Technische Universität Braunschweig

Wigner Crystal phases in bilayer graphene

P.G. Silvestrov & P. Recher (TU,Braunschweig)

- in preparation

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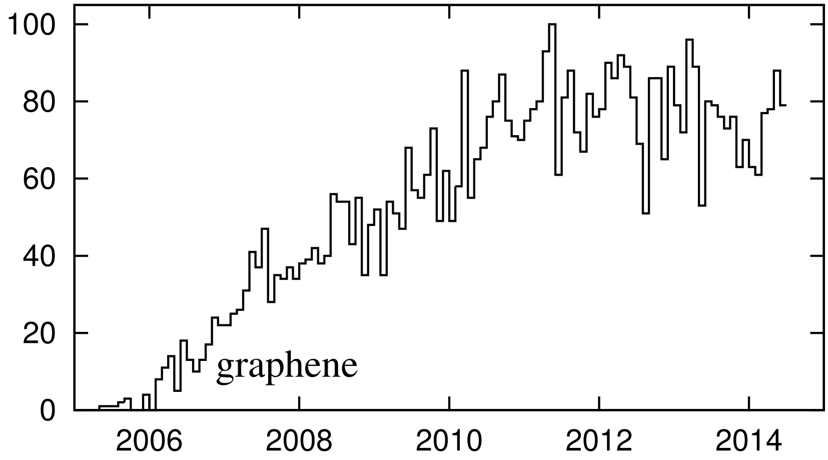
Wigner crystal of a two-dimensional electron gas with a strong spin-orbit interaction, PRB April 2014

P.G.S. & O. Entin-Wohlman (BGU,Beer Sheva + TU,Tel Aviv)

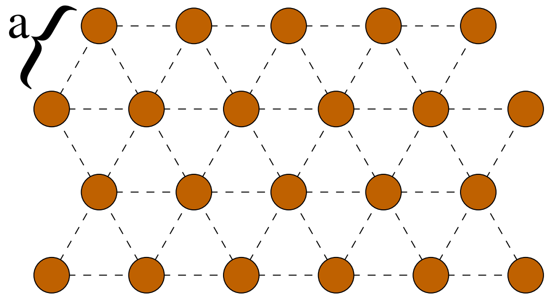
discussions: Y. Imry (Weizmann,Israel)
E. Bergholtz (FU,Berlin)
P. Brouwer (FU,Berlin)



Outline

1. Introduction. Wigner crystal stability
2. Double-layer graphene. Spectrum and screening
3. Intermediate density Wigner crystal in bilayer
4. Low energy bilayer = Rashba
   a. zero point energy and proper ground state
   b. phonons, squeezing the crystal
5. Conclusions

1. Introduction.
Wigner crystal:



The low density phase of electron gas, Wigner 1934

Interaction energy vs. Kinetic energy (per electron)

$$U \sim \frac{e^2}{a}\ , \quad K \sim \frac{p^2}{2m} \sim \frac{\hbar^2}{2ma^2}$$

$$U > K \quad \text{at} \quad a > a_B = \hbar^2/me^2$$

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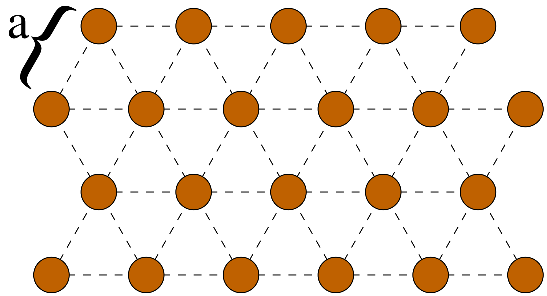

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Triangular lattice for 2-dimensional electron gas

Bonsall & Maradudin 1977

Very low density phase!

Tanatar & Ceperley 1989

$\pi r_s^2 = 1/n a_B^2$, $r_s \approx a/a_B$, $a_B = \hbar^2/me^2$,

$r_s > 35$, i.e. $a \gg a_B$

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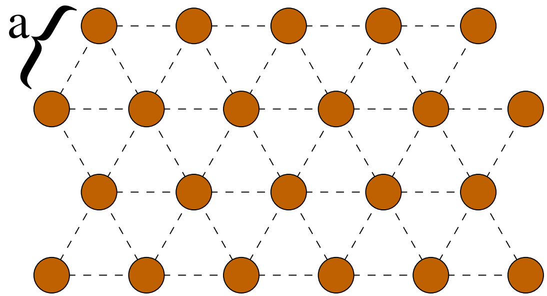

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Experiment: liquid Helium surface - Crimes, Adams 1979

GaAs, electrons in magnetic field - Eva Andrey, et al 1988

heavy holes - Yoon, Shahar, Tsui, Shaegyan 1999

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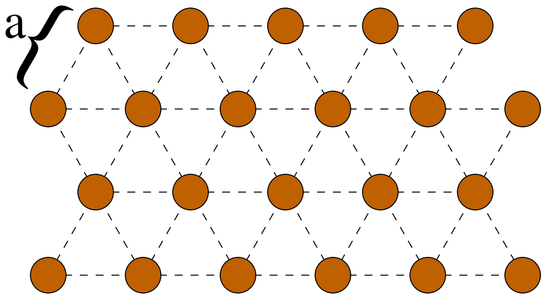

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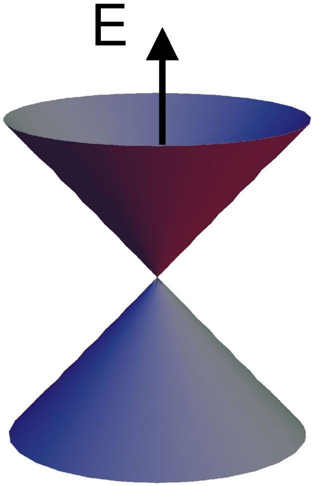
No Wigner crystal in graphene:



$$U \sim \frac{e^2}{a}\,, \quad K \sim v_F p \sim \frac{v_F \hbar}{a}$$

$U \sim K$ for any density!

Dahal, Joglekar, Beddel, Balatsky, PRB 2006

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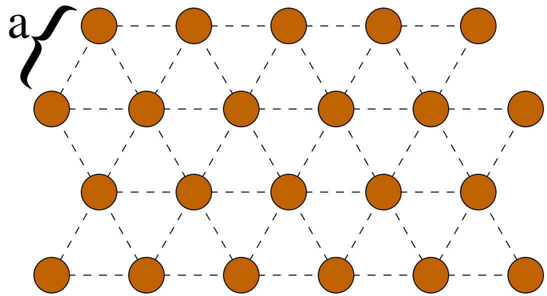

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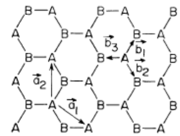

FIG. 1. The honeycomb lattice as a superposition of two triangular sublattices. The basis vectors are $\vec{a}_1 = (\sqrt{3}/2, -\frac{1}{2})a$; $\vec{a}_2 = (0,1)a$ and the sublattices are connected by $\vec{b}_1 = (1/2\sqrt{3}, \frac{1}{2})a$; $\vec{b}_2 = (1/2\sqrt{3}, -\frac{1}{2})a$; $\vec{b}_3 = (-1/\sqrt{3}, 0)a$.

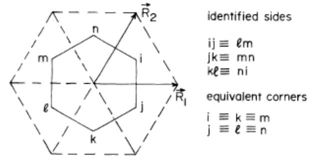

FIG. 2. The Brillouin zone. The reciprocal-lattice basis vectors are $\vec{R}_1 = (4\pi/\sqrt{3}a)(1,0)$; $\vec{R}_2 = (4\pi/\sqrt{3}a) \times (\frac{1}{2}, \frac{1}{2}\sqrt{3})$. The degeneracy points occur at the corners, *ijklmn*, of the Brillouin zone. Two of these are inequivalent; we have chosen $\vec{q}_1 = (4\pi/\sqrt{3}a)(\frac{1}{2}, 1/2\sqrt{3})$ at point *i* and $\vec{q}_2 = -\vec{q}_1$ at point *l*.

