

A Note on the Gauge Invariance of Perturbation Theory

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Standard perturbation theory of quantum mechanical systems is shown to yield eigenvalues which are invariant under gauge transformations when using the vector potential as the expansion parameter. This clarifies a misconception proposed by earlier researchers claiming that the motion of a charged particle in a magnetic field cannot be unequivocally computed via the standard perturbation method. The importance of choosing a suitable boundary condition for the invariance to hold is also emphasized.

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The finite size effect of the diamagnetic susceptibility of a quantum mechanical system has been studied by many researchers with, unfortunately, disagreeing predictions [1-3]. In an attempt to clarify this matter, Klama and Musial[4] claimed that the standard perturbation scheme should not be adopted for the computation of the eigenvalues of the associated Hamiltonian, because the gauge freedom in the choice of the vector potential will reflect itself manifestly in the perturbation series, thus introducing arbitrariness in the series solution for the eigenvalues, which is clearly absurd. In this paper I will explicitly show that their conclusion is misleading. Specifically, I will show that gauge freedom will not appear in the eigenvalues when one chooses to use the vector potential as the expansion parameter, provided *that the Dirichlet condition is imposed*.

Let us consider the following eigenvalue problem for a charged particle moving in a magnetic field $\vec{B} \equiv \nabla \times \vec{A}$:

$$\left(\frac{1}{i}\nabla - \vec{A}\right)^2 \Psi + V\Psi = \lambda\Psi, \quad (1)$$

where V is a non-magnetic external potential and Ψ is an eigenfunction with the associated eigenvalue λ . In the above we have absorbed all the constants to simplify the equation. It is well-known and easy to verify that Ψ' as defined in $\Psi' \equiv e^{i\phi}\Psi$ for any given function ϕ satisfies

$$\left(\frac{1}{i}\nabla - (\vec{A} + \nabla\phi)\right)^2 \Psi' + V\Psi' = \lambda\Psi'.$$

This equation merely tells us that, so long as one imposes Dirichlet boundary condition for the wavefunctions, gauge freedom in the choice of \vec{A} affects only the form of the eigenfunctions but not the eigenvalues. However, this invariance is destroyed at any finite order if one expands out Eq. (1) to yield

$$-\nabla^2\Psi + V\Psi + \left(\vec{A}^2 - \frac{2}{i}\vec{A}\cdot\nabla - \frac{1}{i}\nabla\cdot\vec{A}\right)\Psi = \lambda\Psi,$$

and then performs regular perturbation calculation using the quantity in the parentheses as the expansion parameter. This is the basic premis of Klama and Musial's paper. In view of the fact that the zero-field diamagnetic susceptibility actually deals with energies proportional to the square of the imposed vanishingly small magnetic field, one sees that a more appropriate perturbation scheme should use \vec{A} instead of the parenthesized quantity as the expansion parameter, because the various terms in the parentheses are of different order in the magnetic field. In the following I will show that, in fact, gauge invariance is preserved to any order if one chooses to solve Eq. (1) using the standard perturbation theory with \vec{A} as the (small) expansion parameter.

Writing out

$$\Psi \equiv \Psi_0 + \Psi_1 + \Psi_2 + \dots$$

$$\lambda \equiv \lambda_0 + \lambda_1 + \lambda_2 + \dots,$$

as the true solution to Eq. (1), one immediately obtains

$$\begin{aligned} (-\nabla^2 + V)\Psi_k - \frac{1}{i}(2\vec{A}\cdot\nabla + \nabla\cdot\vec{A})\Psi_{k-1} + \vec{A}^2\Psi_{k-2} \\ = \lambda_0\Psi_k + \lambda_1\Psi_{k-1} + \dots + \lambda_k\Psi_0, \end{aligned}$$

where Ψ_k and λ_k are the k -th order perturbation to the eigenfunction and the eigenvalue, respectively. (They both are of order $|\vec{A}|^k$.) We shall assume that for a definite choice of \vec{A} this set of equations is exactly solved and ask ourselves what difference it makes if someone else tries to solve instead the following equation:

$$\left(\frac{1}{i}\nabla - (\vec{A}' + \nabla\phi)\right)^2 \Psi' + V\Psi' = \lambda'\Psi'.$$

Clearly, this person will use $\vec{A}' \equiv \vec{A} + \nabla\phi$ as his/her expansion parameter and, as a consequence, obtain the following perturbation equation:

$$\begin{aligned} (-\nabla^2 + V)\Psi'_k - \frac{1}{i}(2(\vec{A}' + \nabla\phi)\cdot\nabla + \nabla\cdot(\vec{A}' + \nabla\phi))\Psi'_{k-1} + (\vec{A}' + \nabla\phi)^2\Psi'_{k-2} \\ = \lambda'_0\Psi'_k + \lambda'_1\Psi'_{k-1} + \dots + \lambda'_k\Psi'_0. \end{aligned} \quad (2)$$

