White dwarf cooling: electron-phonon coupling and the metallization of solid helium

Bartomeu Monserrat

University of Cambridge

QMC in the Apuan Alps VIII
31 July 2013
Outline

White dwarf stars overview

Theoretical background
  Anharmonic energy
  Phonon expectation values

Results

Conclusions
Outline

White dwarf stars overview

Theoretical background
   Anharmonic energy
   Phonon expectation values

Results

Conclusions
Star formation

- Virial theorem: $K = -1/2 V_g$.
- Energy expressions:
  
  $$K \propto Nk_B T \quad \text{and} \quad V_g \propto -\frac{GM^2}{R}$$

- Temperature increases as the star gravitationally collapses.
Main sequence star

- Thermonuclear reactions: hydrogen burning.
- Gravitation balanced by nuclear reactions.
- Main sequence star (e.g. the Sun).
White dwarf formation

- Burning material exhausted.
- Gravitational contraction resumes.
- High density leads to degenerate electron gas (DEG).
- White dwarf star balanced by DEG.
- Complications: mass loss (red giant), further burning cycles, ...
White dwarf structure

- Degenerate core: He or C/O.
- Atmosphere: H, He and traces of other elements.
- Atmosphere represents $10^{-4} - 10^{-2}$ of the total mass.
- Atmosphere stratification due to strong gravity.
- Weak energy sources: crystallization, . . .
- Energy transport: conduction, radiation and convection.
White dwarf cooling
White dwarf cooling
White dwarf cooling: metallization of solid helium (I)

Helium

Degenerate electron gas

Degenerate electron gas: isothermal
Core to surface: temperature gradient
Helium phase diagram

- Solid $^4\text{He}$
- Fluid $^4\text{He}$
- $^4\text{He}^0$
- $^4\text{He}^+$
- $^4\text{He}^{++}$
- Metallization

Pressure (TPa) vs. Temperature (K)
White dwarf cooling: metallization of solid helium (II)

Degenerate electron gas: isothermal
Core to surface: temperature gradient
Metallization pressure

- DFT: 17 TPa at zero temperature.
- DMC and \( GW \): 25.7 TPa at zero temperature.
- Electron-phonon coupling: ?
Outline

White dwarf stars overview

Theoretical background

Anharmonic energy

Phonon expectation values

Results

Conclusions
Harmonic approximation

- Vibrational Hamiltonian in \( \{ r_\alpha \} \) (or \( \{ u_\alpha \} \)):

\[
\hat{H}_{\text{vib}} = -\frac{1}{2} \sum_{R_p,\alpha} \frac{1}{m_\alpha} \nabla^2 p_\alpha + \frac{1}{2} \sum_{R_p,\alpha;R_p',\beta} u_{p\alpha} \Phi_{p\alpha;p'\beta} u_{p'\beta}
\]

- Normal mode analysis: \( \{ u_{p\alpha} \} \rightarrow \{ q_{ks} \} \)

\[
u_{p\alpha; i} = \frac{1}{\sqrt{N_0 m_\alpha}} \sum_{k,s} q_{ks} e^{ik \cdot R_p w_{ks; i\alpha}}
\]

\[
q_{ks} = \frac{1}{\sqrt{N_0}} \sum_{R_p,\alpha, i} \sqrt{m_\alpha} u_{p\alpha; i} e^{-ik \cdot R_p w_{-ks; i\alpha}}
\]

- Vibrational Hamiltonian in \( \{ q_{ks} \} \):

\[
\hat{H}_{\text{vib}} = \sum_{k,s} \left( -\frac{1}{2} \frac{\partial^2}{\partial q_{ks}^2} + \frac{1}{2} \omega_{ks}^2 q_{ks}^2 \right)
\]
Principal axes approximation to the BO energy surface

\[
V(\{q_{ks}\}) = V(0) + \sum_{k,s} V_{ks}(q_{ks}) + \frac{1}{2} \sum_{k,s} \sum_{k',s'} V_{ks;k' s'}(q_{ks}, q_{k's'}) + \cdots
\]

- Static lattice DFT total energy
- DFT total energy along frozen independent phonon
- DFT total energy along frozen coupled phonons
Vibrational self-consistent field equations

