Vacancies-Excitons
Mechanism of Supersolidity
(in helium?)

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Intriguing possibility for quantum crystal:

- $\rho(r) = \rho_0 \cos(G \cdot r)$
- *but* atoms mobile
- mobile atoms (bosons) can Bose condense
- exhibit superfluidity
- SUPERSOLID

- NCRI observed in solid He4 by 3 groups
- Bulk, equilibrium property?
Vacancy mechanism of supersolid

- Andreev and Lifshitz - quantum fluctuations favor finite density of vacancies even at $T=0$. Vacancies are mobile and can Bose condense.

- Chester - Jastrow wavefunctions generally have ODLRO, including ones describing solid order. Speculate due to vacancy condensation.

- Presence of vacancies in supersolids necessary provided there is no vacancy-interstitial symmetry, shown by Prokofev and Svistunov recently.
data fit to $c(T) \sim \exp\left(-\frac{f}{kT}\right)$

$E_v \sim 10$ K
- Supersolid He4 not observed until Kim and Chan’s expt.

- Previous expts and theoretical calculations place strict limit on vacancy density in normal solid.

- High activation energies for defects:
  \[ E_v \sim 10 - 15 \text{ K} \quad E_i \sim 50 \text{ K} \]

**Quandary:**
How can defects of such high activation energies condense at low temperature, \( T_c \sim 0.2 \text{ K} \)?

We provide one resolution to this quandary. New mechanism for vacancy condensation.
Proposed Resolution

- **First order transition**
  At $T=0$, $n_v = 0$ in normal solid
  finite in supersolid

- **“Vacuum” switching**
  vacancies condense in background of another type
  of defectons called “excitons”

- **Normal-Supersolid transition accompanied by**
  Commensurate-incommensurate transition
  Change in local density profile
Andreev-Lifshitz Vacancy Model

Defect free solid - Mott insulator
Andreev-Lifshitz Vacancy Model
If $E_v < 0$, spontaneous creation of vacancies at $T = 0$
Such vacancies will Bose condense

$E_v = \varepsilon_a - zt_a$

$E_v < 0$ not supported by expts or theories
Interstitial condensation even more unfavorable.

\[ E_b = \epsilon_b - z t_b \]

\[ t_b > t_a \text{, but } \epsilon_b >> \epsilon_a \text{, so } E_b > E_a \]

Interstitial condensation even more unfavorable.
Have Your Cake and Eat it Too

Model

Third type of defect: bound vacancy-interstitial or “exciton”

\[ \Delta \epsilon_a > \epsilon_b \]

\[ \epsilon_b >> \epsilon_a > \Delta \]
Key physics:
Vacancies can Bose condense easier over exciton background than over defect free background

- activation energy $\epsilon_a - \Delta < \epsilon_a$
- vacancy hops with $t_b$, not $t_a$

Instability criteria $\epsilon_a - \Delta - z t_b$

If condensation amplitude sufficiently large, condensation energy $> \Delta$
vacancies Bose condense
stable normal solid
defect free
\[ n_{\text{ex}} = n_{\text{v}} = 0 \]

unstable normal solid
defect rich
\[ n_{\text{ex}} \neq 0, n_{\text{v}} = 0 \]

stable supersolid
defect rich
\[ n_{\text{ex}} \neq 0, n_{\text{v}} \neq 0 \]

- \( T = 0 \) transition first order
- normal - supersolid transition
  \textit{commensurate - incommensurate transition}
  \textit{change in local density profile}
Change in Local Density Profile

Normal Solid

Supersolid
Microscopic Wavefunction

Normal solid \( \psi = \prod_{i=1}^{N} b_i^+ |\text{vacuum}\rangle \)

\( b_i^+ \) creates a He atom in localized state \( \phi_i = \phi(r-R_i) \)

commensurate
\( \phi \) has single peak

Supersolid \( \psi_{ss} = \prod_{i=1}^{N_0} (u + va_i^+) |\text{vacuum}\rangle \)