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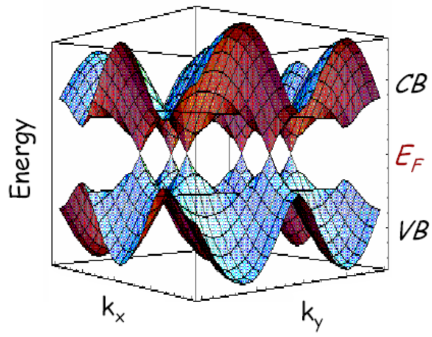

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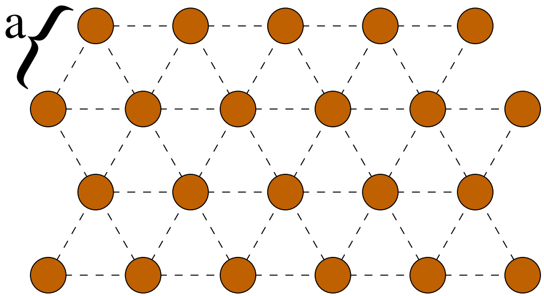

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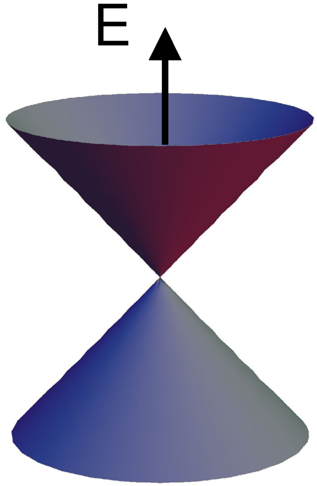

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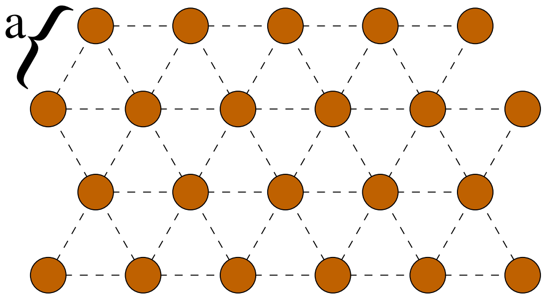

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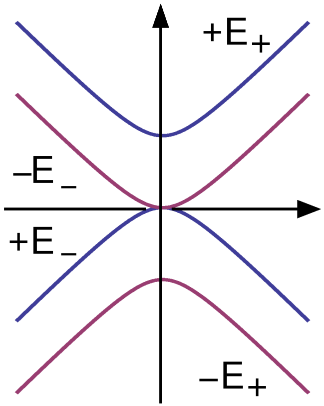
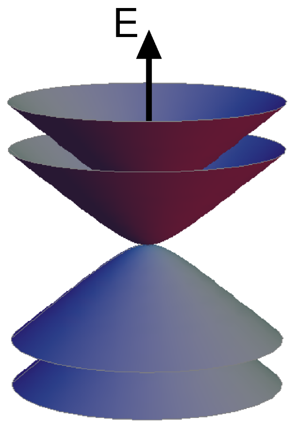
Wigner crystal in bilayer graphene?





$$K \sim p^2 \sim \frac{1}{a^2}$$

But interaction is screened!
Hwang, Das Sarma, PRL 2008

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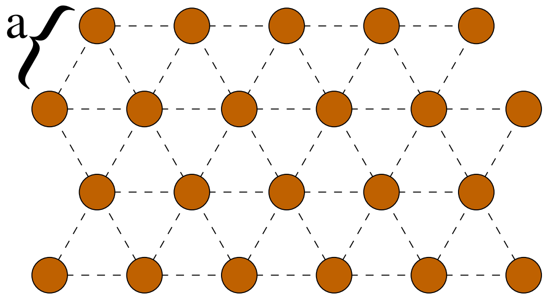

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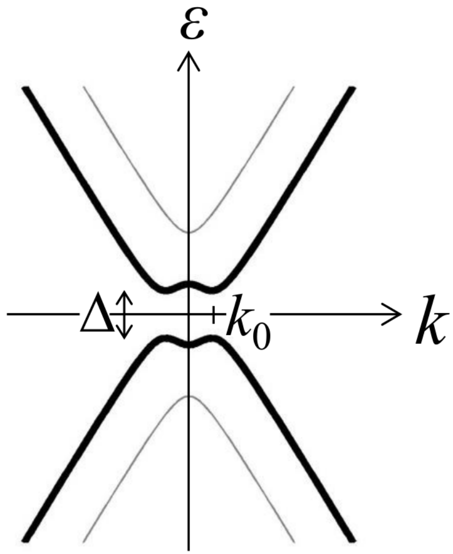
Gated bilayer graphene?

Slightly doped gated bilayer graphene



Gap opens = dielectric

+ Mexican hat potential

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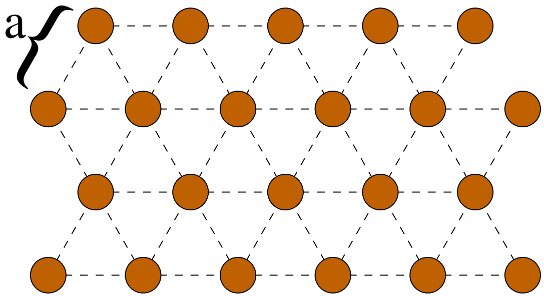

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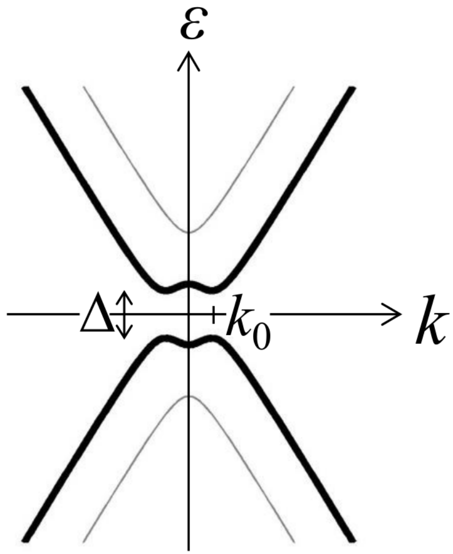

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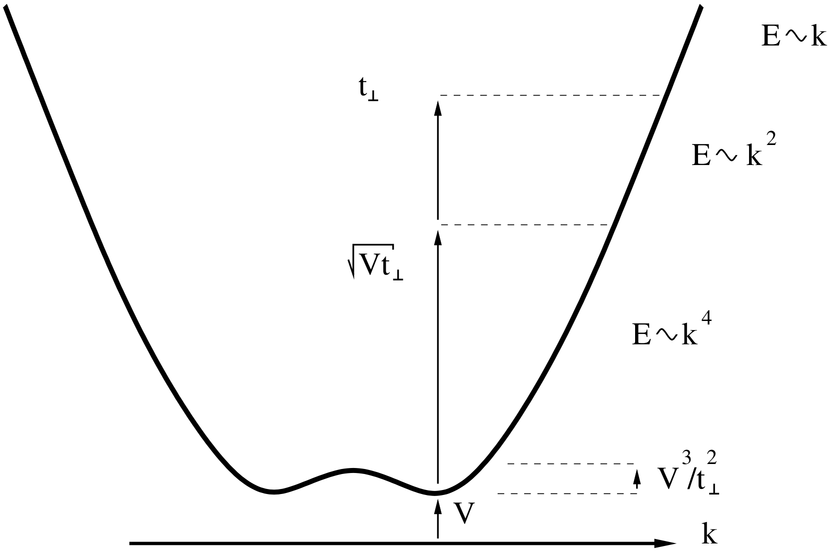
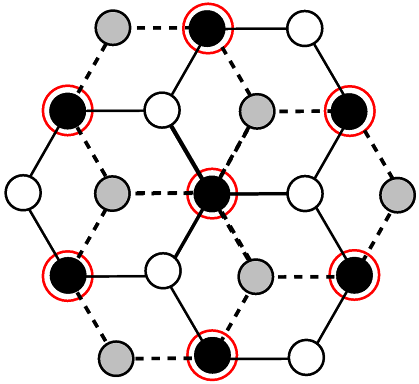
Bound state energy of a Coulomb impurity in gapped bilayer graphene: "Hydrogen atom with a Mexican hat". Brian Skinner, B. I. Shklovskii, M. B. Voloshin, PRB 2014