- Phonon Schrödinger equation:

\[
\left( \sum_{k,s} -\frac{1}{2} \frac{\partial^2}{\partial q_{ks}^2} + V(\{q_{ks}\}) \right) \Phi(\{q_{ks}\}) = E \Phi(\{q_{ks}\})
\]

- Ground state ansatz: \( \Phi(\{q_{ks}\}) = \prod_{k,s} \phi_{ks}(q_{ks}) \)

- Self-consistent equations:

\[
\left( -\frac{1}{2} \frac{\partial^2}{\partial q_{ks}^2} + V_{ks}(q_{ks}) \right) \phi_{ks}(q_{ks}) = \lambda_{ks} \phi_{ks}(q_{ks})
\]

\[
V_{ks}(q_{ks}) = \left\langle \prod_{k',s'}^' \phi_{k's'}(q_{k's'}) \left| V(\{q_{k''s''}\}) \right| \prod_{k',s'}^' \phi_{k's'}(q_{k's'}) \right\rangle
\]
Approximate vibrational excited states:

$$|\Phi^S(Q)\rangle = \prod_{k,s} |\phi^{S_ks}(q_{ks})\rangle$$

where $S$ is a vector with elements $S_{ks}$.

Anharmonic free energy:

$$F = -\frac{1}{\beta} \ln \sum_S e^{-\beta E_S}$$
Diamond independent phonon term (I)

\[ V(\{q_{ks}\}) = V(0) + \sum_{k,s} V_{ks}(q_{ks}) + \frac{1}{2} \sum_{k,s} \sum'_{k',s'} V_{ks; k's'}(q_{ks}, q_{k's'}) + \cdots \]
Diamond independent phonon term (II)
Diamond coupled phonons term

\[ V(\{q_{ks}\}) = V(0) + \sum_{k,s} V_{ks}(q_{ks}) + \frac{1}{2} \sum_{k,s} \sum_{k',s'} V_{ks;k's'}(q_{ks}, q_{k's'}) + \cdots \]
LiH independent phonon term (I)

\[ V(\{q_{ks}\}) = V(0) + \sum_{k,s} V_{ks}(q_{ks}) + \frac{1}{2} \sum_{k,s} \sum' V_{ks;k's'}(q_{ks}, q_{k's'}) + \cdots \]
LiH independent phonon term (II)

Harmonic
Anharmonic

Mode wave function (arb. units)

Mode amplitude (a.u.)
LiH coupled phonons term

\[ V(\{q_{ks}\}) = V(0) + \sum_{k,s} V_{ks}(q_{ks}) + \frac{1}{2} \sum_{k,s} \sum_{k',s'} V_{ks;k's'}(q_{ks}, q_{k's'}) + \cdots \]
Anharmonic ZPE correction
General phonon expectation value

▶ Phonon expectation value at inverse temperature $\beta$:

$$\langle \hat{O}(Q) \rangle_{\Phi,\beta} = \frac{1}{Z} \sum_{S} \langle \Phi^{S}(Q)|\hat{O}(Q)|\Phi^{S}(Q)\rangle e^{-\beta E_{S}}$$

▶ Evaluation:

▶ Standard theories (Allen-Heine, Grüneisen):

$$\hat{O}(Q) = \hat{O}(0) + \sum_{k,s} a_{ks} q_{ks}^{2}$$

▶ Principal axes expansion:

$$\hat{O}(Q) = \hat{O}(0) + \sum_{k,s} \hat{O}_{ks}(q_{ks}) + \frac{1}{2} \sum_{k,s} \sum_{k',s'} \hat{O}_{ks;k's'}(q_{ks}, q_{k's'}) + \cdots$$

▶ Monte Carlo sampling
Band gap renormalization

- Band gap problem (LDA, PBE, ...): underestimation of gaps.
- Caused by the lack of a discontinuity in approximate \( xc \)-functionals with respect to particle number: correction \( \Delta xc \) to band gap.
- Approximate systematic shift in all displaced configurations.
- Error disappears in change in band gap.
Diamond thermal band gap (I)
Diamond thermal band gap (II)

