A charge density wave in the hidden order state of URu$_2$Si$_2$

Jung-Jung Su$^{1,2}$, Yonatan Dubi$^1$, Peter Wölfe$^3$ and Alexander V Balatsky$^{1,2}$

$^1$ Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
$^2$ Center for Integrated Nanotechnologies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
$^3$ Institute for Theory of Condensed Matter and Center for Functional Nanostructures, Karlsruhe Institute of Technology, D-76128 Karlsruhe, Germany

E-mail: jungksu@lanl.gov

Received 31 August 2010, in final form 5 December 2010
Published 17 February 2011
Online at stacks.iop.org/JPhysCM/23/094214

Abstract

We argue that the hidden order (HO) state in URu$_2$Si$_2$ will induce a charge density wave. The modulation vector of the charge density wave will be twice that of the hidden order state, $Q_{\text{CDW}} = 2Q_{\text{HO}}$. To illustrate how the charge density wave arises we use a Ginzburg–Landau theory that contains a coupling of the charge density wave amplitude to the square of the HO order parameter $\Delta_1$. This simple analysis allows us to predict the intensity and temperature dependence of the charge density wave order parameter in terms of the susceptibilities and coupling constants used in the Ginzburg–Landau analysis.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

The exact nature of the hidden order (HO) in URu$_2$Si$_2$ has been a well documented puzzle for more than 20 years [1–3]. The onset of HO is seen in the specific heat as a sharp mean field like transition at $T_{\text{HO}} = 17.5$ K. However, a systematic search for any magnetic or structural transition at $T_{\text{HO}}$ yielded negative results, thus suggesting the term ‘hidden order’ to highlight the missing connection between textbook mean field features, e.g. in the specific heat and the lack of any observable order parameter. The various proposals made to account for this phase generally fall within two categories that can be broadly summed up as (i) localized intra unit cell ordering and (ii) extended momentum space ordering. The first category, in which speculations were made to the effect that the HO is characterized by some local ordering [4–9], was prompted by the large specific heat change and large entropy release at the HO transition, the latter on the scale of $\delta S \approx 0.2 R \ln 2$. Alternatively, the HO transition was viewed as an ordering of itinerant degrees of freedom, thus intrinsically being a momentum space phenomenon with the ordering occurring in momentum space [10–15].

We still do not know which of these models is closer to the true nature of the HO state. New hints emerging from momentum resolved spectroscopies point to the existence of a momentum space instability as an important ingredient, if not a key ingredient, in the HO puzzle. First, the new as well as old neutron scattering data [16–18] provide tantalizing hints that indeed the spin dynamics drastically changes in the HO state. New sharp resonant features appear to develop in the HO state in the spin susceptibility as seen by inelastic neutron scattering, at both commensurate momenta $Q = (1, 0), (0, 1)\pi/a$ [19] at $\omega = 2$ meV and incommensurate momenta $Q^* = (0, 6, 0), (0, 0, 6)\pi/a$ at $\omega_i = 5$ meV [19, 17, 12], indicating changes in the spin dynamics below $T_{\text{HO}}$. Second, recent scanning tunneling microscopy (STM) results revealed the onset of a gap like feature in the tunneling spectra, and quasiparticle interference (QPI) data reveal the onset of a hybridization feature in the quasiparticle band structure of URu$_2$Si$_2$ [20] that develops near or at the incommensurate vector $Q^*$. The hybridization features seen in the tunneling spectra, in quasiparticle dispersion in STM and in neutron scattering resonance, all have the same energy scale of $\sim 5$ meV at characteristic momentum transfers $Q^*$. Therefore, it is at least a plausible suggestion that the HO is a phenomenon that is controlled by momentum space instability. Such a momentum space instability at $Q^*$ would produce a modulation of the order parameter $\Delta_{\text{HO}}(x) = \Delta_{\text{HO}} \exp(iQ^*x)$. 

| 0953-8984/11/094214+04$\times$33.00 | 1 |

© 2011 IOP Publishing Ltd Printed in the UK & the USA
Figure 1. Illustration of the onset of CDW amplitude \( \rho_{q,\ast} \sim |T - T_{\text{HO}}| \) and HO parameter \( \Delta_{\text{HO}} \sim |T - T_{\text{HO}}|^{1/2} \) below the HO transition. The CDW order is induced by the onset of HO and opens up with higher power of \( |T - T_{\text{HO}}| \).

