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Acknowledgments

One of the symptoms of an approaching nervous breakdown is the belief that one's work is terribly important.
BERTRAND RUSSELL (1872-1970) in "Conquest of Happiness"

We are like dwarfs on the shoulders of giants, so that we can see more than they, and things at a great distance, not by virtue of any sight on our part, or any physical distinction, but because we are carried high and raised up by their giant size.
BERNARD OF CHARTRES (12th Century)

It is without any hesitation that I assent to Chartres' and Russel's points of view. In the end, my PhD thesis, no matter how important or unimportant for the world of science, constitutes a piece of work which has profitted greatly from the presence of a number of people around me. It is my pleasure to be able to thank these "giants," who have frequently carried me on their shoulders in various ways.

First and foremost I would like to thank my PhD adviser Prof. Felix von Oppen. I had just started my PhD when he advised me to read Steven Weinberg's "Four golden lessons" [1]. At that time, Weinberg's "oceanographic metaphore" of a PhD student facing the "vast, unexplored ocean" of physics that he still has to learn, felt all too familiar to me. Indeed, it was "sink or swim." All along the way, Prof. von Oppen's encouragement and support provided the water wings needed for succeeding. I have come to appreciate and learn from his great intuition and way of thinking about physics. I am indebted to Prof. von Oppen for the large amounts of time that he spent with me discussing the progress as well as the dead ends I experienced while working on my thesis.

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Citations to Previously Published Work

Large portions of Chapter 3 have appeared in the following two papers:

> *Franck-Condon Blockade and Giant Fano Factors in Transport through Single Molecules*, J. Koch and F. von Oppen, Phys. Rev. Lett. **94**, 206804 (2005), `cond-mat/0409667`;
>
> *Full counting statistics of strongly non-Ohmic transport through single molecules*, J. Koch, M. E. Raikh, and F. von Oppen, Phys. Rev. Lett. **95**, 056801 (2005), `cond-mat/0501065`.

Chapters 5 and 6 are based upon

> *Effects of charge-dependent vibrational frequencies and anharmonicities in transport through molecules*, J. Koch and F. von Oppen, Phys. Rev. B **72**, 113308 (2005), `cond-mat/0508011`;
>
> *Current-induced nonequilibrium vibrations in single-molecule devices*, J. Koch, M. Semmelhack, F. von Oppen, and A. Nitzan, Phys. Rev. B **73**, 155306 (2006), `cond-mat/0504095`.

Chapter 7 appears in its entirety as

> *Thermopower of Single-Molecule Devices*, J. Koch, F. von Oppen, Y. Oreg, and E. Sela, Phys. Rev. B **70**, 195107 (2004), `cond-mat/0405453`.

Central parts of Chapter 8 have been published as

> *Pair tunneling through single molecules*, J. Koch, M. E. Raikh, and F. von Oppen, Phys. Rev. Lett. **96**, 056803 (2006), `cond-mat/0510249`;
>
> *Fractional Shot Noise in the Kondo Regime*, E. Sela, Y. Oreg, F. von Oppen, and J. Koch, `cond-mat/0603442` (submitted to Phys. Rev. Lett.)

A compact review of the topics discussed in Chapters 3 and 8 has also been published as

> *Novel quantum transport effects in single-molecule transistors*, F. von Oppen and J. Koch, Advances in Solid State Physics **46** (Springer-Verlag Berlin, 2006).

Finally, publications on the material presented in Chapter 4 (together with F. von Oppen and A. V. Andreev) and Chapter 8 (together with E. Sela, Y. Oreg, and F. von Oppen) are currently in preparation.
Electronic preprints (shown in `typewriter font`) are available on the Internet at the following URL:

> `http://arXiv.org`

Notation

In order to avoid unneccessarily complicated notation, we have refrained from marking operators with "hats." The c-number vs. operator nature of quantities should be clear from the context. Vectors are denoted in bold face, e.g. $\mathbf{v}$, matrices are indicated by sans-serif font, e.g. W. For the convenience of the reader, we provide a list of the symbols and abbreviations most frequently used throughout the text.

Symbol	**Description**
$\lfloor x \rfloor$	floor function, gives the largest integer less than or equal to x
a	index for the left and right lead ($a = L, R$)
b, $b^\dagger$	annihilation and creation operator for a vibrational excitation of the molecule
β_m	parameter for the inverse width of the Morse potential
$c_{a\mathbf{p}\sigma}$, $c^\dagger_{a\mathbf{p}\sigma}$	annihilation and creation operator for an electron in lead a with momentum $\mathbf{p}$ and spin projection σ
D	parameter for the depth of the Morse potential
d_σ, $d^\dagger_\sigma$	annihilation and creation operator for a spin-σ electron in the molecular orbital
ε_d	one-particle energy of the molecular orbital which dominates the transport
E^n_q	eigenenergy of the molecular state $\vert\, n, q \,\rangle$
F, F_{ex}	(zero-frequency) Fano factor, excess noise Fano factor
$f(\epsilon)$	Dirac-Fermi distribution, $f(\epsilon) = (e^{\beta\epsilon} + 1)^{-1}$
$f_a(\epsilon)$	Dirac-Fermi distribution for lead a, $f_a(\epsilon) = f(\epsilon - \mu_a)$
G	linear conductance
G_T	thermal linear-response coefficient
Γ	total tunneling-induced level width, $\Gamma = \sum_a \Gamma_a$
Γ_a	partial level width induced by tunneling in junction a, $\Gamma_a = 2\pi\rho \vert t_a\vert^2$
$\mathrm{H}_n(x)$	Hermite polynomial
$\mathrm{I}_\nu(x)$	modified Bessel function
λ	dimensionless parameter characterizing the electron-phonon coupling strength
ℓ_{osc}	harmonic oscillator length (measure of the spatial extent of the vibrational ground state)
$\mathrm{L}^m_n(x)$	generalized Laguerre polynomial
μ_a	chemical potential of lead a
$M_{qq'}$	Franck-Condon matrix element for a phonon transition $q \to q'$
n	electronic occupation number of the molecule
$n_B(\epsilon)$	Bose function, $n_B(\epsilon) = (e^{\beta\epsilon} - 1)^{-1}$
$n_{d\sigma}$, n_d	spin-resolved and total occupation-number operator for the molecular orbital
ω	(angular) frequency in the noise-power spectrum
ω_0	(angular) frequency for the vibrational mode of the molecule
P^{eq}_q	thermal equilibrium distribution for vibrational excitations
P^n_q	stationary occupation probability for the molecular state $\vert\, n, q \,\rangle$
$\psi(x)$	digamma function (logarithmic derivative of the Γ function)
q	vibrational excitation number for the molecule
ρ	density of states of the leads (constant in the wide-band limit)
σ	S_z component of the electronic spin ($\sigma = \uparrow, \downarrow$)
$s(n, n')$	spin factor
S	thermopower
$S(\omega)$	noise power spectrum for the current shot noise
T, β	temperature, $\beta = 1/k_B T$
τ	vibrational relaxation rate
t_a	tunneling matrix element for junction a
U	charging energy of the relevant molecular orbital
V	bias voltage
$W^{nn'}_{qq'}$	rate for the tunneling-induced transition $\vert\, n, q \,\rangle \to \vert\, n', q' \,\rangle$

Abbreviation	**Description**
FC	Franck-Condon
HOMO	highest occupied molecular orbital
IV	current-voltage
LUMO	lowest unoccupied molecular orbital
MC	Monte-Carlo
NDC, NDR	negative differential conductance, negative differential resistance
PHLR	particle-hole/left-right
STM	scanning tunneling microscope
WHM	width at half maximum