2. Bilayer graphene.





$t \approx 2.7eV$ - in-plane hopping, $\hbar v_F = 3dt/2$

$t_\perp \approx .3eV \ll t$ - plane-to-plane hopping; $V \ll t_\perp$ - bias.

Easy to "measure" if $V \sim t_\perp$, but rich theory if V is small

$$\mathcal{H}_k = \begin{pmatrix} -V & v_F\tilde{k} & 0 & 0 \\ v_F\tilde{k}^* & -V & t_\perp & 0 \\ 0 & t_\perp & V & v_F\tilde{k} \\ 0 & 0 & v_F\tilde{k}^* & V \end{pmatrix}$$

Spectrum(ugly):

$$\varepsilon_k = \pm\sqrt{V^2 + v_F^2k^2 + \frac{t_\perp^2}{2} \pm \sqrt{4V^2v_F^2k^2 + v_F^2k^2t_\perp^2 + \frac{t_\perp^4}{4}}}$$

$$\tilde{k} = k_x + ik_y$$

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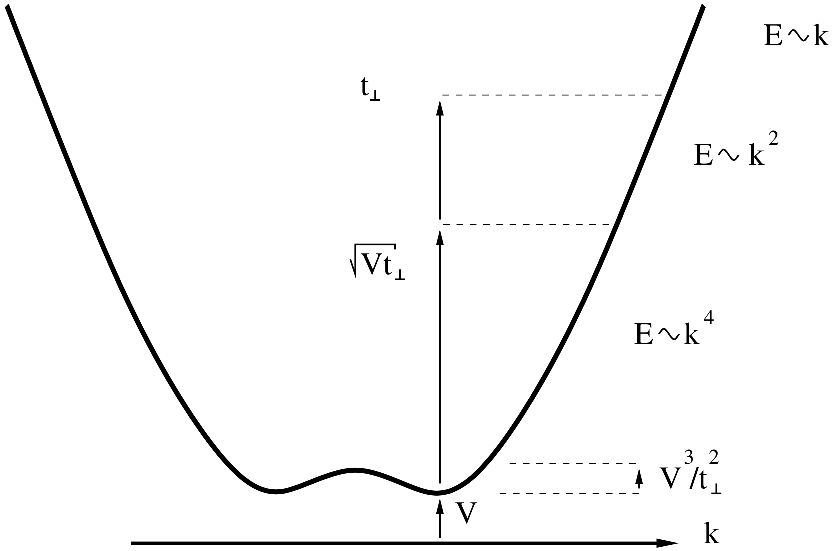

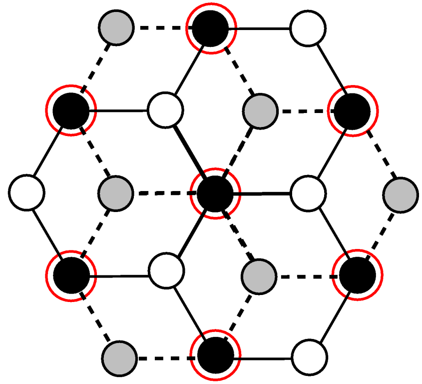

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$\tilde{k} = k_x + ik_y$

For $v_F k \ll \sqrt{Vt_\perp}$:

$$\varepsilon_k \approx V - 2V\frac{v_F^2k^2}{t_\perp^2} + \frac{v_F^4k^4}{2Vt_\perp^2}$$

For $V \ll v_F k \ll t_\perp$:

$$\varepsilon_k \approx \sqrt{V^2 + \frac{v_F^4k^4}{t_\perp^2}}$$

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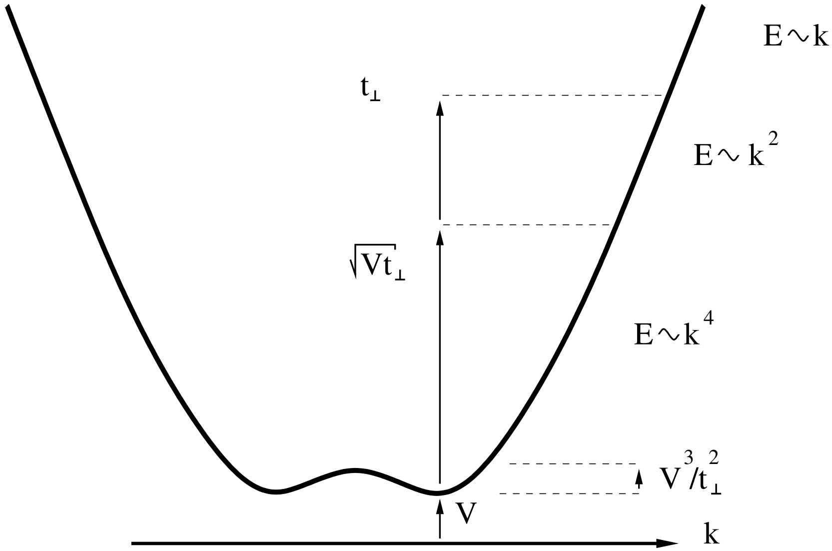
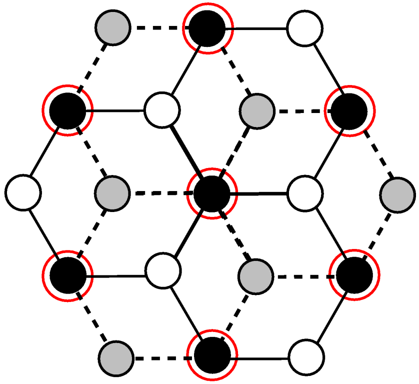




Screening.