A question that naturally arises from these observations is whether the HO is an incommensurate (or a commensurate) wave phenomenon of some sort and whether this wave would produce a charge density wave (CDW). In this paper we prove that a spatially modulated HO parameter will indeed lead to a CDW in the HO state. To prove this point we employ a Ginzburg–Landau (GL) analysis including a coupling between the local charge density modulation \( \rho(x) \) and the square of the HO order parameter \( \Delta_{\text{HO}} \). We use the fact that for any order parameter its square amplitude will be a simple scalar and hence in the free energy analysis it can couple to the charge density via

\[
F_{\text{int}} = - \int d^d x \lambda \rho(x) \Delta_{\text{HO}}(x) \Delta_{\text{HO}}^\ast(x) \tag{1}
\]

with coupling strength \( \lambda \) that can be of either sign. \( \rho(x) \) and \( \Delta_{\text{HO}}(x) \) are the charge density and hidden order parameters at position \( x \). This term can be understood as the change in the chemical potential energy \( \int d^d x \rho(x) \delta \mu(x) \) where \( \delta \mu \) is the effective change in the chemical potential when the hidden order induces generating. More precisely, \( \delta \mu = (\partial \mu / \partial E_f)|_{E_f=\delta E_f} \) where \( \delta E_f \) is the shift in Fermi energy:

\[
\sqrt{E_f^2 + |\Delta_{\text{HO}}(x)|^2} \bigg|_{E_f} = E_f + |\Delta_{\text{HO}}(x)|^2 / (2 E_f)
\]

\[
\equiv E_f + \delta E_f. \tag{2}
\]

Relating the chemical potential energy with the HO–CDW coupling (equation (1)), we obtain that the coupling constant \( \lambda \) is essentially proportional to \( (\partial \mu / \partial E_f)|_{E_f=\delta E_f} \).

On the other hand, the charge stiffness free energy is given by the form

\[
F_{\text{CDW}} = \sum_q f_q |\rho_q|^2 \tag{3}
\]

where \( f_q = a_1 q^2 + a_2 q^2 + a_3 > 0 \) for all momenta [21]. The \( a_1 \) term describes the Coulomb repulsion, the \( a_2 \) term describes the gradient energy costs for density modulations and the \( a_3 \) term describes a short range term. The positivity of \( f_q \) ensures that there is no CDW in the absence of the coupling. From this point on we take \( f_q = \chi/2 > 0 \) for simplicity. As we show below, the amplitude of the induced CDW modulation is proportional to \( \lambda \) and inversely proportional to the charge stiffness \( \chi \). Minimization of the total free energy \( F = F_{\text{CDW}} + F_{\text{HO}} + F_{\text{int}} \) leads to

\[
\rho_{q,\ast} = \frac{\lambda}{\chi} \Delta_{\text{HO}}^\ast(q), \tag{4}
\]

which implies that the modulation wavevector of the CDW is double that of the HO modulation in real space. This observation is the main result of the paper. If the HO modulation is commensurate with the lattice then the CDW will also be commensurate (case of \( Q \) modulation). For instance, if the HO state is a single unit cell order phenomenon without translational symmetry breaking, the CDW momenta are identical with the main Bragg peaks of the lattice. On the other hand if the HO state is incommensurate, so will be the CDW (case of \( Q^\ast \) modulation). For the HO modulated at an incommensurate wavevector like \( Q^\ast = (0.6, 0), (0, 0.65)\pi/a \) the CDW modulation will be at \( Q_{\text{CDW}} = (1.2, 0), (0, 1.2)\pi/a \).

Another immediate consequence of the GL analysis is that the intensity of the CDW will scale as \( \rho_{q,\ast} \sim \Delta_{\text{HO}}^\ast(q) \sim |T - T_{\text{HO}}| \) (figure 1), since the HO order parameter sets in as at a well defined mean field transition.

