta(t_1 - t_2)\langle B_{kl}(t_2) Q_i(t) A_j(t_1) \rangle \\
- \theta(t - t_1)\theta(t_1 - t_2)\langle A_j(t_1) Q_i(t) B_{kl}(t_2) \rangle \\
+ \theta(t - t_1)\theta(t_1 - t_2)\langle Q_i(t) A_j(t_1) B_{kl}(t_2) \rangle.
\]

Now using the identity

\[
\theta(t - t_2)\theta(t_2 - t_1) + \theta(t - t_1)\theta(t_1 - t_2) = \theta(t - t_2)\theta(t - t_1),
\]

(A.3)

the sum of second and seventh terms simplifies to

\[-\theta(t - t_2)\theta(t - t_1)\langle AQB \rangle,
\]

(A.4)

while the sum of third and sixth terms becomes

\[-\theta(t - t_2)\theta(t - t_1)\langle BQA \rangle,
\]

(A.5)
so that we obtain

\[
\phi_{ijkl}^{R}(t; t_1, t_2) = \\
+ \theta(t - t_2)\theta(t_2 - t_1)\langle A_j(t_1)B_{kl}(t_2)Q_i(t) \rangle \\
+ \theta(t - t_2)\theta(t_2 - t_1)\langle Q_i(t)B_{kl}(t_2)A_j(t_1) \rangle \\
+ \theta(t - t_1)\theta(t_1 - t_2)\langle B_{kl}(t_2)A_j(t_1)Q_i(t) \rangle \\
+ \theta(t - t_1)\theta(t_1 - t_2)\langle Q_i(t)A_j(t_1)B_{kl}(t_2) \rangle \\
- \theta(t - t_1)\theta(t - t_2)\langle A_j(t_1)Q_i(t)B_{kl}(t_2) \rangle \\
- \theta(t - t_1)\theta(t - t_2)\langle B_{kl}(t_2)Q_i(t)A_j(t_1) \rangle. 
\]  

(A-6)

Now apart from the \(\theta\) function that determines the analytical structure, the time ordered and retarded nested commutators have similar structures. Therefore one can obtain the expectation value of fully retarded nested commutator by appropriate analytic continuation of the corresponding time ordered one. So, let us obtain the spectral representations of the retarded and time ordered expectation values and compare them.

Our conventions for Fourier transforms are

\[
f(t) = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega t} \tilde{f}(\omega) \Leftrightarrow \tilde{f}(\omega) = \int_{-\infty}^{+\infty} dt e^{i\omega t} f(t).
\]

(A-7)

\[
\chi(\omega; \omega_1, \omega_2) = \int \frac{d\omega}{2\pi} \int \frac{d\omega_2}{2\pi} e^{i\omega_1 t_1} e^{i\omega_2 t_2} \chi(t; t_1, t_2).
\]

Note that the operator \(B(t_2)\) acting at time \(t_2\) couples the second power of the external perturbation to the system. Therefore, in principle it could involve two frequencies \(\omega_2, \omega_3\). But since the external fields are supposed to act at the same time, we always have the combination \(\omega_2 + \omega_3\). Therefore here we have dropped the \(\omega_3\) in our calculations. Using the representation

\[
\theta(t) = i \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} \frac{e^{-i\omega t}}{\omega + i\eta}.
\]

(A-8)
for the step function, after some algebra we get

\[
\chi_T(\omega; \omega_1, \omega_2) = 2\pi \delta(\omega + \omega_\sigma) \sum_{a,b} A_i^{0a} B_{kl}^{ab} Q_i^{b0} \\
- \frac{(\omega_\sigma + E_{b0} - i\eta)(\omega_1 - E_{a0} - i\eta)}{Q_i^{0a} B_{kl}^{ab} A_j^{b0}} \\
- \frac{(\omega_\sigma + E_{a0} + i\eta)(\omega_1 - E_{b0} + i\eta)}{B_{kl}^{0a} A_i^{ab} Q_i^{b0}} \\
- \frac{(\omega_\sigma + E_{b0} + i\eta)(\omega_2 - E_{a0} + i\eta)}{Q_i^{0a} A_j^{ab} B_{kl}^{b0}} \\
+ \frac{(\omega_\sigma + E_{a0} + i\eta)(\omega_2 - E_{b0} + i\eta)}{A_j^{0a} Q_i^{ab} B_{kl}^{b0}} \\
+ \frac{(\omega_\sigma + E_{b0} + i\eta)(\omega_1 - E_{b0} + i\eta)}{B_{kl}^{0a} Q_i^{ab} A_j^{b0}},
\]