Small - to - large distances

$$\frac{e^2}{r} \to \frac{e^2 a_1^2}{r^3} \to \frac{e^2 a_1^2}{r a_2^2}$$

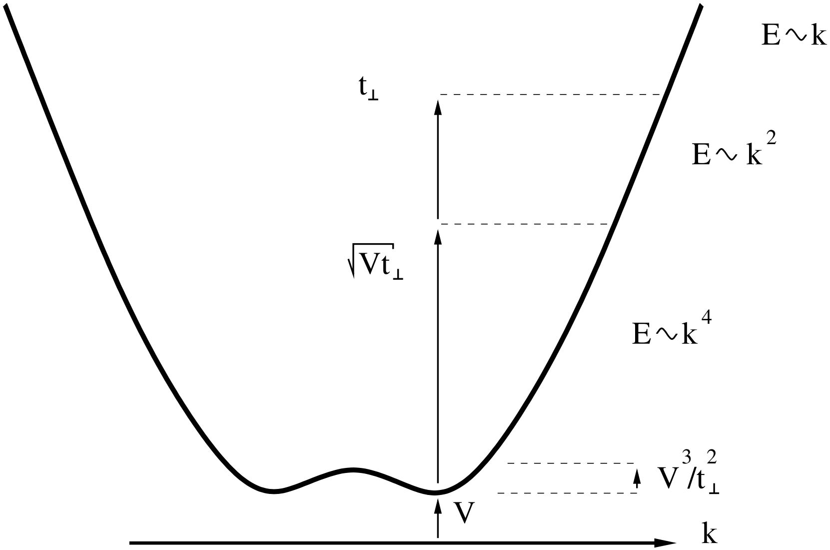
gives

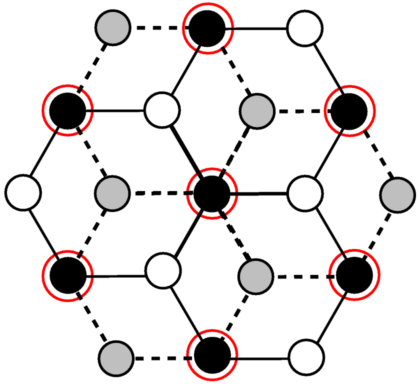
$$a_1 \sim d\frac{t}{t_\perp}, \quad a_2 \sim d\frac{t}{\sqrt{Vt_\perp}}$$

and finally

$$\frac{e^2}{r} \to \frac{V}{t_\perp}\frac{e^2}{r}$$

Coefficients? Never calculated?





3. Intermediate densities.

$$H = \sum \lambda p_j^4 + \sum \frac{e^2}{|r_i - r_j|}$$

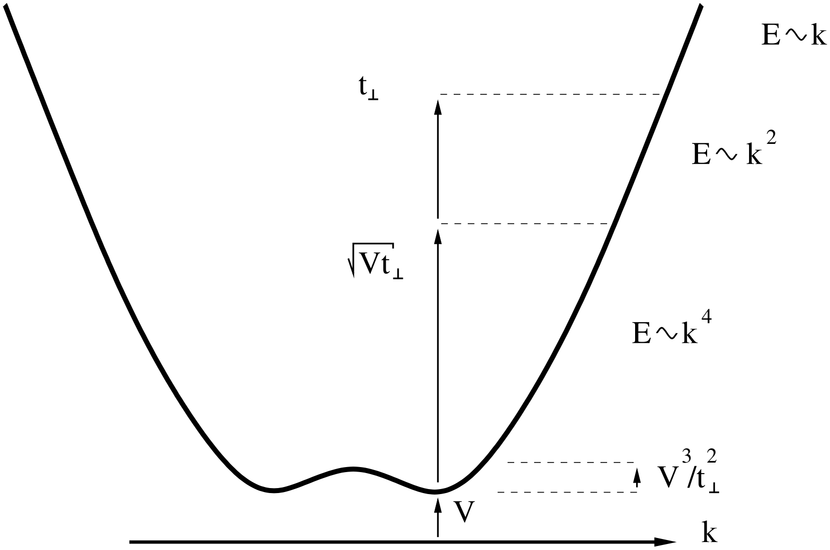
Virial theorem $\langle \lambda p^4 \rangle \sim e^2 \langle \Delta r^2 \rangle / a^3 \ll e^2/a$

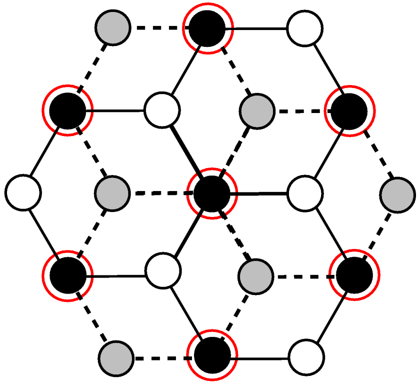
Valid for

$$\left(\frac{V}{t_\perp}\right)^{\frac{2}{3}} \left(\frac{V}{t}\right)^{\frac{2}{3}} \left(\frac{t_\perp}{t}\right)^{\frac{1}{3}} \frac{1}{d} \ll \frac{1}{a} \ll \left(\frac{V}{t}\right)^{\frac{2}{3}} \left(\frac{t_\perp}{t}\right)^{\frac{1}{3}} \frac{1}{d}$$

Here: a-lattice spacing for the Wigner crystal, d-graphene lattice spacing.

At larger a symmetry of the Wigner crystal breaks (Mexican hat).





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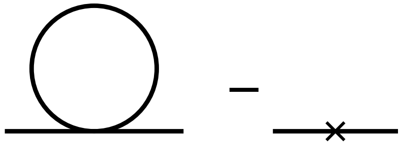
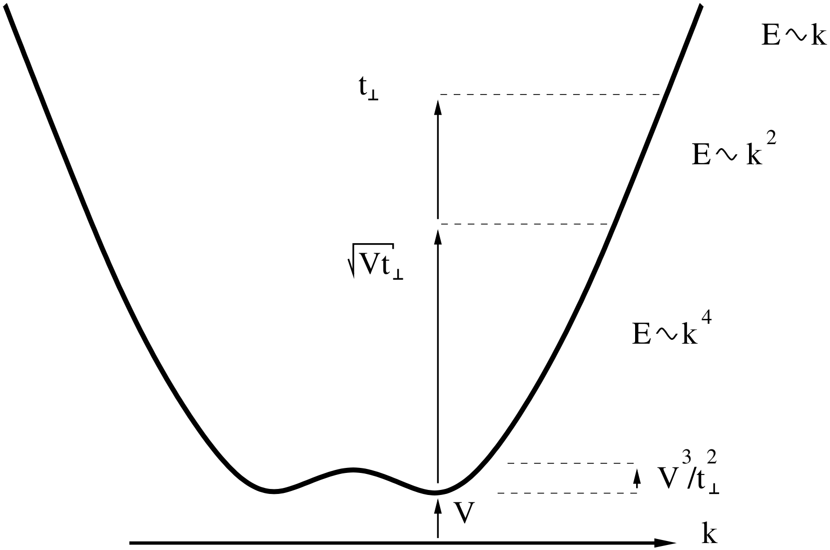


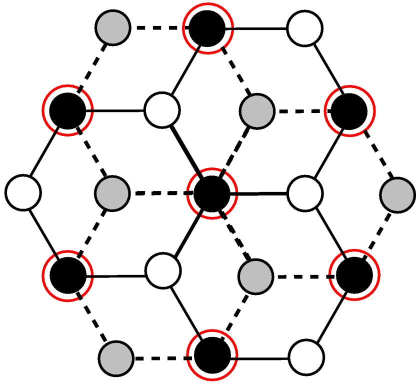
Don't know, what to do?

Mean field: $\sum \lambda p_j^4 \to \sum \lambda p_j^2 \langle p^2 \rangle$

The best possible phonon approximation!

$$\frac{1}{m_{eff}} = \left(2\lambda\hbar \sum_k \frac{\sqrt{m_{eff}\omega_k^2}}{N} \right)^{2/3}$$





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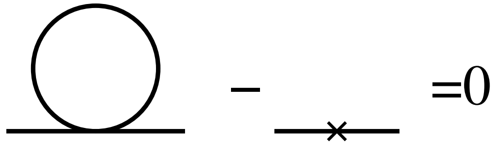


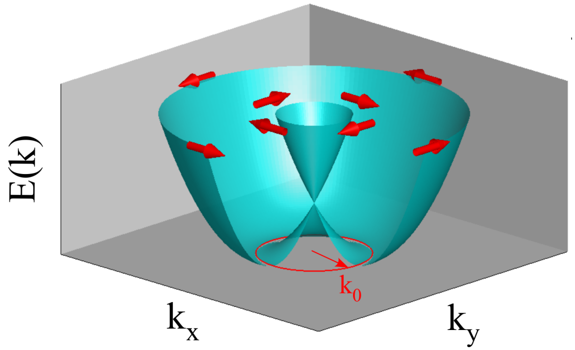
Still phonons are strongly interacting.
And what about the low energy excitations? Plasmons?