2. Ginzburg–Landau model for the CDW

Recently two of us proposed that the HO is a hybridization wave with a modulation of \( Q^\ast \) [14, 15]. In our model the HO in URu2Si2 originates from an indirect excitonic condensation of d-band holes bound to local f-band electrons. In general, such hybridization order takes the form

\[
\Delta_{\text{HO}}(k) = \sum_q V_{q+k} \langle c_{q+k}^\dagger c_{q+k} \rangle. \tag{5}
\]

In particular, we argue that the coupling is mainly between electrons (and holes) with momenta \( Q^\ast/2 \) (and \( -Q^\ast/2 \)) and vice versa, where \( Q^2/4 = (0.5)\pi/a \). This coupling induces a modulation wavevector of \( Q^\ast \) in the hidden order state. In total there are four incommensurate wavevectors \( Q_i, Q_{i1} = Q^\ast \) and the three equivalent vectors in tetragonal symmetry, rotated in the \((a,b)\)-plane by multiples of \( \pi/2 \). We will assume in the following that the HO phase forms a monodomain characterized by a single wavevector direction such that \( Q_i = \pm Q^\ast \). The corresponding Ginzburg–Landau (GL) energy functional for the HO is [21]

\[
F_{\text{HO}} = \sum_k c_k |\Delta_{\text{HO}}(k)|^2 + \frac{1}{2} \alpha |\Delta_{\text{HO}}(k)|^2 + \frac{1}{2} \beta |\Delta_{\text{HO}}(k)|^4 \tag{6}
\]

where the first term is the kinetic energy and \( c_k = c \sum_q (k - Q)^i \) is the stiffness of the hidden order field, the coefficient of the second order term changes sign at \( T = T_{\text{HO}} \), \( \alpha = a(T - T_{\text{HO}}) \), and \( \beta \) is a positive constant. It is clear that without the coupling with other degrees of freedom, \( F_{\text{HO}} \) favors a modulation with momentum \( \pm Q^\ast \), noting that \( T_{\text{HO}} \) is largest for these momentum values. The free energy associated with a charge density modulation is given by

\[
F_{\text{CDW}} = \sum_e \frac{1}{2} \chi |\rho_q|^2. \tag{7}
\]
The HO and the charge degrees of freedom are coupled through

$$F_{\text{int}} = -\lambda \sum_{k,q} \rho_k \Delta_{\text{HO}}(k-q)\Delta_{\text{HO}}^*(k) + \text{c.c.}. \quad (8)$$

which is simply the Fourier transform of equation (1). The total energy functional is

$$F = F_{\text{HO}} + F_{\text{CDW}} + F_{\text{int}}. \quad (9)$$

Minimizing the energy functional yields the equation set

$$0 = \frac{\partial F}{\partial \Delta_{\text{HO}}^R} = -\lambda \sum_q \rho_q \left( \Delta_{\text{HO}}^S(k+q) + \Delta_{\text{HO}}^S(k-q) \right) + 2C(k-q)^2 \Delta_{\text{HO}}^S(k) + \alpha \Delta_{\text{HO}}^S(k) + \beta |\Delta_{\text{HO}}(k)|^2 \Delta_{\text{HO}}^S(k) \quad (10)$$

$$0 = \frac{\partial F}{\partial \rho_q} = \chi \rho_q - \lambda \sum_k \Re \{ \Delta_{\text{HO}}(k+q)\Delta_{\text{HO}}^*(k) \}. \quad (11)$$

We can argue from the above equation sets that the amplitude of the CDW is linear of $T_c - T$ at the vicinity of the critical temperature. In such a regime, the only components of the HO parameter are $\Delta_{\text{HO}}(+Q^*)$ and $\Delta_{\text{HO}}(-Q^*)$, yielding possible momentum values for $q$ in equation (8) of $q = \pm 2Q^*$, and therefore a single Fourier component for the charge modulation $\rho_{2Q^*}$. More precisely, the only nonvanishing contributions to $\Delta_{\text{HO}}(q)$ and $\rho_q$ are

$$|\Delta_{\text{HO}}(\pm Q^*)| = \left( -\frac{\alpha}{\beta - \lambda^2/\chi} \right)^{1/2}$$

$$|\rho_{2Q^*}| = -\frac{\alpha \lambda}{\beta \chi - \lambda^2} = \frac{\lambda}{\chi} |\Delta_{\text{HO}}(Q^*)|^2. \quad (12)$$

The amplitude of $\Delta_{\text{HO}}(\pm Q^*)$ increases with respect to the $\lambda = 0$, $\rho = 0$ solution, resulting in a decrease of the free energy (for negative $\lambda$), indicating that a CDW is formed. This linear in $T_c - T$ amplitude is a direct experimental prediction.

