4 Time-independent quantum systems

4.1 Gauge transformation and Aharonov-Bohm effect

Consider the Hamiltonian of an electron in a magnetic field $\boldsymbol{B}(\boldsymbol{r}) = \nabla \times \boldsymbol{A}(\boldsymbol{r})$,

$$H = \frac{1}{2m}[\boldsymbol{p} - e\boldsymbol{A}(\boldsymbol{r})]^2.$$

a) Show that the gauge transformation $\boldsymbol{A}'(\boldsymbol{r}) = \boldsymbol{A}(\boldsymbol{r}) + \nabla\chi(\boldsymbol{r})$ of the vector potential is equivalent to a unitary transformation $H = UHU^{-1}$ of the Hamiltonian, so it leaves all physical properties invariant.

A ring enclosing a line of magnetic flux Φ at the origin has vector potential $\boldsymbol{A}(r,\phi) = (\Phi/2\pi r)\hat{\phi}$ in polar coordinates. Because $\boldsymbol{B} = 0$ for all $r \neq 0$, we can perform a gauge transformation with $\chi(r,\phi) = (\Phi/2\pi)\phi$ that removes the vector potential from the ring, $\boldsymbol{A}' = \boldsymbol{A} + \nabla\chi = 0$ for $r \neq 0$.

b) Explain why this does not invalidate the existence of the Aharonov-Bohm effect.

4.2 Persistent currents

Consider a ring (radius R) enclosing a magnetic flux Φ. For simplicity, we assume that the ring is one-dimensional and take the coordinate x along the ring, $0 < x < L$ ($L = 2\pi R$). The single-electron Hamiltonian is

$$\hat{H} = \frac{1}{2m}(\hat{p} - eA)^2 + V(\hat{x}),$$

with vector potential $A = \Phi/L$ and electrical potential $V(\hat{x})$. The first term in the Hamiltonian is the kinetic energy $\frac{1}{2}m\hat{v}^2$, with velocity operator $\hat{v} = (\hat{p} - eA)/m$. The corresponding electrical[1] current operator is $\hat{I} = e\hat{v}/L$.

a) Use the Feynman-Hellman theorem to prove that the expectation value $I_0 = \langle\hat{I}\rangle_0$ of the electrical current operator in the ground state equals the derivative of the ground state energy E_0 with respect to the flux,

$$I_0 = -\frac{dE_0}{d\Phi}.$$

[1] To avoid confusion with minus signs, we take the electron charge as e.

This current will not decay, because the ground state is time-independent, so it is a *persistent* current even if the electron is scattered as it moves along the ring (an unexpected discovery in a non-superconducting system by Büttiker, Imry, and Landauer).

b) Show that the persistent current $I_0(\Phi)$ is periodic in Φ with period h/e, as required by the Byers-Yang theorem.
Hint: Examine the effect of the unitary transformation $\hat{H} \mapsto \hat{U}\hat{H}\hat{U}^{-1}$ with $\hat{U} = \exp(2\pi i\hat{x}/L)$.

c) Calculate the magnitude of the persistent current in the simplest case $V \equiv 0$ of a free particle. At what value of Φ is it largest?
Hint: Take notice of the periodic boundary condition $\psi(x) = \psi(x+L)$ when searching for a plane-wave eigenstate $\psi(x) = L^{-1/2}e^{ikx}$.

4.3 Variational principle

The MATHEMATICA notebook 10.1 of Konishi and Paffuti[2] shows how to calculate the ground state energy of the harmonic oscillator using the variational principle, with a Gaussian trial wave function.

a) Repeat the calculation of the ground state energy with a Lorentzian trial wave function, $\psi(x) = 1/(x^2 + a^2)$. Compare and discuss the difference.

b) Extend the calculation to obtain the energy of the first excited state and explain your calculation.
Hint: Use trial wave function $\psi(x) = xe^{-ax^2}$. Why will this give you the first excited state?

A particle of mass m bounces vertically on a perfectly reflecting, rigid floor, under the action of the gravitational potential $V(z) = mgz$ for $z > 0$. (We may take $V(z) = \infty$ for $z < 0$.)

c) Use the variational principle to calculate the ground state energy E_0.
Hint: Use trial wave function $\psi(z) = ze^{-az}$. Why must it vanish at $z = 0$?

The exact answer in this case involves the first zero of the Airy function, $E_0 = 2.33811\,(mg^2\hbar^2/2)^{1/3}$. How accurate is the variational estimate?

[2] download `NB-10.1-Elem-Examples.nb` and `Style07.nb` from
`http://www.df.unipi.it/~paffuti/QuantumMechanics%5bO.P.%5d/Mathematica7/Chap10/`
If you prefer not to use MATHEMATICA, you can also do it "by hand", the integrals are simple enough that using a computer is not strictly needed.