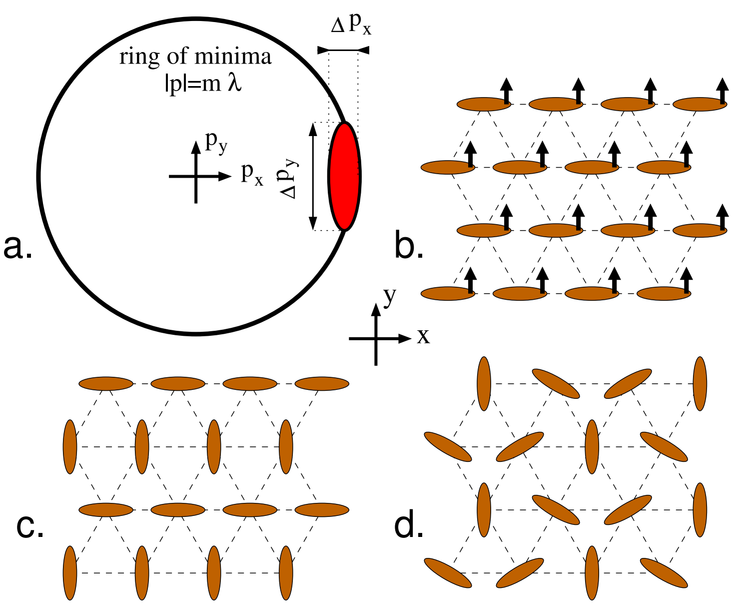
$$\omega_k = [4\pi e^2 k/(\sqrt{3} m a^2)]^{1/2}$$

4. Very low density.

Mexican hat kinetic energy.

Spatial symmetry is broken due to the crystal. Via the uncertainty relation this makes different points at the circle of minima inequivalent. To minimize the interaction (vibrational) energy each electron chooses a particular momentum at the ring of minima!





Absolutely counterintuitive choice of minima distribution: **C.** - is the best! i.e. has the smallest zero point energy

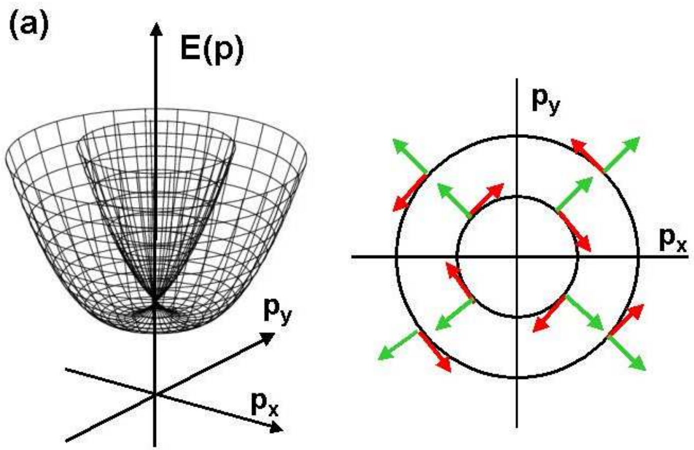
arXiv:1309.2307,
Wigner crystal of a two-dimensional electron gas with a strong spin-orbit interaction,
P.G. Silvestrov, O. Entin-Wohlman, PRB 2014

Spin-orbit interaction

Relativistic correction $\sim \frac{\hbar e}{c^2}(\vec{E} \cdot [\vec{p} \times \vec{\sigma}])$.

Asymmetric quantum well $\langle E_z \rangle \neq 0 \rightarrow$ Rashba Spin-Orbit interaction Hamiltonian

$$H_0 = \frac{p^2}{2m} + \lambda(p_y \sigma_x - p_x \sigma_y).,\qquad E_{p\pm} = \frac{(p \pm m\lambda)^2}{2}.$$



$p^2/2m \sim n,\ \lambda p \sim \lambda\sqrt{n}$ - Spin-orbit is more important at low density, and the Wigner crystal exists only at low density!

Wigner + Spin-orbit

Rashba Spin-Orbit interaction Hamiltonian

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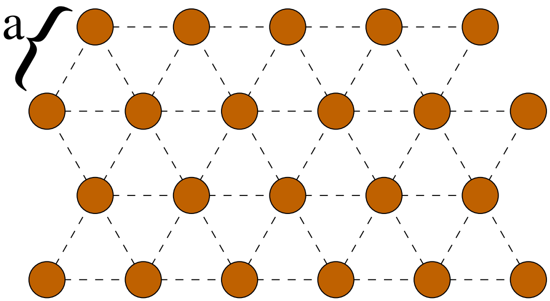
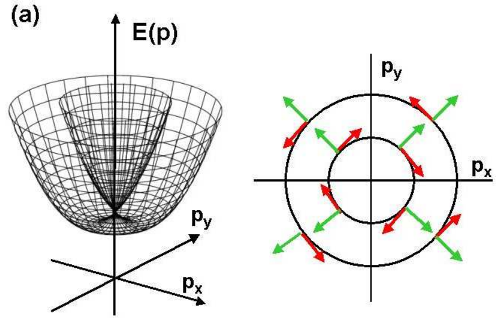
Relativistic correction $\sim \frac{\hbar e}{c^2}(\vec{E} \cdot [\vec{p} \times \vec{\sigma}])$, asymmetric quantum





$$H = \sum_i H_{0i} + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

Subband splitting is large compared to fluctuation energy, $m\lambda^2 \gg \hbar\sqrt{e^2/ma^3}$**.**

Electron may choose a point at the degenerate minimum.

Wigner + Spin-orbit

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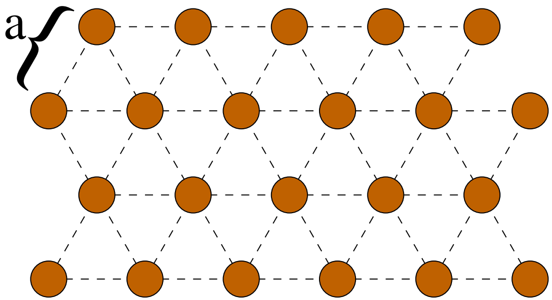
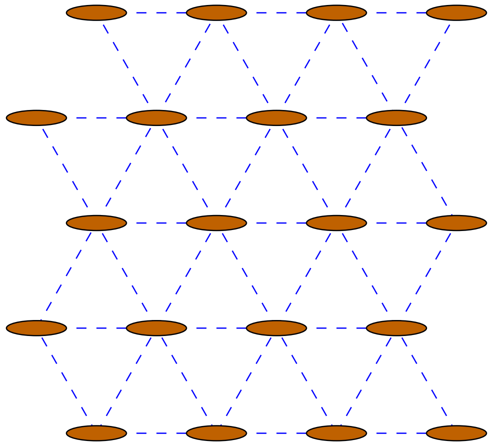
$$H_0 = \frac{p^2}{2m} + \lambda(p_y\sigma_x - p_x\sigma_y), \qquad E_{p\pm} = \frac{(p \pm m\lambda)^2}{2}.$$

Relativistic correction $\sim \frac{\hbar e}{c^2}(\vec{E}\cdot[\vec{p}\times\vec{\sigma}])$, asymmetric quantum well $\langle E_z \rangle \neq 0$.





$$H = \sum_i H_{0i} + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

Subband splitting is large compared to fluctuation energy, $m\lambda^2 \gg \hbar\sqrt{e^2/ma^3}$**.**

Electron may choose a point at the degenerate minimum.

Let us save some energy!