- Static lattice: 0.462 eV
- Including el-ph coupling

Temperature (K):
- 5.1
- 5.2
- 5.3
- 5.4
- 5.5
- 5.6
- 5.7
- 5.8
- 5.9
- 6.0

Energy gap ($E_g$, eV):
- 5.9
- 5.8
- 5.7
- 5.6
- 5.5
- 5.4
- 5.3
- 5.2
- 5.1

Temperature (K):
- 0
- 200
- 400
- 600
- 800
- 1000

B. Monserrat – QMC Apuan Alps VIII – July 2013
Diamond thermal band gap (III)

Thermal expansion (I)

- Gibbs free energy:

\[ dG = dF_{el} + dF_{vib} - \Omega \sum_{i,j} \sigma_{ij}^{\text{ext}} d\epsilon_{ij} \]

- Vibrational stress:

\[ dF_{vib} = -\Omega \sum_{i,j} \sigma_{ij}^{\text{vib}} d\epsilon_{ij} \]

- Effective stress:

\[ dG = dF_{el} - \Omega \sum_{i,j} \sigma_{ij}^{\text{eff}} d\epsilon_{ij} \]

where \( \sigma_{ij}^{\text{eff}} = \sigma_{ij}^{\text{ext}} + \sigma_{ij}^{\text{vib}} \).
Thermal expansion (II)

- Potential part of vibrational stress tensor:

\[ \sigma_{ij}^{\text{vib},V} = \langle \Phi(\mathbf{Q})|\sigma_{ij}^{\text{el}}|\Phi(\mathbf{Q}) \rangle \]

- Kinetic part of vibrational stress tensor:

\[ \sigma_{ij}^{\text{vib},T} = -\frac{1}{\Omega} \left\langle \Phi \right| \sum_{\mathbf{R}_p,\alpha} m_\alpha \ddot{\mathbf{u}}_{p\alpha;i} \ddot{\mathbf{u}}_{p\alpha;j} \left| \Phi \right\rangle \]

- Total vibrational stress tensor:

\[ \sigma_{ij}^{\text{vib}} = \sigma_{ij}^{\text{vib},V} + \sigma_{ij}^{\text{vib},T} \]
LiH and LiD thermal expansion coefficient

Outline

White dwarf stars overview

Theoretical background
  Anharmonic energy
  Phonon expectation values

Results

Conclusions
Solid helium structural phase diagram

![Solid helium structural phase diagram](image.png)
Solid helium electron-phonon gap correction (I)

![Graph showing electron-phonon correction vs. pressure for different temperatures.]

- $T = 0$ K
- $T = 2500$ K
- $T = 5000$ K
- $T = 7500$ K
- $T = 10000$ K

Electron-phonon correction (eV) vs. Pressure (TPa)
Solid helium electron-phonon gap correction (II)
Solid helium equilibrium density

\[ \frac{\rho}{\rho_{\text{static}}} \]

Temperature Dependence:
- \( T = 0 \) K
- \( T = 2500 \) K
- \( T = 5000 \) K
- \( T = 7500 \) K
- \( T = 10000 \) K

\[ \text{Pressure (TPa)} \]

\[ \{0.86, 0.88, 0.90, 0.92, 0.94, 0.96, 0.98, 1.00\} \]

B. Monserrat – QMC Apuan Alps VIII – July 2013
Solid helium metallization pressure

DMC and GW from PRL 101, 106407 (2008)
Helium phase diagram revisited
White dwarf cooling revisited: metallization of solid helium

Higher metallization pressure

Thinner electron-transport layer
Outline

White dwarf stars overview

Theoretical background
  Anharmonic energy
  Phonon expectation values

Results

Conclusions
Conclusions

▶ Theory for anharmonic vibrational energy of solids.
▶ General framework for phonon-dependent expectation values.
▶ Metallization of solid helium.
▶ White dwarf energy transport and cooling.
Acknowledgements:

Prof. Richard J. Needs
Dr Neil D. Drummond
Dr Gareth J. Conduit
Prof. Chris J. Pickard
TCM group
EPSRC

References:

B. Monserrat, N.D. Drummond, R.J. Needs
B. Monserrat, N.D. Drummond, C.J. Pickard, R.J. Needs
Helium paper, in preparation (2013)