\( a_i^+ \) creates a He atom in localized state \( \chi_i = \chi(r-R_i) \)

\( |u^2| = \text{vacancy fraction} \)

\( N < N_0 \), incommensurate
\( \chi \) less localized than \( \phi \), perhaps even multiippeak

\( \text{SS} = (u + v a_i^+) \prod_{i=1}^{N_0} |\text{vacuum}\rangle \)
Equivalence between Jastrow and Nosanow-Jastrow wavefunctions with vacancies

\[ \psi_{SS} = \prod_{i=1}^{N_0} (u + v a_i^+) |\text{vacuum}\rangle \]

\[ \approx P_G \left( \sum_{i=1}^{N_0} \frac{v}{u} a_i^+ \right)^N |\text{vacuum}\rangle \]

\[ \sim P_G \left( \int dr \sum_{i=1}^{N_0} \chi(r - R_i) \psi^+(r) \right)^N |\text{vacuum}\rangle \]

\[ = P_G \prod_{\alpha} \left( \sum_{i=1}^{N_0} \chi(r_\alpha - R_i) \right) \]
Single-Site Mean Field Theory

- Decouple K.E.
  \[ t a^+ a \rightarrow t \langle a^+ a \rangle + t a^+ \langle a \rangle - t \langle a^+ \rangle \langle a \rangle \]
  \( \langle a \rangle \) solved self-consistently to give Bose condensed amplitude

- \( E = E_{MF} + \) elastic energy for change in lattice constant

- Respect strong on-site correlations (hard core)

- Successful for other lattice boson models for \( d \geq 2 \) at \( T=0 \)

- Gives exact instability criteria for Andreev-Lifshitz Model

- Key results for \( T=0 \) strengthened by quantum fluctuations
$T = 0$ Phase Diagram

$\varepsilon_b = 4 \varepsilon_a \quad \Delta = 0.2 \varepsilon_a$
Finite $T$

Illustrate with $\varepsilon_b = \infty$, $t_a = 0$, $\Delta = \varepsilon_a$

Two coupled order parameters:

- $n = \langle n \rangle$, defect concentration
- $b = \langle b \rangle$, condensate amplitude
Finite T Phase Diagram (schematic)
These are transition curves for $n$. NCRI is related to transition in $b$. 
NCRI transition occurs below defect density transition transition second order
NCRI transition occurs with defect density transition first order
Casual Comparison to Experiments
T=0 Superfluid Density

- Kim and Chan reported max $\rho_s/\rho \sim 1\%$
  Our MFT gives 3 - 9%
  Value should be reduced by quantum (phase) fluctuations
  Fluctuations stabilize supersolid vs. defect free state

- More recent data shows $\rho_s$ increasing then decreasing with pressure/density
  Within our model, $\rho_s$ favored by small $\Delta$, $\varepsilon_a$, large $t_{a,b}$
  $t_{a,b}$ may be non-monotonic with $\rho$
Penn State data
Finite $T \rho_s$

- data suggests transition smeared by disorder
- specific heat shows no critical behavior

Two possibilities for pure system:
- second order transition \textit{not} in X-Y universality class
- first order transition

Transition is first order at $T=0$ in our model
May also be first order at finite $T$
He 3 Impurities

Expt, with increasing He3 concentration (ppm):
- $T_c$ increases
- low $T \rho_s$ decreases
- NCRI not observable beyond 0.1% He3 concentration

Qualitative agreement:
- He 3 favors defects due to its smaller mass
  $\Rightarrow T_c$ increases
- Impurities localize vacancies
  $\Rightarrow$ reduce $\rho_s$ and eventually destroys Bose condensation
  (dirty bosons)
Conclusions

- Vacancies can condense in solid He4 in spite of negative evidence from normal state
- Normal solid defect free, supersolid defect rich
  -- first order transition
  -- commensurate - incommensurate
  -- change in local density profile
- No intrinsic contradiction between Kim and Chan’s observation and existing normal solid data