Wigner + Spin-orbit

Rashba Spin-Orbit interaction Hamiltonian

$$H_0 = \frac{p^2}{2m} + \lambda(p_y\sigma_x - p_x\sigma_y), \quad E_{p\pm} = \frac{(p \pm m\lambda)^2}{2}.$$

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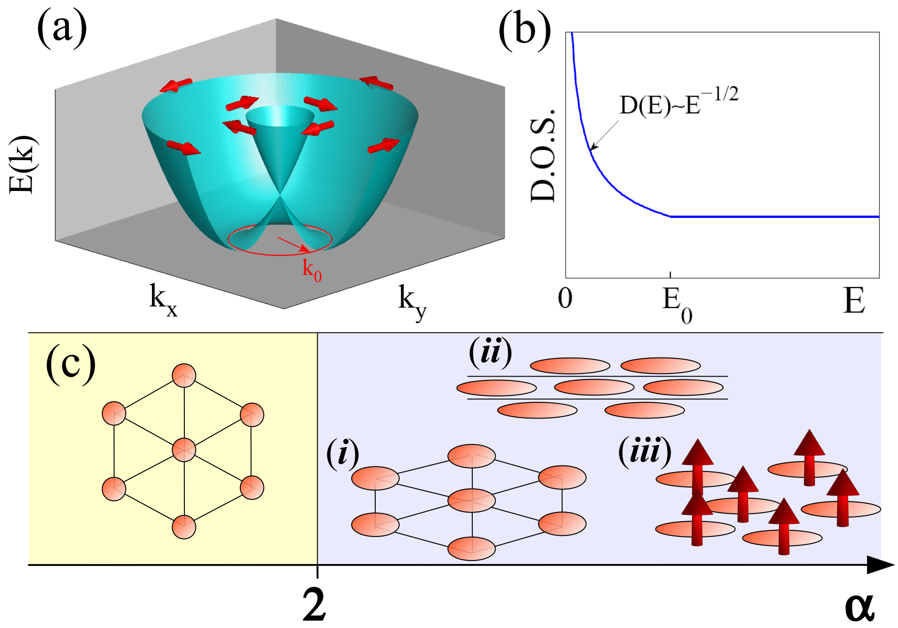

Berg,Rudner,Kivelson, PRB 2012

Spin-orbit stabilizes a (very asymmetric) Wigner crystal even for short range interaction

$$V \sim 1/r^{\alpha}, \ \alpha > 2$$

Wigner + Spin-orbit

Rashba Spin-Orbit interaction Hamiltonian

$$H_0 = \frac{p^2}{2m} + \lambda(p_y\sigma_x - p_x\sigma_y), \quad E_{p\pm} = \frac{(p \pm m\lambda)^2}{2}.$$

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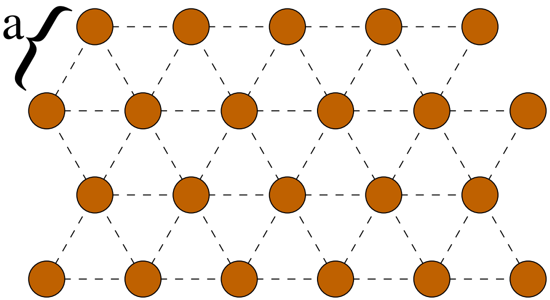
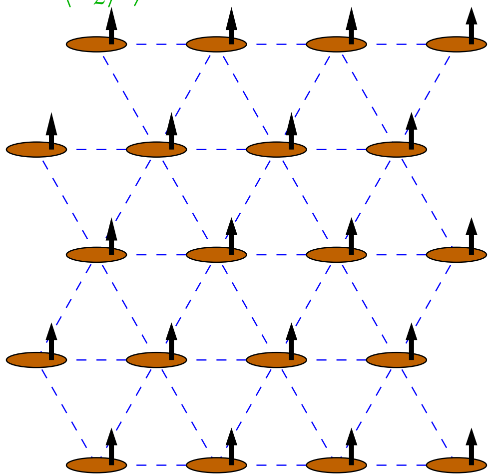




$$H = \sum_i H_{0i} + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

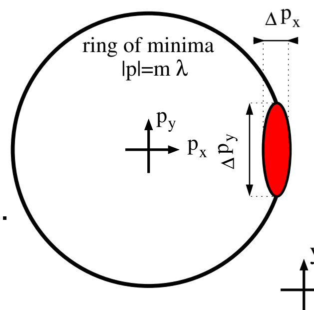
Let the subband splitting be large compared to the fluctuation energy, and

$$m\lambda^2 \gg \hbar\sqrt{e^2/ma^3}, \quad |p_x - m\lambda| \lesssim \Delta p_x, \quad |p_y| \lesssim \Delta p_y, \quad \Delta p_x \ll \Delta p_y \ll m\lambda$$

$$\Delta x \sim \hbar/\Delta p_x \gg \Delta y \sim \hbar/\Delta p_y$$

Similar to the system with anisotropic mass, one light and another very heavy!

a.



Wigner + Spin-orbit

Rashba Spin-Orbit interaction Hamiltonian

$$H_0 = \frac{p^2}{2m} + \lambda(p_y\sigma_x - p_x\sigma_y), \qquad E_{p\pm} = \frac{(p \pm m\lambda)^2}{2}.$$

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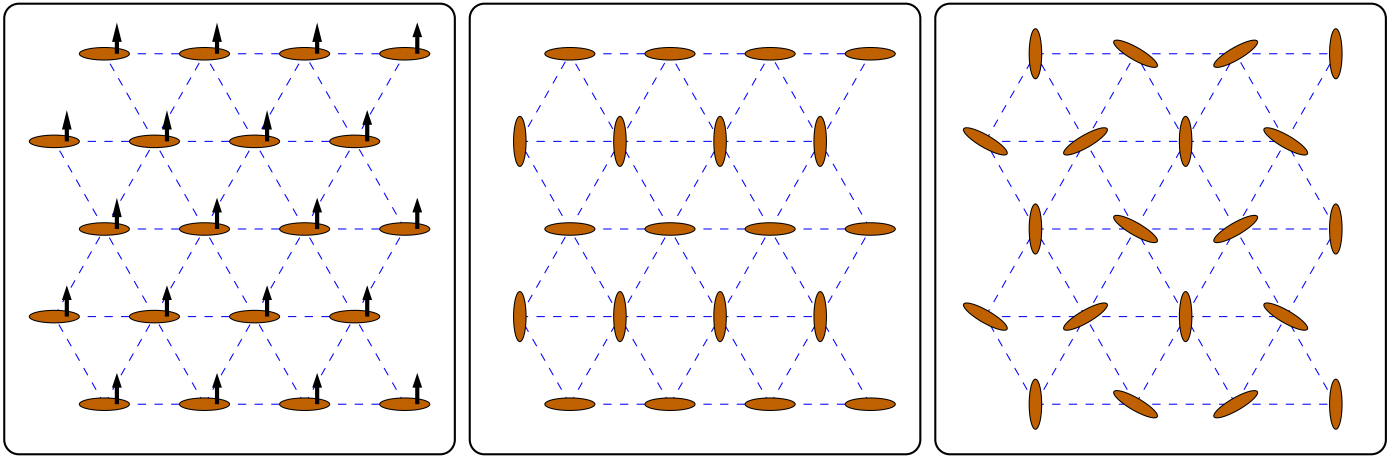
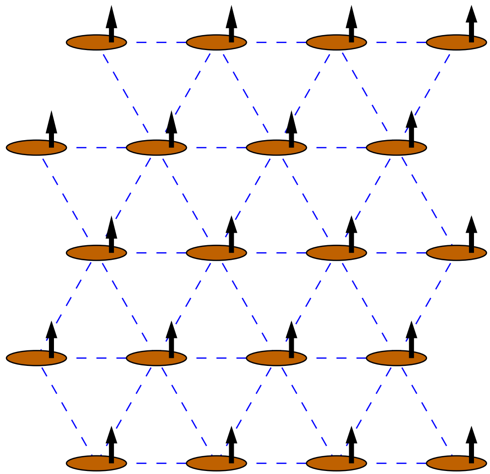


$$H = \sum_i H_{0i} + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

Similar to the system with anisotropic mass, one light and another very heavy!

