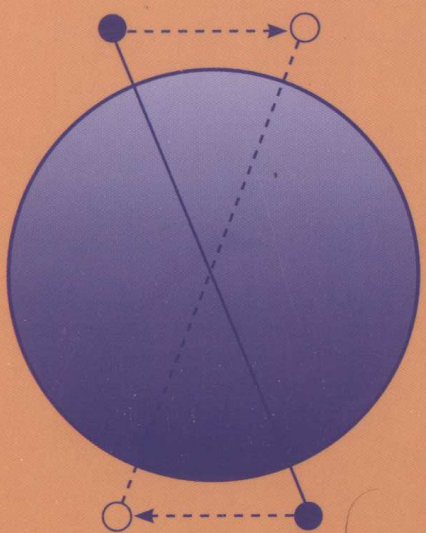
Alexandre M. Zagoskin

Quantum Theory of Many-Body Systems

Techniques and Applications

多体系统的量子理论



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To my parents

Preface

This book grew out of lectures that I gave in the framework of a graduate course in quantum theory of many-body systems at the Applied Physics Department of Chalmers University of Technology and Göteborg University (Göteborg, Sweden) in the years 1992–1995. Its purpose is to give a compact and self-contained account of basic ideas and techniques of the theory from the "condensed matter" point of view. The book is addressed to graduate students with knowledge of standard quantum mechanics and statistical physics. (Hopefully, physicists working in other fields may also find it useful.)

The approach is – quite traditionally – based on a quasiparticle description of many-body systems and its mathematical apparatus – the method of Green's functions. In particular, I tried to bring together all the main versions of diagram techniques for normal and superconducting systems, in and out of equilibrium (i.e., zero-temperature, Matsubara, Keldysh, and Nambu–Gor'kov formalisms) and present them in just enough detail to enable the reader to follow the original papers or more comprehensive monographs, or to apply the techniques to his own problems. Many examples are drawn from mesoscopic physics – a rapidly developing chapter of condensed matter theory and experiment, which deals with macroscopic systems small enough to preserve quantum coherence throughout their volume; this seems to me a natural ground to discuss quantum theory of many-body systems.

The plan of the book is as follows.

In Chapter 1, after a semi-qualitative discussion of the quasiparticle concept, Green's function is introduced in the case of one-body quantum theory, using Feynman path integrals. Then its relation to the S-operator is established, and the

general perturbation theory is developed based on operator formalism. Finally, the second quantization method is introduced.

Chapter 2 contains the usual zero-temperature formalism, beginning with the definition, properties and physical meaning of Green's function in the many-body system, and then buiilding up the diagram technique of the perturbation theory.

In Chapter 3, I present equilibrium Green's functions at finite temperature, and then the Matsubara formalism. Their applications are discussed in relation to linear response theory. Then Keldysh technique is introduced as a means to handle essentially nonequilibrium situations, illustrated by an example of quantum conductivity of a point contact. This gives me an opportunity to discuss both Landauer and tunneling Hamiltonian approaches to transport in mesoscopic systems.

Finally, Chapter 4 is devoted to applications of the theory to the superconductors. Here the Nambu–Gor'kov technique is employed to describe superconducting phase transition, elementary excitations, and current-carrying state of a superconductor. Special attention is paid to the Andreev reflection and to transport in mesoscopic superconductor–normal metal–superconductor (SNS) Josephson junctions.

Each chapter is followed by a set of problems. Their solution will help the reader to obtain a better feeling for how the formalism works.

I did not intend to provide a complete bibliography, which would be far beyond the scope of this book. The *original papers* are cited when the results they contain are either recent or not widely known in the context, and in a few cases where interesting results would require too lengthy a derivation to be presented in full detail (those sections are marked by a star*). For references on more traditional material I have referred the reader to existing **monographs or reviews.**

For a course in quantum many-body theory based on this book I would suggest the following tentative schedule:[1]

Lecture 1 (Sect. 1.1); Lecture 2 (Sect. 1.2.1); Lecture 3 (Sect. 1.2.2, 1.2.3); Lecture 4 (Sect. 1.3); Lecture 5 (Sect. 1.4); Lecture 6 (Sect. 2.1.1); Lecture 7 (Sect. 2.1.2); Lecture 8 (Sect. 2.1.3, 2.1.4); Lecture 9 (Sect. 2.2.1, 2.2.2); Lecture 10 (Sect. 2.2.3); Lectures 11–12 (Sect. 2.2.4); Lecture 13 (Sect. 3.1); Lecture 14 (Sect. 3.2); Lecture 15 (Sect. 3.3); Lecture 16 (Sect. 3.4); Lecture 17 (Sect. 3.5); Lecture 18 (Sect. 3.6); Lecture 19 (Sect. 3.7); Lecture 20 (Sect. 4.1); Lecture 21 (Sect. 4.2); Lecture 22 (Sect. 4.3.1, 4.3.2); Lecture 23 (Sect. 4.3.3, 4.3.4); Lecture 24 (Sect. 4.4.1, 4.4.2); Lectures 25–26 (Sect. 4.4.3–5); Lecture 27 (Sect. 4.5.1); Lecture 28 (Sect. 4.5.2–4); Lecture 29 (Sect. 4.6).