where we have defined \( \omega_\sigma = \omega_2 + \omega_1 \). We see the exact parallelism between the time ordered and fully retarded expectation values. The important difference is due to the nature of step functions that give rise to \( \omega_n + i\eta \) \( (n = 1, 2, \sigma) \) structure in the retarded function. This is what was expected from causality imposed by appropriate \( \theta \) functions in fully retarded one. However, as a consequence of having \( \theta \) functions along with commutators, equal time contractions in diagrammatic perturbation theory do not contribute, and should be excluded.

We can also write the above result in a more compact form if we note that the frequencies are associated with operators as \((A, \omega_1), (B, \omega_2), (Q, -\omega_\sigma)\). If we ignore the \( i\eta \) factor, the above
result can be written as

\[
\chi_R(\omega; \omega_1, \omega_2) = 2\pi \delta(\omega + \omega_\sigma) \sum_{a,b} \sum_{P} \frac{A_{0a}^0 B_{kl}^{ab} Q_{i0}^{\alpha}}{(-\omega_\sigma + E_{0b})(\omega_1 - E_{0a})},
\]  

(A-11)

where \(P\) stands for all different permutations of \((A, \omega_1), (B, \omega_2), (Q, -\omega_\sigma)\). At the end we must remember to use the appropriate \(i\eta\) factors to ensure \(\omega_n + i\eta\) structure. One can easily see that this prescription gives the correct spectral representation in case of two-current correlation with \(A = B = j\):

\[
\chi_R(\omega; \omega_1) = 2\pi \delta(\omega + \omega_1) \sum_{a} \frac{|\langle 0|j|a\rangle|^2}{\omega_1 - (E_a - E_0) + i0^+}.
\]

We can derive a similar prescription for higher order correlation functions of fully retarded nature in a straightforward way:

\[
\chi_R(\omega; \omega_1, \omega_2, \omega_3) = 2\pi \delta(\omega + \omega_\sigma) \sum_{a,b,c} \sum_{P} \frac{A_{0a}^0 B_{kl}^{ab} C_{bc}^{\alpha} Q_{i0}^{\alpha}}{(-\omega_\sigma + E_{0c})(\omega_2 + \omega_1 - E_{0b})(\omega_1 - E_{0a})},
\]  

(A-12)

Appendix B: Tight binding coordinates

In this appendix, we denote the \(k_x\) and \(k_y\) coordinates in the reciprocal space by \(x, y\) for convenience. Since constant energy surfaces \(\cos x + \cos y\) appear very frequently in calculations related to 2D tight binding systems, it is useful to define a natural orthogonal transformation, \((x, y) \rightarrow (\lambda, \xi)\), so that constant coordinate surfaces correspond to constant energy surfaces. The first coordinate obviously must be

\[
\lambda = \cos x + \cos y.
\]  

(B-1)

In order to guess an appropriate form for the second coordinate \(\xi\), we require the constant \(\xi\) surfaces to be orthogonal to the constant \(\lambda\) surfaces, that is

\[
\vec{v}_\xi \propto \nabla \lambda = -\sin x \ \hat{e}_x - \sin y \ \hat{e}_y,
\]  

(B-2)

where \(\vec{v}_\xi\) is a ‘velocity’ tangent to the constant \(\xi\) surface. This equation implies that

\[
\frac{dx}{dt} = -\sin x, \quad \frac{dy}{dt} = -\sin y,
\]  

(B-3)

the division of which gives

\[
\frac{dx}{\sin x} = \frac{dy}{\sin y} \Rightarrow d\ln (\tan(x/2)) = d\ln (\tan(y/2)).
\]  

(B-4)

Integrating the above equation gives \(\tan(y/2) = \text{const} \times \tan(x/2)\), where we define this constant to be \(\tan \xi\):

\[
\tan \xi = \tan(y/2) \cot(x/2).
\]  

(B-5)

Equations (B-1) and (B-5) imply that

\[
dxdy = Jd\lambda d\xi, \quad J = \frac{1}{\sqrt{1 - \beta \cos^2(2\xi)}}.
\]  

(B-6)
with $\beta = 1 - \lambda^2/4$. As a cross check for this formula, one can calculate the area of the BZ ($\int dx dy = 4\pi^2$) in the new coordinate system. A straightforward numerical integration reassures us that the above Jacobian is correct and the intervals $0 < \xi < 2\pi$, $-2 < \lambda < 2$ count the original BZ only once.