But which is which?

Phonon spectrum



Effective Hamiltonian for the spontaneously broken symmetry phase of the Wigner crystal

$$H = \sum_i H_{0i} + \sum_{i<j} \frac{e^2}{|r_i - r_j|}$$

Reduced Hilbert space (lower subband).
After shift of momentum $p_x \to p_x + m\lambda$
we get $H_{0i} \to H_{0i}^{eff} = p_x^2/2m$, and

$$\frac{e^2}{|r_i - r_j|} \to \frac{e^2}{|R_{ij} + r_{ij}|} \approx \frac{e^2}{R_{ij}} - \frac{e^2(\vec{r}_{ij} \cdot \vec{R}_{ij})}{R_{ij}^2} - \frac{e^2 r_{ij}^2}{2R_{ij}^3} + 3e^2 \frac{(\vec{r}_{ij} \cdot \vec{R}_{ij})^2}{2R_{ij}^5}$$

where $\vec{r}_{ij} = \vec{r}_i - \vec{r}_j$, $\vec{R}_{ij} = \vec{R}_i - \vec{R}_j$. Since where is no p_y^2 in the Hamiltonian, $y_i \equiv 0$.

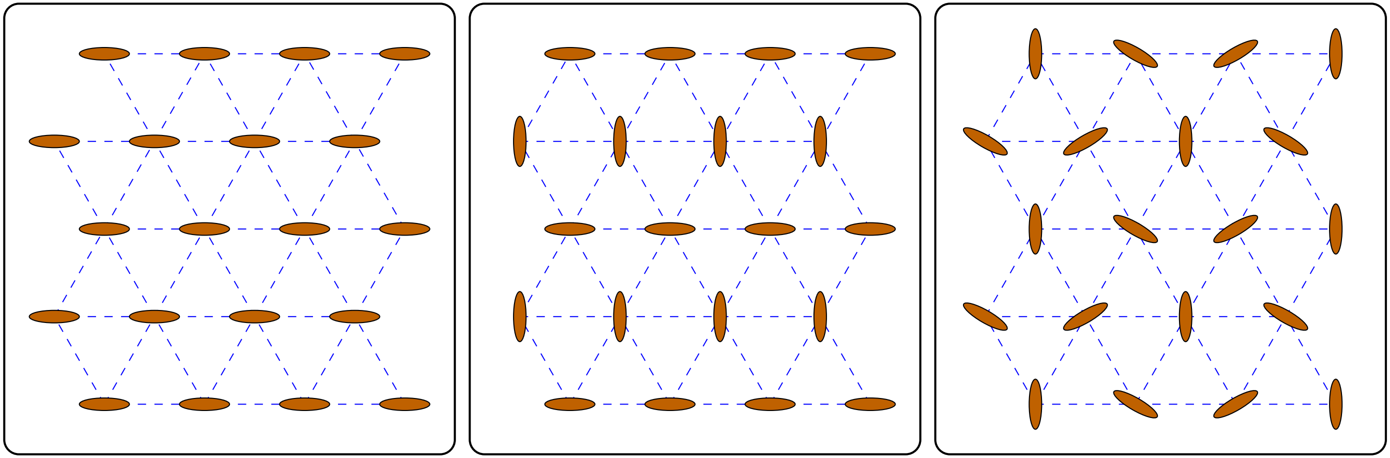
$$\mathcal{H}_{\text{eff}} = \sum_i \left(\frac{p_{x_i}^2}{2m} + \frac{m\omega_0^2 x_i^2}{2} \right) + e^2 \sum_{i<j} \frac{x_i x_j}{R_{ij}^3} \left(1 - 3\frac{X_{ij}^2}{R_{ij}^2} \right)$$

$\omega_0 = \sqrt{\gamma e^2/(ma^3)}$, where $\gamma = \sum_{i \neq 0} a^3/(2R_i^3) = 5.5171$.

Twice less degrees of freedom! Will tell nothing about the rest!

Standard calculation of the phonon $n = 0$ fluctuation energy.

Phonon spectrum



Fluctuation energy per electron!

$0.951\hbar\omega_0$	$0.939\hbar\omega_0$	$0.971\hbar\omega_0$
$1-0.049$	$1-0.061$	$1-0.029$

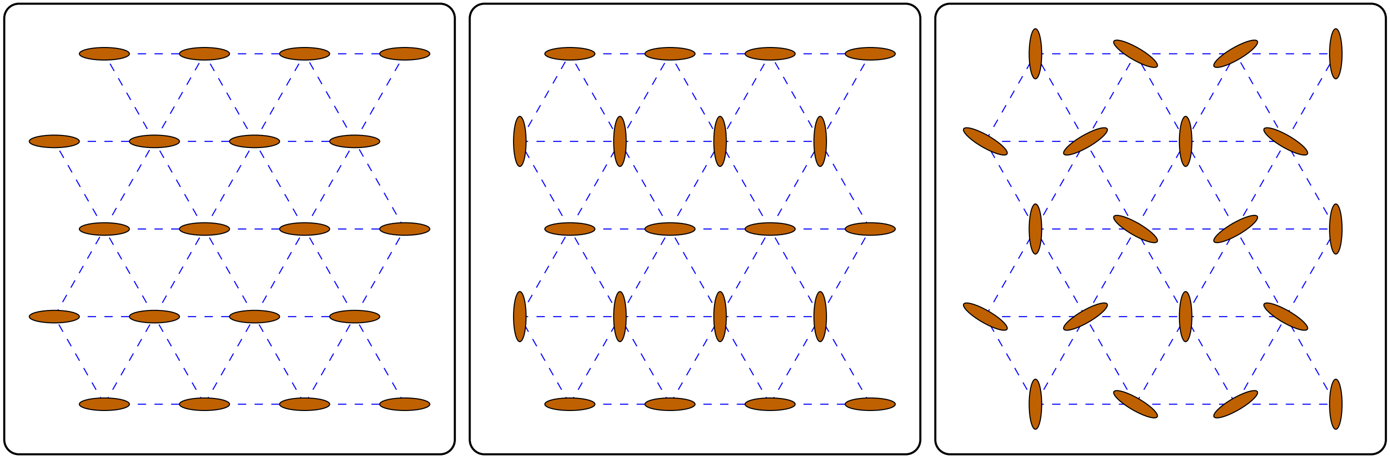
(numerical) averaging of the phonon energy $\hbar\omega(\mathrm{k})$ over the Brillouin zone

90-degrees happens to be a minimum

We are minimizing the total vibrational energy, not the electrostatic energy of charged rods!

In fact: Minimizing the vibrational energy for 1-parameter, 2-parameter, 3-parameter distribution of soft directions.

Phonon spectrum



Fluctuation energy per electron!

