What is Solid State Physics?

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PHYS 624: Introduction to Solid State Physics
http://www.physics.udel.edu/~bnikolic/teaching/phys624/phys624.html
The general theory of quantum mechanics is now almost complete. The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble."

P. A. M. Dirac 1929

$\hat{H} = \sum_{n=1}^{N_N} \frac{P_n^2}{2M_n} + \frac{e^2}{2} \sum_{n\neq m=1}^{N_N} \frac{Z_nZ_m}{|R_n - R_m|}$

$T_N$: motion of nuclei $V_{N-N}$: interaction between nuclei

$+ \sum_{i=1}^{N_e} \frac{p_i^2}{2M_i} + \frac{e^2}{2} \sum_{i \neq j=1}^{N_e} \frac{1}{|r_i - r_j|} - e^2 \sum_{n=1}^{N_N} \sum_{i=1}^{N_e} \frac{Z_n}{|R_n - r_i|}$

$T_e$: motion of electrons $V_{e-e}$: interaction between electrons $V_{e-N}$: interaction between electrons and nuclei

Quantum Hamiltonian of Solid State Physics
Even for chemist, the task of solving the Schrödinger equation for modest multi-electron atoms proves insurmountable without bold approximations.

The problem facing condensed matter physicist is qualitatively more severe:

\[ N_N \sim N_e \sim 10^{23} \]

Energy scales: \(10^{-2}\) eV \(-10^4\) eV

CM Theorist is entrapped in the “thermodynamic limit”
The Way Out:
Separate Length and Energy Scales

- **Energy:** \( \omega, T < 1 \text{ eV} \)

- **Time:** \( \Delta \tau \sim \frac{\hbar}{1 \text{ eV}} \sim \frac{\hbar}{10^{-19} \text{ J}} \sim 10^{-15} \text{ s} \)

- **Length:** \( |x_i - x_j|, q^{-1} \gg 1 \text{ Å} \)

forget about atom formation + forget about crystal formation

+ Born-Oppenheimer approximation for \( \frac{m_e}{m_N} \ll 1 \)

\[ \hat{H}_{\text{electronic}} = \hat{T}_e + \hat{V}_{e-I} + \hat{V}_{e-e}, \quad \hat{V}_{e-I}(\mathbf{r} + \mathbf{r}_n) = \hat{V}_{e-I}(\mathbf{r}), \quad \mathbf{r}_n = n_1 \mathbf{a}_1 + n_2 \mathbf{a}_2 + n_3 \mathbf{a}_3 \]
“Non-Interacting” Electrons in Solids: Band Structure Calculations

In band structure calculations electron-electron interaction is approximated in such a way that the resulting problem becomes an effective single-particle quantum mechanical problem ...

\[ \hat{H}_{\text{IE,H,LDA}}(\mathbf{r}) \phi_{k\mathbf{b}}^{\text{IE,H,LDA}}(\mathbf{r}) = \varepsilon_{\text{IE,H,LDA}}(\mathbf{k}, b) \phi_{k\mathbf{b}}^{\text{IE,H,LDA}}(\mathbf{r}) \]

\[ \hat{H}_{\text{electronic}} = \hat{T}_e + \hat{V}_{e-I} + \hat{V}_{e-e} \]

\[ \hat{H}_{\text{IE}} = \hat{T}_e + \hat{V}_{e-I} = \sum_{i=1}^{N_e} H_{\text{IE}}(\mathbf{r}_i) \]

\[ \hat{H}_{\text{Hartree}} = \hat{T}_e + \hat{V}_{e-I} + e^2 \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}, \quad n(\mathbf{r}) = \sum_{\varepsilon^H(\mathbf{k}, b) \leq E_F} |\phi_{k\mathbf{b}}^H(\mathbf{r})|^2 = n(\mathbf{r} + \mathbf{r}_n) \]

\[ \hat{H}_{\text{LDA}} = \hat{H}_{\text{IE}}(\mathbf{r}) + e^2 \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\delta E_{\text{xc}}^{\text{LDA}}[n_e]}{\delta n(\mathbf{r})}, \quad E_{\text{xc}}^{\text{LDA}}[n_e] = \int d\mathbf{r} n(\mathbf{r}) e_{\text{xc}}^{\text{LDA}}(n(\mathbf{r})) \]
From Many-Body Problem to Density Functional Theory (and its LDA approximation)

“Classical” Schrödinger equation approach:

\[ V(\mathbf{r}) \Rightarrow \Psi(r_1,\ldots,r_{N_e}) \Rightarrow \text{average of observables} \]

Example: Particle density

\[ n(\mathbf{r}) = N \int dr_2 \int dr_3 \cdots \int dr_N \Psi^*(\mathbf{r},\ldots,r_{N_e}) \Psi(\mathbf{r},\ldots,r_{N_e}) \]

DFT approach (Kohn-Hohenberg):

\[ n_0(\mathbf{r}) \Rightarrow \Psi_0(r_1,\ldots,r_{N_e}) \Rightarrow V(\mathbf{r}) \]

\[ \Psi_0(r_1,\ldots,r_{N_e}) \equiv \Psi_0[n_0(\mathbf{r})] \]
Many-Body Wave Function of Fermions

"It is with a heavy heart, I have decided that Fermi-Dirac, and not Einstein is the correct statistics, and I have decided to write a short note on paramagnetism."  
W. Pauli in a letter to Schrödinger (1925).