Acknowledgments

I am deeply grateful to Professor R. Shekhter, collaboration with whom in preparing and giving the course on quantum theory of many-body system significantly influenced this book.

I wish to express my sincere thanks to the Institute for Low Temperature Physics and Engineering (Kharkov, Ukraine) and Professor I.O. Kulik, who first taught me

[1] Based on a "two hours" (90 min) lecture length.

what condensed matter theory is about; to the Applied Physics Department of Chalmers University of Technology and Göteborg University (Göteborg, Sweden) and Professor M. Jonson, and to the Physics and Astronomy Department of the University of British Columbia (Vancouver, Canada) and Professor I. Affleck for support and encouragement.

I thank Drs. S. Gao, S. Rashkeev, P. Hessling, R. Gatt, and Y. Andersson for many helpful comments and discussions.

Last, but not least, I am grateful to my wife Irina for her unwavering support and for actually starting this project by the comment, "Well, if you are spending this much time on preparing these handouts, you should rather be writing a book," and to my daughter Ekaterina for critical appreciation of the illustrations.

Vancouver, British Columbia *Alexandre M. Zagoskin*

Contents

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Basic Concepts

When asked to calculate the stability of a dinner table with four legs, a theorist rather quickly produces the results for tables with one leg and with an infinite number of legs. He spends the rest of his life in futile attempts to solve the problem for a table with an arbitrary number of legs.

A popular wisdom.
From the book "Physicists keep joking."

1.1 Introduction: Whys and Hows of Quantum Many-Body Theory

Technically speaking, physics deals only with one-body and many-body problems (because the two-body problem reduces to the one-body case, and the three-body problem does not, and is already insolvable). Still, what an average physicist thinks of as "many" in this context is probably something of the order of 10^{19} - 10^{23}, the number of particles in a cubic centimeter of a gas or a solid, respectively. When you have this many particles on your hands, you need a many-body theory. At these densities, the particles will spend enough time at several de Broglie wavelengths from each other, and therefore we need a quantum many-body theory. (A good thing too: What we really should not mess with is the classical chaos!)

The real reason why you want to deal with such a large collection of particles in the first place, instead of quietly discussing a helium atom, is of course that 10^{23} is much closer to infinity. The epigraph, or intuition, or both, tell us that the infinite number of particles (or legs) is almost as easy to handle as one, and much, much easier than, say, 3, 4, or 7.

The basic idea of the approach is that instead of following a large number of strongly interacting real particles, we should try to get away with considering a relatively small number of weakly interacting *quasiparticles*, or *elementary excitations*.

An elementary excitation is what its name implies: something that appears in the system after it has suffered an external perturbation, and to which the reaction of

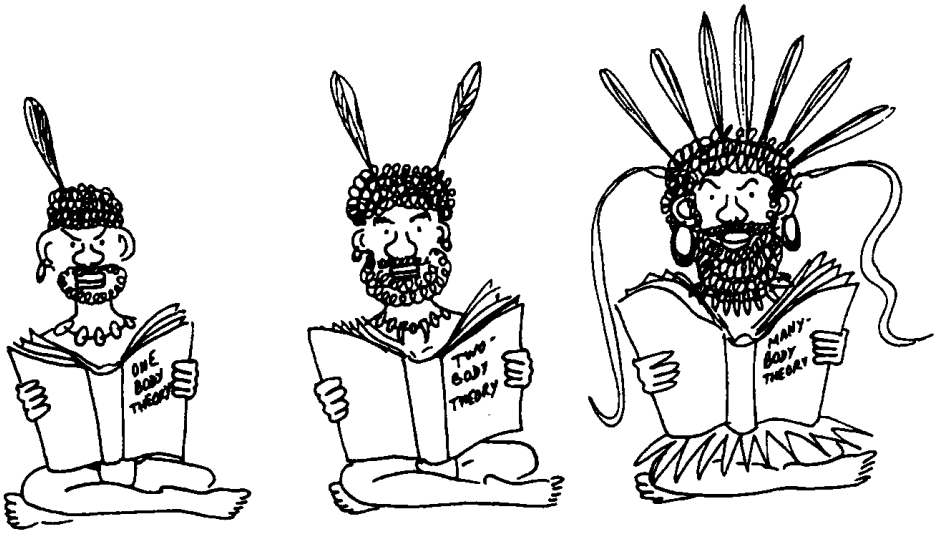

FIGURE 1.1. One, two, many....

the system to this perturbation can be almost completely ascribed – like a ripple on the surface of a pond, only in quantum theory those ripples will be quantized. In a crystal lattice, such quantized ripples are *phonons*, sound quanta, which carry both energy and *quasi*momentum, and only weakly interact with each other and, e.g., electrons. Strike a solid, or heat it, and you excite (that is, generate) a whole bunch of phonons, which will carry away the energy and momentum of your influence.