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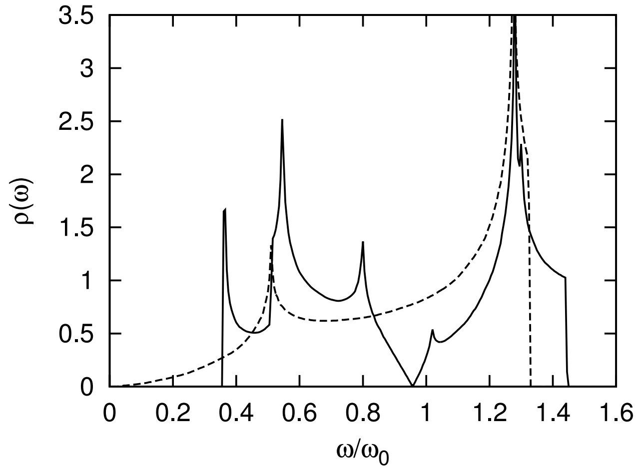
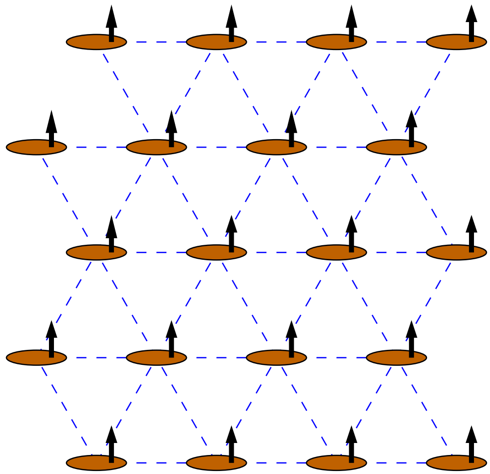


Density of phonons vs. frequency
(also experimentally measurable)

Van Hove singularities:
$\Theta(\omega)$ - edge
$\ln(\omega)$ - saddle point
$1/\sqrt{\omega}$ - non-existing in 2d?
+ Dirac crossing point

Still does not explain, why one is better than another?

Phonon spectrum



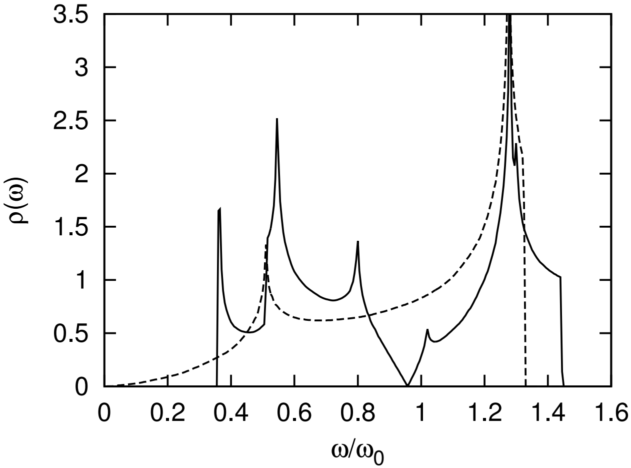
Metastable state

Plasmon spectrum

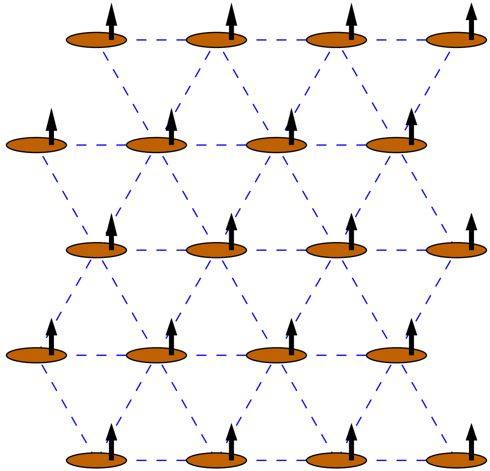
The only configuration having acoustic plasmons!

$$\omega_k = [8\pi e^2/(\sqrt{3}ma^2)]^{1/2}|k_x|/\sqrt{k}$$

$\omega \sim \sqrt{k}$ - known. Anisotropy, $\omega \sim k_x/k$ - new!



Squeezing the crystal



Squeezing - natural, after the symmetry was broken.
Want to preserve the charge density (α - a small number)

$$\vec{R}_i = (R_{x_i}, R_{y_i}) \to \tilde{\vec{R}}_i = ((1+\alpha)R_{x_i}, R_{y_i}/(1+\alpha)),$$

Coulomb energy per electron

$$U(\alpha) = \frac{e^2}{a}(c_0 + \alpha^2 c_2 + \cdots) \approx \frac{e^2}{a}(c_0 + .527\,\alpha^2 + \cdots)$$

Phonon zero-point energy per electron

$$K(\alpha) = \hbar\omega(d_0 - \alpha d_1 + ...) \approx \hbar\omega(0.482 - 0.236\,\alpha)$$

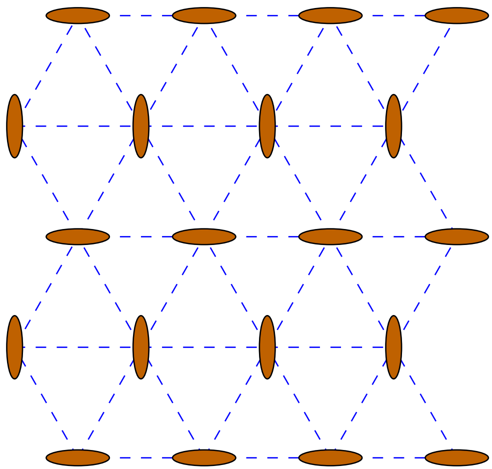
Minimizing the total energy, $U(\alpha) + K(\alpha)$, we find

$$\alpha_c = \frac{\hbar\omega}{2e^2/a}\frac{d_1}{c_2} = \sqrt{\frac{\gamma a_B}{4a}}\frac{d_1}{c_2} \neq 0$$

α_c, scales like $a^{-1/2} \sim n^{1/4}$, but since $m\lambda^2 \gg \hbar\omega$

$$\alpha_c \ll \left(\frac{\hbar\lambda}{e^2}\right)^{2/3},$$

unlike in the case of Berg *et. al*



5. Conclusions

1. Wigner crystal exists in gated bilayer graphene.

2. There exist two! different phases of the crystal.

3. Plenty of open problems. Both for Mexican hat and for p^4 regimes.

4. What to do with $\lambda \sum \mathrm{p}^4$? May be numerics?

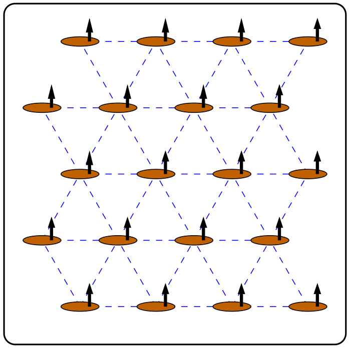
5. Eh, $\cdots$ Experiment of course $\cdots$

5. Conclusions: What to do?

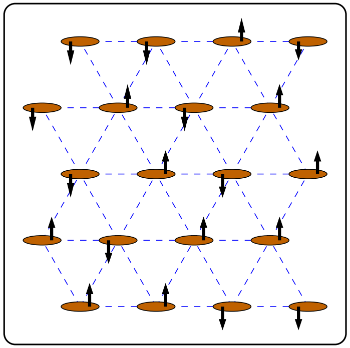
1. Soft modes. What about fluctuations in light masses direction = ellipses orientations?

Acoustic modes are here.

2. Spin flips



or



?

Even what is the spin ground state?

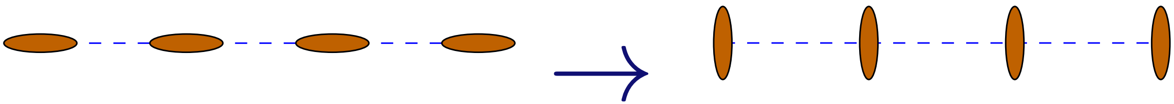
Next:

3. Perturbation theory in Spin-orbit. How this all started?

4. Magnetic field. If I would be experimentalist?

5. 1-dimensional Wigner crystal.

1-dimensional chanel with parabolic confinement. Phase transition.



6. Even, what happens with $r_s = 35$ in case of spin-orbit?