Also the inverse transformation is given by

$$\cos x = \frac{\lambda}{2} + \frac{J^{-1} - 1}{\cos(2\xi)}, \quad (B\cdot7)$$

$$\cos y = \frac{\lambda}{2} - \frac{J^{-1} - 1}{\cos(2\xi)}, \quad (B\cdot8)$$

where the Jacobian $J$ is already defined in equation (B-6). The variable $\xi$ can be interpreted as an angle. In fact near the $\Gamma$ point where $x, y \approx 0$ and hence, $\tan x \sim x$, $\tan y \sim y$, we can actually see that $\tan \xi \sim y/x$ and hence near to $\Gamma$ point $\xi$ can be identified with the polar coordinate $\phi$. In this limit also we can write $\lambda \approx 2 - (x^2 + y^2)/2 = 2 - r^2/2$. Therefore our coordinate system is a natural extension of polar coordinates $(r, \phi)$. Near the zone center the energy contours become circular, but near the Fermi energy $\lambda = 0$, the contours are rectangular.

As an example of the application of this coordinate system, let us calculate the exact DOS for SDW systems in 2D. All we have to do is to switch to the new coordinate system so that

$$\rho^{2D}(\nu) = \int \int dxdy 4\pi^2 \delta(\nu - \epsilon) = \int_0^{2\pi} d\xi \int_0^2 d\lambda \frac{\delta(\nu - \epsilon)}{4\pi^2 \sqrt{1 - \beta \cos^2(2\xi)}}. \quad (B\cdot9)$$

The $\lambda$ integration can be performed by changing to the new variable $\epsilon = \sqrt{\Delta^2 + \lambda^2}$ that gives $d\lambda = \epsilon d\epsilon/\lambda$. Hence the final result is

$$\rho^{2D}(\nu) = \frac{\nu}{\pi^2 \sqrt{\nu^2 - \Delta^2}} K \left( \sqrt{1 - \frac{\nu^2 - \Delta^2}{4}} \right), \quad (B\cdot10)$$

where $K$ is the elliptic integral of first kind, and the restriction $0 < \lambda < 2$ translates to $\Delta < \nu < w_2$, with $w_2^2 = 4 + \Delta^2$ defining the upper band edge. This result in the limit of $\Delta \to 0$ reduces to the appropriate result for the tight binding bands. In this limit we have a log($\nu$) singularity at the Fermi surface. But for $\Delta \neq 0$, the nature of singularity near the lower band edge for 2D SDW system is log($\nu - \Delta$)/$\sqrt{\nu - \Delta}$. In 1D, the logarithmic contribution is absent. Hence the lower band edge in 2D spin density wave systems offers more DOS than 1D case. We see in the text that this simple observation has profound implications on third order nonlinearity in SDW systems.

Calculation of DOS in 1D is much easier. We need to calculate the following:

$$\rho(\omega) = \sum_k \delta(\epsilon_k - \omega) = \int d\epsilon \rho_0(\epsilon) \delta(\epsilon - \omega). \quad (B\cdot11)$$

The DOS corresponding to gapless situation $\Delta = 0$, is given by $\rho_0(\omega) = 1/\sqrt{1 - \omega^2}$. Now we use the relation $\epsilon = \sqrt{\epsilon^2 - \Delta^2}$ between energies $\epsilon$ and $\epsilon$ corresponding to $\Delta = 0$ and $\Delta \neq 0$. 

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situations, respectively. This change of variables gives:

$$\rho(\omega) = \int \frac{\varepsilon d\varepsilon}{\sqrt{\varepsilon^2 - \Delta^2}} \frac{\delta(\varepsilon - \omega)}{\sqrt{w_1^2 - \varepsilon^2}} \sqrt{w_1^2 - \omega^2},$$

where $w_1 = \sqrt{1 + \Delta^2}$. For SDW insulator, the gap parameter $\Delta = -Um$ is determined by Coulomb correlation.
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