All electrons in the Universe are identical → two physical situations that differ only by interchange of identical particles are indistinguishable!

\[ P_{ij} \Psi(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_n) = P_{ij} \Psi(x_1, \ldots, x_j, \ldots, x_i, \ldots, x_n) \]

\[ \hat{P}_{ij} \hat{H} = \hat{H} \hat{P}_{ij} \leftarrow \langle \Psi | \hat{A} | \Psi \rangle = \langle \Psi | \hat{P}_{ij}^\dagger \hat{A} \hat{P} | \Psi \rangle \iff \hat{P}_{ij} \hat{A} = \hat{A} \hat{P} \]

\[ \left| \Psi_S \right> \quad \left| \Psi_A \right> \]

\[ \hat{P}_\alpha \left| \Psi_S \right> = \left| \Psi_S \right>, \quad \hat{P}_\alpha \left| \Psi_A \right> = \begin{cases} + \left| \Psi_A \right>, & \hat{P}_\alpha \text{ is even} \\ - \left| \Psi_A \right>, & \hat{P}_\alpha \text{ is odd} \end{cases} \]

\[ \hat{P}_\alpha \hat{A} \left| \Psi \right> = \hat{A} \left| \Psi \right>, \quad \hat{A} = \frac{1}{N!} \sum_{\alpha} \varepsilon_\alpha \hat{P}_\alpha \]

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Pauli Exclusion Principle

"There is no one fact in the physical world which has greater impact on the way things are, than the Pauli exclusion principle." I. Duck and E. C. G. Sudarshan, “Pauli and the Spin-Statistics Theorem” (World Scientific, Singapore, 1998).

Two identical fermions cannot occupy the same quantum-mechanical state:

\[ \hat{H} = \hat{h}_1 + \hat{h}_2 + \ldots + \hat{h}_N \]

\[ \hat{h}_i \left| \phi_i \right\rangle = e_i \left| \phi_i \right\rangle \Rightarrow \hat{H} \left| \Phi_{1,2,\ldots,N_e} \right\rangle = E_{1,2,\ldots,N_e} \left| \Phi_{1,2,\ldots,N_e} \right\rangle \]

\[ E_{1,2,\ldots,N_e} = e_1 + e_2 + \ldots + e_{N_e} \]

\[ \left| \Phi_{1,2,\ldots,N_e} \right\rangle = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(1) & \ldots & \phi_{N_e}(1) \\ \vdots & \ddots & \vdots \\ \phi_1(N_e) & \ldots & \phi_{N_e}(N_e) \end{vmatrix} \Rightarrow n_{k\sigma} = \frac{1}{e^{(\varepsilon_{k\sigma} - \mu)/k_B T} + 1} \]
QUESTION: In QM we learn that the ground state must have the symmetry of the Hamiltonian - so there can't be a dipole moment (interactions between ions and electrons have no preferred direction in space). On the other hand, ammonia molecule obviously has dipole moment? 

RESOLUTION: The ammonia molecule ground state is a superposition of states, so as to recover the symmetry of the Hamiltonian. However, at short time-scale molecule can be trapped in one of the states (due to large potential barrier for tunneling between the states), and we measure non-zero dipole moment.

QUESTION: What about larger molecules (> 10 atoms) which have definite three-dimensional structures which break the symmetry of the Hamiltonian?

RESOLUTION: We cannot understand the structure of molecules starting from Quantum Mechanics of elementary particles - we need additional theoretical ideas (emergent phenomena)!
Phases of matter often exhibit much less symmetry than underlying microscopic equations.

**Example:** Water exhibits full translational and rotational symmetry of Newton’s or Schrödinger’s equations; Ice, however, is only invariant under the discrete translational and rotational group of its crystal lattice → translational and rotational symmetry of the microscopic equations have been spontaneously broken!

**Order Parameter Paradigm (L. D. Landau, 1940s):** Development of phases in a material can be described by the emergence of an "order parameter" (which fluctuates strongly at classical critical points):

\[ M, \quad \Psi(r) = \sqrt{\rho_s} e^{i\phi}, \quad \rho_{\text{typical}}(\omega, r) \]
Positive ions arrange to break translational and rotational symmetry – it is energetically favorable to break the symmetry in the same way in different parts of the system → because of broken symmetries the solids are rigid (i.e., solid).

In crystalline solids discrete subgroups of the translational and rotational group are preserved:

- **Metals**: $T \to 0 \Rightarrow \sigma \neq 0$
- **Insulators**: $T \to 0 \Rightarrow \sigma = 0$
- **Superconductors**: $T < T_c \Rightarrow \sigma \to \infty$ + Meissner effect

All of these three phases can be further subdivided into ferromagnets or antiferromagnets, which break the spin rotational invariance.

