4 Time-independent quantum systems

4.1 Gauge transformation and Aharonov-Bohm effect

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

\[
H = \frac{1}{2m} \left( p - eA(r) \right)^2.
\]

a) Show that the gauge transformation \( A'(r) = A(r) + \nabla \chi(r) \) 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 \( \Phi \) at the origin has vector potential \( A(r, \phi) = (\Phi/2\pi r) \hat{\phi} \) in polar coordinates. Because \( B = 0 \) 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, \( A' = A + \nabla \chi = 0 \) 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 \( \Phi \). 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 \( \frac{1}{2m} \hat{v}^2 \), with velocity operator \( \hat{v} = (\hat{p} - eA)/m \). The corresponding electrical 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,

\[
I_0 = -\frac{dE_0}{d\Phi}.
\]

1To 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 $\Phi$ with period $h/e$, as required by the Byers-Yang theorem. 

Hint: Examine the effect of the unitary transformation $\hat{H} \rightarrow \hat{U} \hat{H} \hat{U}^{-1}$ 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 $\Phi$ 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 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, $E_0 = 2.33811 (mg^2h^2/2)^{1/3}$. How accurate is the variational estimate?

\[ \text{download NB-10.1-Elem-Examples.nb and Style07.nb from http://www.df.unipi.it/~paffuti/QuantumMechanics/5b0.P.5d/Mathematica/Chap10/} \]

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.