Technische Universität Berlin
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http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/

Theoretical Material Science: exercise sheet 11

Return: Monday, July 7th in the exercise

Exercise 25 (8 points): *Master equation*
The master equation for an N-state system reads

$$\frac{d}{dt}P_n(t) = \sum_{m=1}^{N} \Big(W_{nm}P_m(t) - W_{mn}P_n(t) \Big), \tag{1}$$

where $P_n(t)$ is the probability of finding the system in state n at time t and W_{nm} are the transition rates from state m to state n.

(a) Show that the master equation conserves probability.

(b) Write Eq. (1) as a matrix equation, $\dot{\mathbf{P}} = \mathbf{T} \cdot \mathbf{P}$ and give the elements of matrix $\mathbf{T}$. What is physical significance of the null-space of $\mathbf{T}$?

A single-electron transitor consists of a quantum dot coupled to two leads through tunnel barriers. Consider a situation in which there is just a single relevant electronic state on the quantum dot, which can be either empty or occupied, and assume that electrons tunnel from the left lead to the dot with rate Γ_L, and from the dot to the right lead with rate Γ_R.

(c) Construct a master equation for $P_0(t)$ and $P_1(t)$, the probabilities of finding the dot empty and occupied at time t.

(d) Solve this master equation for probability $P_0(t)$ starting from an empty dot at $t = 0$.

(e) Calculate the steady state of the system. What is the corresponding steady-state current?

Exercise 26 (4 points): *Hund's rules*

(a) Show that Hund's rules for a shell of angular momentum l containing n electrons can be summarised in the formulae:

$$\begin{aligned} S &= \frac{1}{2}\left[(2l+1) - |2l+1-n|\right], \\ L &= S|2l+1-n|, \\ J &= |2l-n|S. \end{aligned}$$

(b) Verify that the two ways of counting the degeneracy of given LS-multiplet give the same answer; i.e. verify that

$$(2L+1)(2S+1) = \sum_{|L-S|}^{L+S} (2J+1)$$

Please turn over!⟶

- **Webpage of the lecture:** http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/
- **Lecture:** Tue. & Fri., 10:00 a.m.-12:00 p.m. in room EW 203, TU Berlin
- **Exercise:** Mon., 14:00 a.m. in room H 1029
- **Literature:**
  - Ashcroft, Mermin, David: Solid state physics, Saunders College, Philadelphia, 1981
  - Kittel: Quantum theory of solids,Wiley, New York, 1963
  - Ziman: Principles of the theory of solids, Cambridge University Press, Cambridge, 1964
  - Ibach, Lueth: Solid-state physics: an introduction to principles of materials science, Springer, Berlin, 1995
  - Madelung: Festkörpertheorie, Springer, Berlin, 1972
  - Scherz: Quantenmechanik, Teubner, Stuttgart, 1999
  - Dreizler, Gross: Density functional theory: an approach to the quantum many-body problem, Springer, Berlin, 1990
  - Parr, Yang: Density-functional theory of atoms and molecules, Oxford University Press, Oxford, 1994
  - Anderson: Basic notations of condensed matter physics, Benjamin/Cummings, London, 1984
  - Marder: Condensed matter physics, Wiley, New York, 2000
  - Martin: Electronic Structure, Cambridge University Press, Cambridge, 2004
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler: on appointment
  - Dr. Volker Blum: on appointment
  - Philipp Zedler: Wed, 11:00 - 12:00 a.m. in room EW 711
  - Dr. Clive Emary, Wed, 16:00 - 17:00 in room EW 705