Other hard matter: quasicrystals (translational order completely broken; rotational symmetry broken to 5-fold discrete subgroup) and glasses (rigid but random arrangement of atoms; in fact, they are “non-equilibrium phase” – a ‘snapshot’ of liquids).
- **Liquids** (full translational and rotational group preserved) vs. **Solids** (preserve only a discrete subgroups).

- **Liquid crystalline phase** - translational and rotational symmetry is broken to a combination of discrete and continuous subgroups.

- **Polymers** - extremely long molecules that can exist in solution or a chemical reaction can take place which cross-links them, thereby forming a gel.
Complexity and Diversity of Crystalline Phases

- No. inequivalent Atoms/unit cell
  - 1: Si, Elemental Insulator
  - 2: MgB$_2$
  - 3: UPd$_2$Al$_3$
  - 4: YBa$_2$Cu$_3$O$_7$
- Complexity: Simplest Biological Molecules

- # different types of compound:
  - 10$^2$
  - 10$^4$
  - 10$^6$
  - 10$^8$
Broken Symmetries and Rigidity

- Phase of a Cooper pair develops a rigidity → it costs energy to bend phase → superflow of particles is directly proportional to gradient of phase:

\[ U(x) \sim \frac{1}{2} \rho_s [\nabla \phi(x)]^2 \Rightarrow j_s = \rho_s \nabla \phi_s \]

<table>
<thead>
<tr>
<th>Phase</th>
<th>Broken Symmetry</th>
<th>Rigidity/Superflow</th>
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<tbody>
<tr>
<td>crystal superfluid</td>
<td>translation gauge</td>
<td>Momentum (sheer stress)</td>
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<tr>
<td>superconductivity</td>
<td>EM gauge spin rotation</td>
<td>matter charge spin (x-y magnets only)</td>
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<tr>
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<td>angular momentum</td>
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<td>translation</td>
<td>Energy?</td>
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<td>?</td>
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High Energy Physics: Lessons from Low Energy Experiments

Anderson Higgs Mechanism

Asymptotic Freedom in the Physics of Quark Confinement
Experimental Probes of Condensed Matter Phases

- **Scattering**: Send neutrons or X-rays into the system with prescribed energy and momentum; measure the energy and momentum of the outgoing neutrons or X-rays.

- **NMR**: Apply static magnetic field $B$ and measure absorption and emission of magnetic radiation at frequencies of the order of $\omega_c = \frac{geB}{m}$.

- **Thermodynamics**: Measure the response of macroscopic variables (energy, volume, etc.) to variations of the temperature, pressure, etc.

- **Transport**: Set up a potential $\nabla \varphi$ or thermal gradient $\nabla T$ and measure the electrical or heat current. The gradients can be held constant or made to oscillate at finite frequency.
Weakly vs. Strongly Correlated Electrons

- Exchange and Correlation in 3D gas of noninteracting fermions:
  \[ g_{\sigma,\sigma}(\mathbf{r},\mathbf{r}') = -\left[ \frac{3n}{2} \frac{\sin x - x \cos x}{x^3} \right]^2 \]
  \[ g_{\sigma,-\sigma}(\mathbf{r},\mathbf{r}') = 0, \quad x = k_F |\mathbf{r} - \mathbf{r}'| \]

- Correlated Electron System: \( g_{\sigma,-\sigma}(\mathbf{r},\mathbf{r}') \neq 0 \)

- Strongly Correlated Electron System: \( g_{\sigma,\sigma}(\mathbf{r},\mathbf{r}') \sim g_{\sigma,-\sigma}(\mathbf{r},\mathbf{r}') \)

- Example of new strongly correlated matter:
  Fractional Quantum Hall Effect
Bloch theory of electrons in metals: completely independent particles (e.g., even more sophisticated Hartree-Fock fails badly because dynamic correlations cancel miraculously exchange effects).

Why is long-range strong Coulomb interaction marginal in metals?

1. In system with itinerant electrons, Coulomb interaction is very effectively screened on the length scale of $k_F^{-1}$.

2. In the presence of Fermi surface the scattering rate between electrons with energy $E_F + \omega$ vanished proportional to $\omega^2$ since the Pauli principle strongly reduces the number of scattering channels that are compatible with energy and momentum conservations – Landau “quasielectrons” live very long!
Bohm and Pines (1953): separate strongly interacting gas into two independent sets of excitations (progenitor of the idea of renormalization!)

\[ \hbar \omega_p \sim 6 \text{eV} \]

- High energy \( \omega \) plasmon modes
- E-Quasiparticles

- Electron-hole continuum
- \( q = 2k_F \)

\[ \vec{k} \rightarrow \vec{k} + \vec{Q} \]

- High energy \( \rightarrow \) plasmon
- Low energy \( \rightarrow \) electron-hole pairs
Quantum Criticality in Your Car Bumper

\[ \tau \sim \frac{\hbar}{k_B T} \]

- $\rho(T)$
- $T_0(x)$
- Critical Point
- AFM
- Heavy electrons
- Quantum Critical Point
- $X_c$
Quantum Criticality: Example of High Tc Superconductors