Phonons form a rather dilute Bose gas, and therefore are much easier to deal with, than the actual particles – atoms or ions – that constitute the lattice. The phonons are called quasiparticles not only because they don't exist outside the lattice; they also have finite lifetime, unlike the stable "proper" particles. A key point here is that the quasiparticles must be stable enough: if they decay faster than they can be created, the whole description loses sense.

Let us now consider a system of interacting electrons in a metal lattice (which we will describe by the standard "jelly" model of uniformly distributed positive charge, neutralizing the total charge of free electrons). Here we have real particles, which interact through strong Coulomb forces, which moreover have an infinite radius (because they decay only as $1/r^2$). For a given electron, we must thus take into account influences of all the other electrons. Therefore, nothing actually depends on the details of behavior of any of those electrons! We can safely replace their action by some average field, depending on averaged electronic density $n(\mathbf{r})$, thus arriving at the *mean field approximation* (MFA). We immediately use it to calculate the screening of Coulomb interaction, to see that not only particles, but interactions as well, are changed in the many-body systems.

1.1.1 Screening of Coulomb Potential in Metal

Suppose we place an external charge Q in the system. It will create a potential $\Phi(\mathbf{r})$, which will change the initial uniform distribution of electronic density,

$$n = \frac{p_F^3}{3\pi^2\hbar^3}. \tag{1.1}$$

Here $p_F = \sqrt{2m\mu}$ is the Fermi momentum, and we have used the well-known relation between p_F and density of the electron gas. Of course, if the electronic density becomes coordinate dependent, so is the Fermi momentum: $p_F \to p_F(n(\mathbf{r}))$. In equilibrium, the electrochemical potential of the electrons must be constant, that is,

$$\mu = \frac{p_F^2(n(\mathbf{r}))}{2m} + e\Phi(\mathbf{r}) = \text{const}, \tag{1.2}$$

and we easily find that

$$n(\mathbf{r}) = \frac{(2m(\mu - e\Phi(\mathbf{r})))^{3/2}}{3\pi^2\hbar^3}. \tag{1.3}$$

If there is no external potential, we return to the unperturbed case (1.1).

Now let us employ the electrostatics. The potential must satisfy Poisson's equation,

$$\nabla^2\Phi(\mathbf{r}) = 4\pi\rho \equiv 4\pi e\Delta n,$$

where ρ is the charge density induced on the neutral background by the probe charge, and $\Delta n(\mathbf{r}) = n(\mathbf{r}) - n$ is the change in electronic density. (The positive "jelly" neutralized the negative charge of the electrons, remember? Besides, we assume that it has unit dielectric permeability, $\varepsilon = 1$.) Therefore, we can write

$$\nabla^2\Phi(\mathbf{r}) = 4\pi e\left[\frac{(2m(\mu - e\Phi(\mathbf{r})))^{3/2} - (2m\mu)^{3/2}}{3\pi^2\hbar^3}\right]. \tag{1.4}$$

This is the *Thomas–Fermi equation*, first obtained in the theory of electron density distribution in atoms.

Generally, this nonlinear equation can be solved only numerically. If, though, we assume that $e\Phi$ is much smaller than the Fermi energy, μ, and expand the right-hand side of (1.4) in powers of Φ to the lowest order – that is, taking

$$\Delta n(\mathbf{r}) = -\frac{3}{2}\frac{e\Phi(\mathbf{r})n}{\mu}, \tag{1.5}$$

we obtain a linear equation,

$$\nabla^2\Phi(\mathbf{r}) = \frac{1}{\lambda_{TF}^2}\Phi(\mathbf{r}). \tag{1.6}$$

Here λ_{TF} is the *Thomas–Fermi screening length*,

$$\lambda_{TF} = \frac{\mu^{1/2}}{\sqrt{6\pi}en^{1/2}} = \frac{\pi^{1/6}}{2\cdot 3^{1/6}}\frac{\hbar}{em^{1/2}}n^{-1/6}. \tag{1.7}$$

To find the physical meaning of λ_{TF}, let us solve (1.6) for $\Phi(\mathbf{r})$, imposing the condition that at small distances $\Phi(\mathbf{r}) \approx Q/r$. This is reasonable, because close