While the above argument corresponds essentially to the weak coupling regime, we can consider the more general cases by solving the equation set numerically without assumptions in $q = \pm 2Q^*$. Here we consider cases of various levels of coupling strength. In figures 2-4 we plot the numerical solutions for equations (10) and (11) for the parameters $\alpha = -0.005$, $\beta = 0.001$, $\chi = 1.0$, $\lambda = -0.05$ and $c = 50, 10, 2$ respectively (which effectively correspond to the weak, intermediate and strong coupling regimes). The numerical calculations are consistent with the results obtained above. In the weak coupling regime, we obtain a CDW oscillating with wavevectors around $2Q^*$ in all three cases. For large stiffness (figure 2), $\Delta_{\text{HO}}$ oscillates with a single wavevector $Q^*$ and is not affected significantly by the coupling with the CDW. The CDW oscillates with a rapid oscillation $2Q^*$ on top of a slow modulation. When the stiffness decreases (figures 3 and 4), the peaks in $\Delta_{\text{HO}}(q)$ and $\rho_q$ broaden. Interferences between momenta within the peak width cause the modulation to vanish at large $r$.

3. Conclusions

In this paper we showed that in the presence of an HO parameter with modulation wavevector $Q^*$, a charge density wave with modulation wavevector $2Q^*$ emerges, provided a coupling between the HO parameter amplitude (squared) and the charge density modulation exists in the free energy. We predict that the amplitude of the resulting CDW grows linearly in temperature below $T_{\text{HO}}$. We hope that our results will stimulate a detailed search for the proposed CDW. The natural techniques that would allow for CDW observation would be neutron scattering, x-ray scattering and local probes. In principle, the optical conductivity and ARPES might also see effects of band changes due to CDW formation. If CDW is observed it may shed further light on the nature of the hidden order state in URu$_2$Si$_2$. 
Acknowledgments

The authors enjoyed fruitful discussions with J C Davis, M J Graf, B Gaulin, G Kotliar, G Luke, E Hassinger and J Mydosh. This work was supported by the US Department of Energy at Los Alamos National Laboratory under contract No. DE-AC52-06NA25396 and by UCOP TR01 and by the DFG research unit ‘Quantum phase transitions’ (PW).

References

[1] Palstra T T M et al 1985 Phys. Rev. Lett. 55 2727
[2] Schlabitz W et al 1986 Z. Phys. B 62 171–7
[3] Maple M B et al 1986 Phys. Rev. Lett. 56 185–8
[4] Chandra P, Coleman P, Mydosh J A and Tripathi V 2002 Nature 417 831
[5] Santini P 1998 Phys. Rev. B 57 5191
[6] Kasuya T 1997 J. Phys. Soc. Japan 66 3348–51
[7] Sikkema A E, Buyers W J L, Affleck I and Gan J 1996 Phys. Rev. B 54 9322
[8] Cricchio F, Bultmark F, Gránäo O and Nordström L 2009 Phys. Rev. Lett. 103 107202
[9] Haule K and Kotliar G 2009 Nat. Phys. 5 796
[10] Ikeda H and Ohashi Y 1998 Phys. Rev. Lett. 81 3723
[11] Varma C M and Zhu L 2006 Phys. Rev. Lett. 96 036405
[12] Balatsky A V, Chantis A, Dahal H P, Parker D and Zhu J X 2009 Phys. Rev. B 79 214413
[13] Elgazzar S, Rusz J, Amft M, Oppeneer P M and Mydosh J A 2009 Nat. Mater. 8 337
[14] Wölffle P, Dubi Y and Balatsky A V 2010 Phys. Rev. Lett. 105 246401
[15] Wölffle P, Dubi Y and Balatsky A V 2010 arXiv:1008.4923
[16] Broholm C et al 1987 Phys. Rev. Lett. 58 1467
[17] Wiebe C R et al 2007 Nat. Phys. 3 96
[18] Ikeda Y et al 2010 J. Phys.: Conf. Ser. 200 012065
[19] Bourdarot F et al 2010 arXiv:cond-mat:1004.1899
[20] Schmidt A R et al 2010 Nature 465 570
[21] Turgut S and Falicov L M 1994 Phys. Rev. B 50 8221