We now show that, up to an overall normalization constant, the primed solution is related to the unprimed solution by the formulas below:

$$\Psi'_k = \sum_{j=0}^k \frac{(i\phi)^j}{j!} \Psi_{k-j}, \quad (3)$$

and

$$\lambda'_k = \lambda_k. \quad (4)$$

The proof can be simplified by noting that it suffices to show that all terms of order ϕ^l must cancel exactly for any non-negative integer l when we substitute Eqs. (3) and (4) into Eq.(2), because ϕ is arbitrary in this problem. Indeed, after the substitution the terms of order ϕ^l read

$$\begin{aligned} & (-\nabla^2 + V) \frac{1}{l!} (i\phi)^l \Psi_{k-l} - \frac{1}{i} (2\vec{A} \cdot \nabla + \nabla \cdot \vec{A}) \frac{1}{l!} (i\phi)^l \Psi_{k-l-1} \\ & - \frac{1}{i} (2\nabla\phi \cdot \nabla + \nabla^2\phi) \frac{1}{(l-1)!} (i\phi)^{l-1} \Psi_{k-l} + \vec{A}^2 \frac{1}{l!} (i\phi)^l \Psi_{k-l-2} \\ & + (2\vec{A} \cdot \nabla\phi) \frac{1}{(l-1)!} (i\phi)^{l-1} \Psi_{k-l-1} + (\nabla\phi)^2 \frac{1}{(l-2)!} (i\phi)^{l-2} \Psi_{k-l} \\ & - \frac{1}{l!} (i\phi)^l \sum_{j=0}^{k-l} \lambda_j \Psi_{k-l-j}, \end{aligned}$$

which can be verified to add up to zero after one carries out the differentiations and utilizes Eq. (2). This then completes our proof, because the only remaining arbitrariness in the solution is a normalization constant, which never affects the computed eigenvalues. Incidentally, we note that Friedman's result [2] cannot be rejected based solely on his use of non-gauge invariant perturbation series. This is because he correctly discarded all terms of order higher than \vec{A}^2 , an act effectively brings back the desirable gauge invariance of the eigenvalues. However, his computed eigenvalues still are gauge-dependent for a different reason: His adoption of periodic boundary condition in one direction suffers the indicated difficulty.

At this point, it is of interest to note that gauge freedom does not affect the eigenvalues computed through the JWKB scheme, either. (Again, this assertion holds to every order of the JWKB series.) To see it, one can consider the time-dependent Schrodinger's equation in the following form:

$$\left(\frac{\alpha}{i} \nabla - \vec{A} \right)^2 \Psi + V\Psi = i\alpha \frac{\partial \Psi}{\partial t},$$

where α is a small parameter (to be identified with the Planck's constant). In the JWKB scheme [5,6], one starts with the assumption that the wavefunction is a linear combination of "general solutions" of the form

$$\Psi_G = e^{\frac{iy}{\alpha}},$$

with functions y expanded in a power series of α :

$$\mathbf{y} \equiv \mathbf{y}_0 + \alpha y_1 + \alpha^2 y_2 + \dots.$$

After substituting this ansatz into the Schrodinger's equation and collecting terms of like power in α , we obtain:

$$\begin{aligned} -\frac{\partial y_0}{\partial t} &= (\nabla y_0 - \vec{A})^2 + V \\ -\frac{\partial y_1}{\partial t} &= -i \nabla \cdot (\nabla y_0 - \vec{A}) + 2(\nabla y_0 - \vec{A}) \cdot \nabla y_1 \\ -\frac{\partial y_2}{\partial t} &= -i \nabla^2 y_1 + 2(\nabla y_0 - \vec{A}) \cdot \nabla y_2 + \nabla y_1 \cdot \nabla y_1 \\ -\frac{\partial y_3}{\partial t} &= -i \nabla^2 y_2 + 2(\nabla y_0 - \vec{A}) \cdot \nabla y_3 + 2 \nabla y_1 \cdot \nabla y_2 \end{aligned}$$

Since we are solving for the eigenvalues, each $-\frac{\partial y_k}{\partial t}$ should be replaced by λ_k , the k -th order perturbation to the eigenvalue. Then it is obviously true in view of the equations above that replacing the vector potential \vec{A} by $\vec{A} + \nabla \phi$ merely adds the gauge function ϕ to every solution for y_0 . Since the quantization condition is derived by imposing single-valuedness as well as the correct boundary condition (the Dirichlet condition) on the whole wavefunction [5], we immediately see that the introduction of the extra ϕ causes no change in form of the quantization rule, because it simply factors out --

$$\Psi' = e^{\frac{i\phi}{\alpha}} \Psi.$$

(This, of course, is nothing but the well-known result we mentioned in the beginning.) Thus, gauge freedom can never show up in the expression for eigenvalues -- just as one would have expected.

Again, I would like to emphasize that this conclusion is valid only when one imposes the Dirichlet condition. Since it has been a common practice in the literature to use periodic boundary condition in the theoretical analysis of Landau diamagnetism, the results contained in previous works must be subjected to more critical scrutiny before a correct picture can emerge. Our investigation of this and related issues will be reported elsewhere.

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